



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 12:07 AM GMT

PDB ID : 1ZPU  
Title : Crystal Structure of Fet3p, a Multicopper Oxidase that Functions in Iron Import  
Authors : Taylor, A.B.; Stoj, C.S.; Ziegler, L.; Kosman, D.J.; Hart, P.J.  
Deposited on : 2005-05-17  
Resolution : 2.80 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

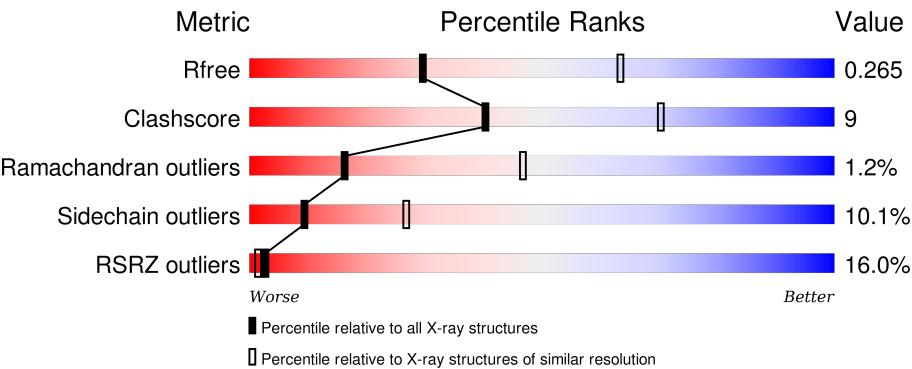
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.80 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.




Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R <sub>free</sub>	91344	2393 (2.80-2.80)
Clashscore	102246	2827 (2.80-2.80)
Ramachandran outliers	100387	2782 (2.80-2.80)
Sidechain outliers	100360	2784 (2.80-2.80)
RSRZ outliers	91569	2404 (2.80-2.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	534	<div><div>8%</div><div><div></div><div></div><div></div><div></div></div><div>74%</div><div>21%</div><div></div><div></div></div>
1	B	534	<div><div>7%</div><div><div></div><div></div><div></div><div></div></div><div>70%</div><div>25%</div><div></div><div></div></div>
1	C	534	<div><div>12%</div><div><div></div><div></div><div></div><div></div></div><div>72%</div><div>23%</div><div></div><div></div></div>
1	D	534	<div><div>13%</div><div><div></div><div></div><div></div><div></div></div><div>72%</div><div>23%</div><div></div><div></div></div>
1	E	534	<div><div>23%</div><div><div></div><div></div><div></div><div></div></div><div>77%</div><div>20%</div><div></div><div></div></div>

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Mol	Chain	Length	Quality of chain
1	F	534	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	NAG	D	2007	X	-	-	-
2	NAG	E	2007	X	-	-	X
2	NAG	F	2007	-	-	-	X
3	NAG	A	2003	X	-	-	-
3	NAG	B	2003	X	-	-	-
3	NAG	D	2003	X	-	-	-
3	NAG	F	2003	X	-	-	-
4	NAG	C	2008	-	-	-	X
4	NAG	D	2009	X	-	-	-
5	NAG	A	2006	X	-	-	-
5	NAG	A	2012	X	-	-	X
5	NAG	B	2006	X	-	-	-
5	NAG	B	2012	X	-	-	X
5	NAG	B	2014	-	-	-	X
5	NAG	B	2018	X	-	-	-
5	NAG	C	2012	X	-	-	X
5	NAG	C	2018	X	-	-	-
5	NAG	D	2006	X	-	-	-
5	NAG	D	2008	-	-	-	X
5	NAG	D	2012	-	-	-	X
5	NAG	D	2014	-	-	-	X
5	NAG	E	2005	-	-	-	X
5	NAG	E	2008	-	-	-	X
5	NAG	E	2012	X	-	-	-
5	NAG	F	2005	X	-	-	X
5	NAG	F	2006	X	-	-	-
5	NAG	F	2009	X	-	-	-
5	NAG	F	2012	X	-	-	-
6	NAG	A	2010	X	-	-	-
6	NAG	C	2010	X	-	-	-
6	NAG	D	2010	X	-	-	X
6	NAG	E	2010	X	-	-	-
6	NAG	F	2010	X	-	-	X
8	NAG	B	2010	X	-	-	-
9	NAG	C	2003	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
9	NAG	E	2003	X	-	-	-

## 2 Entry composition [i](#)

There are 10 unique types of molecules in this entry. The entry contains 27659 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Iron transport multicopper oxidase FET3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	529	Total	C	N	O	S	0	0	0
			4254	2701	695	838	20			
1	B	529	Total	C	N	O	S	0	0	0
			4254	2701	695	838	20			
1	C	529	Total	C	N	O	S	0	0	0
			4254	2701	695	838	20			
1	D	529	Total	C	N	O	S	0	0	0
			4254	2701	695	838	20			
1	E	529	Total	C	N	O	S	0	0	0
			4254	2701	695	838	20			
1	F	529	Total	C	N	O	S	0	0	0
			4254	2701	695	838	20			

- Molecule 2 is a polymer of unknown type called SUGAR (5-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	5	Total	C	N	O	0	0
			61	34	2	25		
2	A	5	Total	C	N	O	0	0
			61	34	2	25		
2	B	5	Total	C	N	O	0	0
			61	34	2	25		
2	B	5	Total	C	N	O	0	0
			61	34	2	25		
2	C	5	Total	C	N	O	0	0
			61	34	2	25		
2	C	5	Total	C	N	O	0	0
			61	34	2	25		
2	D	5	Total	C	N	O	0	0
			61	34	2	25		
2	D	5	Total	C	N	O	0	0
			61	34	2	25		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	E	5	Total	C	N	O	0	0
			61	34	2	25		
2	E	5	Total	C	N	O	0	0
			61	34	2	25		
2	F	5	Total	C	N	O	0	0
			61	34	2	25		
2	F	5	Total	C	N	O	0	0
			61	34	2	25		

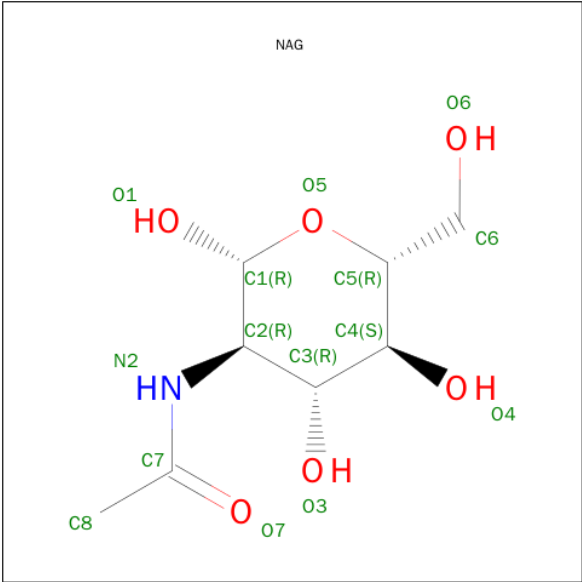
- Molecule 3 is a polymer of unknown type called SUGAR (6-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	6	Total	C	N	O	0	0
			72	40	2	30		
3	B	6	Total	C	N	O	0	0
			72	40	2	30		
3	D	6	Total	C	N	O	0	0
			72	40	2	30		
3	F	6	Total	C	N	O	0	0
			72	40	2	30		

- Molecule 4 is a polymer of unknown type called SUGAR (2-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	2	Total	C	N	O	0	0
			28	16	2	10		
4	B	2	Total	C	N	O	0	0
			28	16	2	10		
4	B	2	Total	C	N	O	0	0
			28	16	2	10		
4	C	2	Total	C	N	O	0	0
			28	16	2	10		
4	D	2	Total	C	N	O	0	0
			28	16	2	10		
4	E	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 5 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula:  $C_8H_{15}NO_6$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	N	O	0	0
			14	8	1	5		
5	A	1	Total	C	N	O	0	0
			14	8	1	5		
5	A	1	Total	C	N	O	0	0
			14	8	1	5		
5	A	1	Total	C	N	O	0	0
			14	8	1	5		
5	B	1	Total	C	N	O	0	0
			14	8	1	5		
5	B	1	Total	C	N	O	0	0
			14	8	1	5		
5	B	1	Total	C	N	O	0	0
			14	8	1	5		
5	B	1	Total	C	N	O	0	0
			14	8	1	5		
5	C	1	Total	C	N	O	0	0
			14	8	1	5		
5	C	1	Total	C	N	O	0	0
			14	8	1	5		
5	C	1	Total	C	N	O	0	0
			14	8	1	5		
5	C	1	Total	C	N	O	0	0
			14	8	1	5		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	D	1	Total	C	N	O	0	0
			14	8	1	5		
5	D	1	Total	C	N	O	0	0
			14	8	1	5		
5	D	1	Total	C	N	O	0	0
			14	8	1	5		
5	D	1	Total	C	N	O	0	0
			14	8	1	5		
5	D	1	Total	C	N	O	0	0
			14	8	1	5		
5	E	1	Total	C	N	O	0	0
			14	8	1	5		
5	E	1	Total	C	N	O	0	0
			14	8	1	5		
5	E	1	Total	C	N	O	0	0
			14	8	1	5		
5	E	1	Total	C	N	O	0	0
			14	8	1	5		
5	E	1	Total	C	N	O	0	0
			14	8	1	5		
5	F	1	Total	C	N	O	0	0
			14	8	1	5		
5	F	1	Total	C	N	O	0	0
			14	8	1	5		
5	F	1	Total	C	N	O	0	0
			14	8	1	5		
5	F	1	Total	C	N	O	0	0
			14	8	1	5		
5	F	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 6 is a polymer of unknown type called SUGAR (3-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	3	Total	C	N	O	0	0
			39	22	2	15		
6	A	3	Total	C	N	O	0	0
			39	22	2	15		
6	C	3	Total	C	N	O	0	0
			39	22	2	15		

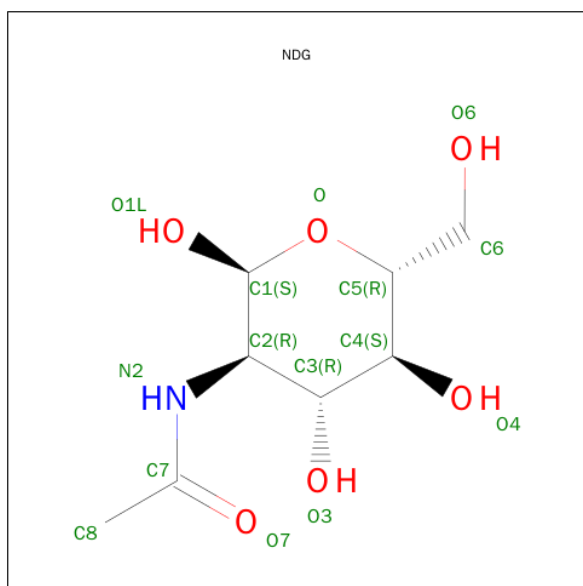
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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	C	3	Total	C	N	O	0	0
			39	22	2	15		
6	D	3	Total	C	N	O	0	0
			39	22	2	15		
6	E	3	Total	C	N	O	0	0
			39	22	2	15		
6	F	3	Total	C	N	O	0	0
			39	22	2	15		

- Molecule 7 is SUGAR (2-(ACETYLAMINO)-2-DEOXY-A-D-GLUCOPYRANOSE) (three-letter code: NDG) (formula: C<sub>8</sub>H<sub>15</sub>NO<sub>6</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	A	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 8 is a polymer of unknown type called SUGAR (4-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	B	4	Total	C	N	O	0	0
			50	28	2	20		

- Molecule 9 is a polymer of unknown type called SUGAR (7-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
9	C	7	Total	C	N	O	0	0
			83	46	2	35		
9	E	7	Total	C	N	O	0	0
			83	46	2	35		

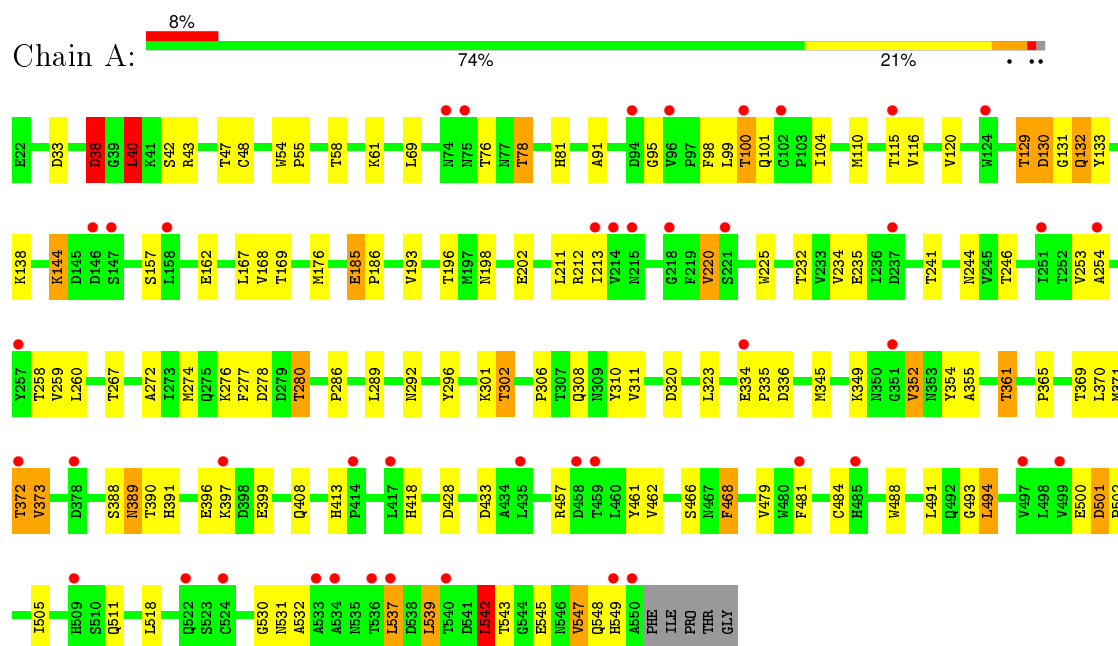
- Molecule 10 is COPPER (I) ION (three-letter code: CU1) (formula: Cu).

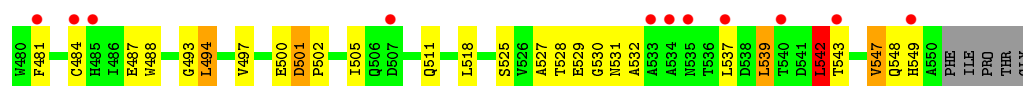
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	D	4	Total	Cu	0	0
			4	4		
10	E	4	Total	Cu	0	0
			4	4		
10	B	4	Total	Cu	0	0
			4	4		
10	C	4	Total	Cu	0	0
			4	4		
10	A	4	Total	Cu	0	0
			4	4		
10	F	4	Total	Cu	0	0
			4	4		

### 3 Residue-property plots

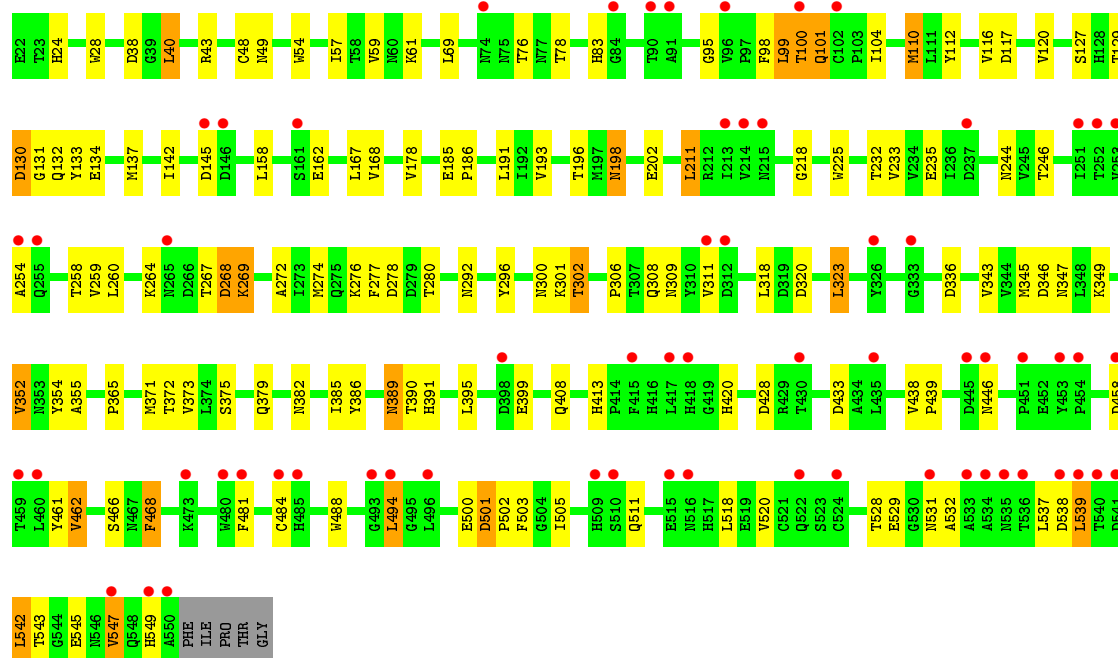
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

#### • Molecule 1: Iron transport multicopper oxidase FET3

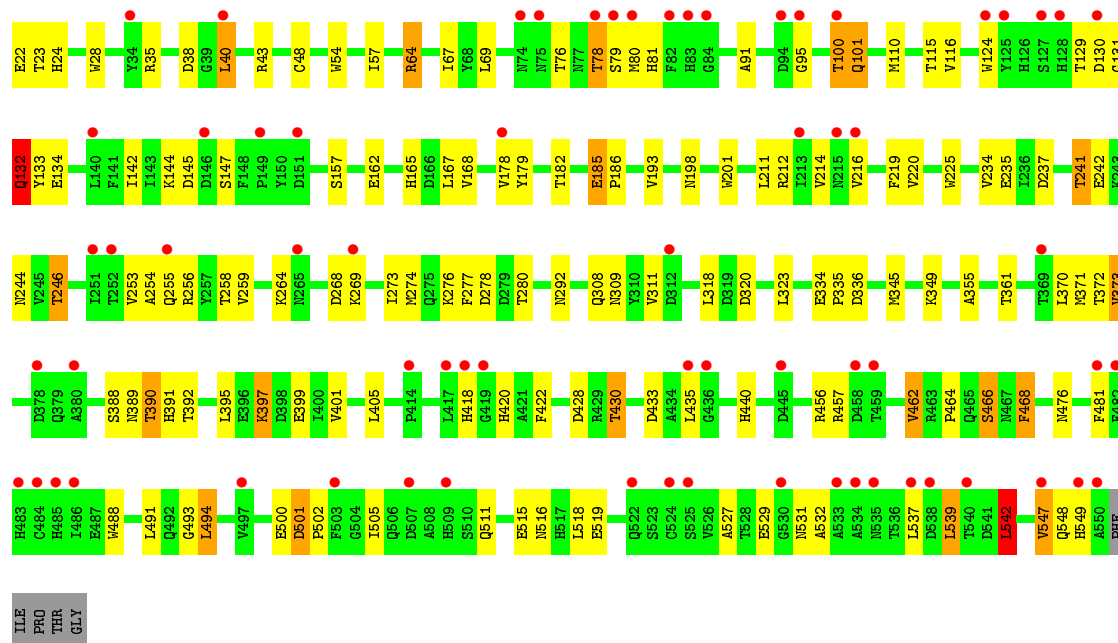




• Molecule 1: Iron transport multicopper oxidase FET3



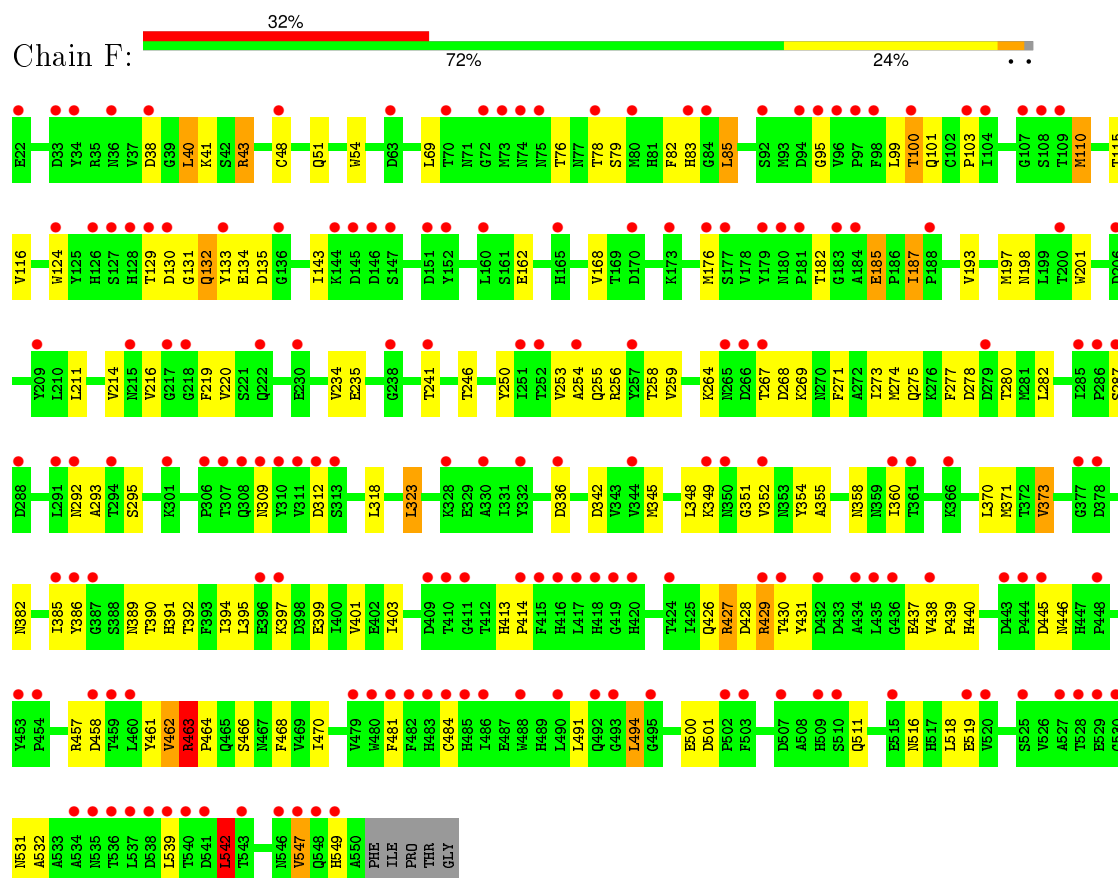
• Molecule 1: Iron transport multicopper oxidase FET3



## Chain E:



## Chain F:



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 32	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	168.53Å 168.53Å 174.60Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	50.00 – 2.80 36.72 – 2.80	Depositor EDS
% Data completeness (in resolution range)	98.2 (50.00-2.80) 98.2 (36.72-2.80)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.08	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.09 (at 2.81Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.226 , 0.257 0.235 , 0.265	Depositor DCC
$R_{free}$ test set	6726 reflections (5.28%)	DCC
Wilson B-factor (Å <sup>2</sup> )	62.6	Xtriage
Anisotropy	0.138	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.29 , 68.1	EDS
Estimated twinning fraction	0.000 for -h,-k,l 0.010 for h,-h-k,-l 0.000 for -k,-h,-l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.35$	Xtriage
Outliers	0 of 134170 reflections	Xtriage
$F_o, F_c$ correlation	0.90	EDS
Total number of atoms	27659	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	69.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 30.19 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 1.3641e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<sup>1</sup> Intensities estimated from amplitudes.

<sup>2</sup> Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: CU1, BMA, NAG, NDG, MAN

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	A	0.50	0/4373	0.66	2/5981 (0.0%)
1	B	0.50	0/4373	0.66	3/5981 (0.1%)
1	C	0.55	5/4373 (0.1%)	0.64	2/5981 (0.0%)
1	D	0.51	3/4373 (0.1%)	0.60	2/5981 (0.0%)
1	E	0.44	1/4373 (0.0%)	0.58	1/5981 (0.0%)
1	F	0.99	20/4373 (0.5%)	0.77	11/5981 (0.2%)
All	All	0.61	29/26238 (0.1%)	0.65	21/35886 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	F	0	1
2	D	1	0
2	E	1	0
3	A	1	0
3	B	1	0
3	D	1	0
3	F	1	0
4	D	1	0
6	A	1	0
6	C	1	0
6	D	1	0
6	E	1	0
6	F	1	0
8	B	1	0
9	C	1	0
9	E	1	0
All	All	15	1

All (29) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	463	ARG	CZ-NH1	40.06	1.85	1.33
1	F	250	TYR	CE2-CZ	15.67	1.58	1.38
1	F	250	TYR	CG-CD2	15.35	1.59	1.39
1	D	515	GLU	CD-OE1	13.48	1.40	1.25
1	F	250	TYR	CE1-CZ	13.27	1.55	1.38
1	F	250	TYR	CG-CD1	11.36	1.53	1.39
1	F	358	ASN	CG-OD1	10.61	1.47	1.24
1	F	445	ASP	CG-OD2	9.77	1.47	1.25
1	F	431	TYR	CE1-CZ	9.44	1.50	1.38
1	C	538	ASP	CG-OD2	9.41	1.47	1.25
1	D	515	GLU	CD-OE2	8.80	1.35	1.25
1	D	35	ARG	CZ-NH1	8.75	1.44	1.33
1	F	431	TYR	CG-CD2	7.97	1.49	1.39
1	F	312	ASP	CG-OD2	7.86	1.43	1.25
1	F	431	TYR	CG-CD1	7.78	1.49	1.39
1	F	426	GLN	CD-OE1	7.58	1.40	1.24
1	F	446	ASN	CG-OD1	7.40	1.40	1.24
1	C	379	GLN	CG-CD	7.34	1.68	1.51
1	C	538	ASP	CB-CG	7.01	1.66	1.51
1	F	429	ARG	NE-CZ	6.76	1.41	1.33
1	C	503	PHE	CD2-CE2	6.44	1.52	1.39
1	F	463	ARG	CD-NE	6.35	1.57	1.46
1	F	312	ASP	CG-OD1	6.22	1.39	1.25
1	F	463	ARG	NE-CZ	5.97	1.40	1.33
1	F	445	ASP	CG-OD1	5.95	1.39	1.25
1	F	437	GLU	CD-OE1	5.86	1.32	1.25
1	F	437	GLU	CD-OE2	5.60	1.31	1.25
1	C	379	GLN	CD-NE2	5.29	1.46	1.32
1	E	396	GLU	CD-OE1	5.10	1.31	1.25

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	463	ARG	NE-CZ-NH2	-25.91	107.34	120.30
1	F	463	ARG	NE-CZ-NH1	10.71	125.66	120.30
1	F	445	ASP	CB-CG-OD2	-9.31	109.92	118.30
1	F	429	ARG	NE-CZ-NH2	-8.88	115.86	120.30
1	F	463	ARG	NH1-CZ-NH2	-8.13	110.46	119.40
1	F	250	TYR	CB-CG-CD1	-7.12	116.73	121.00
1	C	458	ASP	CB-CA-C	-7.02	96.35	110.40
1	F	250	TYR	CD1-CG-CD2	6.90	125.49	117.90
1	D	542	LEU	CA-CB-CG	6.81	130.96	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	542	LEU	CA-CB-CG	6.34	129.88	115.30
1	F	312	ASP	CB-CG-OD2	-6.21	112.71	118.30
1	F	431	TYR	CG-CD2-CE2	-5.88	116.60	121.30
1	F	250	TYR	CG-CD1-CE1	-5.71	116.73	121.30
1	B	462	VAL	CB-CA-C	-5.59	100.79	111.40
1	E	40	LEU	CA-CB-CG	5.54	128.04	115.30
1	A	38	ASP	CB-CG-OD1	-5.52	113.33	118.30
1	D	35	ARG	NE-CZ-NH2	-5.51	117.55	120.30
1	B	99	LEU	CA-CB-CG	5.43	127.79	115.30
1	F	250	TYR	CB-CG-CD2	-5.38	117.77	121.00
1	A	40	LEU	CA-CB-CG	5.35	127.61	115.30
1	C	99	LEU	CA-CB-CG	5.16	127.16	115.30

All (15) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	A	2003	NAG	C1
6	A	2010	NAG	C1
3	B	2003	NAG	C1
8	B	2010	NAG	C1
9	C	2003	NAG	C1
6	C	2010	NAG	C1
3	D	2003	NAG	C1
2	D	2007	NAG	C1
4	D	2009	NAG	C1
6	D	2010	NAG	C1
9	E	2003	NAG	C1
2	E	2007	NAG	C1
6	E	2010	NAG	C1
3	F	2003	NAG	C1
6	F	2010	NAG	C1

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	F	463	ARG	Sidechain

## 5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen

atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4254	0	3960	72	0
1	B	4254	0	3960	97	0
1	C	4254	0	3961	78	0
1	D	4254	0	3960	76	0
1	E	4254	0	3962	62	0
1	F	4254	0	3960	78	0
2	A	122	0	104	2	0
2	B	122	0	104	1	0
2	C	122	0	104	1	0
2	D	122	0	104	2	0
2	E	122	0	104	2	0
2	F	122	0	104	1	0
3	A	72	0	61	0	0
3	B	72	0	61	1	0
3	D	72	0	61	0	0
3	F	72	0	61	1	0
4	A	28	0	25	2	0
4	B	56	0	50	0	0
4	C	28	0	25	0	0
4	D	28	0	25	0	0
4	E	28	0	25	0	0
5	A	56	0	52	0	0
5	B	70	0	65	3	0
5	C	70	0	65	2	0
5	D	70	0	64	2	0
5	E	70	0	65	2	0
5	F	84	0	78	4	0
6	A	78	0	68	2	0
6	C	78	0	68	4	0
6	D	39	0	34	0	0
6	E	39	0	34	1	0
6	F	39	0	34	0	0
7	A	14	0	13	0	0
8	B	50	0	43	0	0
9	C	83	0	70	1	0
9	E	83	0	70	2	0
10	A	4	0	0	0	0
10	B	4	0	0	0	0
10	C	4	0	0	0	0
10	D	4	0	0	0	0
10	E	4	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
10	F	4	0	0	0	0
All	All	27659	0	25604	464	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 9.

All (464) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:2006:NAG:C7	5:F:2006:NAG:C8	1.80	1.60
1:F:463:ARG:NH1	1:F:463:ARG:CZ	1.85	1.37
5:F:2005:NAG:C6	5:F:2005:NAG:O6	1.74	1.32
6:C:3013:BMA:C6	6:C:3013:BMA:O6	1.75	1.32
1:F:427:ARG:HD2	1:F:463:ARG:NH1	1.56	1.20
1:C:246:THR:HG21	1:C:318:LEU:HB2	1.43	1.00
1:F:246:THR:HG21	1:F:318:LEU:HB2	1.44	0.98
1:F:427:ARG:HD2	1:F:463:ARG:HH11	1.12	0.95
1:D:78:THR:HG23	1:D:132:GLN:OE1	1.70	0.91
1:F:427:ARG:CD	1:F:463:ARG:HH11	1.82	0.91
1:E:131:GLY:HA3	1:E:168:VAL:HG11	1.52	0.90
1:A:78:THR:HG23	1:A:132:GLN:OE1	1.71	0.90
1:E:420:HIS:NE2	1:E:500:GLU:OE1	2.05	0.90
1:B:131:GLY:HA3	1:B:168:VAL:HG11	1.51	0.89
1:C:244:ASN:HD22	5:C:2005:NAG:H83	1.38	0.89
1:A:131:GLY:HA3	1:A:168:VAL:HG11	1.56	0.87
1:A:302:THR:HG23	1:B:55:PRO:HB3	1.55	0.86
1:D:131:GLY:HA3	1:D:168:VAL:HG11	1.55	0.86
1:A:272:ALA:HB1	1:A:274:MET:HE1	1.56	0.85
1:F:131:GLY:HA3	1:F:168:VAL:HG11	1.59	0.84
1:C:131:GLY:HA3	1:C:168:VAL:HG11	1.60	0.82
1:B:78:THR:HG23	1:B:132:GLN:OE1	1.79	0.82
1:B:395:LEU:HD12	1:B:500:GLU:HG3	1.63	0.81
1:A:129:THR:HG22	1:A:130:ASP:H	1.45	0.80
1:D:246:THR:HG21	1:D:318:LEU:HB2	1.63	0.79
1:A:244:ASN:HD22	4:A:2005:NAG:H83	1.48	0.78
1:A:278:ASP:OD2	1:A:280:THR:HB	1.84	0.77
1:C:395:LEU:HD12	1:C:500:GLU:HG3	1.68	0.75
1:B:38:ASP:OD2	1:B:165:HIS:NE2	2.19	0.74
1:C:276:LYS:HG3	1:C:292:ASN:HB3	1.68	0.74
1:B:235:GLU:HB3	1:B:258:THR:HB	1.70	0.73
1:B:278:ASP:OD2	1:B:280:THR:HB	1.91	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:129:THR:HG22	1:B:130:ASP:H	1.56	0.70
1:A:302:THR:CG2	1:B:55:PRO:HB3	2.21	0.70
1:C:129:THR:HG22	1:C:130:ASP:H	1.56	0.69
1:B:246:THR:HG21	1:B:318:LEU:HB2	1.72	0.69
1:D:116:VAL:HG12	1:D:116:VAL:O	1.93	0.69
1:B:67:ILE:HG21	1:B:80:MET:CE	2.24	0.68
1:F:395:LEU:HD12	1:F:500:GLU:HG3	1.75	0.68
1:A:272:ALA:HB1	1:A:274:MET:CE	2.23	0.68
1:D:178:VAL:HG11	1:F:440:HIS:CD2	2.29	0.68
1:B:116:VAL:O	1:B:116:VAL:HG12	1.94	0.67
1:B:349:LYS:HD2	1:B:547:VAL:HG23	1.77	0.67
1:D:388:SER:H	1:D:542:LEU:HD21	1.59	0.67
1:A:129:THR:HG22	1:A:130:ASP:N	2.11	0.66
1:D:349:LYS:HD2	1:D:547:VAL:HG23	1.76	0.66
1:F:542:LEU:H	1:F:542:LEU:HD13	1.61	0.65
1:B:185:GLU:HG3	1:B:219:PHE:CZ	2.31	0.65
1:E:246:THR:HG21	1:E:318:LEU:HB2	1.77	0.65
1:B:505:ILE:HG23	1:B:511:GLN:HG2	1.78	0.65
1:F:116:VAL:HG11	1:F:143:ILE:HD13	1.78	0.65
1:C:272:ALA:HB1	1:C:274:MET:CE	2.27	0.64
1:A:505:ILE:HG23	1:A:511:GLN:HG2	1.79	0.64
1:A:38:ASP:HB3	1:A:40:LEU:H	1.63	0.64
1:D:235:GLU:HB3	1:D:258:THR:HB	1.77	0.64
1:B:372:THR:HB	1:B:530:GLY:HA2	1.80	0.64
1:D:167:LEU:H	1:D:167:LEU:HD12	1.62	0.64
1:C:296:TYR:HD2	1:C:306:PRO:HG2	1.62	0.64
1:C:116:VAL:O	1:C:116:VAL:HG12	1.97	0.64
1:D:395:LEU:HD12	1:D:500:GLU:HG3	1.81	0.63
1:D:220:VAL:HG21	1:D:277:PHE:HD2	1.63	0.63
1:B:272:ALA:HB1	1:B:274:MET:HE1	1.79	0.63
1:B:244:ASN:HD22	5:B:2005:NAG:H83	1.64	0.62
1:D:274:MET:CE	1:D:309:ASN:H	2.13	0.62
1:C:38:ASP:HB3	1:C:40:LEU:H	1.63	0.62
1:B:67:ILE:HG21	1:B:80:MET:HE1	1.82	0.62
1:D:185:GLU:HG3	1:D:219:PHE:CZ	2.35	0.61
1:D:225:TRP:CZ2	1:D:274:MET:HG2	2.36	0.61
1:B:38:ASP:HB3	1:B:40:LEU:H	1.64	0.61
1:A:537:LEU:HD23	1:A:539:LEU:HB2	1.83	0.61
1:F:116:VAL:HG11	1:F:143:ILE:CD1	2.30	0.61
1:C:244:ASN:HD22	5:C:2005:NAG:C8	2.10	0.60
1:C:278:ASP:OD2	1:C:280:THR:HB	2.01	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:116:VAL:CG1	1:A:116:VAL:O	2.49	0.60
2:A:3001:BMA:H3	2:A:3007:MAN:H3	1.83	0.60
1:F:318:LEU:HD21	1:F:323:LEU:HD11	1.82	0.60
1:C:420:HIS:NE2	1:C:500:GLU:OE1	2.27	0.60
1:E:278:ASP:OD2	1:E:280:THR:HB	2.01	0.60
1:B:428:ASP:HB3	1:B:466:SER:OG	2.01	0.60
1:F:274:MET:CE	1:F:309:ASN:H	2.15	0.60
1:F:427:ARG:CD	1:F:463:ARG:NH1	2.45	0.59
1:C:134:GLU:OE2	1:C:218:GLY:HA3	2.01	0.59
1:D:95:GLY:H	1:D:100:THR:HG21	1.67	0.59
1:C:235:GLU:HB3	1:C:258:THR:HB	1.84	0.59
1:A:95:GLY:H	1:A:100:THR:HG21	1.67	0.59
1:B:129:THR:HG22	1:B:130:ASP:N	2.18	0.58
1:F:78:THR:HG23	1:F:132:GLN:OE1	2.02	0.58
1:C:48:CYS:HB2	1:C:54:TRP:CD2	2.38	0.58
1:C:100:THR:HG22	1:C:101:GLN:HG2	1.86	0.58
1:F:235:GLU:HB3	1:F:258:THR:HB	1.86	0.58
1:D:430:THR:HG23	1:D:464:PRO:HD2	1.84	0.58
1:F:360:ILE:HD11	5:F:2012:NAG:H82	1.86	0.58
1:A:116:VAL:O	1:A:116:VAL:HG12	2.03	0.58
1:F:78:THR:HG22	1:F:79:SER:H	1.67	0.58
1:B:134:GLU:OE2	1:B:218:GLY:HA3	2.04	0.57
6:C:3013:BMA:O6	6:C:3013:BMA:C5	2.51	0.57
1:C:272:ALA:HB1	1:C:274:MET:HE1	1.86	0.57
1:F:220:VAL:HG21	1:F:277:PHE:HD2	1.69	0.57
1:F:214:VAL:HG13	1:F:256:ARG:HG3	1.87	0.57
1:E:352:VAL:HG22	1:E:354:TYR:CE1	2.39	0.57
1:A:95:GLY:HA2	1:A:101:GLN:OE1	2.04	0.57
1:F:274:MET:HE1	1:F:309:ASN:H	1.70	0.57
1:C:202:GLU:OE1	1:C:301:LYS:HD3	2.05	0.57
1:F:403:ILE:HD12	1:F:470:ILE:HD11	1.87	0.57
1:B:103:PRO:HG2	2:B:2007:NAG:H61	1.87	0.57
1:A:361:THR:HG22	1:A:493:GLY:HA3	1.87	0.57
1:D:23:THR:HG23	1:D:64:ARG:HG2	1.87	0.56
1:A:157:SER:OG	1:A:212:ARG:HD2	2.04	0.56
1:E:308:GLN:HE22	6:E:2010:NAG:H2	1.68	0.56
1:A:267:THR:HG22	1:A:267:THR:O	2.05	0.56
1:B:99:LEU:HD13	1:B:497:VAL:HG13	1.86	0.56
1:E:438:VAL:HG21	1:F:351:GLY:HA3	1.87	0.56
1:B:355:ALA:HB1	1:B:494:LEU:HG	1.88	0.56
1:D:395:LEU:HD13	1:D:401:VAL:HG21	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:390:THR:HG23	1:B:392:THR:OG1	2.05	0.56
1:A:235:GLU:HB3	1:A:258:THR:HB	1.87	0.56
1:D:124:TRP:CE3	1:D:216:VAL:HG12	2.41	0.56
1:B:527:ALA:HB1	1:B:529:GLU:HG3	1.86	0.56
1:A:61:LYS:HD3	1:A:120:VAL:HG23	1.88	0.55
1:A:234:VAL:C	1:A:241:THR:HG22	2.26	0.55
1:C:129:THR:HG22	1:C:130:ASP:N	2.19	0.55
1:B:272:ALA:HB1	1:B:274:MET:CE	2.36	0.55
1:D:274:MET:HE1	1:D:309:ASN:H	1.72	0.55
1:F:78:THR:HG22	1:F:79:SER:N	2.21	0.55
1:A:211:LEU:HD22	1:A:213:ILE:CG1	2.37	0.55
1:B:81:HIS:CE1	1:B:418:HIS:CE1	2.94	0.55
1:A:48:CYS:HB2	1:A:54:TRP:CD2	2.41	0.55
1:F:95:GLY:H	1:F:100:THR:HG21	1.70	0.55
1:A:296:TYR:HD2	1:A:306:PRO:HG2	1.70	0.55
1:A:276:LYS:HG3	1:A:292:ASN:HB3	1.87	0.55
1:D:537:LEU:HD23	1:D:539:LEU:HB2	1.89	0.55
1:B:276:LYS:HG3	1:B:292:ASN:HB3	1.89	0.55
1:F:386:TYR:O	1:F:390:THR:HG21	2.07	0.55
1:C:267:THR:O	1:C:267:THR:HG22	2.07	0.55
1:C:300:ASN:OD1	1:C:302:THR:HG22	2.06	0.55
1:B:234:VAL:C	1:B:241:THR:HG22	2.28	0.55
5:F:2005:NAG:O6	5:F:2005:NAG:C5	2.54	0.54
1:A:225:TRP:CZ2	1:A:274:MET:HG2	2.42	0.54
1:D:100:THR:HG22	1:D:101:GLN:HG2	1.90	0.54
1:B:48:CYS:HB2	1:B:54:TRP:CD2	2.42	0.54
1:D:38:ASP:OD2	1:D:165:HIS:NE2	2.34	0.54
1:F:131:GLY:CA	1:F:168:VAL:HG11	2.35	0.54
1:B:244:ASN:HD22	5:B:2005:NAG:C8	2.19	0.54
1:B:95:GLY:H	1:B:100:THR:HG21	1.73	0.54
1:E:274:MET:CE	1:E:309:ASN:H	2.20	0.54
1:B:276:LYS:HE2	1:B:292:ASN:HD22	1.73	0.54
1:D:67:ILE:HG21	1:D:80:MET:HE1	1.90	0.54
1:E:386:TYR:O	1:E:390:THR:HG21	2.07	0.54
1:B:388:SER:H	1:B:542:LEU:HD21	1.72	0.54
1:C:349:LYS:HD2	1:C:547:VAL:HG23	1.89	0.54
1:B:120:VAL:HG21	1:B:145:ASP:HB3	1.89	0.54
1:F:336:ASP:HB2	1:F:399:GLU:HB2	1.90	0.54
1:B:83:HIS:CE1	1:B:254:ALA:HB1	2.42	0.54
1:D:48:CYS:HB2	1:D:54:TRP:CD2	2.43	0.53
1:B:28:TRP:HH2	1:B:57:ILE:HD11	1.73	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:361:THR:HG23	1:D:493:GLY:HA3	1.89	0.53
1:C:95:GLY:H	1:C:100:THR:HG21	1.73	0.53
1:E:95:GLY:HA2	1:E:101:GLN:OE1	2.09	0.53
1:F:462:VAL:HG22	1:F:468:PHE:CE1	2.44	0.53
1:F:429:ARG:HA	1:F:463:ARG:HD2	1.90	0.53
1:A:244:ASN:HD22	4:A:2005:NAG:C8	2.19	0.53
1:E:355:ALA:HB1	1:E:494:LEU:HG	1.90	0.53
1:D:142:ILE:HD12	2:D:2002:NAG:H81	1.90	0.52
1:E:438:VAL:HG21	1:F:351:GLY:CA	2.40	0.52
1:D:48:CYS:HB2	1:D:54:TRP:CE2	2.43	0.52
1:E:95:GLY:H	1:E:100:THR:HG21	1.75	0.52
1:B:244:ASN:HB2	5:B:2005:NAG:H83	1.92	0.52
1:B:120:VAL:CG2	1:B:145:ASP:HB3	2.40	0.52
1:B:214:VAL:HG13	1:B:256:ARG:HG3	1.90	0.52
1:C:537:LEU:HD23	1:C:539:LEU:HB2	1.91	0.52
1:C:352:VAL:HG22	1:C:354:TYR:CE1	2.45	0.52
1:A:211:LEU:HD22	1:A:213:ILE:HG13	1.92	0.51
1:B:78:THR:CG2	1:B:132:GLN:OE1	2.54	0.51
1:D:167:LEU:HD12	1:D:167:LEU:N	2.24	0.51
1:C:110:MET:HB2	1:C:520:VAL:HG21	1.91	0.51
1:C:462:VAL:HG13	1:C:468:PHE:CD1	2.46	0.51
1:A:428:ASP:HB3	1:A:466:SER:OG	2.11	0.51
1:D:157:SER:OG	1:D:212:ARG:HD2	2.10	0.51
1:E:244:ASN:HB2	5:E:2005:NAG:H83	1.93	0.51
1:D:186:PRO:HG2	1:D:488:TRP:CZ2	2.45	0.51
1:B:130:ASP:O	1:B:487:GLU:OE1	2.28	0.51
1:D:502:PRO:HA	1:D:505:ILE:HD12	1.93	0.51
1:B:468:PHE:C	1:B:468:PHE:CD2	2.84	0.51
1:A:308:GLN:OE1	6:A:2010:NAG:H83	2.11	0.51
1:E:199:LEU:HD21	2:E:2001:NAG:H82	1.92	0.51
1:A:349:LYS:HD2	1:A:547:VAL:HG23	1.93	0.51
1:B:225:TRP:CZ2	1:B:274:MET:HG2	2.46	0.50
1:E:272:ALA:HB1	1:E:274:MET:CE	2.40	0.50
1:E:276:LYS:HG3	1:E:292:ASN:HB3	1.93	0.50
1:C:336:ASP:HB2	1:C:399:GLU:HB2	1.93	0.50
1:E:237:ASP:OD1	1:E:457:ARG:HB2	2.11	0.50
1:C:274:MET:CE	1:C:309:ASN:H	2.24	0.50
1:B:386:TYR:O	1:B:390:THR:HG21	2.12	0.50
1:D:220:VAL:HG21	1:D:277:PHE:CD2	2.45	0.50
1:C:95:GLY:HA2	1:C:101:GLN:OE1	2.10	0.50
1:A:389:ASN:OD1	1:A:545:GLU:HG2	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:370:LEU:HA	1:B:373:VAL:HG13	1.92	0.50
1:F:348:LEU:HD12	1:F:354:TYR:CD1	2.47	0.50
1:F:95:GLY:N	1:F:100:THR:HG21	2.26	0.50
1:A:352:VAL:HG22	1:A:354:TYR:CE1	2.46	0.50
1:D:22:GLU:OE1	1:D:24:HIS:NE2	2.45	0.50
1:E:104:ILE:HG12	1:E:110:MET:HE2	1.94	0.50
1:B:33:ASP:HB2	1:B:47:THR:HG21	1.94	0.50
1:F:103:PRO:HG2	2:F:2007:NAG:H61	1.93	0.50
1:F:100:THR:HG22	1:F:101:GLN:HG2	1.92	0.49
1:A:370:LEU:HA	1:A:373:VAL:HG13	1.93	0.49
1:D:179:TYR:HE2	1:F:428:ASP:OD2	1.95	0.49
1:B:78:THR:HG22	1:B:79:SER:H	1.77	0.49
1:A:186:PRO:HG2	1:A:488:TRP:CZ2	2.48	0.49
1:D:276:LYS:HE2	1:D:292:ASN:HD22	1.77	0.49
1:E:527:ALA:HB1	1:E:529:GLU:HG3	1.94	0.49
1:D:78:THR:HG22	1:D:79:SER:H	1.75	0.49
1:F:82:PHE:HB3	1:F:85:LEU:HD22	1.93	0.49
1:E:390:THR:HG23	1:E:392:THR:OG1	2.12	0.49
1:B:468:PHE:HD2	1:B:468:PHE:C	2.16	0.49
1:B:197:MET:HB2	3:B:2003:NAG:HN2	1.77	0.49
1:A:484:CYS:HB2	1:A:494:LEU:HD13	1.94	0.49
1:F:220:VAL:HG11	1:F:277:PHE:CE2	2.48	0.49
1:D:278:ASP:OD2	1:D:280:THR:HB	2.12	0.49
1:C:274:MET:HE1	1:C:309:ASN:H	1.77	0.48
1:A:253:VAL:O	1:A:254:ALA:HB3	2.13	0.48
1:C:505:ILE:HG23	1:C:511:GLN:HG2	1.94	0.48
1:B:336:ASP:HB2	1:B:399:GLU:HB2	1.95	0.48
1:C:83:HIS:CE1	1:C:254:ALA:HB1	2.49	0.48
1:B:227:GLU:HG2	1:B:271:PHE:HD2	1.78	0.48
1:A:91:ALA:N	1:A:511:GLN:OE1	2.46	0.48
1:C:413:HIS:O	1:C:461:TYR:HA	2.13	0.48
1:A:502:PRO:HA	1:A:505:ILE:HD12	1.96	0.48
1:E:48:CYS:HB2	1:E:54:TRP:CD2	2.49	0.48
1:B:186:PRO:HG2	1:B:488:TRP:CZ2	2.49	0.48
1:C:225:TRP:CZ2	1:C:274:MET:HG2	2.49	0.48
1:A:372:THR:HB	1:A:530:GLY:HA2	1.95	0.48
1:B:413:HIS:O	1:B:461:TYR:HA	2.14	0.47
1:F:430:THR:HG23	1:F:464:PRO:HD2	1.95	0.47
1:D:38:ASP:HB3	1:D:40:LEU:H	1.79	0.47
1:C:127:SER:HB2	1:C:137:MET:SD	2.54	0.47
1:B:296:TYR:HD2	1:B:306:PRO:HG2	1.78	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:82:PHE:HB3	1:B:85:LEU:HD22	1.96	0.47
1:C:134:GLU:OE2	1:C:218:GLY:CA	2.61	0.47
1:C:468:PHE:CD2	1:C:468:PHE:C	2.88	0.47
1:D:237:ASP:OD1	1:D:457:ARG:HB2	2.14	0.47
1:F:255:GLN:HB2	1:F:457:ARG:NH2	2.29	0.47
1:E:272:ALA:HB1	1:E:274:MET:HE2	1.97	0.47
1:F:355:ALA:HB1	1:F:494:LEU:HG	1.97	0.47
1:C:48:CYS:HB2	1:C:54:TRP:CE2	2.49	0.47
1:F:278:ASP:OD2	1:F:280:THR:HB	2.14	0.47
1:A:388:SER:H	1:A:542:LEU:HD21	1.78	0.47
1:D:516:ASN:O	1:D:519:GLU:HB3	2.15	0.47
1:B:124:TRP:CE3	1:B:216:VAL:HG12	2.50	0.47
1:F:390:THR:HG23	1:F:392:THR:OG1	2.14	0.47
1:A:98:PHE:HB3	1:A:365:PRO:HD2	1.97	0.47
1:B:352:VAL:HG22	1:B:354:TYR:CE1	2.50	0.47
2:A:2013:NAG:H83	2:A:2013:NAG:H3	1.97	0.47
1:F:413:HIS:O	1:F:461:TYR:HA	2.15	0.47
1:C:158:LEU:HG	1:C:211:LEU:HD21	1.95	0.47
1:A:55:PRO:HB3	1:C:302:THR:HG23	1.97	0.47
1:B:191:LEU:HG	1:B:277:PHE:CE1	2.50	0.47
1:F:48:CYS:HB2	1:F:54:TRP:CD2	2.51	0.46
1:A:542:LEU:HB2	1:A:543:THR:H	1.33	0.46
1:C:61:LYS:HD3	1:C:120:VAL:HG23	1.97	0.46
1:E:185:GLU:OE2	1:E:489:HIS:NE2	2.47	0.46
1:B:28:TRP:CH2	1:B:57:ILE:HD11	2.49	0.46
1:C:272:ALA:HB1	1:C:274:MET:HE2	1.95	0.46
1:E:225:TRP:CZ2	1:E:274:MET:HG2	2.50	0.46
1:C:110:MET:HG2	1:C:112:TYR:CE1	2.51	0.46
1:E:104:ILE:CG1	1:E:110:MET:HE2	2.45	0.46
1:D:390:THR:HG23	1:D:392:THR:OG1	2.16	0.46
1:B:388:SER:H	1:B:542:LEU:CD2	2.28	0.46
1:D:505:ILE:HG23	1:D:511:GLN:HG2	1.96	0.46
1:F:201:TRP:HE3	1:F:273:ILE:HD11	1.80	0.46
1:F:176:MET:HE3	1:F:491:LEU:HB3	1.97	0.46
1:C:542:LEU:HB2	1:C:543:THR:H	1.52	0.46
1:A:413:HIS:O	1:A:461:TYR:HA	2.15	0.46
1:E:129:THR:HG22	1:E:130:ASP:H	1.80	0.46
6:C:2016:NAG:O3	6:C:2016:NAG:H83	2.15	0.46
1:C:24:HIS:CD2	1:C:59:VAL:HG12	2.50	0.46
1:E:91:ALA:O	1:E:100:THR:HG23	2.16	0.46
1:C:428:ASP:HB3	1:C:466:SER:OG	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:501:ASP:HA	1:E:502:PRO:HD2	1.72	0.46
1:A:336:ASP:HB2	1:A:399:GLU:HB2	1.97	0.46
1:F:48:CYS:HB2	1:F:54:TRP:CE2	2.51	0.46
1:D:336:ASP:HB2	1:D:399:GLU:HB2	1.98	0.46
1:D:244:ASN:HB2	5:D:2005:NAG:H83	1.97	0.46
1:D:476:ASN:HB2	5:D:2008:NAG:H82	1.96	0.46
1:E:336:ASP:HB2	1:E:399:GLU:HB2	1.97	0.45
1:B:134:GLU:OE2	1:B:218:GLY:CA	2.64	0.45
1:F:395:LEU:HD22	1:F:401:VAL:HG21	1.97	0.45
1:A:95:GLY:N	1:A:100:THR:HG21	2.31	0.45
1:F:197:MET:HB2	3:F:2003:NAG:HN2	1.79	0.45
1:C:198:ASN:OD1	9:C:2003:NAG:H83	2.16	0.45
1:C:232:THR:HB	1:C:260:LEU:HB2	1.98	0.45
1:D:274:MET:HE3	1:D:309:ASN:H	1.80	0.45
1:E:131:GLY:CA	1:E:168:VAL:HG11	2.36	0.45
1:E:395:LEU:HD12	1:E:500:GLU:HG2	1.97	0.45
1:A:369:THR:HB	1:A:479:VAL:HG11	1.98	0.45
1:B:116:VAL:HG11	1:B:143:ILE:HD13	1.99	0.45
1:A:355:ALA:HB1	1:A:494:LEU:HG	1.97	0.45
1:C:167:LEU:H	1:C:167:LEU:HD12	1.82	0.45
1:F:253:VAL:O	1:F:254:ALA:HB3	2.17	0.45
1:C:355:ALA:HB1	1:C:494:LEU:HG	1.98	0.45
1:E:375:SER:OG	1:E:529:GLU:O	2.33	0.45
1:A:468:PHE:C	1:A:468:PHE:CD2	2.90	0.45
1:D:355:ALA:HB1	1:D:494:LEU:HG	1.98	0.45
1:A:104:ILE:HG12	1:A:110:MET:HE2	1.98	0.45
5:E:2006:NAG:O7	5:E:2006:NAG:H5	2.17	0.44
1:B:116:VAL:CG1	1:B:143:ILE:HD13	2.47	0.44
1:F:110:MET:HE2	1:F:110:MET:HB2	1.73	0.44
1:D:320:ASP:OD2	1:D:457:ARG:NH1	2.50	0.44
1:A:286:PRO:HG2	1:A:289:LEU:HB2	2.00	0.44
1:C:142:ILE:HD12	2:C:2002:NAG:H81	1.98	0.44
1:E:235:GLU:HB3	1:E:258:THR:HB	1.99	0.44
1:D:28:TRP:HH2	1:D:57:ILE:HD11	1.82	0.44
1:D:167:LEU:H	1:D:167:LEU:CD1	2.30	0.44
1:E:48:CYS:HB2	1:E:54:TRP:CE2	2.53	0.44
1:E:40:LEU:HB3	9:E:2004:NAG:H61	1.99	0.44
1:F:382:ASN:O	1:F:385:ILE:HG12	2.18	0.44
1:B:267:THR:HG22	1:B:299:TYR:O	2.17	0.44
1:B:484:CYS:HB2	1:B:494:LEU:HD13	2.00	0.44
1:F:187:ILE:HG23	1:F:282:LEU:HD22	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:308:GLN:HE22	6:C:2010:NAG:H2	1.82	0.44
1:B:417:LEU:HD23	1:B:422:PHE:HD1	1.83	0.44
1:B:232:THR:HB	1:B:260:LEU:HB2	1.99	0.44
1:A:274:MET:HE3	1:A:274:MET:HB2	1.76	0.43
1:F:414:PRO:HD2	1:F:484:CYS:SG	2.57	0.43
1:A:388:SER:H	1:A:542:LEU:CD2	2.31	0.43
1:B:537:LEU:HD23	1:B:539:LEU:HB2	2.00	0.43
1:A:185:GLU:H	1:A:185:GLU:HG2	1.25	0.43
1:A:334:GLU:HA	1:A:335:PRO:HD3	1.83	0.43
1:B:91:ALA:N	1:B:511:GLN:OE1	2.41	0.43
1:D:527:ALA:HB1	1:D:529:GLU:HG3	2.00	0.43
1:C:386:TYR:O	1:C:390:THR:HG21	2.18	0.43
1:C:501:ASP:HA	1:C:502:PRO:HD2	1.80	0.43
1:F:116:VAL:CG1	1:F:143:ILE:HD13	2.47	0.43
1:E:83:HIS:CE1	1:E:254:ALA:HB1	2.54	0.43
1:E:214:VAL:HG13	1:E:256:ARG:HG3	2.01	0.43
1:D:214:VAL:HG13	1:D:256:ARG:HG3	2.00	0.43
1:C:382:ASN:O	1:C:385:ILE:HG12	2.18	0.43
1:F:516:ASN:O	1:F:519:GLU:HB3	2.19	0.43
1:E:98:PHE:HB3	1:E:365:PRO:HD2	2.01	0.43
1:D:542:LEU:H	1:D:542:LEU:HD12	1.84	0.43
1:D:255:GLN:HB2	1:D:457:ARG:NH2	2.34	0.43
1:B:361:THR:HG23	1:B:493:GLY:HA3	2.00	0.43
1:A:176:MET:CE	1:A:491:LEU:HB3	2.49	0.43
1:F:511:GLN:HA	1:F:511:GLN:OE1	2.18	0.43
1:A:167:LEU:H	1:A:167:LEU:HD12	1.84	0.43
1:D:95:GLY:N	1:D:100:THR:HG21	2.31	0.43
1:E:505:ILE:HG23	1:E:511:GLN:HG2	2.01	0.43
1:E:255:GLN:HB2	1:E:457:ARG:HH21	1.82	0.43
1:E:320:ASP:HA	1:E:323:LEU:HD22	2.00	0.43
1:C:98:PHE:HB3	1:C:365:PRO:HD2	2.00	0.43
1:E:144:LYS:HB2	1:E:144:LYS:HE2	1.70	0.43
1:A:133:TYR:O	1:A:138:LYS:HD3	2.18	0.43
1:B:144:LYS:HB2	1:B:144:LYS:HE2	1.75	0.43
1:F:370:LEU:HA	1:F:373:VAL:HG13	2.01	0.43
1:E:334:GLU:HA	1:E:335:PRO:HD3	1.83	0.43
1:E:274:MET:HE1	1:E:309:ASN:H	1.84	0.43
1:B:253:VAL:O	1:B:254:ALA:HB3	2.18	0.43
1:D:405:LEU:HD22	1:D:462:VAL:HG21	2.01	0.43
1:E:103:PRO:HG2	2:E:2007:NAG:H61	2.01	0.43
1:F:386:TYR:HE1	1:F:394:ILE:HD11	1.83	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:185:GLU:H	1:F:185:GLU:HG2	1.62	0.42
1:D:428:ASP:HB3	1:D:466:SER:OG	2.19	0.42
1:C:28:TRP:HH2	1:C:57:ILE:HD11	1.83	0.42
1:D:370:LEU:HA	1:D:373:VAL:HG13	2.01	0.42
1:E:220:VAL:HG21	1:E:277:PHE:HD2	1.85	0.42
1:D:274:MET:HE1	1:D:308:GLN:HA	2.01	0.42
1:A:310:TYR:HE2	6:A:2010:NAG:H82	1.85	0.42
1:E:40:LEU:N	1:E:40:LEU:HD23	2.33	0.42
1:D:144:LYS:NZ	2:D:3008:MAN:H2	2.34	0.42
1:B:127:SER:HB2	1:B:137:MET:SD	2.60	0.42
1:B:474:ALA:HB1	1:B:500:GLU:HG2	2.01	0.42
1:A:220:VAL:HG11	1:A:277:PHE:CD2	2.54	0.42
1:B:220:VAL:HG21	1:B:277:PHE:HD2	1.85	0.42
1:E:38:ASP:HB3	1:E:40:LEU:H	1.83	0.42
1:B:150:TYR:CD2	1:B:243:LYS:HE3	2.54	0.42
1:C:274:MET:HE3	1:C:309:ASN:HB3	2.01	0.42
1:B:81:HIS:CE1	1:B:418:HIS:ND1	2.88	0.42
1:F:43:ARG:NH2	1:F:135:ASP:OD1	2.52	0.42
1:B:318:LEU:HD21	1:B:323:LEU:HD11	2.02	0.42
1:F:395:LEU:HD12	1:F:500:GLU:CG	2.47	0.42
1:D:95:GLY:HA2	1:D:101:GLN:OE1	2.19	0.42
1:C:49:ASN:HD22	1:E:302:THR:HA	1.85	0.42
1:D:234:VAL:HA	1:D:241:THR:HG22	2.00	0.42
1:D:241:THR:HG23	1:D:242:GLU:O	2.19	0.42
1:D:253:VAL:O	1:D:254:ALA:HB3	2.19	0.42
1:F:234:VAL:C	1:F:241:THR:HG22	2.40	0.42
1:A:320:ASP:OD2	1:A:457:ARG:NH1	2.49	0.42
1:E:91:ALA:N	1:E:511:GLN:OE1	2.51	0.42
1:B:422:PHE:O	1:B:456:ARG:HA	2.19	0.42
1:C:268:ASP:OD1	1:C:269:LYS:HB2	2.19	0.42
1:D:468:PHE:CD2	1:D:468:PHE:C	2.93	0.42
1:C:233:VAL:HG21	1:C:318:LEU:HD22	2.01	0.42
1:B:274:MET:HB2	1:B:274:MET:HE3	1.94	0.42
1:D:234:VAL:C	1:D:241:THR:HG22	2.40	0.42
1:C:191:LEU:HG	1:C:277:PHE:CE1	2.54	0.42
1:C:28:TRP:CH2	1:C:57:ILE:HD11	2.55	0.42
1:A:232:THR:HB	1:A:260:LEU:HB2	2.02	0.42
1:E:413:HIS:O	1:E:461:TYR:HA	2.20	0.42
1:F:438:VAL:HB	1:F:439:PRO:CD	2.49	0.42
1:B:320:ASP:HA	1:B:323:LEU:HD22	2.02	0.41
1:C:134:GLU:OE2	1:C:218:GLY:N	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:542:LEU:HB2	1:B:543:THR:H	1.51	0.41
1:F:176:MET:CE	1:F:491:LEU:HB3	2.50	0.41
1:D:201:TRP:HE3	1:D:273:ILE:HD11	1.85	0.41
1:C:186:PRO:HG2	1:C:488:TRP:CZ2	2.55	0.41
1:F:428:ASP:OD1	1:F:429:ARG:N	2.52	0.41
1:D:420:HIS:NE2	1:D:500:GLU:OE1	2.42	0.41
1:F:255:GLN:HB2	1:F:457:ARG:HH21	1.85	0.41
1:E:185:GLU:H	1:E:185:GLU:HG2	1.23	0.41
1:B:334:GLU:HA	1:B:335:PRO:HD3	1.85	0.41
1:C:389:ASN:OD1	1:C:545:GLU:HG2	2.21	0.41
1:E:28:TRP:CH2	1:E:57:ILE:HD11	2.56	0.41
1:C:375:SER:OG	1:C:529:GLU:O	2.37	0.41
1:A:396:GLU:H	1:A:399:GLU:CD	2.24	0.41
1:F:264:LYS:HD2	1:F:271:PHE:CZ	2.56	0.41
1:A:33:ASP:HB2	1:A:47:THR:HG21	2.01	0.41
1:F:124:TRP:CE3	1:F:216:VAL:HG12	2.55	0.41
1:E:410:THR:HA	1:E:465:GLN:HG3	2.03	0.41
1:D:500:GLU:O	1:D:501:ASP:C	2.59	0.41
1:F:95:GLY:HA2	1:F:101:GLN:OE1	2.21	0.41
1:F:185:GLU:HG3	1:F:219:PHE:CZ	2.56	0.41
1:F:349:LYS:HD2	1:F:547:VAL:HG23	2.02	0.41
1:C:95:GLY:N	1:C:100:THR:HG21	2.34	0.41
1:C:543:THR:HG23	1:C:543:THR:O	2.21	0.41
1:B:361:THR:CG2	1:B:493:GLY:HA3	2.50	0.41
1:D:234:VAL:CA	1:D:241:THR:HG22	2.50	0.41
1:B:178:VAL:HG11	1:D:440:HIS:NE2	2.35	0.41
1:B:131:GLY:HA2	1:B:487:GLU:OE1	2.21	0.41
1:F:220:VAL:HG21	1:F:277:PHE:CD2	2.53	0.41
1:A:48:CYS:HB2	1:A:54:TRP:CE2	2.55	0.41
1:B:48:CYS:HB2	1:B:54:TRP:CE2	2.55	0.41
1:F:83:HIS:CE1	1:F:254:ALA:HB1	2.55	0.41
9:E:2003:NAG:H62	9:E:2004:NAG:HN2	1.86	0.41
1:F:275:GLN:HG3	1:F:293:ALA:HB3	2.03	0.41
1:B:501:ASP:HA	1:B:502:PRO:HD2	1.83	0.41
1:B:67:ILE:HD13	1:B:80:MET:HE1	2.03	0.41
1:B:33:ASP:HB2	1:B:47:THR:CG2	2.50	0.41
1:D:81:HIS:CE1	1:D:418:HIS:CE1	3.09	0.41
1:E:405:LEU:HD22	1:E:462:VAL:HG21	2.03	0.41
1:D:334:GLU:HA	1:D:335:PRO:HD3	1.81	0.41
1:E:428:ASP:O	1:E:463:ARG:NH1	2.53	0.41
1:B:500:GLU:O	1:B:501:ASP:C	2.58	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:91:ALA:N	1:D:511:GLN:OE1	2.52	0.41
1:C:484:CYS:HB2	1:C:494:LEU:HD13	2.02	0.41
1:C:346:ASP:OD2	1:C:347:ASN:N	2.54	0.41
1:A:500:GLU:O	1:A:501:ASP:C	2.59	0.41
1:C:500:GLU:O	1:C:501:ASP:C	2.60	0.40
1:E:255:GLN:HB2	1:E:457:ARG:NH2	2.36	0.40
1:B:264:LYS:HE2	1:B:264:LYS:HB3	1.90	0.40
1:A:202:GLU:OE1	1:A:301:LYS:HD3	2.20	0.40
1:A:58:THR:CG2	1:A:144:LYS:HD2	2.51	0.40
1:E:542:LEU:H	1:E:542:LEU:HD23	1.86	0.40
1:C:343:VAL:HG13	1:C:494:LEU:HD21	2.02	0.40
1:F:38:ASP:HB3	1:F:40:LEU:H	1.86	0.40
1:C:320:ASP:HA	1:C:323:LEU:HD22	2.02	0.40
1:C:438:VAL:HB	1:C:439:PRO:CD	2.51	0.40
1:D:422:PHE:O	1:D:456:ARG:HA	2.22	0.40
1:E:96:VAL:HA	1:E:97:PRO:HD2	1.90	0.40
1:E:468:PHE:CD2	1:E:468:PHE:C	2.94	0.40
1:B:67:ILE:HG21	1:B:80:MET:HE2	2.02	0.40
1:C:104:ILE:HG12	1:C:110:MET:HE2	2.04	0.40
1:F:484:CYS:HB2	1:F:494:LEU:HD13	2.03	0.40
1:E:302:THR:O	1:E:302:THR:HG22	2.21	0.40
1:A:81:HIS:CE1	1:A:418:HIS:CE1	3.08	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	527/534 (99%)	497 (94%)	23 (4%)	7 (1%)	15	44
1	B	527/534 (99%)	498 (94%)	23 (4%)	6 (1%)	17	50
1	C	527/534 (99%)	495 (94%)	27 (5%)	5 (1%)	21	55

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	527/534 (99%)	497 (94%)	22 (4%)	8 (2%)	13	40
1	E	527/534 (99%)	497 (94%)	24 (5%)	6 (1%)	17	50
1	F	527/534 (99%)	498 (94%)	23 (4%)	6 (1%)	17	50
All	All	3162/3204 (99%)	2982 (94%)	142 (4%)	38 (1%)	16	47

All (38) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	130	ASP
1	B	531	ASN
1	C	130	ASP
1	D	130	ASP
1	E	130	ASP
1	E	531	ASN
1	F	130	ASP
1	A	531	ASN
1	B	130	ASP
1	B	542	LEU
1	C	531	ASN
1	D	531	ASN
1	D	542	LEU
1	F	531	ASN
1	A	542	LEU
1	C	542	LEU
1	E	542	LEU
1	F	542	LEU
1	A	132	GLN
1	A	501	ASP
1	B	501	ASP
1	B	532	ALA
1	C	501	ASP
1	D	501	ASP
1	E	501	ASP
1	E	532	ALA
1	F	501	ASP
1	B	132	GLN
1	C	532	ALA
1	D	129	THR
1	D	132	GLN
1	D	397	LYS
1	D	532	ALA

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Mol	Chain	Res	Type
1	E	129	THR
1	F	532	ALA
1	A	129	THR
1	A	532	ALA
1	F	129	THR

### 5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	477/481 (99%)	430 (90%)	47 (10%)	10	28
1	B	477/481 (99%)	425 (89%)	52 (11%)	8	23
1	C	477/481 (99%)	431 (90%)	46 (10%)	10	29
1	D	477/481 (99%)	425 (89%)	52 (11%)	8	23
1	E	477/481 (99%)	432 (91%)	45 (9%)	11	31
1	F	477/481 (99%)	429 (90%)	48 (10%)	9	27
All	All	2862/2886 (99%)	2572 (90%)	290 (10%)	9	27

All (290) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	38	ASP
1	A	40	LEU
1	A	42	SER
1	A	43	ARG
1	A	69	LEU
1	A	76	THR
1	A	78	THR
1	A	99	LEU
1	A	100	THR
1	A	115	THR
1	A	144	LYS
1	A	162	GLU
1	A	169	THR

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Mol	Chain	Res	Type
1	A	185	GLU
1	A	193	VAL
1	A	196	THR
1	A	198	ASN
1	A	220	VAL
1	A	246	THR
1	A	259	VAL
1	A	280	THR
1	A	302	THR
1	A	311	VAL
1	A	323	LEU
1	A	345	MET
1	A	352	VAL
1	A	361	THR
1	A	371	MET
1	A	372	THR
1	A	373	VAL
1	A	389	ASN
1	A	390	THR
1	A	391	HIS
1	A	397	LYS
1	A	408	GLN
1	A	433	ASP
1	A	462	VAL
1	A	468	PHE
1	A	481	PHE
1	A	494	LEU
1	A	518	LEU
1	A	537	LEU
1	A	539	LEU
1	A	542	LEU
1	A	547	VAL
1	A	548	GLN
1	A	549	HIS
1	B	33	ASP
1	B	38	ASP
1	B	40	LEU
1	B	42	SER
1	B	43	ARG
1	B	69	LEU
1	B	76	THR
1	B	78	THR

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Mol	Chain	Res	Type
1	B	99	LEU
1	B	100	THR
1	B	120	VAL
1	B	133	TYR
1	B	145	ASP
1	B	162	GLU
1	B	185	GLU
1	B	193	VAL
1	B	196	THR
1	B	198	ASN
1	B	211	LEU
1	B	259	VAL
1	B	264	LYS
1	B	267	THR
1	B	268	ASP
1	B	269	LYS
1	B	292	ASN
1	B	302	THR
1	B	311	VAL
1	B	323	LEU
1	B	345	MET
1	B	352	VAL
1	B	371	MET
1	B	372	THR
1	B	373	VAL
1	B	389	ASN
1	B	391	HIS
1	B	397	LYS
1	B	408	GLN
1	B	433	ASP
1	B	435	LEU
1	B	438	VAL
1	B	462	VAL
1	B	468	PHE
1	B	481	PHE
1	B	494	LEU
1	B	518	LEU
1	B	525	SER
1	B	528	THR
1	B	539	LEU
1	B	542	LEU
1	B	547	VAL

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Mol	Chain	Res	Type
1	B	548	GLN
1	B	549	HIS
1	C	40	LEU
1	C	43	ARG
1	C	69	LEU
1	C	76	THR
1	C	78	THR
1	C	99	LEU
1	C	100	THR
1	C	101	GLN
1	C	110	MET
1	C	117	ASP
1	C	132	GLN
1	C	133	TYR
1	C	145	ASP
1	C	162	GLU
1	C	178	VAL
1	C	185	GLU
1	C	193	VAL
1	C	196	THR
1	C	198	ASN
1	C	211	LEU
1	C	259	VAL
1	C	264	LYS
1	C	268	ASP
1	C	269	LYS
1	C	302	THR
1	C	311	VAL
1	C	323	LEU
1	C	345	MET
1	C	352	VAL
1	C	371	MET
1	C	372	THR
1	C	373	VAL
1	C	389	ASN
1	C	391	HIS
1	C	408	GLN
1	C	433	ASP
1	C	446	ASN
1	C	462	VAL
1	C	468	PHE
1	C	481	PHE

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Mol	Chain	Res	Type
1	C	494	LEU
1	C	518	LEU
1	C	528	THR
1	C	539	LEU
1	C	547	VAL
1	C	549	HIS
1	D	40	LEU
1	D	43	ARG
1	D	64	ARG
1	D	69	LEU
1	D	76	THR
1	D	78	THR
1	D	100	THR
1	D	101	GLN
1	D	110	MET
1	D	115	THR
1	D	132	GLN
1	D	133	TYR
1	D	134	GLU
1	D	145	ASP
1	D	147	SER
1	D	162	GLU
1	D	182	THR
1	D	185	GLU
1	D	193	VAL
1	D	198	ASN
1	D	211	LEU
1	D	241	THR
1	D	246	THR
1	D	259	VAL
1	D	264	LYS
1	D	268	ASP
1	D	269	LYS
1	D	311	VAL
1	D	323	LEU
1	D	345	MET
1	D	371	MET
1	D	372	THR
1	D	373	VAL
1	D	389	ASN
1	D	390	THR
1	D	391	HIS

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Mol	Chain	Res	Type
1	D	397	LYS
1	D	430	THR
1	D	433	ASP
1	D	435	LEU
1	D	462	VAL
1	D	466	SER
1	D	468	PHE
1	D	481	PHE
1	D	491	LEU
1	D	494	LEU
1	D	518	LEU
1	D	539	LEU
1	D	542	LEU
1	D	547	VAL
1	D	548	GLN
1	D	549	HIS
1	E	33	ASP
1	E	40	LEU
1	E	43	ARG
1	E	69	LEU
1	E	76	THR
1	E	78	THR
1	E	99	LEU
1	E	101	GLN
1	E	133	TYR
1	E	145	ASP
1	E	146	ASP
1	E	162	GLU
1	E	185	GLU
1	E	193	VAL
1	E	196	THR
1	E	211	LEU
1	E	228	ASP
1	E	246	THR
1	E	268	ASP
1	E	269	LYS
1	E	292	ASN
1	E	311	VAL
1	E	312	ASP
1	E	315	ASP
1	E	323	LEU
1	E	345	MET

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Mol	Chain	Res	Type
1	E	352	VAL
1	E	371	MET
1	E	373	VAL
1	E	389	ASN
1	E	391	HIS
1	E	397	LYS
1	E	408	GLN
1	E	435	LEU
1	E	441	SER
1	E	462	VAL
1	E	468	PHE
1	E	481	PHE
1	E	494	LEU
1	E	501	ASP
1	E	523	SER
1	E	525	SER
1	E	538	ASP
1	E	543	THR
1	E	547	VAL
1	F	40	LEU
1	F	41	LYS
1	F	43	ARG
1	F	51	GLN
1	F	69	LEU
1	F	76	THR
1	F	85	LEU
1	F	99	LEU
1	F	100	THR
1	F	110	MET
1	F	115	THR
1	F	132	GLN
1	F	133	TYR
1	F	134	GLU
1	F	162	GLU
1	F	182	THR
1	F	185	GLU
1	F	187	ILE
1	F	193	VAL
1	F	198	ASN
1	F	211	LEU
1	F	259	VAL
1	F	267	THR

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Mol	Chain	Res	Type
1	F	268	ASP
1	F	269	LYS
1	F	287	SER
1	F	292	ASN
1	F	295	SER
1	F	323	LEU
1	F	342	ASP
1	F	345	MET
1	F	352	VAL
1	F	371	MET
1	F	373	VAL
1	F	389	ASN
1	F	391	HIS
1	F	397	LYS
1	F	427	ARG
1	F	458	ASP
1	F	462	VAL
1	F	466	SER
1	F	481	PHE
1	F	494	LEU
1	F	518	LEU
1	F	539	LEU
1	F	542	LEU
1	F	547	VAL
1	F	549	HIS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	101	GLN
1	A	255	GLN
1	B	222	GLN
1	B	255	GLN
1	B	275	GLN
1	B	324	GLN
1	B	517	HIS
1	C	51	GLN
1	C	66	GLN
1	C	517	HIS
1	D	324	GLN
1	E	195	ASN
1	E	382	ASN

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Mol	Chain	Res	Type
1	E	549	HIS
1	F	309	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

## 5.5 Carbohydrates ⓘ

135 carbohydrates are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
2	NAG	A	2001	1,2	14,14,15	0.69	0	15,19,21	1.32	2 (13%)
2	NAG	A	2002	2	14,14,15	0.52	0	15,19,21	0.99	1 (6%)
3	NAG	A	2003	1,3	14,14,15	0.75	0	15,19,21	1.95	4 (26%)
3	NAG	A	2004	3	14,14,15	0.61	0	15,19,21	0.96	0
4	NAG	A	2005	1,4	14,14,15	0.61	0	15,19,21	1.86	4 (26%)
2	NAG	A	2007	1,2	14,14,15	0.69	0	15,19,21	1.74	3 (20%)
6	NAG	A	2009	1,6	14,14,15	0.49	0	15,19,21	1.67	2 (13%)
6	NAG	A	2010	1,6	14,14,15	0.48	0	15,19,21	1.92	3 (20%)
6	NAG	A	2011	6	14,14,15	0.52	0	15,19,21	1.04	1 (6%)
2	NAG	A	2013	2	14,14,15	0.60	0	15,19,21	2.16	3 (20%)
4	NAG	A	2015	4	14,14,15	1.06	2 (14%)	15,19,21	1.33	1 (6%)
6	NAG	A	2016	6	14,14,15	0.45	0	15,19,21	0.88	0
2	BMA	A	3001	2	11,11,12	0.80	0	14,15,17	1.94	2 (14%)
6	BMA	A	3002	6	11,11,12	0.62	0	14,15,17	2.23	2 (14%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	BMA	A	3003	2	11,11,12	0.71	0	14,15,17	1.56	2 (14%)
3	BMA	A	3004	3	11,11,12	0.76	0	14,15,17	2.07	3 (21%)
2	MAN	A	3005	2	11,11,12	0.71	0	14,15,17	1.85	3 (21%)
2	MAN	A	3006	2	11,11,12	0.68	0	14,15,17	1.89	1 (7%)
2	MAN	A	3007	2	11,11,12	0.58	0	14,15,17	1.42	1 (7%)
2	MAN	A	3008	2	11,11,12	0.70	0	14,15,17	2.27	2 (14%)
3	MAN	A	3009	3	11,11,12	0.67	0	14,15,17	1.75	3 (21%)
3	MAN	A	3010	3	11,11,12	0.58	0	14,15,17	1.13	1 (7%)
3	MAN	A	3011	3	11,11,12	0.69	0	14,15,17	1.17	1 (7%)
6	BMA	A	3013	6	11,11,12	0.91	0	14,15,17	1.24	1 (7%)
2	NAG	B	2001	1,2	14,14,15	0.69	0	15,19,21	0.97	0
2	NAG	B	2002	2	14,14,15	0.59	0	15,19,21	1.16	1 (6%)
3	NAG	B	2003	1,3	14,14,15	0.67	0	15,19,21	1.27	2 (13%)
3	NAG	B	2004	3	14,14,15	0.55	0	15,19,21	1.04	1 (6%)
2	NAG	B	2007	1,2	14,14,15	0.54	0	15,19,21	1.84	3 (20%)
4	NAG	B	2008	1,4	14,14,15	0.54	0	15,19,21	0.86	0
4	NAG	B	2009	1,4	14,14,15	0.45	0	15,19,21	1.87	4 (26%)
8	NAG	B	2010	1,8	14,14,15	0.72	0	15,19,21	1.18	1 (6%)
8	NAG	B	2011	8	14,14,15	0.61	0	15,19,21	1.26	2 (13%)
2	NAG	B	2013	2	14,14,15	0.71	0	15,19,21	1.24	2 (13%)
4	NAG	B	2016	4	14,14,15	0.46	0	15,19,21	1.26	1 (6%)
4	NAG	B	2017	4	14,14,15	0.48	0	15,19,21	1.02	2 (13%)
2	BMA	B	3001	2	11,11,12	0.74	0	14,15,17	1.03	1 (7%)
8	BMA	B	3002	8	11,11,12	0.53	0	14,15,17	1.06	1 (7%)
2	BMA	B	3003	2	11,11,12	0.72	0	14,15,17	1.73	5 (35%)
3	BMA	B	3004	3	11,11,12	0.77	0	14,15,17	1.60	2 (14%)
2	MAN	B	3005	2	11,11,12	0.59	0	14,15,17	2.19	5 (35%)
2	MAN	B	3006	2	11,11,12	1.70	2 (18%)	14,15,17	2.39	3 (21%)
2	MAN	B	3007	2	11,11,12	0.68	0	14,15,17	2.86	5 (35%)
2	MAN	B	3008	2	11,11,12	0.43	0	14,15,17	1.44	3 (21%)
3	MAN	B	3009	3	11,11,12	0.55	0	14,15,17	1.18	2 (14%)
3	MAN	B	3010	3	11,11,12	0.59	0	14,15,17	2.19	2 (14%)
3	MAN	B	3011	3	11,11,12	0.54	0	14,15,17	1.35	2 (14%)
8	MAN	B	3014	8	11,11,12	0.53	0	14,15,17	2.28	4 (28%)
2	NAG	C	2001	1,2	14,14,15	0.71	0	15,19,21	1.17	3 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	NAG	C	2002	2	14,14,15	0.61	0	15,19,21	1.46	3 (20%)
9	NAG	C	2003	1,9	14,14,15	0.88	1 (7%)	15,19,21	1.75	6 (40%)
9	NAG	C	2004	9	14,14,15	0.43	0	15,19,21	0.82	0
2	NAG	C	2007	1,2	14,14,15	0.46	0	15,19,21	2.15	2 (13%)
4	NAG	C	2008	1,4	14,14,15	0.50	0	15,19,21	1.18	1 (6%)
6	NAG	C	2009	1,6	14,14,15	1.97	3 (21%)	15,19,21	0.88	0
6	NAG	C	2010	1,6	14,14,15	0.47	0	15,19,21	1.48	4 (26%)
6	NAG	C	2011	6	14,14,15	0.41	0	15,19,21	1.15	1 (6%)
2	NAG	C	2013	2	14,14,15	0.72	0	15,19,21	1.00	2 (13%)
6	NAG	C	2016	6	14,14,15	1.73	3 (21%)	15,19,21	2.37	4 (26%)
4	NAG	C	2017	4	14,14,15	1.19	2 (14%)	15,19,21	1.49	2 (13%)
2	BMA	C	3001	2	11,11,12	0.54	0	14,15,17	2.03	4 (28%)
6	BMA	C	3002	6	11,11,12	0.65	0	14,15,17	0.95	0
2	BMA	C	3003	2	11,11,12	0.68	0	14,15,17	1.40	2 (14%)
9	BMA	C	3004	9	11,11,12	0.57	0	14,15,17	2.04	3 (21%)
2	MAN	C	3005	2	11,11,12	0.75	0	14,15,17	1.67	2 (14%)
2	MAN	C	3006	2	11,11,12	0.59	0	14,15,17	1.69	2 (14%)
2	MAN	C	3007	2	11,11,12	0.55	0	14,15,17	1.53	3 (21%)
2	MAN	C	3008	2	11,11,12	0.62	0	14,15,17	1.43	3 (21%)
9	MAN	C	3009	9	11,11,12	0.76	0	14,15,17	1.95	3 (21%)
9	MAN	C	3010	9	11,11,12	0.58	0	14,15,17	1.37	1 (7%)
9	MAN	C	3011	9	11,11,12	0.69	0	14,15,17	0.83	0
9	MAN	C	3012	9	11,11,12	0.56	0	14,15,17	2.24	3 (21%)
6	BMA	C	3013	6	11,11,12	2.42	1 (9%)	14,15,17	1.92	4 (28%)
2	NAG	D	2001	1,2	14,14,15	0.52	0	15,19,21	0.78	0
2	NAG	D	2002	2	14,14,15	0.57	0	15,19,21	1.28	2 (13%)
3	NAG	D	2003	1,3	14,14,15	0.60	0	15,19,21	1.74	2 (13%)
3	NAG	D	2004	3	14,14,15	0.67	0	15,19,21	0.89	1 (6%)
2	NAG	D	2007	1,2	14,14,15	0.40	0	15,19,21	1.29	1 (6%)
4	NAG	D	2009	1,4	14,14,15	1.39	2 (14%)	15,19,21	1.41	1 (6%)
6	NAG	D	2010	1,6	14,14,15	0.51	0	15,19,21	1.04	0
6	NAG	D	2011	6	14,14,15	0.52	0	15,19,21	0.74	0
2	NAG	D	2013	2	14,14,15	0.56	0	15,19,21	0.84	1 (6%)
4	NAG	D	2016	4	14,14,15	0.49	0	15,19,21	0.72	0
2	BMA	D	3001	2	11,11,12	0.56	0	14,15,17	1.46	3 (21%)
6	BMA	D	3002	6	11,11,12	0.53	0	14,15,17	1.01	2 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	BMA	D	3003	2	11,11,12	0.65	0	14,15,17	1.30	2 (14%)
3	BMA	D	3004	3	11,11,12	0.72	0	14,15,17	1.97	4 (28%)
2	MAN	D	3005	2	11,11,12	0.52	0	14,15,17	1.79	3 (21%)
2	MAN	D	3006	2	11,11,12	0.60	0	14,15,17	1.59	2 (14%)
2	MAN	D	3007	2	11,11,12	0.56	0	14,15,17	1.36	1 (7%)
2	MAN	D	3008	2	11,11,12	0.62	0	14,15,17	1.23	2 (14%)
3	MAN	D	3009	3	11,11,12	1.05	1 (9%)	14,15,17	2.16	3 (21%)
3	MAN	D	3010	3	11,11,12	0.58	0	14,15,17	1.18	1 (7%)
3	MAN	D	3011	3	11,11,12	0.61	0	14,15,17	1.00	1 (7%)
2	NAG	E	2001	1,2	14,14,15	0.58	0	15,19,21	1.01	0
2	NAG	E	2002	2	14,14,15	0.53	0	15,19,21	0.74	0
9	NAG	E	2003	1,9	14,14,15	0.55	0	15,19,21	0.90	0
9	NAG	E	2004	9	14,14,15	0.48	0	15,19,21	1.30	2 (13%)
2	NAG	E	2007	1,2	14,14,15	0.53	0	15,19,21	1.30	3 (20%)
4	NAG	E	2009	1,4	14,14,15	0.52	0	15,19,21	1.06	1 (6%)
6	NAG	E	2010	1,6	14,14,15	0.58	0	15,19,21	1.75	4 (26%)
6	NAG	E	2011	6	14,14,15	0.59	0	15,19,21	1.05	2 (13%)
2	NAG	E	2013	2	14,14,15	0.49	0	15,19,21	0.91	1 (6%)
4	NAG	E	2016	4	14,14,15	0.56	0	15,19,21	1.01	1 (6%)
2	BMA	E	3001	2	11,11,12	0.77	0	14,15,17	2.23	4 (28%)
6	BMA	E	3002	6	11,11,12	0.87	0	14,15,17	2.03	4 (28%)
2	BMA	E	3003	2	11,11,12	0.61	0	14,15,17	1.13	1 (7%)
9	BMA	E	3004	9	11,11,12	0.61	0	14,15,17	1.62	4 (28%)
2	MAN	E	3005	2	11,11,12	0.54	0	14,15,17	1.48	2 (14%)
2	MAN	E	3006	2	11,11,12	0.56	0	14,15,17	1.52	2 (14%)
2	MAN	E	3007	2	11,11,12	0.58	0	14,15,17	0.66	0
2	MAN	E	3008	2	11,11,12	0.53	0	14,15,17	1.49	1 (7%)
9	MAN	E	3009	9	11,11,12	0.53	0	14,15,17	1.66	1 (7%)
9	MAN	E	3010	9	11,11,12	0.62	0	14,15,17	1.60	3 (21%)
9	MAN	E	3011	9	11,11,12	0.54	0	14,15,17	1.01	1 (7%)
9	MAN	E	3012	9	11,11,12	0.69	0	14,15,17	1.64	2 (14%)
2	NAG	F	2001	1,2	14,14,15	0.59	0	15,19,21	0.95	0
2	NAG	F	2002	2	14,14,15	0.58	0	15,19,21	1.21	1 (6%)
3	NAG	F	2003	1,3	14,14,15	0.61	0	15,19,21	1.07	2 (13%)
3	NAG	F	2004	3	14,14,15	0.71	0	15,19,21	1.47	2 (13%)
2	NAG	F	2007	1,2	14,14,15	0.50	0	15,19,21	1.33	1 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
6	NAG	F	2010	1,6	14,14,15	0.49	0	15,19,21	1.11	1 (6%)
6	NAG	F	2011	6	14,14,15	0.56	0	15,19,21	1.39	3 (20%)
2	NAG	F	2013	2	14,14,15	0.53	0	15,19,21	1.09	2 (13%)
2	BMA	F	3001	2	11,11,12	0.63	0	14,15,17	1.50	3 (21%)
6	BMA	F	3002	6	11,11,12	1.81	2 (18%)	14,15,17	1.10	0
2	BMA	F	3003	2	11,11,12	0.69	0	14,15,17	1.36	1 (7%)
3	BMA	F	3004	3	11,11,12	0.78	0	14,15,17	1.03	2 (14%)
2	MAN	F	3005	2	11,11,12	0.65	0	14,15,17	0.92	1 (7%)
2	MAN	F	3006	2	11,11,12	1.54	1 (9%)	14,15,17	1.90	2 (14%)
2	MAN	F	3007	2	11,11,12	0.62	0	14,15,17	1.84	2 (14%)
2	MAN	F	3008	2	11,11,12	0.47	0	14,15,17	1.69	1 (7%)
3	MAN	F	3009	3	11,11,12	0.58	0	14,15,17	1.80	2 (14%)
3	MAN	F	3010	3	11,11,12	1.16	1 (9%)	14,15,17	1.50	2 (14%)
3	MAN	F	3011	3	11,11,12	0.93	1 (9%)	14,15,17	1.02	1 (7%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	A	2001	1,2	-	0/6/23/26	0/1/1/1
2	NAG	A	2002	2	-	0/6/23/26	0/1/1/1
3	NAG	A	2003	1,3	1/1/5/7	0/6/23/26	0/1/1/1
3	NAG	A	2004	3	-	0/6/23/26	0/1/1/1
4	NAG	A	2005	1,4	-	0/6/23/26	0/1/1/1
2	NAG	A	2007	1,2	-	0/6/23/26	0/1/1/1
6	NAG	A	2009	1,6	-	2/6/23/26	0/1/1/1
6	NAG	A	2010	1,6	1/1/5/7	0/6/23/26	0/1/1/1
6	NAG	A	2011	6	-	0/6/23/26	0/1/1/1
2	NAG	A	2013	2	-	0/6/23/26	0/1/1/1
4	NAG	A	2015	4	-	0/6/23/26	0/1/1/1
6	NAG	A	2016	6	-	0/6/23/26	0/1/1/1
2	BMA	A	3001	2	-	0/2/19/22	0/1/1/1
6	BMA	A	3002	6	-	0/2/19/22	0/1/1/1
2	BMA	A	3003	2	-	0/2/19/22	0/1/1/1
3	BMA	A	3004	3	-	0/2/19/22	0/1/1/1
2	MAN	A	3005	2	-	0/2/19/22	0/1/1/1
2	MAN	A	3006	2	-	0/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	MAN	A	3007	2	-	0/2/19/22	0/1/1/1
2	MAN	A	3008	2	-	0/2/19/22	1/1/1/1
3	MAN	A	3009	3	-	0/2/19/22	0/1/1/1
3	MAN	A	3010	3	-	0/2/19/22	0/1/1/1
3	MAN	A	3011	3	-	0/2/19/22	0/1/1/1
6	BMA	A	3013	6	-	0/2/19/22	0/1/1/1
2	NAG	B	2001	1,2	-	0/6/23/26	0/1/1/1
2	NAG	B	2002	2	-	0/6/23/26	0/1/1/1
3	NAG	B	2003	1,3	1/1/5/7	0/6/23/26	0/1/1/1
3	NAG	B	2004	3	-	0/6/23/26	0/1/1/1
2	NAG	B	2007	1,2	-	0/6/23/26	0/1/1/1
4	NAG	B	2008	1,4	-	0/6/23/26	0/1/1/1
4	NAG	B	2009	1,4	-	0/6/23/26	0/1/1/1
8	NAG	B	2010	1,8	1/1/5/7	0/6/23/26	0/1/1/1
8	NAG	B	2011	8	-	0/6/23/26	0/1/1/1
2	NAG	B	2013	2	-	0/6/23/26	0/1/1/1
4	NAG	B	2016	4	-	0/6/23/26	0/1/1/1
4	NAG	B	2017	4	-	0/6/23/26	0/1/1/1
2	BMA	B	3001	2	-	0/2/19/22	0/1/1/1
8	BMA	B	3002	8	-	0/2/19/22	0/1/1/1
2	BMA	B	3003	2	-	0/2/19/22	0/1/1/1
3	BMA	B	3004	3	-	0/2/19/22	0/1/1/1
2	MAN	B	3005	2	-	0/2/19/22	0/1/1/1
2	MAN	B	3006	2	-	0/2/19/22	0/1/1/1
2	MAN	B	3007	2	-	0/2/19/22	0/1/1/1
2	MAN	B	3008	2	-	0/2/19/22	1/1/1/1
3	MAN	B	3009	3	-	0/2/19/22	0/1/1/1
3	MAN	B	3010	3	-	0/2/19/22	0/1/1/1
3	MAN	B	3011	3	-	0/2/19/22	0/1/1/1
8	MAN	B	3014	8	-	0/2/19/22	0/1/1/1
2	NAG	C	2001	1,2	-	0/6/23/26	0/1/1/1
2	NAG	C	2002	2	-	0/6/23/26	0/1/1/1
9	NAG	C	2003	1,9	1/1/5/7	0/6/23/26	0/1/1/1
9	NAG	C	2004	9	-	0/6/23/26	0/1/1/1
2	NAG	C	2007	1,2	-	0/6/23/26	0/1/1/1
4	NAG	C	2008	1,4	-	0/6/23/26	0/1/1/1
6	NAG	C	2009	1,6	-	0/6/23/26	0/1/1/1
6	NAG	C	2010	1,6	1/1/5/7	0/6/23/26	0/1/1/1
6	NAG	C	2011	6	-	0/6/23/26	0/1/1/1
2	NAG	C	2013	2	-	0/6/23/26	0/1/1/1
6	NAG	C	2016	6	-	1/6/23/26	0/1/1/1
4	NAG	C	2017	4	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	BMA	C	3001	2	-	0/2/19/22	0/1/1/1
6	BMA	C	3002	6	-	0/2/19/22	0/1/1/1
2	BMA	C	3003	2	-	0/2/19/22	0/1/1/1
9	BMA	C	3004	9	-	0/2/19/22	0/1/1/1
2	MAN	C	3005	2	-	0/2/19/22	0/1/1/1
2	MAN	C	3006	2	-	0/2/19/22	0/1/1/1
2	MAN	C	3007	2	-	0/2/19/22	0/1/1/1
2	MAN	C	3008	2	-	0/2/19/22	0/1/1/1
9	MAN	C	3009	9	-	0/2/19/22	0/1/1/1
9	MAN	C	3010	9	-	0/2/19/22	0/1/1/1
9	MAN	C	3011	9	-	0/2/19/22	0/1/1/1
9	MAN	C	3012	9	-	0/2/19/22	0/1/1/1
6	BMA	C	3013	6	-	0/2/19/22	0/1/1/1
2	NAG	D	2001	1,2	-	0/6/23/26	0/1/1/1
2	NAG	D	2002	2	-	0/6/23/26	0/1/1/1
3	NAG	D	2003	1,3	1/1/5/7	0/6/23/26	0/1/1/1
3	NAG	D	2004	3	-	0/6/23/26	0/1/1/1
2	NAG	D	2007	1,2	1/1/5/7	0/6/23/26	0/1/1/1
4	NAG	D	2009	1,4	1/1/5/7	0/6/23/26	0/1/1/1
6	NAG	D	2010	1,6	1/1/5/7	0/6/23/26	0/1/1/1
6	NAG	D	2011	6	-	0/6/23/26	0/1/1/1
2	NAG	D	2013	2	-	0/6/23/26	0/1/1/1
4	NAG	D	2016	4	-	0/6/23/26	0/1/1/1
2	BMA	D	3001	2	-	0/2/19/22	0/1/1/1
6	BMA	D	3002	6	-	0/2/19/22	0/1/1/1
2	BMA	D	3003	2	-	0/2/19/22	0/1/1/1
3	BMA	D	3004	3	-	0/2/19/22	0/1/1/1
2	MAN	D	3005	2	-	0/2/19/22	0/1/1/1
2	MAN	D	3006	2	-	0/2/19/22	0/1/1/1
2	MAN	D	3007	2	-	0/2/19/22	0/1/1/1
2	MAN	D	3008	2	-	0/2/19/22	0/1/1/1
3	MAN	D	3009	3	-	0/2/19/22	0/1/1/1
3	MAN	D	3010	3	-	0/2/19/22	0/1/1/1
3	MAN	D	3011	3	-	0/2/19/22	0/1/1/1
2	NAG	E	2001	1,2	-	0/6/23/26	0/1/1/1
2	NAG	E	2002	2	-	0/6/23/26	0/1/1/1
9	NAG	E	2003	1,9	1/1/5/7	0/6/23/26	0/1/1/1
9	NAG	E	2004	9	-	0/6/23/26	0/1/1/1
2	NAG	E	2007	1,2	1/1/5/7	0/6/23/26	0/1/1/1
4	NAG	E	2009	1,4	-	1/6/23/26	0/1/1/1
6	NAG	E	2010	1,6	1/1/5/7	0/6/23/26	0/1/1/1
6	NAG	E	2011	6	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	E	2013	2	-	0/6/23/26	0/1/1/1
4	NAG	E	2016	4	-	0/6/23/26	0/1/1/1
2	BMA	E	3001	2	-	0/2/19/22	0/1/1/1
6	BMA	E	3002	6	-	0/2/19/22	0/1/1/1
2	BMA	E	3003	2	-	0/2/19/22	0/1/1/1
9	BMA	E	3004	9	-	0/2/19/22	0/1/1/1
2	MAN	E	3005	2	-	0/2/19/22	1/1/1/1
2	MAN	E	3006	2	-	0/2/19/22	0/1/1/1
2	MAN	E	3007	2	-	0/2/19/22	0/1/1/1
2	MAN	E	3008	2	-	0/2/19/22	0/1/1/1
9	MAN	E	3009	9	-	0/2/19/22	0/1/1/1
9	MAN	E	3010	9	-	0/2/19/22	0/1/1/1
9	MAN	E	3011	9	-	0/2/19/22	0/1/1/1
9	MAN	E	3012	9	-	0/2/19/22	0/1/1/1
2	NAG	F	2001	1,2	-	0/6/23/26	0/1/1/1
2	NAG	F	2002	2	-	0/6/23/26	0/1/1/1
3	NAG	F	2003	1,3	1/1/5/7	0/6/23/26	0/1/1/1
3	NAG	F	2004	3	-	0/6/23/26	0/1/1/1
2	NAG	F	2007	1,2	-	2/6/23/26	0/1/1/1
6	NAG	F	2010	1,6	1/1/5/7	0/6/23/26	0/1/1/1
6	NAG	F	2011	6	-	0/6/23/26	0/1/1/1
2	NAG	F	2013	2	-	0/6/23/26	0/1/1/1
2	BMA	F	3001	2	-	0/2/19/22	0/1/1/1
6	BMA	F	3002	6	-	0/2/19/22	0/1/1/1
2	BMA	F	3003	2	-	0/2/19/22	0/1/1/1
3	BMA	F	3004	3	-	0/2/19/22	0/1/1/1
2	MAN	F	3005	2	-	0/2/19/22	0/1/1/1
2	MAN	F	3006	2	-	0/2/19/22	1/1/1/1
2	MAN	F	3007	2	-	0/2/19/22	0/1/1/1
2	MAN	F	3008	2	-	0/2/19/22	1/1/1/1
3	MAN	F	3009	3	-	0/2/19/22	0/1/1/1
3	MAN	F	3010	3	-	0/2/19/22	0/1/1/1
3	MAN	F	3011	3	-	0/2/19/22	0/1/1/1

All (22) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	C	2003	NAG	O5-C1	-2.16	1.40	1.43
4	A	2015	NAG	C8-C7	2.03	1.54	1.50
4	A	2015	NAG	C1-C2	2.40	1.55	1.52
6	C	2016	NAG	C7-N2	2.45	1.43	1.34
6	F	3002	BMA	C4-C3	2.47	1.58	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	2009	NAG	O7-C7	2.47	1.28	1.23
4	C	2017	NAG	O7-C7	2.53	1.29	1.23
3	F	3011	MAN	O6-C6	2.55	1.53	1.42
4	C	2017	NAG	C8-C7	2.69	1.55	1.50
3	D	3009	MAN	O6-C6	2.77	1.54	1.42
6	C	2009	NAG	O6-C6	3.04	1.55	1.42
6	C	2016	NAG	O7-C7	3.29	1.30	1.23
3	F	3010	MAN	O6-C6	3.46	1.57	1.42
2	B	3006	MAN	C2-C3	3.52	1.57	1.52
2	B	3006	MAN	O6-C6	3.74	1.58	1.42
4	D	2009	NAG	C8-C7	4.18	1.58	1.50
6	C	2009	NAG	O7-C7	4.33	1.33	1.23
6	C	2016	NAG	C8-C7	4.69	1.60	1.50
6	F	3002	BMA	O6-C6	4.70	1.62	1.42
6	C	2009	NAG	C8-C7	4.74	1.60	1.50
2	F	3006	MAN	O6-C6	4.77	1.63	1.42
6	C	3013	BMA	O6-C6	7.58	1.75	1.42

All (258) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	C	2016	NAG	C2-N2-C7	-6.72	114.40	123.04
2	D	3005	MAN	C1-C2-C3	-5.11	103.50	109.54
2	B	3005	MAN	C1-C2-C3	-4.85	103.81	109.54
2	A	3005	MAN	C1-C2-C3	-4.51	104.20	109.54
9	C	3009	MAN	O5-C1-C2	-4.34	103.82	110.86
2	C	3005	MAN	C1-C2-C3	-4.26	104.50	109.54
2	B	3003	BMA	O3-C3-C2	-4.04	102.71	110.00
6	C	2016	NAG	O7-C7-N2	-3.88	113.95	121.86
3	A	3009	MAN	O5-C1-C2	-3.79	104.71	110.86
6	C	3013	BMA	O6-C6-C5	-3.69	99.13	111.33
2	B	2007	NAG	C2-N2-C7	-3.68	118.31	123.04
2	C	2002	NAG	O4-C4-C3	-3.42	102.65	110.34
2	C	2002	NAG	C2-N2-C7	-3.33	118.76	123.04
3	A	3004	BMA	C3-C4-C5	-3.25	104.53	110.20
2	C	3008	MAN	C1-C2-C3	-3.24	105.71	109.54
2	C	2007	NAG	C2-N2-C7	-3.20	118.92	123.04
9	E	3004	BMA	C1-C2-C3	-3.12	105.85	109.54
6	A	2010	NAG	C3-C4-C5	-3.01	104.95	110.20
2	D	3003	BMA	O3-C3-C2	-3.00	104.58	110.00
6	F	2011	NAG	C2-N2-C7	-2.98	119.21	123.04
3	D	3004	BMA	C3-C4-C5	-2.89	105.15	110.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	C	2010	NAG	C3-C4-C5	-2.86	105.22	110.20
2	A	3003	BMA	O3-C3-C2	-2.84	104.86	110.00
2	C	3003	BMA	O3-C3-C2	-2.81	104.92	110.00
9	C	2003	NAG	C3-C4-C5	-2.72	105.45	110.20
2	B	3008	MAN	C2-C3-C4	-2.63	106.57	111.04
2	C	3008	MAN	O5-C1-C2	-2.57	106.68	110.86
8	B	2011	NAG	O4-C4-C3	-2.56	104.58	110.34
6	C	2010	NAG	O7-C7-C8	-2.49	117.50	122.06
2	C	2001	NAG	O7-C7-C8	-2.45	117.57	122.06
8	B	2011	NAG	C1-O5-C5	-2.44	109.16	112.25
2	C	3007	MAN	C1-C2-C3	-2.41	106.69	109.54
2	A	2007	NAG	C2-N2-C7	-2.40	119.96	123.04
3	A	2003	NAG	C3-C2-N2	-2.37	104.87	110.56
6	F	2011	NAG	C4-C3-C2	-2.34	107.59	111.23
2	A	2001	NAG	C6-C5-C4	-2.32	107.28	113.02
9	C	2003	NAG	C3-C2-N2	-2.30	105.06	110.56
2	E	3003	BMA	O3-C3-C2	-2.28	105.87	110.00
2	B	3005	MAN	O3-C3-C2	-2.27	105.90	110.00
2	D	2002	NAG	O4-C4-C3	-2.26	105.25	110.34
2	C	3001	BMA	O3-C3-C2	-2.26	105.92	110.00
8	B	2010	NAG	C2-N2-C7	-2.25	120.15	123.04
2	D	3001	BMA	O3-C3-C2	-2.22	105.99	110.00
4	A	2005	NAG	O4-C4-C3	-2.20	105.38	110.34
6	A	2010	NAG	O7-C7-C8	-2.16	118.09	122.06
6	E	2010	NAG	O7-C7-C8	-2.16	118.11	122.06
3	A	2003	NAG	C3-C4-C5	-2.12	106.50	110.20
2	C	3007	MAN	O5-C1-C2	-2.12	107.42	110.86
2	D	3005	MAN	O5-C1-C2	-2.10	107.45	110.86
2	C	2001	NAG	O4-C4-C3	-2.09	105.63	110.34
2	E	3005	MAN	C1-C2-C3	-2.08	107.08	109.54
3	B	3009	MAN	O5-C1-C2	-2.02	107.58	110.86
6	E	3002	BMA	O5-C1-C2	-2.02	107.59	110.86
4	B	2009	NAG	C4-C3-C2	-2.01	108.10	111.23
9	C	3012	MAN	C1-C2-C3	-2.01	107.16	109.54
2	E	2013	NAG	C1-O5-C5	2.00	114.79	112.25
4	B	2017	NAG	C1-O5-C5	2.01	114.80	112.25
2	A	3005	MAN	C1-O5-C5	2.01	114.80	112.25
3	B	2004	NAG	C2-N2-C7	2.01	125.62	123.04
2	C	2001	NAG	C4-C3-C2	2.02	114.36	111.23
2	D	3008	MAN	C1-O5-C5	2.02	114.81	112.25
6	E	2011	NAG	C1-O5-C5	2.04	114.84	112.25
2	E	2007	NAG	C1-O5-C5	2.05	114.85	112.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	3005	MAN	O5-C5-C6	2.05	111.79	107.35
2	E	3001	BMA	O5-C5-C6	2.06	111.81	107.35
2	B	3003	BMA	O5-C5-C6	2.06	111.81	107.35
2	C	3008	MAN	O2-C2-C1	2.07	113.36	109.21
3	B	3011	MAN	C1-C2-C3	2.08	112.00	109.54
9	C	2003	NAG	C8-C7-N2	2.08	120.08	116.11
6	A	2009	NAG	C3-C4-C5	2.08	113.82	110.20
9	E	3004	BMA	C1-O5-C5	2.09	114.90	112.25
2	C	3001	BMA	O5-C1-C2	2.10	114.26	110.86
3	A	2003	NAG	C8-C7-N2	2.10	120.12	116.11
6	C	2016	NAG	C1-O5-C5	2.10	114.92	112.25
3	B	2003	NAG	C1-O5-C5	2.12	114.93	112.25
9	C	3009	MAN	C2-C3-C4	2.12	114.65	111.04
6	D	3002	BMA	C1-O5-C5	2.13	114.95	112.25
3	F	2003	NAG	C8-C7-N2	2.15	120.22	116.11
9	E	2004	NAG	C3-C4-C5	2.16	113.97	110.20
2	B	3008	MAN	O5-C5-C6	2.18	112.07	107.35
2	C	2013	NAG	C2-N2-C7	2.18	125.84	123.04
3	F	3010	MAN	C3-C4-C5	2.18	114.00	110.20
9	C	3012	MAN	O2-C2-C1	2.18	113.58	109.21
2	D	2013	NAG	C3-C4-C5	2.19	114.02	110.20
2	B	3003	BMA	C3-C4-C5	2.20	114.03	110.20
2	D	3005	MAN	O2-C2-C1	2.21	113.63	109.21
3	F	3004	BMA	C1-O5-C5	2.22	115.06	112.25
2	A	3008	MAN	O5-C5-C6	2.22	112.16	107.35
6	E	2010	NAG	C8-C7-N2	2.24	120.38	116.11
2	B	3003	BMA	C1-C2-C3	2.24	112.19	109.54
3	B	3004	BMA	O3-C3-C4	2.27	115.45	110.34
2	B	3007	MAN	C1-C2-C3	2.27	112.23	109.54
2	F	2013	NAG	C2-N2-C7	2.28	125.97	123.04
6	D	3002	BMA	C1-C2-C3	2.28	112.24	109.54
2	B	3001	BMA	C1-O5-C5	2.29	115.15	112.25
2	B	2013	NAG	C4-C3-C2	2.29	114.78	111.23
3	B	2003	NAG	C2-N2-C7	2.31	126.01	123.04
2	B	2013	NAG	O7-C7-N2	2.31	126.58	121.86
2	B	2007	NAG	O5-C5-C6	2.32	112.37	107.35
4	A	2005	NAG	C8-C7-N2	2.33	120.56	116.11
2	E	3006	MAN	C1-C2-C3	2.33	112.30	109.54
3	D	2004	NAG	C1-O5-C5	2.33	115.21	112.25
4	E	2009	NAG	C2-N2-C7	2.33	126.04	123.04
4	B	2017	NAG	C3-C4-C5	2.33	114.27	110.20
3	B	3009	MAN	C1-O5-C5	2.33	115.21	112.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	C	3013	BMA	C1-O5-C5	2.35	115.23	112.25
2	D	3001	BMA	O5-C5-C6	2.36	112.45	107.35
2	C	2002	NAG	C1-O5-C5	2.36	115.25	112.25
2	D	3008	MAN	C3-C4-C5	2.37	114.33	110.20
6	C	2010	NAG	C1-O5-C5	2.38	115.26	112.25
8	B	3014	MAN	O5-C5-C6	2.38	112.50	107.35
2	C	3005	MAN	O2-C2-C1	2.40	114.01	109.21
2	C	2013	NAG	C1-O5-C5	2.40	115.30	112.25
6	E	2011	NAG	C4-C3-C2	2.41	114.97	111.23
4	C	2017	NAG	C3-C4-C5	2.41	114.39	110.20
2	F	2013	NAG	C4-C3-C2	2.41	114.97	111.23
9	E	3010	MAN	C3-C4-C5	2.42	114.42	110.20
6	C	3013	BMA	C2-C3-C4	2.43	115.16	111.04
9	C	2003	NAG	C4-C3-C2	2.46	115.06	111.23
9	E	3004	BMA	O3-C3-C4	2.48	115.92	110.34
9	C	2003	NAG	C6-C5-C4	2.49	119.15	113.02
2	E	2007	NAG	C3-C4-C5	2.50	114.56	110.20
2	B	3007	MAN	C2-C3-C4	2.56	115.39	111.04
3	F	2003	NAG	C2-N2-C7	2.56	126.33	123.04
2	B	3003	BMA	O3-C3-C4	2.56	116.11	110.34
3	F	3004	BMA	C1-C2-C3	2.60	112.61	109.54
4	E	2016	NAG	C4-C3-C2	2.60	115.27	111.23
3	D	3004	BMA	C1-O5-C5	2.63	115.59	112.25
2	A	2002	NAG	C1-O5-C5	2.67	115.64	112.25
4	B	2009	NAG	C1-O5-C5	2.67	115.64	112.25
2	F	3001	BMA	C3-C4-C5	2.69	114.89	110.20
2	A	2007	NAG	O5-C5-C6	2.71	113.20	107.35
3	D	3011	MAN	C1-O5-C5	2.71	115.69	112.25
3	D	3009	MAN	C1-O5-C5	2.72	115.70	112.25
8	B	3002	BMA	C1-C2-C3	2.72	112.76	109.54
8	B	3014	MAN	C3-C4-C5	2.72	114.95	110.20
6	A	2011	NAG	C1-O5-C5	2.73	115.72	112.25
6	F	2010	NAG	C1-O5-C5	2.74	115.72	112.25
2	A	2013	NAG	C8-C7-N2	2.75	121.38	116.11
6	C	2010	NAG	C8-C7-N2	2.75	121.38	116.11
3	D	3004	BMA	O3-C3-C4	2.76	116.55	110.34
2	D	3003	BMA	O3-C3-C4	2.77	116.57	110.34
2	F	3001	BMA	C1-O5-C5	2.83	115.83	112.25
3	F	3011	MAN	C1-O5-C5	2.85	115.86	112.25
2	B	3005	MAN	O2-C2-C1	2.86	114.93	109.21
9	C	3004	BMA	O3-C3-C4	2.88	116.82	110.34
2	E	2007	NAG	C4-C3-C2	2.90	115.74	111.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	3010	MAN	C1-O5-C5	2.91	115.94	112.25
6	C	2016	NAG	O7-C7-C8	2.92	127.42	122.06
9	E	3011	MAN	C1-O5-C5	2.94	115.98	112.25
6	E	2010	NAG	C2-N2-C7	2.94	126.82	123.04
9	E	2004	NAG	C1-O5-C5	2.97	116.02	112.25
3	D	3009	MAN	C2-C3-C4	2.97	116.08	111.04
9	E	3012	MAN	C1-O5-C5	2.99	116.04	112.25
2	A	2013	NAG	C3-C2-N2	3.00	117.76	110.56
3	A	3009	MAN	C1-O5-C5	3.02	116.08	112.25
4	B	2009	NAG	C3-C2-N2	3.03	117.83	110.56
4	B	2016	NAG	C1-O5-C5	3.05	116.12	112.25
2	A	3005	MAN	O2-C2-C1	3.08	115.39	109.21
2	C	3003	BMA	C1-C2-C3	3.08	113.19	109.54
2	A	2001	NAG	C1-O5-C5	3.10	116.18	112.25
2	E	3001	BMA	C3-C4-C5	3.12	115.63	110.20
2	F	3006	MAN	C1-C2-C3	3.14	113.25	109.54
2	B	3005	MAN	C3-C4-C5	3.14	115.68	110.20
9	C	2003	NAG	C2-N2-C7	3.15	127.09	123.04
2	D	2002	NAG	C1-O5-C5	3.16	116.26	112.25
2	B	3006	MAN	C3-C4-C5	3.17	115.72	110.20
3	A	3011	MAN	C1-O5-C5	3.19	116.29	112.25
2	D	3001	BMA	C1-C2-C3	3.19	113.32	109.54
9	E	3004	BMA	O3-C3-C2	3.21	115.79	110.00
2	B	2002	NAG	C1-O5-C5	3.21	116.33	112.25
2	B	3006	MAN	C1-C2-C3	3.22	113.35	109.54
2	D	3006	MAN	C3-C4-C5	3.24	115.84	110.20
3	F	2004	NAG	C2-N2-C7	3.24	127.20	123.04
2	C	3006	MAN	C3-C4-C5	3.25	115.87	110.20
2	F	3001	BMA	C1-C2-C3	3.26	113.40	109.54
9	E	3010	MAN	C1-C2-C3	3.26	113.40	109.54
2	E	3001	BMA	C2-C3-C4	3.28	116.61	111.04
6	F	2011	NAG	C1-O5-C5	3.30	116.44	112.25
4	A	2005	NAG	C2-N2-C7	3.31	127.29	123.04
2	F	3003	BMA	C3-C4-C5	3.31	115.97	110.20
2	C	3007	MAN	C3-C4-C5	3.32	115.99	110.20
3	D	2003	NAG	C1-O5-C5	3.33	116.47	112.25
3	D	3010	MAN	C1-O5-C5	3.34	116.49	112.25
2	B	3005	MAN	C1-O5-C5	3.34	116.49	112.25
2	C	3001	BMA	O5-C5-C6	3.36	114.61	107.35
6	E	3002	BMA	C2-C3-C4	3.36	116.75	111.04
4	C	2008	NAG	C1-O5-C5	3.38	116.53	112.25
3	F	2004	NAG	C4-C3-C2	3.43	116.56	111.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	E	3010	MAN	C1-O5-C5	3.49	116.68	112.25
2	B	3008	MAN	C1-O5-C5	3.50	116.69	112.25
3	A	3009	MAN	C3-C4-C5	3.53	116.34	110.20
6	A	3013	BMA	C1-C2-C3	3.54	113.72	109.54
2	D	3007	MAN	C3-C4-C5	3.57	116.42	110.20
6	C	2011	NAG	C1-O5-C5	3.63	116.85	112.25
3	A	3004	BMA	O3-C3-C4	3.65	118.56	110.34
9	C	3004	BMA	C1-O5-C5	3.65	116.89	112.25
3	B	3011	MAN	C1-O5-C5	3.75	117.01	112.25
4	C	2017	NAG	C4-C3-C2	3.77	117.09	111.23
3	B	3010	MAN	C3-C4-C5	3.80	116.81	110.20
2	F	2002	NAG	C1-O5-C5	3.83	117.11	112.25
6	E	3002	BMA	C3-C4-C5	3.86	116.93	110.20
4	A	2015	NAG	C2-N2-C7	3.88	128.03	123.04
2	B	3007	MAN	O5-C1-C2	3.91	117.20	110.86
3	B	3004	BMA	O3-C3-C2	3.93	117.10	110.00
2	F	3007	MAN	C3-C4-C5	3.96	117.10	110.20
9	E	3012	MAN	C3-C4-C5	3.96	117.10	110.20
2	F	2007	NAG	C1-O5-C5	4.10	117.45	112.25
3	F	3009	MAN	C1-C2-C3	4.10	114.40	109.54
4	A	2005	NAG	C4-C3-C2	4.14	117.67	111.23
2	A	3001	BMA	C1-C2-C3	4.15	114.45	109.54
9	C	3009	MAN	C3-C4-C5	4.16	117.45	110.20
6	C	3013	BMA	C1-C2-C3	4.17	114.48	109.54
2	E	3005	MAN	C1-O5-C5	4.20	117.57	112.25
2	A	3007	MAN	C1-O5-C5	4.21	117.59	112.25
2	D	3006	MAN	C1-O5-C5	4.24	117.63	112.25
6	E	3002	BMA	C1-C2-C3	4.26	114.58	109.54
8	B	3014	MAN	C1-C2-C3	4.29	114.62	109.54
2	A	3003	BMA	C1-C2-C3	4.33	114.66	109.54
2	D	2007	NAG	C1-O5-C5	4.33	117.75	112.25
6	E	2010	NAG	C1-O5-C5	4.34	117.75	112.25
2	E	3006	MAN	C1-O5-C5	4.35	117.76	112.25
2	C	3006	MAN	C1-O5-C5	4.36	117.78	112.25
2	A	3001	BMA	C3-C4-C5	4.47	117.99	110.20
2	A	2007	NAG	C1-O5-C5	4.55	118.03	112.25
3	A	3004	BMA	O3-C3-C2	4.61	118.32	110.00
3	F	3010	MAN	C1-O5-C5	4.62	118.11	112.25
9	C	3004	BMA	O3-C3-C2	4.65	118.40	110.00
9	C	3010	MAN	C1-O5-C5	4.73	118.25	112.25
3	F	3009	MAN	C1-O5-C5	4.75	118.27	112.25
4	D	2009	NAG	C2-N2-C7	4.85	129.27	123.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	3007	MAN	C1-O5-C5	4.86	118.42	112.25
3	D	3004	BMA	O3-C3-C2	4.86	118.79	110.00
6	A	2009	NAG	C2-N2-C7	4.94	129.38	123.04
3	D	2003	NAG	C2-N2-C7	5.01	129.48	123.04
2	E	3008	MAN	C1-O5-C5	5.03	118.63	112.25
2	B	2007	NAG	C1-O5-C5	5.06	118.67	112.25
2	B	3007	MAN	C3-C4-C5	5.07	119.03	110.20
6	A	2010	NAG	C1-O5-C5	5.17	118.81	112.25
4	B	2009	NAG	C2-N2-C7	5.24	129.77	123.04
3	A	2003	NAG	C2-N2-C7	5.34	129.90	123.04
6	A	3002	BMA	C1-C2-C3	5.43	115.96	109.54
2	F	3008	MAN	C1-O5-C5	5.55	119.29	112.25
6	A	3002	BMA	C1-O5-C5	5.55	119.29	112.25
2	C	3001	BMA	C1-C2-C3	5.55	116.11	109.54
8	B	3014	MAN	C1-O5-C5	5.70	119.48	112.25
2	F	3006	MAN	C1-O5-C5	5.76	119.56	112.25
9	E	3009	MAN	C1-O5-C5	5.85	119.67	112.25
2	E	3001	BMA	C1-C2-C3	5.95	116.58	109.54
3	D	3009	MAN	C1-C2-C3	6.00	116.64	109.54
2	A	3006	MAN	C1-O5-C5	6.47	120.46	112.25
2	A	2013	NAG	C2-N2-C7	6.68	131.63	123.04
3	B	3010	MAN	C1-O5-C5	6.74	120.80	112.25
9	C	3012	MAN	C1-O5-C5	6.93	121.04	112.25
2	C	2007	NAG	C1-O5-C5	7.07	121.22	112.25
2	B	3006	MAN	C1-O5-C5	7.17	121.35	112.25
2	B	3007	MAN	C1-O5-C5	7.50	121.77	112.25
2	A	3008	MAN	C1-O5-C5	7.63	121.93	112.25

All (15) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	A	2003	NAG	C1
8	B	2010	NAG	C1
3	D	2003	NAG	C1
3	B	2003	NAG	C1
6	E	2010	NAG	C1
2	D	2007	NAG	C1
6	F	2010	NAG	C1
9	C	2003	NAG	C1
6	A	2010	NAG	C1
6	D	2010	NAG	C1
4	D	2009	NAG	C1

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Mol	Chain	Res	Type	Atom
3	F	2003	NAG	C1
9	E	2003	NAG	C1
6	C	2010	NAG	C1
2	E	2007	NAG	C1

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	E	2009	NAG	O7-C7-N2-C2
6	C	2016	NAG	O7-C7-N2-C2
6	A	2009	NAG	O7-C7-N2-C2
2	F	2007	NAG	O7-C7-N2-C2
6	A	2009	NAG	C8-C7-N2-C2
2	F	2007	NAG	C8-C7-N2-C2

All (5) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	F	3006	MAN	C1-C2-C3-C4-C5-O5
2	A	3008	MAN	C1-C2-C3-C4-C5-O5
2	E	3005	MAN	C1-C2-C3-C4-C5-O5
2	F	3008	MAN	C1-C2-C3-C4-C5-O5
2	B	3008	MAN	C1-C2-C3-C4-C5-O5

21 monomers are involved in 23 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	2005	NAG	2	0
6	A	2010	NAG	2	0
2	A	2013	NAG	1	0
2	A	3001	BMA	1	0
2	A	3007	MAN	1	0
3	B	2003	NAG	1	0
2	B	2007	NAG	1	0
2	C	2002	NAG	1	0
9	C	2003	NAG	1	0
6	C	2010	NAG	1	0
6	C	2016	NAG	1	0
6	C	3013	BMA	2	0
2	D	2002	NAG	1	0
2	D	3008	MAN	1	0
2	E	2001	NAG	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	E	2003	NAG	1	0
9	E	2004	NAG	2	0
2	E	2007	NAG	1	0
6	E	2010	NAG	1	0
3	F	2003	NAG	1	0
2	F	2007	NAG	1	0

## 5.6 Ligand geometry [i](#)

Of 55 ligands modelled in this entry, 24 are monoatomic - leaving 31 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
5	NAG	A	2006	1	14,14,15	0.85	0	15,19,21	0.89	0
5	NAG	A	2008	1	14,14,15	0.46	0	15,19,21	0.75	0
5	NAG	A	2012	1	14,14,15	0.53	0	15,19,21	1.12	1 (6%)
5	NAG	A	2014	1	14,14,15	0.61	0	15,19,21	1.05	1 (6%)
7	NDG	A	2018	1	14,14,15	0.67	0	15,19,21	1.55	2 (13%)
5	NAG	B	2005	1	14,14,15	0.56	0	15,19,21	0.78	0
5	NAG	B	2006	1	14,14,15	0.66	0	15,19,21	0.67	0
5	NAG	B	2012	1	14,14,15	0.52	0	15,19,21	1.23	1 (6%)
5	NAG	B	2014	1	14,14,15	0.45	0	15,19,21	1.83	1 (6%)
5	NAG	B	2018	1	14,14,15	0.76	1 (7%)	15,19,21	1.22	1 (6%)
5	NAG	C	2005	1	14,14,15	0.52	0	15,19,21	1.74	4 (26%)
5	NAG	C	2006	1	14,14,15	0.45	0	15,19,21	1.44	1 (6%)
5	NAG	C	2012	1	14,14,15	0.51	0	15,19,21	1.70	2 (13%)
5	NAG	C	2014	1	14,14,15	0.53	0	15,19,21	1.90	2 (13%)
5	NAG	C	2018	1	14,14,15	5.02	3 (21%)	15,19,21	2.16	4 (26%)
5	NAG	D	2005	1	14,14,15	0.51	0	15,19,21	1.00	0
5	NAG	D	2006	1	14,14,15	3.78	3 (21%)	15,19,21	1.98	3 (20%)
5	NAG	D	2008	1	14,14,15	0.47	0	15,19,21	0.91	0
5	NAG	D	2012	1	14,14,15	0.65	0	15,19,21	0.82	0



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
5	NAG	D	2014	1	14,14,15	0.51	0	15,19,21	0.85	0
5	NAG	E	2005	1	14,14,15	0.54	0	15,19,21	0.85	0
5	NAG	E	2006	1	14,14,15	0.64	0	15,19,21	1.74	3 (20%)
5	NAG	E	2008	1	14,14,15	0.50	0	15,19,21	0.83	0
5	NAG	E	2012	1	14,14,15	3.46	2 (14%)	15,19,21	1.52	3 (20%)
5	NAG	E	2014	1	14,14,15	0.46	0	15,19,21	1.93	2 (13%)
5	NAG	F	2005	1	14,14,15	4.21	4 (28%)	15,19,21	2.01	3 (20%)
5	NAG	F	2006	1	14,14,15	4.19	4 (28%)	15,19,21	1.86	3 (20%)
5	NAG	F	2008	1	14,14,15	0.53	0	15,19,21	1.23	1 (6%)
5	NAG	F	2009	1	14,14,15	0.85	0	15,19,21	1.43	2 (13%)
5	NAG	F	2012	1	14,14,15	0.47	0	15,19,21	1.57	3 (20%)
5	NAG	F	2014	1	14,14,15	0.44	0	15,19,21	1.21	1 (6%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	A	2006	1	1/1/5/7	0/6/23/26	0/1/1/1
5	NAG	A	2008	1	-	0/6/23/26	0/1/1/1
5	NAG	A	2012	1	1/1/5/7	0/6/23/26	0/1/1/1
5	NAG	A	2014	1	-	0/6/23/26	0/1/1/1
7	NDG	A	2018	1	-	0/6/23/26	0/1/1/1
5	NAG	B	2005	1	-	0/6/23/26	0/1/1/1
5	NAG	B	2006	1	1/1/5/7	0/6/23/26	0/1/1/1
5	NAG	B	2012	1	1/1/5/7	0/6/23/26	0/1/1/1
5	NAG	B	2014	1	-	0/6/23/26	0/1/1/1
5	NAG	B	2018	1	1/1/5/7	0/6/23/26	0/1/1/1
5	NAG	C	2005	1	-	0/6/23/26	0/1/1/1
5	NAG	C	2006	1	-	0/6/23/26	0/1/1/1
5	NAG	C	2012	1	1/1/5/7	0/6/23/26	0/1/1/1
5	NAG	C	2014	1	-	0/6/23/26	0/1/1/1
5	NAG	C	2018	1	1/1/5/7	0/6/23/26	0/1/1/1
5	NAG	D	2005	1	-	0/6/23/26	0/1/1/1
5	NAG	D	2006	1	1/1/5/7	0/6/23/26	0/1/1/1
5	NAG	D	2008	1	-	0/6/23/26	0/1/1/1
5	NAG	D	2012	1	-	0/6/23/26	0/1/1/1
5	NAG	D	2014	1	-	2/6/23/26	0/1/1/1
5	NAG	E	2005	1	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	E	2006	1	-	0/6/23/26	0/1/1/1
5	NAG	E	2008	1	-	0/6/23/26	0/1/1/1
5	NAG	E	2012	1	1/1/5/7	0/6/23/26	0/1/1/1
5	NAG	E	2014	1	-	0/6/23/26	0/1/1/1
5	NAG	F	2005	1	1/1/5/7	0/6/23/26	0/1/1/1
5	NAG	F	2006	1	1/1/5/7	0/6/23/26	0/1/1/1
5	NAG	F	2008	1	-	0/6/23/26	0/1/1/1
5	NAG	F	2009	1	1/1/5/7	0/6/23/26	0/1/1/1
5	NAG	F	2012	1	1/1/5/7	0/6/23/26	0/1/1/1
5	NAG	F	2014	1	-	0/6/23/26	0/1/1/1

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	F	2006	NAG	O7-C7	-3.29	1.15	1.23
5	F	2006	NAG	C1-C2	2.10	1.55	1.52
5	B	2018	NAG	C1-C2	2.16	1.55	1.52
5	D	2006	NAG	C1-C2	2.37	1.55	1.52
5	F	2006	NAG	C7-N2	2.51	1.44	1.34
5	C	2018	NAG	O6-C6	2.92	1.55	1.42
5	F	2005	NAG	C2-N2	4.89	1.55	1.46
5	D	2006	NAG	C8-C7	6.85	1.64	1.50
5	E	2012	NAG	O7-C7	7.07	1.39	1.23
5	F	2005	NAG	O6-C6	7.46	1.74	1.42
5	F	2005	NAG	C1-C2	8.22	1.63	1.52
5	F	2005	NAG	C8-C7	9.46	1.69	1.50
5	E	2012	NAG	C8-C7	10.71	1.72	1.50
5	D	2006	NAG	O7-C7	11.50	1.49	1.23
5	C	2018	NAG	C8-C7	11.83	1.74	1.50
5	C	2018	NAG	O7-C7	14.02	1.55	1.23
5	F	2006	NAG	C8-C7	14.84	1.80	1.50

All (44) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	D	2006	NAG	C8-C7-N2	-4.60	107.31	116.11
5	F	2006	NAG	C2-N2-C7	-4.51	117.24	123.04
5	C	2018	NAG	O7-C7-N2	-4.40	112.90	121.86
5	F	2006	NAG	O7-C7-N2	-3.95	113.82	121.86
5	D	2006	NAG	C2-N2-C7	-3.58	118.44	123.04
5	F	2005	NAG	O6-C6-C5	-3.57	99.55	111.33
5	F	2005	NAG	O7-C7-N2	-2.59	116.59	121.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	E	2012	NAG	C8-C7-N2	-2.19	111.91	116.11
5	C	2014	NAG	C6-C5-C4	-2.15	107.71	113.02
5	E	2014	NAG	C6-C5-C4	-2.12	107.79	113.02
5	C	2005	NAG	O7-C7-C8	-2.09	118.22	122.06
5	A	2014	NAG	C1-O5-C5	2.02	114.82	112.25
5	F	2012	NAG	C3-C2-N2	2.06	115.48	110.56
5	C	2012	NAG	C4-C3-C2	2.30	114.81	111.23
5	E	2006	NAG	C4-C3-C2	2.30	114.81	111.23
7	A	2018	NDG	C3-C4-C5	2.51	114.58	110.20
5	E	2012	NAG	C1-O5-C5	2.62	115.58	112.25
5	F	2012	NAG	C1-O5-C5	2.68	115.64	112.25
5	D	2006	NAG	C1-O5-C5	2.69	115.67	112.25
5	F	2006	NAG	O7-C7-C8	2.93	127.43	122.06
5	C	2018	NAG	C3-C4-C5	3.00	115.42	110.20
5	F	2009	NAG	C1-O5-C5	3.00	116.05	112.25
5	C	2005	NAG	C8-C7-N2	3.02	121.88	116.11
5	E	2006	NAG	C2-N2-C7	3.03	126.93	123.04
5	A	2012	NAG	C1-O5-C5	3.29	116.42	112.25
5	F	2014	NAG	C1-O5-C5	3.37	116.53	112.25
5	C	2005	NAG	C1-O5-C5	3.46	116.64	112.25
5	E	2012	NAG	O7-C7-C8	3.50	128.48	122.06
5	B	2012	NAG	C1-O5-C5	3.55	116.75	112.25
5	F	2009	NAG	C2-N2-C7	3.59	127.66	123.04
5	B	2018	NAG	C4-C3-C2	3.64	116.89	111.23
5	F	2008	NAG	C1-O5-C5	3.69	116.92	112.25
5	C	2005	NAG	C2-N2-C7	3.96	128.13	123.04
5	F	2012	NAG	C2-N2-C7	4.00	128.17	123.04
5	C	2018	NAG	C4-C3-C2	4.06	117.54	111.23
7	A	2018	NDG	C4-C3-C2	4.21	117.77	111.23
5	C	2006	NAG	C1-O5-C5	4.22	117.61	112.25
5	C	2018	NAG	O7-C7-C8	4.25	129.86	122.06
5	E	2006	NAG	C1-O5-C5	4.75	118.28	112.25
5	C	2012	NAG	C1-O5-C5	4.86	118.41	112.25
5	B	2014	NAG	C1-O5-C5	5.49	119.22	112.25
5	F	2005	NAG	C1-O5-C5	5.72	119.51	112.25
5	C	2014	NAG	C1-O5-C5	6.26	120.19	112.25
5	E	2014	NAG	C1-O5-C5	6.67	120.71	112.25

All (13) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
5	A	2012	NAG	C1

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Mol	Chain	Res	Type	Atom
5	B	2012	NAG	C1
5	F	2012	NAG	C1
5	B	2018	NAG	C1
5	B	2006	NAG	C1
5	F	2009	NAG	C1
5	E	2012	NAG	C1
5	C	2018	NAG	C1
5	D	2006	NAG	C1
5	F	2006	NAG	C1
5	F	2005	NAG	C1
5	A	2006	NAG	C1
5	C	2012	NAG	C1

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	D	2014	NAG	C8-C7-N2-C2
5	D	2014	NAG	O7-C7-N2-C2

There are no ring outliers.

9 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	2005	NAG	3	0
5	C	2005	NAG	2	0
5	D	2005	NAG	1	0
5	D	2008	NAG	1	0
5	E	2005	NAG	1	0
5	E	2006	NAG	1	0
5	F	2005	NAG	2	0
5	F	2006	NAG	1	0
5	F	2012	NAG	1	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å <sup>2</sup> )	Q<0.9
1	A	529/534 (99%)	0.71	44 (8%)	14 7	67, 69, 71, 74	0
1	B	529/534 (99%)	0.70	39 (7%)	17 9	67, 69, 71, 74	0
1	C	529/534 (99%)	0.80	64 (12%)	6 3	67, 69, 71, 74	0
1	D	529/534 (99%)	0.86	67 (12%)	5 2	67, 69, 71, 73	0
1	E	529/534 (99%)	1.31	121 (22%)	1 1	68, 69, 71, 73	0
1	F	529/534 (99%)	1.63	172 (32%)	1 0	68, 69, 71, 73	0
All	All	3174/3204 (99%)	1.00	507 (15%)	3 1	67, 69, 71, 74	0

All (507) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	549	HIS	10.2
1	F	266	ASP	8.7
1	F	443	ASP	8.1
1	E	536	THR	7.2
1	E	549	HIS	7.2
1	F	435	LEU	7.1
1	E	378	ASP	7.1
1	F	535	ASN	7.0
1	D	535	ASN	6.8
1	C	540	THR	6.6
1	F	312	ASP	6.4
1	F	313	SER	6.4
1	F	529	GLU	6.4
1	F	179	TYR	6.4
1	D	534	ALA	6.2
1	A	533	ALA	6.2
1	E	454	PRO	6.2
1	E	540	THR	6.2
1	F	286	PRO	6.0

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Mol	Chain	Res	Type	RSRZ
1	E	451	PRO	6.0
1	F	547	VAL	5.9
1	F	287	SER	5.8
1	C	538	ASP	5.8
1	E	538	ASP	5.7
1	D	549	HIS	5.6
1	A	550	ALA	5.6
1	F	436	GLY	5.5
1	F	536	THR	5.5
1	D	533	ALA	5.4
1	F	528	THR	5.4
1	E	397	LYS	5.4
1	C	534	ALA	5.4
1	E	537	LEU	5.4
1	E	384	GLU	5.3
1	B	535	ASN	5.3
1	E	535	ASN	5.2
1	E	96	VAL	5.2
1	F	438	VAL	5.2
1	C	515	GLU	5.2
1	E	507	ASP	5.0
1	F	540	THR	4.9
1	F	534	ALA	4.9
1	F	144	LYS	4.9
1	E	333	GLY	4.8
1	F	74	ASN	4.8
1	F	503	PHE	4.8
1	D	312	ASP	4.8
1	C	549	HIS	4.8
1	F	307	THR	4.7
1	F	485	HIS	4.7
1	C	524	CYS	4.7
1	F	109	THR	4.7
1	F	444	PRO	4.7
1	F	265	ASN	4.6
1	E	267	THR	4.6
1	F	165	HIS	4.6
1	F	481	PHE	4.5
1	E	481	PHE	4.5
1	F	410	THR	4.5
1	E	334	GLU	4.5
1	E	453	TYR	4.4

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Mol	Chain	Res	Type	RSRZ
1	A	459	THR	4.4
1	B	146	ASP	4.4
1	F	484	CYS	4.3
1	F	434	ALA	4.3
1	F	414	PRO	4.2
1	E	416	HIS	4.2
1	A	549	HIS	4.2
1	F	173	LYS	4.2
1	E	502	PRO	4.2
1	F	397	LYS	4.2
1	E	444	PRO	4.2
1	F	84	GLY	4.1
1	F	151	ASP	4.1
1	C	146	ASP	4.1
1	F	301	LYS	4.1
1	F	483	HIS	4.1
1	E	150	TYR	4.1
1	F	215	ASN	4.1
1	F	537	LEU	4.0
1	E	75	ASN	4.0
1	F	366	LYS	4.0
1	F	170	ASP	4.0
1	E	529	GLU	4.0
1	E	530	GLY	4.0
1	F	417	LEU	4.0
1	F	509	HIS	4.0
1	F	454	PRO	3.9
1	F	75	ASN	3.9
1	F	453	TYR	3.9
1	F	387	GLY	3.9
1	F	124	TRP	3.8
1	C	536	THR	3.8
1	F	230	GLU	3.8
1	D	378	ASP	3.8
1	C	522	GLN	3.8
1	E	214	VAL	3.8
1	C	453	TYR	3.8
1	F	378	ASP	3.8
1	A	537	LEU	3.8
1	B	215	ASN	3.8
1	E	147	SER	3.8
1	F	184	ALA	3.8

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Mol	Chain	Res	Type	RSRZ
1	E	389	ASN	3.8
1	F	416	HIS	3.8
1	F	385	ILE	3.8
1	E	550	ALA	3.8
1	F	22	GLU	3.7
1	B	534	ALA	3.7
1	F	445	ASP	3.7
1	D	503	PHE	3.7
1	E	547	VAL	3.7
1	E	184	ALA	3.7
1	F	310	TYR	3.7
1	C	446	ASN	3.6
1	F	107	GLY	3.6
1	E	206	ASP	3.6
1	C	531	ASN	3.6
1	E	299	TYR	3.6
1	C	509	HIS	3.6
1	E	417	LEU	3.6
1	F	176	MET	3.6
1	D	215	ASN	3.6
1	E	480	TRP	3.6
1	E	385	ILE	3.6
1	B	417	LEU	3.5
1	A	397	LYS	3.5
1	E	527	ALA	3.5
1	F	482	PHE	3.5
1	F	510	SER	3.5
1	B	74	ASN	3.5
1	F	418	HIS	3.5
1	F	495	GLY	3.5
1	C	481	PHE	3.5
1	A	536	THR	3.5
1	D	540	THR	3.5
1	F	306	PRO	3.4
1	E	287	SER	3.4
1	F	291	LEU	3.4
1	F	415	PHE	3.4
1	C	417	LEU	3.4
1	B	459	THR	3.4
1	E	479	VAL	3.4
1	D	481	PHE	3.4
1	D	417	LEU	3.4

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Mol	Chain	Res	Type	RSRZ
1	F	218	GLY	3.4
1	F	188	PRO	3.4
1	B	537	LEU	3.3
1	E	376	SER	3.3
1	F	95	GLY	3.3
1	E	97	PRO	3.3
1	F	72	GLY	3.3
1	E	130	ASP	3.3
1	F	78	THR	3.2
1	B	34	TYR	3.2
1	E	386	TYR	3.2
1	C	252	THR	3.2
1	F	146	ASP	3.2
1	D	484	CYS	3.2
1	D	537	LEU	3.2
1	E	146	ASP	3.2
1	F	411	GLY	3.2
1	C	445	ASP	3.2
1	C	510	SER	3.2
1	C	533	ALA	3.2
1	D	525	SER	3.2
1	F	525	SER	3.2
1	E	522	GLN	3.2
1	D	435	LEU	3.2
1	F	285	ILE	3.1
1	D	509	HIS	3.1
1	E	112	TYR	3.1
1	D	497	VAL	3.1
1	E	254	ALA	3.1
1	C	535	ASN	3.1
1	D	100	THR	3.1
1	F	34	TYR	3.1
1	C	459	THR	3.1
1	F	308	GLN	3.1
1	E	100	THR	3.1
1	C	145	ASP	3.1
1	B	96	VAL	3.1
1	F	344	VAL	3.1
1	F	252	THR	3.1
1	F	432	ASP	3.1
1	B	434	ALA	3.1
1	E	124	TRP	3.1

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Mol	Chain	Res	Type	RSRZ
1	B	205	PRO	3.1
1	E	62	GLY	3.0
1	C	454	PRO	3.0
1	D	151	ASP	3.0
1	C	484	CYS	3.0
1	F	459	THR	3.0
1	F	519	GLU	3.0
1	D	507	ASP	3.0
1	E	424	THR	3.0
1	E	482	PHE	3.0
1	E	408	GLN	3.0
1	D	459	THR	3.0
1	A	146	ASP	3.0
1	A	497	VAL	3.0
1	E	473	LYS	3.0
1	F	548	GLN	3.0
1	E	260	LEU	3.0
1	F	460	LEU	3.0
1	A	540	THR	3.0
1	F	206	ASP	3.0
1	E	432	ASP	2.9
1	B	484	CYS	2.9
1	C	214	VAL	2.9
1	F	541	ASP	2.9
1	D	269	LYS	2.9
1	F	360	ILE	2.9
1	A	102	CYS	2.9
1	F	183	GLY	2.9
1	E	336	ASP	2.9
1	F	336	ASP	2.9
1	E	145	ASP	2.9
1	A	378	ASP	2.9
1	F	63	ASP	2.9
1	F	100	THR	2.9
1	C	473	LYS	2.9
1	A	509	HIS	2.9
1	F	98	PHE	2.9
1	E	426	GLN	2.9
1	F	349	LYS	2.9
1	E	425	ILE	2.9
1	E	183	GLY	2.9
1	C	326	TYR	2.9

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Mol	Chain	Res	Type	RSRZ
1	E	95	GLY	2.9
1	F	279	ASP	2.8
1	D	82	PHE	2.8
1	F	103	PRO	2.8
1	E	349	LYS	2.8
1	E	508	ALA	2.8
1	F	96	VAL	2.8
1	E	431	TYR	2.8
1	C	547	VAL	2.8
1	D	265	ASN	2.8
1	D	547	VAL	2.8
1	D	524	CYS	2.8
1	D	483	HIS	2.8
1	D	485	HIS	2.8
1	E	128	HIS	2.8
1	F	128	HIS	2.8
1	E	377	GLY	2.8
1	F	38	ASP	2.8
1	E	253	VAL	2.8
1	B	397	LYS	2.8
1	C	333	GLY	2.8
1	E	496	LEU	2.8
1	E	337	HIS	2.8
1	F	217	GLY	2.8
1	A	257	TYR	2.8
1	F	492	GLN	2.8
1	D	94	ASP	2.7
1	F	241	THR	2.7
1	D	255	GLN	2.7
1	E	436	GLY	2.7
1	D	458	ASP	2.7
1	F	507	ASP	2.7
1	E	22	GLU	2.7
1	E	311	VAL	2.7
1	F	530	GLY	2.7
1	D	213	ILE	2.7
1	A	334	GLU	2.7
1	F	350	ASN	2.7
1	F	546	ASN	2.7
1	D	445	ASP	2.7
1	C	84	GLY	2.7
1	F	332	TYR	2.7

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Mol	Chain	Res	Type	RSRZ
1	E	415	PHE	2.7
1	B	479	VAL	2.7
1	F	490	LEU	2.7
1	F	352	VAL	2.7
1	A	254	ALA	2.7
1	E	256	ARG	2.7
1	F	104	ILE	2.6
1	E	315	ASP	2.6
1	F	267	THR	2.6
1	E	328	LYS	2.6
1	F	152	TYR	2.6
1	E	139	GLY	2.6
1	D	124	TRP	2.6
1	C	415	PHE	2.6
1	E	125	TYR	2.6
1	F	94	ASP	2.6
1	F	458	ASP	2.6
1	C	539	LEU	2.6
1	C	237	ASP	2.6
1	D	252	THR	2.6
1	E	459	THR	2.6
1	E	154	GLU	2.6
1	F	419	GLY	2.6
1	F	538	ASP	2.6
1	D	216	VAL	2.6
1	D	251	ILE	2.6
1	D	486	ILE	2.6
1	C	215	ASN	2.6
1	F	33	ASP	2.6
1	F	145	ASP	2.6
1	F	292	ASN	2.6
1	D	125	TYR	2.6
1	F	311	VAL	2.6
1	F	129	THR	2.5
1	C	91	ALA	2.5
1	C	541	ASP	2.5
1	D	146	ASP	2.5
1	E	151	ASP	2.5
1	F	126	HIS	2.5
1	F	48	CYS	2.5
1	D	538	ASP	2.5
1	A	214	VAL	2.5

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Mol	Chain	Res	Type	RSRZ
1	D	482	PHE	2.5
1	A	351	GLY	2.5
1	B	217	GLY	2.5
1	D	95	GLY	2.5
1	C	312	ASP	2.5
1	D	369	THR	2.5
1	A	75	ASN	2.5
1	E	503	PHE	2.5
1	F	133	TYR	2.5
1	C	550	ALA	2.5
1	E	161	SER	2.5
1	F	180	ASN	2.5
1	B	507	ASP	2.5
1	D	84	GLY	2.5
1	F	181	PRO	2.5
1	F	309	ASN	2.5
1	B	257	TYR	2.5
1	B	128	HIS	2.5
1	F	70	THR	2.4
1	F	209	TYR	2.4
1	E	458	ASP	2.4
1	D	74	ASN	2.4
1	E	533	ALA	2.4
1	E	153	ASP	2.4
1	A	100	THR	2.4
1	C	90	THR	2.4
1	F	83	HIS	2.4
1	B	481	PHE	2.4
1	F	502	PRO	2.4
1	C	516	ASN	2.4
1	C	96	VAL	2.4
1	D	40	LEU	2.4
1	E	252	THR	2.4
1	B	549	HIS	2.4
1	E	399	GLU	2.4
1	D	130	ASP	2.4
1	E	497	VAL	2.4
1	A	435	LEU	2.4
1	A	213	ILE	2.4
1	F	136	GLY	2.4
1	F	543	THR	2.4
1	C	435	LEU	2.4

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Mol	Chain	Res	Type	RSRZ
1	E	255	GLN	2.4
1	A	534	ALA	2.4
1	A	221	SER	2.4
1	C	418	HIS	2.4
1	C	458	ASP	2.4
1	A	417	LEU	2.4
1	C	493	GLY	2.4
1	E	113	ASN	2.4
1	F	328	LYS	2.4
1	B	540	THR	2.4
1	B	255	GLN	2.3
1	F	377	GLY	2.3
1	F	127	SER	2.3
1	E	484	CYS	2.3
1	E	465	GLN	2.3
1	A	215	ASN	2.3
1	A	458	ASP	2.3
1	C	494	LEU	2.3
1	E	461	TYR	2.3
1	F	361	THR	2.3
1	C	451	PRO	2.3
1	A	74	ASN	2.3
1	C	255	GLN	2.3
1	B	254	ALA	2.3
1	D	80	MET	2.3
1	F	527	ALA	2.3
1	A	414	PRO	2.3
1	F	520	VAL	2.3
1	F	130	ASP	2.3
1	A	147	SER	2.3
1	E	483	HIS	2.3
1	F	493	GLY	2.3
1	F	429	ARG	2.3
1	F	486	ILE	2.3
1	C	398	ASP	2.3
1	E	441	SER	2.3
1	E	509	HIS	2.3
1	F	36	ASN	2.3
1	F	251	ILE	2.3
1	F	488	TRP	2.3
1	C	102	CYS	2.3
1	C	265	ASN	2.3

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Mol	Chain	Res	Type	RSRZ
1	F	257	TYR	2.3
1	C	213	ILE	2.3
1	C	253	VAL	2.3
1	F	479	VAL	2.3
1	E	94	ASP	2.3
1	E	266	ASP	2.3
1	E	330	ALA	2.3
1	D	128	HIS	2.3
1	F	420	HIS	2.3
1	A	115	THR	2.3
1	E	246	THR	2.3
1	F	424	THR	2.3
1	B	95	GLY	2.3
1	F	539	LEU	2.3
1	A	524	CYS	2.2
1	D	178	VAL	2.2
1	C	74	ASN	2.2
1	E	366	LYS	2.2
1	F	108	SER	2.2
1	E	159	SER	2.2
1	E	513	LEU	2.2
1	A	372	THR	2.2
1	C	430	THR	2.2
1	F	288	ASP	2.2
1	A	481	PHE	2.2
1	C	460	LEU	2.2
1	F	330	ALA	2.2
1	C	100	THR	2.2
1	E	440	HIS	2.2
1	E	490	LEU	2.2
1	D	414	PRO	2.2
1	A	124	TRP	2.2
1	A	499	VAL	2.2
1	E	216	VAL	2.2
1	E	74	ASN	2.2
1	B	221	SER	2.2
1	B	533	ALA	2.2
1	D	380	ALA	2.2
1	B	213	ILE	2.2
1	F	515	GLU	2.2
1	F	294	THR	2.2
1	B	83	HIS	2.2

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Mol	Chain	Res	Type	RSRZ
1	D	75	ASN	2.2
1	A	485	HIS	2.1
1	D	34	TYR	2.1
1	F	480	TRP	2.1
1	E	541	ASP	2.1
1	B	485	HIS	2.1
1	C	485	HIS	2.1
1	C	161	SER	2.1
1	E	414	PRO	2.1
1	A	96	VAL	2.1
1	A	237	ASP	2.1
1	B	378	ASP	2.1
1	A	522	GLN	2.1
1	A	158	LEU	2.1
1	B	415	PHE	2.1
1	B	153	ASP	2.1
1	E	382	ASN	2.1
1	F	147	SER	2.1
1	F	254	ALA	2.1
1	D	418	HIS	2.1
1	E	372	THR	2.1
1	B	97	PRO	2.1
1	D	149	PRO	2.1
1	F	97	PRO	2.1
1	B	117	ASP	2.1
1	D	419	GLY	2.1
1	E	237	ASP	2.1
1	F	409	ASP	2.1
1	E	257	TYR	2.1
1	F	177	SER	2.1
1	B	253	VAL	2.1
1	C	311	VAL	2.1
1	D	550	ALA	2.1
1	C	251	ILE	2.1
1	D	78	THR	2.1
1	B	435	LEU	2.1
1	C	254	ALA	2.1
1	D	530	GLY	2.0
1	A	251	ILE	2.0
1	F	200	THR	2.0
1	F	430	THR	2.0
1	D	522	GLN	2.0

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Mol	Chain	Res	Type	RSRZ
1	F	222	GLN	2.0
1	E	99	LEU	2.0
1	F	160	LEU	2.0
1	A	218	GLY	2.0
1	F	73	MET	2.0
1	A	94	ASP	2.0
1	F	386	TYR	2.0
1	E	127	SER	2.0
1	F	238	GLY	2.0
1	C	480	TRP	2.0
1	F	80	MET	2.0
1	B	543	THR	2.0
1	E	412	THR	2.0
1	E	446	ASN	2.0
1	E	467	ASN	2.0
1	D	127	SER	2.0
1	D	436	GLY	2.0
1	F	92	SER	2.0
1	F	448	PRO	2.0
1	B	458	ASP	2.0
1	D	83	HIS	2.0
1	C	496	LEU	2.0
1	D	140	LEU	2.0
1	E	327	GLU	2.0
1	F	396	GLU	2.0
1	D	79	SER	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

## 6.3 Carbohydrates [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q < 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
6	NAG	D	2010	14/15	0.85	0.36	3.54	72,73,75,76	0
4	NAG	C	2008	14/15	0.81	0.40	3.22	75,77,78,80	0
2	NAG	E	2007	14/15	0.73	0.47	2.15	72,73,74,74	0
2	NAG	C	2007	14/15	0.75	0.37	1.28	69,73,76,76	0
6	NAG	E	2010	14/15	0.88	0.36	1.26	63,66,69,69	0
6	NAG	F	2010	14/15	0.73	0.44	1.09	75,76,77,77	0
4	NAG	B	2008	14/15	0.88	0.28	1.07	76,79,81,86	0
4	NAG	A	2005	14/15	0.93	0.24	1.04	71,76,80,87	0
2	NAG	F	2007	14/15	0.79	0.41	0.74	71,72,75,76	0
3	NAG	F	2003	14/15	0.84	0.27	0.18	78,81,83,83	0
2	NAG	A	2007	14/15	0.78	0.27	0.13	74,76,80,83	0
3	MAN	F	3011	11/12	0.73	0.32	0.12	75,76,77,77	0
2	NAG	B	2007	14/15	0.86	0.23	0.10	74,77,81,84	0
9	MAN	E	3011	11/12	0.92	0.22	0.00	71,72,73,73	0
6	NAG	C	2010	14/15	0.92	0.22	-0.35	62,64,67,68	0
2	NAG	E	2002	14/15	0.85	0.25	-0.53	75,77,79,79	0
9	NAG	C	2003	14/15	0.92	0.20	-0.71	69,70,76,79	0
2	NAG	D	2007	14/15	0.89	0.22	-0.72	73,75,78,78	0
3	NAG	D	2003	14/15	0.90	0.18	-0.74	64,68,70,71	0
3	MAN	D	3011	11/12	0.93	0.19	-0.84	63,64,65,65	0
8	NAG	B	2010	14/15	0.89	0.22	-1.11	68,69,71,72	0
2	NAG	F	2001	14/15	0.87	0.18	-1.21	70,71,72,72	0
2	NAG	C	2002	14/15	0.90	0.15	-1.38	71,74,78,82	0
3	NAG	B	2003	14/15	0.94	0.18	-1.48	70,74,77,77	0
2	NAG	A	2001	14/15	0.96	0.17	-1.48	63,65,68,68	0
3	NAG	A	2003	14/15	0.93	0.17	-1.51	67,72,78,80	0
2	NAG	D	2001	14/15	0.95	0.14	-1.57	68,69,69,71	0
6	NAG	A	2010	14/15	0.94	0.19	-1.72	64,67,69,70	0
2	NAG	F	2002	14/15	0.92	0.17	-1.79	71,71,74,75	0
2	NAG	A	2002	14/15	0.95	0.15	-1.79	70,72,73,77	0
2	NAG	D	2002	14/15	0.93	0.14	-1.83	70,72,74,74	0
2	NAG	B	2002	14/15	0.92	0.16	-1.85	72,74,76,79	0
2	NAG	B	2001	14/15	0.96	0.17	-1.93	67,68,70,71	0
9	NAG	E	2003	14/15	0.92	0.18	-2.11	76,77,79,79	0
3	MAN	B	3011	11/12	0.95	0.14	-2.24	68,70,71,73	0
2	NAG	C	2001	14/15	0.95	0.13	-2.77	67,69,71,72	0
2	NAG	E	2001	14/15	0.95	0.10	-3.53	70,71,73,75	0
9	MAN	C	3011	11/12	0.97	0.11	-3.96	64,65,66,67	0
3	MAN	A	3011	11/12	0.94	0.13	-4.29	67,72,73,75	0
6	BMA	F	3002	11/12	0.64	0.67	-	81,82,82,83	0
2	BMA	B	3003	11/12	0.84	0.31	-	71,72,73,74	0
9	BMA	C	3004	11/12	0.93	0.21	-	77,81,85,88	0
9	NAG	E	2004	14/15	0.86	0.28	-	80,82,82,83	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
3	NAG	F	2004	14/15	0.72	0.43	-	82,83,85,85	0
2	NAG	F	2013	14/15	0.77	0.45	-	68,70,70,71	0
4	NAG	B	2016	14/15	0.86	0.33	-	74,76,77,78	0
2	NAG	E	2013	14/15	0.86	0.43	-	73,74,74,74	0
6	BMA	C	3013	11/12	0.87	0.50	-	47,49,50,50	0
2	MAN	F	3008	11/12	0.71	0.34	-	82,84,84,85	0
9	NAG	C	2004	14/15	0.95	0.17	-	72,75,77,79	0
2	MAN	B	3005	11/12	0.62	0.28	-	70,73,74,75	0
3	MAN	D	3010	11/12	0.85	0.31	-	67,68,69,69	0
2	BMA	F	3003	11/12	0.68	0.46	-	66,67,68,68	0
2	BMA	C	3003	11/12	0.90	0.29	-	81,83,86,88	0
2	MAN	D	3008	11/12	0.74	0.29	-	77,78,78,78	0
2	BMA	E	3001	11/12	0.82	0.26	-	81,83,86,87	0
2	MAN	D	3007	11/12	0.66	0.47	-	78,78,79,79	0
6	BMA	A	3002	11/12	0.61	0.56	-	78,80,81,81	0
3	BMA	D	3004	11/12	0.91	0.34	-	70,72,73,73	0
2	MAN	C	3006	11/12	0.65	0.51	-	89,90,91,91	0
4	NAG	B	2009	14/15	0.87	0.24	-	70,71,73,74	0
2	MAN	D	3005	11/12	0.70	0.27	-	74,76,76,77	0
2	MAN	A	3007	11/12	0.79	0.26	-	92,93,94,95	0
2	MAN	C	3007	11/12	0.72	0.46	-	96,97,98,99	0
4	NAG	C	2017	14/15	0.69	0.64	-	82,83,84,85	0
9	MAN	C	3009	11/12	0.71	0.29	-	92,95,96,97	0
2	BMA	B	3001	11/12	0.84	0.18	-	82,85,89,90	0
2	NAG	A	2013	14/15	0.90	0.25	-	71,73,75,75	0
2	MAN	C	3008	11/12	0.75	0.30	-	95,95,96,96	0
4	NAG	B	2017	14/15	0.85	0.55	-	89,90,92,93	0
6	NAG	A	2009	14/15	0.90	0.22	-	64,69,71,72	0
4	NAG	D	2009	14/15	0.81	0.32	-	68,69,70,72	0
2	MAN	A	3008	11/12	0.56	0.36	-	90,91,94,94	0
4	NAG	E	2009	14/15	0.83	0.37	-	65,67,67,67	0
2	BMA	E	3003	11/12	0.72	0.28	-	75,76,77,78	0
3	BMA	B	3004	11/12	0.86	0.25	-	79,85,88,92	0
2	NAG	C	2013	14/15	0.83	0.32	-	76,78,80,80	0
2	MAN	E	3006	11/12	0.59	0.56	-	78,79,79,79	0
3	MAN	A	3009	11/12	0.73	0.31	-	98,100,100,100	0
2	BMA	F	3001	11/12	0.86	0.29	-	76,77,79,82	0
6	BMA	D	3002	11/12	0.57	0.66	-	80,80,80,81	0
3	MAN	B	3010	11/12	0.88	0.23	-	73,77,78,79	0
2	MAN	B	3007	11/12	0.79	0.34	-	91,92,93,94	0
3	MAN	D	3009	11/12	0.66	0.36	-	73,75,76,76	0
2	MAN	B	3008	11/12	0.83	0.19	-	93,94,95,95	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
2	MAN	F	3005	11/12	0.60	0.47	-	63,65,65,65	0
4	NAG	D	2016	14/15	0.73	0.56	-	73,74,75,76	0
9	BMA	E	3004	11/12	0.77	0.34	-	82,86,89,92	0
6	NAG	A	2011	14/15	0.92	0.36	-	71,72,73,75	0
2	BMA	C	3001	11/12	0.82	0.39	-	87,90,93,94	0
6	BMA	E	3002	11/12	0.77	0.36	-	65,66,66,66	0
2	MAN	F	3007	11/12	0.79	0.41	-	77,78,79,79	0
9	MAN	C	3010	11/12	0.95	0.20	-	72,76,80,83	0
2	NAG	D	2013	14/15	0.84	0.41	-	71,74,75,77	0
4	NAG	A	2015	14/15	0.58	0.58	-	92,95,96,96	0
3	BMA	F	3004	11/12	0.57	0.66	-	80,82,82,83	0
6	NAG	C	2009	14/15	0.91	0.40	-	58,62,65,66	0
3	BMA	A	3004	11/12	0.94	0.24	-	80,86,89,93	0
9	MAN	E	3010	11/12	0.89	0.22	-	76,80,82,84	0
6	NAG	D	2011	14/15	0.89	0.33	-	75,76,76,78	0
8	BMA	B	3002	11/12	0.53	0.53	-	82,84,85,87	0
3	NAG	B	2004	14/15	0.93	0.24	-	78,79,80,82	0
2	MAN	C	3005	11/12	0.64	0.29	-	82,84,86,86	0
2	BMA	A	3003	11/12	0.89	0.27	-	73,74,75,77	0
3	NAG	A	2004	14/15	0.96	0.23	-	79,82,86,86	0
6	NAG	E	2011	14/15	0.84	0.35	-	65,65,66,66	0
2	MAN	B	3006	11/12	0.78	0.42	-	74,75,75,75	0
3	MAN	F	3010	11/12	0.69	0.36	-	76,78,79,79	0
6	NAG	F	2011	14/15	0.71	0.57	-	77,78,79,81	0
2	BMA	A	3001	11/12	0.84	0.17	-	80,84,88,89	0
3	NAG	D	2004	14/15	0.89	0.21	-	67,68,69,71	0
2	NAG	B	2013	14/15	0.83	0.29	-	68,71,71,72	0
2	MAN	E	3005	11/12	0.65	0.35	-	74,76,76,76	0
2	MAN	E	3008	11/12	0.67	0.41	-	88,89,89,90	0
2	MAN	D	3006	11/12	0.60	0.34	-	81,82,83,83	0
3	MAN	B	3009	11/12	0.78	0.42	-	96,100,100,100	0
6	NAG	C	2016	14/15	0.80	0.43	-	52,53,54,55	0
3	MAN	F	3009	11/12	0.54	0.50	-	80,80,81,82	0
6	NAG	A	2016	14/15	0.81	0.30	-	73,73,74,76	0
2	MAN	E	3007	11/12	0.69	0.45	-	87,88,89,89	0
9	MAN	E	3009	11/12	0.29	0.58	-	95,97,97,97	0
8	NAG	B	2011	14/15	0.90	0.32	-	73,75,76,79	0
2	MAN	F	3006	11/12	0.71	0.54	-	67,69,69,69	0
9	MAN	E	3012	11/12	0.64	0.46	-	83,85,86,87	0
6	BMA	A	3013	11/12	0.76	0.53	-	73,74,75,75	0
8	MAN	B	3014	11/12	0.66	0.54	-	88,88,89,89	0
2	MAN	A	3006	11/12	0.56	0.50	-	77,78,79,79	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
2	BMA	D	3003	11/12	0.67	0.42	-	78,78,80,81	0
4	NAG	E	2016	14/15	0.87	0.36	-	64,65,66,66	0
3	MAN	A	3010	11/12	0.93	0.23	-	74,77,78,79	0
2	BMA	D	3001	11/12	0.87	0.22	-	75,76,77,77	0
9	MAN	C	3012	11/12	0.78	0.37	-	86,87,88,90	0
6	NAG	C	2011	14/15	0.91	0.28	-	68,71,75,76	0
2	MAN	A	3005	11/12	0.64	0.30	-	74,76,77,78	0
6	BMA	C	3002	11/12	0.67	0.51	-	78,80,81,82	0

## 6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
5	NAG	E	2005	14/15	0.69	0.53	5.12	70,71,71,71	0
5	NAG	F	2005	14/15	0.74	0.52	4.77	67,70,71,72	0
5	NAG	B	2014	14/15	0.79	0.36	4.56	67,70,71,71	0
5	NAG	B	2012	14/15	0.90	0.28	3.88	74,75,79,79	0
5	NAG	D	2014	14/15	0.75	0.43	3.82	65,66,67,67	0
5	NAG	E	2008	14/15	0.68	0.43	3.39	72,72,73,73	0
5	NAG	C	2012	14/15	0.84	0.35	2.86	75,77,79,80	0
5	NAG	A	2012	14/15	0.83	0.36	2.31	76,79,80,81	0
5	NAG	D	2012	14/15	0.85	0.33	2.07	73,74,76,77	0
5	NAG	D	2008	14/15	0.83	0.38	2.01	70,71,73,73	0
5	NAG	C	2005	14/15	0.86	0.31	1.84	64,68,70,70	0
5	NAG	A	2014	14/15	0.87	0.25	1.53	67,67,71,72	0
5	NAG	D	2005	14/15	0.86	0.27	1.27	71,72,74,75	0
5	NAG	F	2008	14/15	0.84	0.35	0.99	71,71,72,72	0
5	NAG	F	2014	14/15	0.89	0.31	0.77	59,62,63,64	0
5	NAG	C	2014	14/15	0.89	0.23	0.11	53,55,57,58	0
5	NAG	E	2014	14/15	0.91	0.26	0.02	52,56,57,58	0
5	NAG	A	2008	14/15	0.90	0.22	-0.06	68,69,70,70	0
5	NAG	B	2005	14/15	0.91	0.20	-0.78	64,67,69,70	0
10	CU1	E	1001	1/1	0.92	0.23	-1.10	88,88,88,88	0
10	CU1	E	1004	1/1	0.85	0.17	-2.13	100,100,100,100	0
10	CU1	F	1001	1/1	0.85	0.20	-2.34	90,90,90,90	0
10	CU1	E	1002	1/1	0.95	0.09	-2.79	93,93,93,93	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
10	CU1	A	1001	1/1	0.98	0.12	-2.85	82,82,82,82	0
10	CU1	E	1003	1/1	0.91	0.15	-2.99	99,99,99,99	0
10	CU1	C	1001	1/1	0.97	0.07	-3.12	85,85,85,85	0
10	CU1	B	1002	1/1	0.98	0.17	-3.62	88,88,88,88	0
10	CU1	D	1001	1/1	0.93	0.09	-3.73	86,86,86,86	0
10	CU1	C	1002	1/1	0.98	0.09	-3.80	85,85,85,85	0
10	CU1	C	1004	1/1	0.93	0.11	-3.81	100,100,100,100	0
10	CU1	A	1002	1/1	0.98	0.16	-3.92	87,87,87,87	0
10	CU1	A	1003	1/1	0.99	0.18	-4.20	89,89,89,89	0
10	CU1	F	1003	1/1	0.95	0.09	-4.27	91,91,91,91	0
10	CU1	B	1001	1/1	0.97	0.10	-4.41	87,87,87,87	0
10	CU1	F	1004	1/1	0.95	0.09	-4.53	100,100,100,100	0
10	CU1	F	1002	1/1	0.94	0.07	-4.92	96,96,96,96	0
10	CU1	D	1002	1/1	0.99	0.07	-5.01	87,87,87,87	0
10	CU1	B	1003	1/1	0.98	0.16	-5.05	87,87,87,87	0
10	CU1	D	1004	1/1	0.95	0.07	-5.63	100,100,100,100	0
10	CU1	C	1003	1/1	0.97	0.10	-6.12	83,83,83,83	0
10	CU1	D	1003	1/1	0.96	0.10	-7.02	89,89,89,89	0
10	CU1	A	1004	1/1	0.90	0.12	-9.75	100,100,100,100	0
10	CU1	B	1004	1/1	0.98	0.10	-10.23	100,100,100,100	0
5	NAG	E	2012	14/15	0.54	0.53	-	73,74,77,77	0
7	NDG	A	2018	14/15	0.63	0.44	-	78,80,82,82	0
5	NAG	B	2018	14/15	0.84	0.40	-	80,83,83,83	0
5	NAG	C	2018	14/15	0.69	0.52	-	74,76,77,78	0
5	NAG	D	2006	14/15	0.81	0.33	-	65,68,70,71	0
5	NAG	F	2006	14/15	0.69	0.51	-	67,68,70,70	0
5	NAG	C	2006	14/15	0.84	0.33	-	74,76,77,78	0
5	NAG	B	2006	14/15	0.84	0.27	-	74,76,78,79	0
5	NAG	F	2009	14/15	0.84	0.28	-	66,69,69,69	0
5	NAG	F	2012	14/15	0.69	0.57	-	72,73,75,75	0
5	NAG	A	2006	14/15	0.75	0.30	-	71,73,74,74	0
5	NAG	E	2006	14/15	0.72	0.43	-	73,74,75,76	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.