



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 02:54 PM GMT

PDB ID : 4AUE  
Title : Crystal structure, recombinant expression and mutagenesis studies of the bi-functional catalase-phenol oxidase from *Scytalidium thermophilum*  
Authors : Yuzugullu, Y.; Trinh, C.H.; Smith, M.A.; Pearson, A.R.; Phillips, S.E.V.; Sutay Kocabas, D.; Bakir, U.; Ogel, Z.B.; McPherson, M.J.  
Deposited on : 2012-05-17  
Resolution : 2.70 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

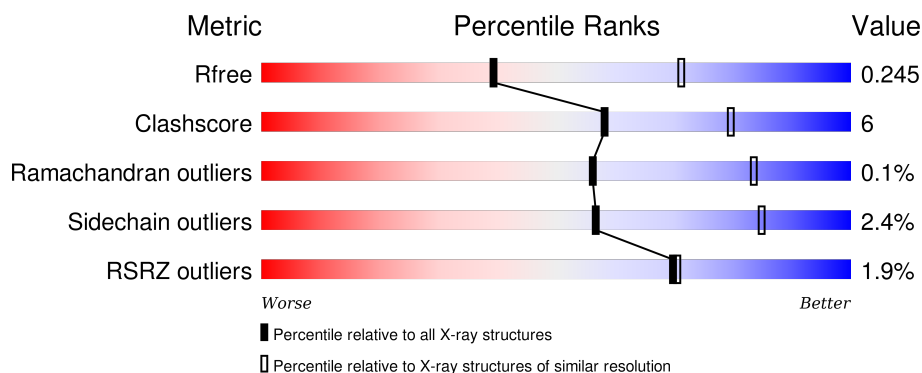
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.70 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))
$R_{free}$	91344	2103 (2.70-2.70)
Clashscore	102246	2422 (2.70-2.70)
Ramachandran outliers	100387	2382 (2.70-2.70)
Sidechain outliers	100360	2382 (2.70-2.70)
RSRZ outliers	91569	2107 (2.70-2.70)

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	717	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 0%, red 1%, orange 1%, orange 79%, yellow 79%, yellow 92%, green 92%, green 100%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span>%</span> <span>79%</span> <span>13%</span> <span>• 7%</span> </div> </div>
1	B	717	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 0%, red 3%, orange 3%, orange 80%, yellow 80%, yellow 93%, green 93%, green 100%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span>3%</span> <span>80%</span> <span>13%</span> <span>• 6%</span> </div> </div>
1	C	717	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 0%, red 2%, orange 2%, orange 81%, yellow 81%, yellow 93%, green 93%, green 100%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span>2%</span> <span>81%</span> <span>12%</span> <span>• 7%</span> </div> </div>
1	D	717	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 0%, red 1%, orange 1%, orange 82%, yellow 82%, yellow 93%, green 93%, green 100%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span>%</span> <span>82%</span> <span>11%</span> <span>• 7%</span> </div> </div>

2 Entry composition ⓘ

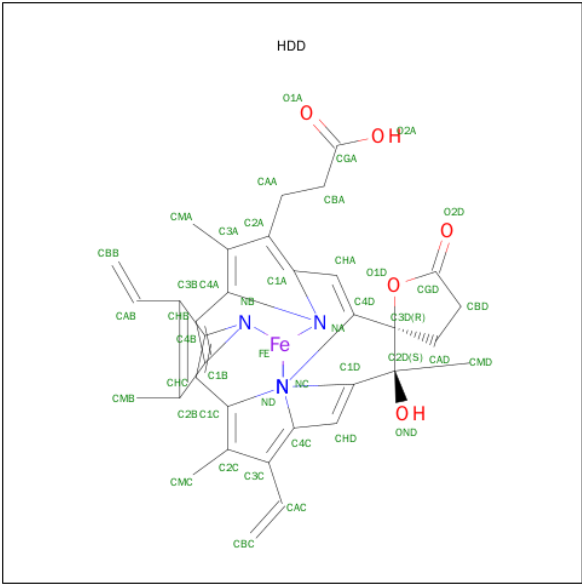
There are 6 unique types of molecules in this entry. The entry contains 21804 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 CATALASE-PHENOL OXIDASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	669	Total	C	N	O	S	0	8	0
			5274	3328	928	1007	11			
1	B	671	Total	C	N	O	S	0	3	0
			5253	3312	921	1009	11			
1	C	670	Total	C	N	O	S	0	4	0
			5258	3316	925	1006	11			
1	D	669	Total	C	N	O	S	0	2	0
			5232	3300	918	1003	11			

- Molecule 2 is CIS-HEME D HYDROXYCHLORIN GAMMA-SPIROLACTONE (three-letter code: HDD) (formula: C<sub>34</sub>H<sub>32</sub>FeN<sub>4</sub>O<sub>5</sub>).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	Fe	N	O	0	0
			44	34	1	4	5		
2	B	1	Total	C	Fe	N	O	0	0
			44	34	1	4	5		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	C	1	Total	C	Fe	N	O	0	0
			44	34	1	4	5		
2	D	1	Total	C	Fe	N	O	0	0
			44	34	1	4	5		

- Molecule 3 is a polymer of unknown type called SUGAR (2-MER).

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

- Molecule 4 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula:  $C_8H_{15}NO_6$ ).



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

- Molecule 5 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	1	Total	Ca	0	0
			1	1		

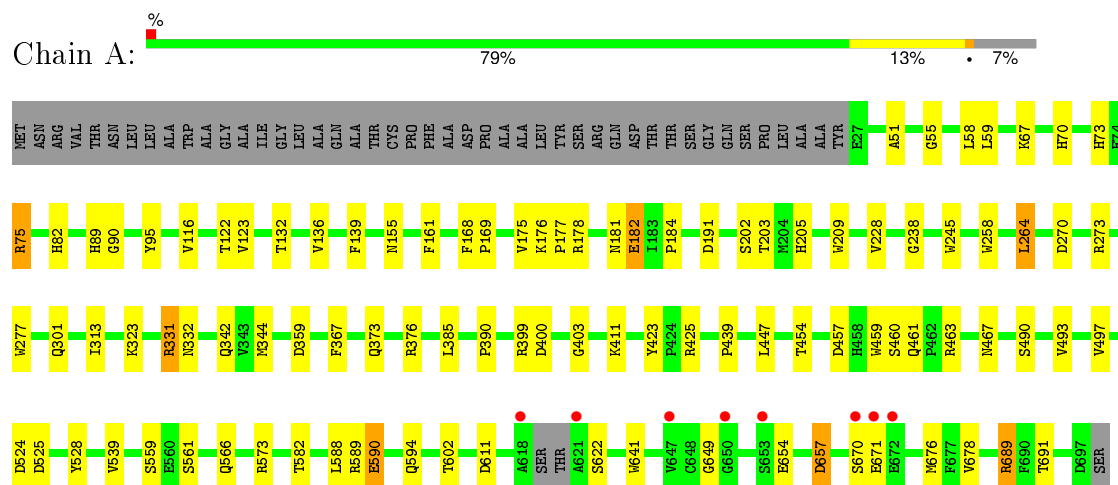
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	128	Total	O	0	0
			128	128		
6	B	75	Total	O	0	0
			75	75		
6	C	51	Total	O	0	0
			51	51		
6	D	62	Total	O	0	0
			62	62		

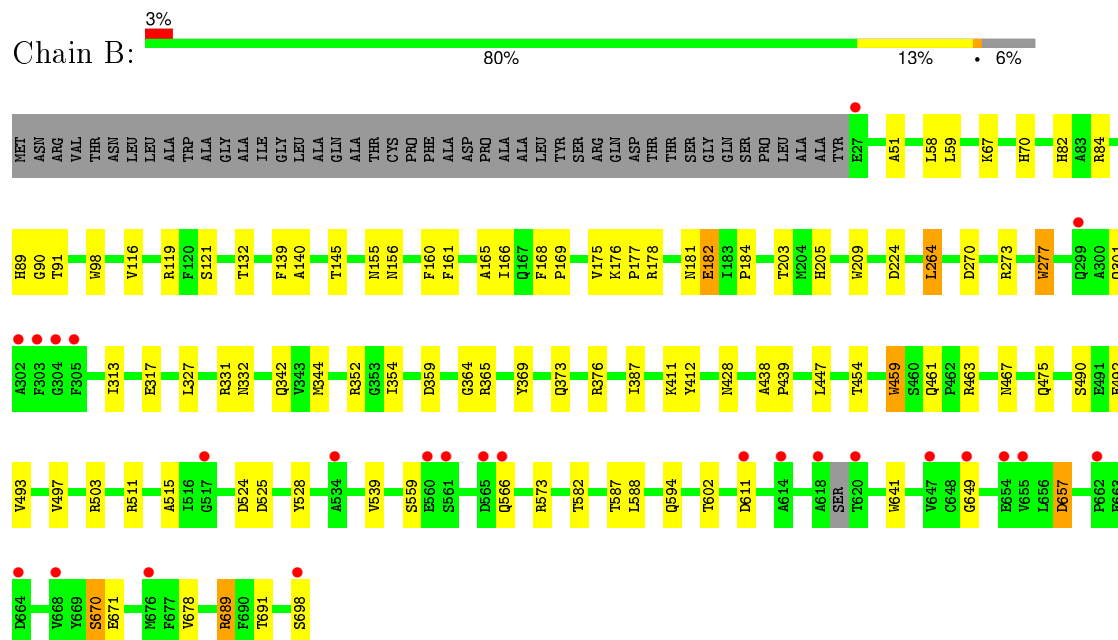
### 3 Residue-property plots

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.

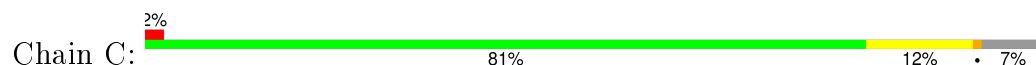
#### • Molecule 1: CATALASE-PHENOL OXIDASE

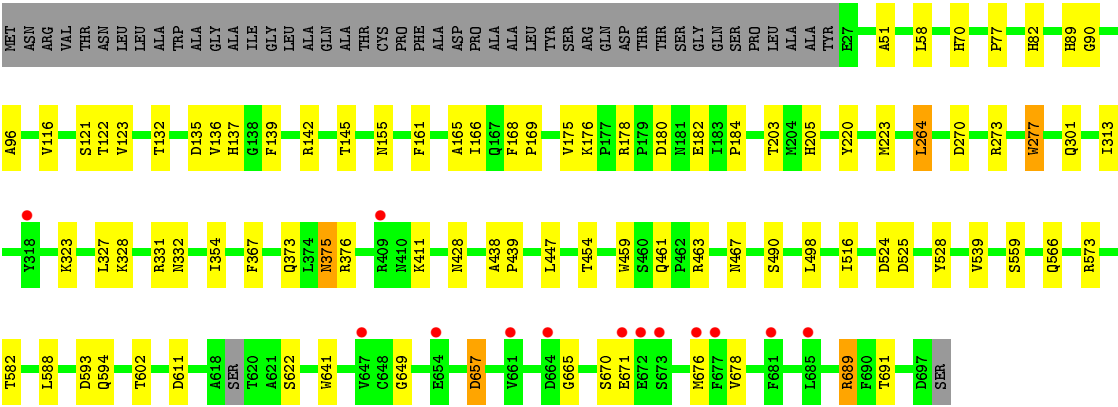


#### • Molecule 1: CATALASE-PHENOL OXIDASE

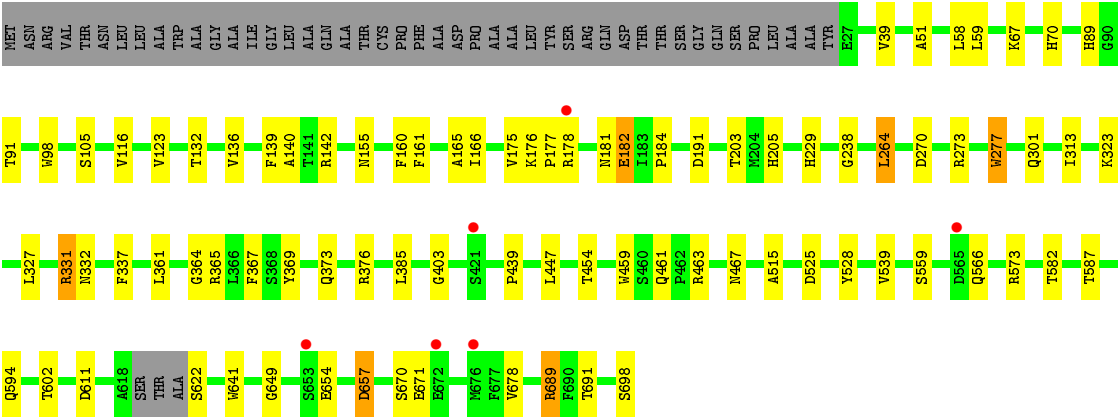
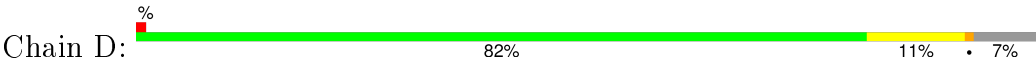


#### • Molecule 1: CATALASE-PHENOL OXIDASE





● Molecule 1: CATALASE-PHENOL OXIDASE



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	185.45Å 216.34Å 68.61Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	141.42 – 2.70 45.33 – 2.70	Depositor EDS
% Data completeness (in resolution range)	99.8 (141.42-2.70) 99.9 (45.33-2.70)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.45 (at 2.69Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, $R_{free}$	0.192 , 0.251 0.188 , 0.245	Depositor DCC
$R_{free}$ test set	3852 reflections (5.29%)	DCC
Wilson B-factor (Å <sup>2</sup> )	49.8	Xtriage
Anisotropy	0.328	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.29 , 29.4	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 76729 reflections	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	21804	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	49.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.74% of the height of the origin peak. No significant pseudotranslation is detected.*

<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

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CA, HDD, NAG

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	0.67	5/5418 (0.1%)	0.70	3/7362 (0.0%)
1	B	0.64	6/5385 (0.1%)	0.68	1/7319 (0.0%)
1	C	0.67	5/5390 (0.1%)	0.70	1/7325 (0.0%)
1	D	0.67	4/5364 (0.1%)	0.69	2/7290 (0.0%)
All	All	0.66	20/21557 (0.1%)	0.69	7/29296 (0.0%)

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	98	TRP	CD2-CE2	5.93	1.48	1.41
1	A	641	TRP	CD2-CE2	5.90	1.48	1.41
1	C	277	TRP	CD2-CE2	5.88	1.48	1.41
1	B	641	TRP	CD2-CE2	5.86	1.48	1.41
1	A	209	TRP	CD2-CE2	5.78	1.48	1.41
1	A	245	TRP	CD2-CE2	5.65	1.48	1.41
1	C	459	TRP	CD2-CE2	5.62	1.48	1.41
1	D	277	TRP	CD2-CE2	5.59	1.48	1.41
1	C	375	ASN	CG-OD1	-5.57	1.11	1.24
1	B	317	GLU	C-N	5.55	1.46	1.34
1	A	258	TRP	CD2-CE2	5.55	1.48	1.41
1	A	459	TRP	CD2-CE2	5.50	1.48	1.41
1	B	209	TRP	CD2-CE2	5.47	1.48	1.41
1	C	641	TRP	CD2-CE2	5.39	1.47	1.41
1	C	375	ASN	CG-ND2	-5.38	1.19	1.32
1	B	98	TRP	CD2-CE2	5.37	1.47	1.41
1	B	277	TRP	CD2-CE2	5.18	1.47	1.41
1	D	641	TRP	CD2-CE2	5.16	1.47	1.41
1	B	459	TRP	CD2-CE2	5.15	1.47	1.41
1	D	459	TRP	CD2-CE2	5.14	1.47	1.41

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	399	ARG	NE-CZ-NH1	5.99	123.30	120.30
1	D	331	ARG	NE-CZ-NH2	-5.56	117.52	120.30
1	B	352	ARG	NE-CZ-NH1	5.37	122.98	120.30
1	D	331	ARG	NE-CZ-NH1	5.25	122.92	120.30
1	A	75	ARG	NE-CZ-NH1	5.14	122.87	120.30
1	A	331	ARG	NE-CZ-NH1	5.02	122.81	120.30
1	C	142	ARG	NE-CZ-NH2	-5.02	117.79	120.30

There are no chirality outliers.

There are no planarity outliers.

## 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	5274	0	5060	76	0
1	B	5253	0	5019	76	0
1	C	5258	0	5037	65	0
1	D	5232	0	5002	65	0
2	A	44	0	31	3	0
2	B	44	0	31	7	0
2	C	44	0	31	3	0
2	D	44	0	31	3	0
3	A	84	0	75	0	0
3	B	56	0	50	0	0
3	C	56	0	50	1	0
3	D	84	0	75	1	0
4	B	14	0	13	0	0
5	B	1	0	0	0	0
6	A	128	0	0	0	0
6	B	75	0	0	2	0
6	C	51	0	0	2	0
6	D	62	0	0	0	0
All	All	21804	0	20505	246	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 6.

All (246) 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)
1:B:689:ARG:HG3	1:B:689:ARG:HH11	1.17	1.10
1:C:689:ARG:HH11	1:C:689:ARG:HG3	1.13	1.08
1:A:689:ARG:HH11	1:A:689:ARG:HG3	1.17	1.06
1:D:689:ARG:HG3	1:D:689:ARG:HH11	1.17	1.05
1:A:590:GLU:HA	1:A:590:GLU:OE1	1.62	0.97
1:C:161:PHE:HB3	1:C:203:THR:HG22	1.51	0.93
1:A:463:ARG:HE	1:A:467:ASN:HD21	1.20	0.89
1:C:463:ARG:HE	1:C:467:ASN:HD21	1.20	0.88
1:B:463:ARG:HE	1:B:467:ASN:HD21	1.17	0.88
1:A:73:HIS:HA	1:C:375:ASN:HD22	1.37	0.87
1:A:161:PHE:HB3	1:A:203:THR:HG22	1.57	0.87
1:C:264:LEU:HG	1:C:602:THR:HB	1.58	0.85
1:B:161:PHE:HB3	1:B:203:THR:HG22	1.58	0.85
1:C:313:ILE:H	1:C:461:GLN:HE22	1.22	0.85
1:A:313:ILE:H	1:A:461:GLN:HE22	1.24	0.84
1:D:161:PHE:HB3	1:D:203:THR:HG22	1.59	0.83
1:D:264:LEU:HG	1:D:602:THR:HB	1.60	0.82
1:C:670:SER:O	1:C:671:GLU:HG2	1.79	0.82
1:B:313:ILE:H	1:B:461:GLN:HE22	1.30	0.79
1:A:264:LEU:HG	1:A:602:THR:HB	1.64	0.79
1:D:463:ARG:HE	1:D:467:ASN:HD21	1.28	0.79
1:B:264:LEU:HG	1:B:602:THR:HB	1.63	0.78
1:D:313:ILE:H	1:D:461:GLN:HE22	1.30	0.77
1:A:689:ARG:HG3	1:A:689:ARG:NH1	1.98	0.76
1:D:566:GLN:HE22	1:D:611:ASP:HB3	1.51	0.76
1:B:566:GLN:HE22	1:B:611:ASP:HB3	1.52	0.74
1:B:689:ARG:NH1	1:B:689:ARG:HG3	1.98	0.73
1:A:566:GLN:HE22	1:A:611:ASP:HB3	1.54	0.73
1:D:670:SER:O	1:D:671:GLU:HG2	1.87	0.73
1:C:689:ARG:HG3	1:C:689:ARG:NH1	1.93	0.72
1:A:670:SER:O	1:A:671:GLU:HG2	1.90	0.72
1:B:670:SER:O	1:B:671:GLU:HG2	1.90	0.71
1:C:566:GLN:HE22	1:C:611:ASP:HB3	1.55	0.70
1:A:411:LYS:NZ	1:B:178:ARG:HE	1.89	0.70
1:A:689:ARG:HH11	1:A:689:ARG:CG	2.02	0.69
1:D:573:ARG:HG2	1:D:678:VAL:HG21	1.74	0.68
1:A:95:TYR:CE2	1:A:323[B]:LYS:HE3	2.29	0.68
1:D:573:ARG:CG	1:D:678:VAL:HG21	2.24	0.67
1:A:155:ASN:CG	2:A:900:HDD:HMB2	2.15	0.67
1:C:670:SER:C	1:C:671:GLU:HG2	2.17	0.65
1:D:373:GLN:HA	1:D:373:GLN:HE21	1.62	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:611:ASP:HB2	1:B:649:GLY:HA3	1.79	0.65
1:C:89:HIS:HB2	1:C:331:ARG:HB3	1.78	0.65
1:A:539:VAL:HG11	1:A:691:THR:HG21	1.78	0.64
1:A:411:LYS:HZ2	1:B:178:ARG:HE	1.44	0.63
1:B:301:GLN:HE22	1:B:454:THR:HG21	1.63	0.63
1:B:582:THR:HG21	1:B:594:GLN:HE21	1.64	0.62
1:C:573[A]:ARG:HG3	1:C:678:VAL:HG21	1.82	0.62
1:D:105:SER:HB2	3:D:903:NAG:H61	1.79	0.62
1:D:301:GLN:HE22	1:D:454:THR:HG21	1.65	0.62
1:D:689:ARG:CG	1:D:689:ARG:HH11	2.02	0.61
1:D:611:ASP:HB2	1:D:649:GLY:HA3	1.83	0.60
2:B:900:HDD:HMC1	2:B:900:HDD:HBC1	1.81	0.60
1:B:689:ARG:CG	1:B:689:ARG:HH11	2.03	0.60
1:C:689:ARG:HH11	1:C:689:ARG:CG	1.99	0.60
1:A:411:LYS:NZ	1:B:178:ARG:NE	2.50	0.59
1:A:58:LEU:HD11	1:C:447:LEU:HD22	1.84	0.59
1:D:689:ARG:HG3	1:D:689:ARG:NH1	1.98	0.59
1:C:539:VAL:HG11	1:C:691:THR:HG21	1.84	0.59
2:A:900:HDD:HBC1	2:A:900:HDD:HMC1	1.85	0.59
1:C:582:THR:HG21	1:C:594:GLN:HE21	1.67	0.59
1:A:611:ASP:HB2	1:A:649:GLY:HA3	1.85	0.59
1:D:539:VAL:HG11	1:D:691:THR:HG21	1.85	0.58
1:B:539:VAL:HG11	1:B:691:THR:HG21	1.84	0.58
1:B:184:PRO:HA	1:D:270:ASP:OD2	2.04	0.58
1:C:611:ASP:HB2	1:C:649:GLY:HA3	1.85	0.58
1:D:670:SER:C	1:D:671:GLU:HG2	2.24	0.57
1:B:155:ASN:CG	2:B:900:HDD:HMB2	2.24	0.57
1:A:155:ASN:ND2	2:A:900:HDD:HMB2	2.20	0.57
1:A:301:GLN:HE22	1:A:454:THR:HG21	1.70	0.57
1:B:573:ARG:HG3	1:B:678:VAL:HG21	1.87	0.56
1:B:573:ARG:CG	1:B:678:VAL:HG21	2.36	0.56
1:C:573[A]:ARG:HG3	1:C:678:VAL:HG11	1.88	0.56
1:C:301:GLN:HE22	1:C:454:THR:HG21	1.71	0.56
1:A:573:ARG:HG2	1:A:678:VAL:HG21	1.86	0.56
1:B:670:SER:C	1:B:671:GLU:HG2	2.27	0.55
1:A:582:THR:HG21	1:A:594:GLN:HE21	1.71	0.55
1:B:182:GLU:HB3	1:D:273:ARG:NH1	2.21	0.55
1:D:582:THR:HG21	1:D:594:GLN:HE21	1.71	0.55
1:A:670:SER:C	1:A:671:GLU:HG2	2.27	0.55
1:B:270:ASP:OD2	1:D:184:PRO:HA	2.06	0.55
1:B:373:GLN:HE21	1:B:373:GLN:HA	1.72	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:205:HIS:CE1	1:D:461:GLN:HE21	2.24	0.54
1:D:525:ASP:HA	1:D:528:TYR:CD2	2.43	0.54
1:C:96:ALA:HB2	3:C:902:NAG:H82	1.90	0.54
1:A:89:HIS:HB2	1:A:331:ARG:HB3	1.88	0.54
1:C:277:TRP:CZ3	1:C:332:ASN:HB3	2.42	0.54
1:D:373:GLN:HA	1:D:373:GLN:NE2	2.23	0.53
1:B:205:HIS:CE1	1:B:461:GLN:HE21	2.26	0.53
1:A:463:ARG:NE	1:A:467:ASN:HD21	1.98	0.53
1:B:119:ARG:HD3	2:B:900:HDD:O1A	2.09	0.53
1:C:313:ILE:H	1:C:461:GLN:NE2	1.99	0.52
1:A:411:LYS:HZ1	1:B:178:ARG:NE	2.07	0.52
1:C:373:GLN:HA	1:C:373:GLN:HE21	1.73	0.52
1:B:67:LYS:HE2	1:D:166:ILE:O	2.10	0.52
1:B:525:ASP:HA	1:B:528:TYR:CD2	2.45	0.52
1:B:182:GLU:HB3	1:D:273:ARG:HH11	1.75	0.52
1:A:123:VAL:HG23	1:A:136:VAL:O	2.11	0.51
1:B:51:ALA:HB2	1:B:58:LEU:HD21	1.92	0.51
1:A:132:THR:HG21	1:A:264:LEU:HD13	1.92	0.51
1:B:89:HIS:HB2	1:B:331:ARG:HB3	1.93	0.51
1:D:132:THR:HG21	1:D:264:LEU:HD13	1.92	0.51
1:C:51:ALA:HB2	1:C:58:LEU:HD21	1.93	0.51
1:C:205:HIS:CE1	1:C:461:GLN:HE21	2.28	0.51
1:A:525:ASP:HA	1:A:528:TYR:CD2	2.46	0.51
1:B:463:ARG:HE	1:B:467:ASN:ND2	1.99	0.51
1:A:67:LYS:HE2	1:C:166:ILE:O	2.11	0.50
1:C:82:HIS:HD2	1:C:121:SER:OG	1.94	0.50
1:B:132:THR:HG21	1:B:264:LEU:HD13	1.94	0.50
1:A:447:LEU:HD22	1:C:58:LEU:HD11	1.93	0.50
1:B:411:LYS:HE2	1:B:412:TYR:CZ	2.47	0.50
1:D:176:LYS:HB3	1:D:177:PRO:CD	2.42	0.49
1:B:176:LYS:HB3	1:B:177:PRO:CD	2.43	0.49
1:B:273:ARG:NH1	1:D:182:GLU:HB3	2.27	0.49
1:B:515:ALA:HA	1:D:587:THR:HG22	1.93	0.49
1:B:447:LEU:HD22	1:D:58:LEU:HD11	1.94	0.49
1:B:84:ARG:HA	6:B:2013:HOH:O	2.11	0.49
1:A:95:TYR:HE2	1:A:323[B]:LYS:HE3	1.75	0.49
1:B:140:ALA:HB2	2:B:900:HDD:HMA3	1.95	0.49
1:A:178:ARG:HD2	1:B:411:LYS:HZ1	1.77	0.49
1:C:525:ASP:HA	1:C:528:TYR:CD2	2.47	0.49
1:B:59:LEU:HD11	1:C:367:PHE:HB2	1.95	0.49
1:D:365:ARG:O	1:D:369:TYR:HD1	1.96	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:373:GLN:HE22	1:C:376:ARG:NH1	2.10	0.48
1:A:178:ARG:HD2	1:B:411:LYS:NZ	2.28	0.48
1:B:475:GLN:OE1	1:B:511:ARG:NH2	2.45	0.48
1:A:205:HIS:CE1	1:A:461:GLN:HE21	2.31	0.48
1:C:665:GLY:HA2	6:C:2051:HOH:O	2.13	0.48
1:C:178:ARG:HG2	1:C:180:ASP:OD1	2.14	0.48
1:A:367:PHE:HB2	1:D:59:LEU:HD11	1.96	0.48
1:C:155:ASN:CG	2:C:900:HDD:HMB2	2.34	0.48
1:A:373:GLN:HE22	1:A:376:ARG:NH1	2.12	0.48
1:B:313:ILE:H	1:B:461:GLN:NE2	2.07	0.48
1:B:373:GLN:HE22	1:B:376:ARG:NH1	2.12	0.48
1:C:411:LYS:NZ	1:D:178:ARG:HD2	2.28	0.47
1:A:182:GLU:HB3	1:C:273:ARG:NH1	2.29	0.47
1:A:51:ALA:HB2	1:A:58:LEU:HD21	1.96	0.47
1:A:463:ARG:HE	1:A:467:ASN:ND2	2.01	0.47
1:D:51:ALA:HB2	1:D:58:LEU:HD21	1.97	0.47
1:A:373:GLN:HE22	1:A:376:ARG:HH11	1.61	0.47
1:A:654:GLU:HG2	1:A:654:GLU:O	2.14	0.47
1:B:428:ASN:HB2	6:B:2060:HOH:O	2.14	0.47
1:B:342:GLN:O	1:B:344:MET:HG3	2.15	0.47
1:A:342:GLN:O	1:A:344:MET:HG3	2.15	0.47
1:B:373:GLN:HA	1:B:373:GLN:NE2	2.30	0.46
1:A:82:HIS:HA	1:A:122:THR:O	2.15	0.46
1:A:90:GLY:C	1:A:116:VAL:HG22	2.36	0.46
1:C:123:VAL:HG23	1:C:136:VAL:O	2.16	0.45
1:B:168:PHE:HB3	1:B:169:PRO:HD3	1.98	0.45
1:A:373:GLN:HE21	1:A:373:GLN:HA	1.82	0.45
1:C:220:TYR:O	1:C:223:MET:HG2	2.16	0.45
1:C:428:ASN:HB2	6:C:2043:HOH:O	2.15	0.45
1:C:373:GLN:NE2	1:C:373:GLN:HA	2.31	0.45
1:C:135:ASP:O	1:C:137:HIS:CE1	2.69	0.45
1:A:566:GLN:HE22	1:A:611:ASP:CB	2.26	0.45
1:C:411:LYS:CE	1:D:178:ARG:HD2	2.47	0.45
1:A:75:ARG:HH21	1:C:176:LYS:HE3	1.81	0.45
1:C:573[A]:ARG:CG	1:C:678:VAL:HG21	2.46	0.45
1:A:168:PHE:HB3	1:A:169:PRO:HD3	1.99	0.45
1:B:58:LEU:HD11	1:D:447:LEU:HD22	1.99	0.45
1:B:365:ARG:O	1:B:369:TYR:HD1	2.00	0.45
1:A:277:TRP:CZ3	1:A:332:ASN:HB3	2.51	0.45
1:C:132:THR:HG21	1:C:264:LEU:HD13	1.99	0.45
1:D:116:VAL:HG21	1:D:327:LEU:CD1	2.47	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:165:ALA:CB	1:D:364:GLY:HA3	2.47	0.45
1:A:176:LYS:HB3	1:A:177:PRO:CD	2.47	0.45
1:C:165:ALA:HB1	2:C:900:HDD:HBC1	1.98	0.44
2:C:900:HDD:HMC1	2:C:900:HDD:HBC1	1.98	0.44
1:A:493:VAL:O	1:A:497:VAL:HG23	2.17	0.44
1:B:587:THR:HG22	1:D:515:ALA:HA	1.99	0.44
1:B:493:VAL:O	1:B:497:VAL:HG23	2.17	0.44
1:B:82:HIS:HD2	1:B:121:SER:OG	2.00	0.44
1:A:385:LEU:HD21	1:D:403:GLY:HA2	1.99	0.44
2:B:900:HDD:HMC1	2:B:900:HDD:CBC	2.48	0.44
1:D:277:TRP:CZ3	1:D:332:ASN:HB3	2.53	0.44
1:A:589:ARG:O	1:A:590:GLU:C	2.55	0.44
1:D:116:VAL:HA	1:D:142:ARG:O	2.17	0.44
1:C:168:PHE:HB3	1:C:169:PRO:HD3	1.99	0.44
1:B:160:PHE:CG	2:B:900:HDD:HAB	2.53	0.44
1:C:498:LEU:HD11	1:C:516:ILE:HD11	2.00	0.44
1:C:90:GLY:HA3	1:C:328:LYS:O	2.18	0.44
1:B:277:TRP:CE3	1:D:181:ASN:HB3	2.53	0.43
1:A:313:ILE:H	1:A:461:GLN:NE2	2.03	0.43
1:C:566:GLN:HE22	1:C:611:ASP:CB	2.26	0.43
1:A:270:ASP:OD2	1:C:184:PRO:HA	2.19	0.43
1:A:461:GLN:HB3	1:A:461:GLN:HE21	1.64	0.43
1:D:140:ALA:HB2	2:D:900:HDD:HMA3	2.01	0.43
1:D:155:ASN:CG	2:D:900:HDD:HMB2	2.39	0.43
1:C:116:VAL:HG21	1:C:327:LEU:CD1	2.48	0.43
1:A:423:TYR:CE1	1:A:425[B]:ARG:HD2	2.53	0.43
1:B:461:GLN:HE21	1:B:461:GLN:HB3	1.57	0.43
1:D:229:HIS:HE1	1:D:361:LEU:HD23	1.84	0.43
1:A:524:ASP:C	1:A:524:ASP:OD1	2.57	0.43
1:A:359:ASP:OD1	1:A:359:ASP:C	2.57	0.43
1:C:82:HIS:HA	1:C:122:THR:O	2.19	0.43
1:A:403:GLY:HA2	1:D:385:LEU:HD21	2.01	0.43
1:C:411:LYS:HZ1	1:D:178:ARG:HD2	1.83	0.43
1:A:181:ASN:HB3	1:C:277:TRP:CE3	2.53	0.42
1:B:277:TRP:CZ3	1:B:332:ASN:HB3	2.53	0.42
1:D:89:HIS:HB2	1:D:331:ARG:HB3	2.01	0.42
1:C:77:PRO:HG2	1:C:375:ASN:OD1	2.19	0.42
1:D:238:GLY:O	1:D:439:PRO:HD2	2.19	0.42
1:B:459:TRP:CD1	1:B:503:ARG:HB3	2.54	0.42
1:A:323[A]:LYS:HB2	1:A:323[A]:LYS:HE3	1.77	0.42
1:A:373:GLN:NE2	1:A:373:GLN:HA	2.35	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:566:GLN:HE22	1:D:611:ASP:CB	2.26	0.42
1:B:155:ASN:ND2	2:B:900:HDD:HMB2	2.34	0.42
1:C:82:HIS:CD2	1:C:121:SER:OG	2.72	0.42
1:A:184:PRO:HA	1:C:270:ASP:OD2	2.20	0.42
1:C:582:THR:HG23	1:C:593:ASP:HB2	2.02	0.42
1:D:657:ASP:OD1	1:D:657:ASP:N	2.53	0.42
1:A:238:GLY:O	1:A:439:PRO:HD2	2.19	0.42
1:B:166:ILE:O	1:D:67:LYS:HE2	2.19	0.41
1:D:373:GLN:HE22	1:D:376:ARG:NH1	2.18	0.41
1:D:160:PHE:CG	2:D:900:HDD:HAB	2.55	0.41
1:B:387:ILE:HG13	1:B:387:ILE:O	2.19	0.41
1:D:205:HIS:HE1	1:D:461:GLN:HE21	1.68	0.41
1:A:588:LEU:HD21	1:A:594:GLN:HA	2.01	0.41
1:B:463:ARG:NE	1:B:467:ASN:HD21	1.99	0.41
1:C:461:GLN:HB3	1:C:461:GLN:HE21	1.64	0.41
1:B:181:ASN:HB3	1:D:277:TRP:CE3	2.55	0.41
1:B:165:ALA:CB	1:B:364:GLY:HA3	2.50	0.41
1:C:657:ASP:N	1:C:657:ASP:OD1	2.53	0.41
1:B:524:ASP:C	1:B:524:ASP:OD1	2.59	0.41
1:C:524:ASP:C	1:C:524:ASP:OD1	2.58	0.41
1:D:123:VAL:HG23	1:D:136:VAL:O	2.21	0.41
1:A:411:LYS:HB2	1:A:411:LYS:HE3	1.82	0.41
1:B:588:LEU:HD21	1:B:594:GLN:HA	2.03	0.41
1:B:90:GLY:C	1:B:116:VAL:HG22	2.41	0.41
1:B:657:ASP:N	1:B:657:ASP:OD1	2.53	0.41
1:A:457:ASP:OD2	1:A:460:SER:OG	2.23	0.41
1:D:654:GLU:O	1:D:654:GLU:HG2	2.21	0.41
1:B:359:ASP:C	1:B:359:ASP:OD1	2.59	0.41
1:B:156:ASN:HA	1:B:224:ASP:O	2.21	0.41
1:A:51:ALA:O	1:A:55:GLY:HA3	2.21	0.40
1:B:181:ASN:HB3	1:D:277:TRP:CZ3	2.56	0.40
1:B:116:VAL:HG21	1:B:327:LEU:CD1	2.51	0.40
1:A:400:ASP:HA	1:D:337:PHE:CD2	2.56	0.40
1:A:390:PRO:HB3	1:D:39:VAL:O	2.22	0.40
1:B:438:ALA:HA	1:B:439:PRO:HD3	1.98	0.40
1:D:161:PHE:CB	1:D:203:THR:HG22	2.41	0.40
1:A:657:ASP:N	1:A:657:ASP:OD1	2.54	0.40
1:C:588:LEU:HD21	1:C:594:GLN:HA	2.02	0.40
1:C:438:ALA:HA	1:C:439:PRO:HD3	1.93	0.40
1:A:59:LEU:HD11	1:D:367:PHE:HB2	2.04	0.40
1:A:273:ARG:NH1	1:C:182:GLU:HB3	2.36	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	673/717 (94%)	645 (96%)	25 (4%)	3 (0%)	39	69
1	B	670/717 (93%)	641 (96%)	29 (4%)	0	100	100
1	C	670/717 (93%)	641 (96%)	29 (4%)	0	100	100
1	D	667/717 (93%)	637 (96%)	30 (4%)	0	100	100
All	All	2680/2868 (93%)	2564 (96%)	113 (4%)	3 (0%)	56	83

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	202	SER
1	A	590	GLU
1	A	228	VAL

### 5.3.2 Protein sidechains [i](#)

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	561/590 (95%)	548 (98%)	13 (2%)	58	85
1	B	558/590 (95%)	543 (97%)	15 (3%)	52	82
1	C	559/590 (95%)	546 (98%)	13 (2%)	58	85
1	D	556/590 (94%)	543 (98%)	13 (2%)	58	85

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	2234/2360 (95%)	2180 (98%)	54 (2%)	57 85

All (54) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	70	HIS
1	A	139	PHE
1	A	175	VAL
1	A	182	GLU
1	A	191	ASP
1	A	264	LEU
1	A	490	SER
1	A	559	SER
1	A	561	SER
1	A	622	SER
1	A	657	ASP
1	A	676	MET
1	A	689	ARG
1	B	70	HIS
1	B	91	THR
1	B	139	PHE
1	B	145	THR
1	B	175	VAL
1	B	182	GLU
1	B	264	LEU
1	B	354	ILE
1	B	490	SER
1	B	492	GLU
1	B	559	SER
1	B	657	ASP
1	B	670	SER
1	B	689	ARG
1	B	698	SER
1	C	70	HIS
1	C	139	PHE
1	C	145	THR
1	C	175	VAL
1	C	264	LEU
1	C	323	LYS
1	C	354	ILE
1	C	490	SER
1	C	559	SER

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Mol	Chain	Res	Type
1	C	622	SER
1	C	657	ASP
1	C	676	MET
1	C	689	ARG
1	D	70	HIS
1	D	91	THR
1	D	139	PHE
1	D	175	VAL
1	D	182	GLU
1	D	191	ASP
1	D	264	LEU
1	D	323	LYS
1	D	559	SER
1	D	622	SER
1	D	657	ASP
1	D	689	ARG
1	D	698	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (33) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	82	HIS
1	A	167	GLN
1	A	246	HIS
1	A	301	GLN
1	A	373	GLN
1	A	375	ASN
1	A	461	GLN
1	A	467	ASN
1	A	594	GLN
1	B	70	HIS
1	B	82	HIS
1	B	301	GLN
1	B	373	GLN
1	B	461	GLN
1	B	467	ASN
1	B	594	GLN
1	C	70	HIS
1	C	82	HIS
1	C	167	GLN
1	C	301	GLN
1	C	373	GLN

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Mol	Chain	Res	Type
1	C	461	GLN
1	C	467	ASN
1	C	594	GLN
1	D	70	HIS
1	D	82	HIS
1	D	167	GLN
1	D	301	GLN
1	D	373	GLN
1	D	461	GLN
1	D	467	ASN
1	D	566	GLN
1	D	594	GLN

### 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 ⓘ

20 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	$\# Z  > 2$
3	NAG	A	901	1,3	14,14,15	0.75	0	15,19,21	2.13	4 (26%)
3	NAG	A	902	3	14,14,15	0.69	0	15,19,21	1.39	2 (13%)
3	NAG	A	903	1,3	14,14,15	0.66	0	15,19,21	1.24	2 (13%)
3	NAG	A	904	3	14,14,15	0.49	0	15,19,21	1.68	4 (26%)
3	NAG	A	905	1,3	14,14,15	0.65	0	15,19,21	1.45	1 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	NAG	A	906	3	14,14,15	1.11	1 (7%)	15,19,21	2.30	6 (40%)
3	NAG	B	901	1,3	14,14,15	0.56	0	15,19,21	1.28	1 (6%)
3	NAG	B	902	3	14,14,15	0.64	0	15,19,21	1.40	2 (13%)
3	NAG	B	903	1,3	14,14,15	0.53	0	15,19,21	1.40	1 (6%)
3	NAG	B	904	3	14,14,15	0.51	0	15,19,21	1.77	3 (20%)
3	NAG	C	901	1,3	14,14,15	0.63	0	15,19,21	1.36	3 (20%)
3	NAG	C	902	3	14,14,15	0.52	0	15,19,21	1.31	1 (6%)
3	NAG	C	903	1,3	14,14,15	0.86	1 (7%)	15,19,21	1.12	0
3	NAG	C	904	3	14,14,15	0.69	1 (7%)	15,19,21	1.76	3 (20%)
3	NAG	D	901	1,3	14,14,15	0.56	0	15,19,21	1.42	1 (6%)
3	NAG	D	902	3	14,14,15	0.52	0	15,19,21	1.10	2 (13%)
3	NAG	D	903	1,3	14,14,15	0.51	0	15,19,21	2.69	4 (26%)
3	NAG	D	904	3	14,14,15	0.54	0	15,19,21	1.99	4 (26%)
3	NAG	D	905	1,3	14,14,15	0.70	0	15,19,21	1.17	1 (6%)
3	NAG	D	906	3	14,14,15	0.76	1 (7%)	15,19,21	1.89	3 (20%)

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
3	NAG	A	901	1,3	-	0/6/23/26	0/1/1/1
3	NAG	A	902	3	-	0/6/23/26	0/1/1/1
3	NAG	A	903	1,3	-	0/6/23/26	0/1/1/1
3	NAG	A	904	3	-	0/6/23/26	0/1/1/1
3	NAG	A	905	1,3	-	0/6/23/26	0/1/1/1
3	NAG	A	906	3	-	0/6/23/26	0/1/1/1
3	NAG	B	901	1,3	-	0/6/23/26	0/1/1/1
3	NAG	B	902	3	-	0/6/23/26	0/1/1/1
3	NAG	B	903	1,3	-	0/6/23/26	0/1/1/1
3	NAG	B	904	3	-	0/6/23/26	0/1/1/1
3	NAG	C	901	1,3	-	0/6/23/26	0/1/1/1
3	NAG	C	902	3	-	0/6/23/26	0/1/1/1
3	NAG	C	903	1,3	-	0/6/23/26	0/1/1/1
3	NAG	C	904	3	-	0/6/23/26	0/1/1/1
3	NAG	D	901	1,3	-	0/6/23/26	0/1/1/1
3	NAG	D	902	3	-	0/6/23/26	0/1/1/1
3	NAG	D	903	1,3	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	D	904	3	-	0/6/23/26	0/1/1/1
3	NAG	D	905	1,3	-	0/6/23/26	0/1/1/1
3	NAG	D	906	3	-	0/6/23/26	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	904	NAG	C1-C2	2.13	1.55	1.52
3	D	906	NAG	C1-C2	2.14	1.55	1.52
3	C	903	NAG	C1-C2	2.35	1.55	1.52
3	A	906	NAG	C1-C2	3.42	1.57	1.52

All (48) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	906	NAG	C3-C4-C5	-4.02	103.19	110.20
3	C	904	NAG	C3-C4-C5	-3.52	104.06	110.20
3	A	901	NAG	O5-C5-C6	-3.22	100.37	107.35
3	D	903	NAG	O3-C3-C4	-2.82	103.98	110.34
3	A	904	NAG	C2-N2-C7	-2.63	119.66	123.04
3	D	906	NAG	C3-C2-N2	-2.56	104.44	110.56
3	A	901	NAG	O4-C4-C3	-2.43	104.86	110.34
3	C	901	NAG	C3-C4-C5	-2.43	105.96	110.20
3	C	901	NAG	C3-C2-N2	-2.33	104.98	110.56
3	C	904	NAG	O7-C7-C8	-2.24	117.94	122.06
3	D	903	NAG	O5-C5-C6	-2.14	102.71	107.35
3	B	904	NAG	O3-C3-C4	-2.14	105.52	110.34
3	A	906	NAG	O7-C7-C8	-2.03	118.34	122.06
3	B	902	NAG	C3-C2-N2	-2.01	105.75	110.56
3	D	902	NAG	C6-C5-C4	-2.01	108.06	113.02
3	A	904	NAG	O5-C5-C6	2.02	111.71	107.35
3	A	901	NAG	C2-N2-C7	2.07	125.70	123.04
3	D	904	NAG	O7-C7-N2	2.08	126.10	121.86
3	D	904	NAG	O4-C4-C5	2.08	114.74	109.24
3	A	903	NAG	C4-C3-C2	2.13	114.55	111.23
3	D	905	NAG	O4-C4-C5	2.20	115.06	109.24
3	C	901	NAG	C6-C5-C4	2.26	118.60	113.02
3	A	904	NAG	O4-C4-C3	2.69	116.38	110.34
3	D	902	NAG	C1-O5-C5	2.77	115.76	112.25
3	A	902	NAG	O4-C4-C5	2.78	116.61	109.24
3	A	904	NAG	C1-O5-C5	3.04	116.11	112.25
3	B	904	NAG	C4-C3-C2	3.09	116.03	111.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	906	NAG	O4-C4-C5	3.17	117.64	109.24
3	A	903	NAG	C1-O5-C5	3.31	116.45	112.25
3	A	902	NAG	C1-O5-C5	3.41	116.58	112.25
3	A	906	NAG	C2-N2-C7	3.42	127.43	123.04
3	D	906	NAG	C4-C3-C2	3.47	116.62	111.23
3	B	901	NAG	C1-O5-C5	3.58	116.79	112.25
3	C	904	NAG	O5-C5-C6	3.63	115.20	107.35
3	A	906	NAG	C1-O5-C5	3.82	117.10	112.25
3	C	902	NAG	C1-O5-C5	3.91	117.22	112.25
3	A	906	NAG	O3-C3-C2	3.92	116.87	109.11
3	D	903	NAG	C3-C4-C5	3.97	117.13	110.20
3	D	901	NAG	C1-O5-C5	3.98	117.31	112.25
3	B	902	NAG	C4-C3-C2	4.08	117.57	111.23
3	D	904	NAG	C2-N2-C7	4.10	128.30	123.04
3	B	903	NAG	C1-O5-C5	4.11	117.46	112.25
3	D	906	NAG	C2-N2-C7	4.33	128.60	123.04
3	D	904	NAG	C1-O5-C5	4.56	118.04	112.25
3	A	905	NAG	C1-O5-C5	4.69	118.20	112.25
3	B	904	NAG	C1-O5-C5	4.73	118.25	112.25
3	A	901	NAG	C1-O5-C5	5.96	119.81	112.25
3	D	903	NAG	C1-O5-C5	7.94	122.33	112.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	902	NAG	1	0
3	D	903	NAG	1	0

## 5.6 Ligand geometry ⓘ

Of 6 ligands modelled in this entry, 1 is monoatomic - leaving 5 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
2	HDD	A	900	1	30,52,52	1.81	8 (26%)	20,89,89	2.52	8 (40%)
2	HDD	B	900	1	30,52,52	2.14	10 (33%)	20,89,89	2.22	13 (65%)
4	NAG	B	905	1	14,14,15	0.62	0	15,19,21	1.75	1 (6%)
2	HDD	C	900	1	30,52,52	2.13	10 (33%)	20,89,89	2.55	10 (50%)
2	HDD	D	900	1	30,52,52	2.13	10 (33%)	20,89,89	2.27	9 (45%)

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	HDD	A	900	1	-	0/3/89/89	0/1/9/9
2	HDD	B	900	1	-	0/3/89/89	0/1/9/9
4	NAG	B	905	1	-	0/6/23/26	0/1/1/1
2	HDD	C	900	1	-	0/3/89/89	0/1/9/9
2	HDD	D	900	1	-	0/3/89/89	0/1/9/9

All (38) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	900	HDD	C4D-ND	-2.30	1.34	1.38
2	D	900	HDD	O1D-C3D	-2.24	1.43	1.46
2	B	900	HDD	C1D-ND	-2.20	1.34	1.38
2	C	900	HDD	C1D-ND	-2.16	1.34	1.38
2	A	900	HDD	O1D-C3D	-2.08	1.43	1.46
2	C	900	HDD	O1D-C3D	-2.08	1.43	1.46
2	D	900	HDD	C1D-ND	-2.01	1.35	1.38
2	A	900	HDD	C1C-CHC	2.09	1.45	1.39
2	C	900	HDD	C4A-CHB	2.38	1.46	1.39
2	B	900	HDD	C4A-CHB	2.41	1.46	1.39
2	A	900	HDD	C4C-CHD	2.44	1.46	1.39
2	C	900	HDD	C1C-CHC	2.50	1.46	1.39
2	D	900	HDD	C1C-CHC	2.53	1.46	1.39
2	C	900	HDD	C4C-CHD	2.53	1.46	1.39
2	D	900	HDD	C1A-CHA	2.58	1.46	1.39
2	D	900	HDD	C4A-CHB	2.72	1.47	1.39
2	B	900	HDD	C4C-CHD	2.74	1.47	1.39
2	D	900	HDD	C4C-CHD	2.79	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	900	HDD	C2A-C3A	2.84	1.46	1.37
2	B	900	HDD	C1C-CHC	3.00	1.48	1.39
2	B	900	HDD	C1A-CHA	3.01	1.48	1.39
2	D	900	HDD	C2A-C3A	3.05	1.46	1.37
2	A	900	HDD	C1A-CHA	3.09	1.48	1.39
2	B	900	HDD	C2A-C3A	3.13	1.46	1.37
2	A	900	HDD	C2A-C3A	3.24	1.47	1.37
2	C	900	HDD	C1A-CHA	3.47	1.49	1.39
2	A	900	HDD	C3B-C2B	3.62	1.45	1.40
2	A	900	HDD	C3C-C2C	4.22	1.45	1.40
2	C	900	HDD	C3C-C2C	4.22	1.45	1.40
2	A	900	HDD	O1D-CGD	4.26	1.42	1.35
2	B	900	HDD	C3C-C2C	4.42	1.46	1.40
2	D	900	HDD	C3B-C2B	4.46	1.46	1.40
2	B	900	HDD	C3B-C2B	4.52	1.46	1.40
2	D	900	HDD	C3C-C2C	4.87	1.46	1.40
2	C	900	HDD	C3B-C2B	5.02	1.46	1.40
2	C	900	HDD	O1D-CGD	5.63	1.45	1.35
2	D	900	HDD	O1D-CGD	5.76	1.45	1.35
2	B	900	HDD	O1D-CGD	6.02	1.45	1.35

All (41) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	900	HDD	CAA-CBA-CGA	-5.18	103.26	112.75
2	A	900	HDD	C3B-CAB-CBB	-5.03	116.03	126.32
2	C	900	HDD	CAA-CBA-CGA	-4.92	103.74	112.75
2	D	900	HDD	C3B-CAB-CBB	-4.72	116.67	126.32
2	C	900	HDD	C3B-CAB-CBB	-4.21	117.71	126.32
2	A	900	HDD	C3C-CAC-CBC	-3.43	119.30	126.32
2	B	900	HDD	CAA-CBA-CGA	-3.34	106.62	112.75
2	A	900	HDD	C2D-C1D-CHD	-3.30	118.34	123.48
2	D	900	HDD	CAA-CBA-CGA	-3.12	107.02	112.75
2	A	900	HDD	OND-C2D-CMD	-2.97	104.05	109.41
2	B	900	HDD	C3C-CAC-CBC	-2.95	120.29	126.32
2	B	900	HDD	C3B-CAB-CBB	-2.61	120.97	126.32
2	C	900	HDD	C3C-CAC-CBC	-2.58	121.05	126.32
2	B	900	HDD	OND-C2D-CMD	-2.55	104.80	109.41
2	D	900	HDD	C3C-CAC-CBC	-2.35	121.51	126.32
2	B	900	HDD	CAD-CBD-CGD	-2.22	100.80	104.64
2	A	900	HDD	CBA-CAA-C2A	-2.20	108.59	112.53
2	B	900	HDD	C2D-C1D-CHD	-2.08	120.24	123.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	900	HDD	C2D-C1D-CHD	-2.01	120.35	123.48
2	B	900	HDD	O1D-CGD-CBD	2.10	112.66	110.20
2	B	900	HDD	CMB-C2B-C3B	2.15	129.30	125.09
2	D	900	HDD	O1D-CGD-O2D	2.19	122.89	120.80
2	C	900	HDD	C3B-C4B-NB	2.26	115.21	110.94
2	D	900	HDD	CMB-C2B-C3B	2.43	129.85	125.09
2	B	900	HDD	C3B-C4B-NB	2.48	115.62	110.94
2	D	900	HDD	CMA-C3A-C4A	2.49	132.48	128.36
2	A	900	HDD	CMA-C3A-C2A	2.49	130.44	125.24
2	B	900	HDD	CMC-C2C-C3C	2.54	130.05	125.09
2	B	900	HDD	CAA-C2A-C1A	2.62	129.85	127.01
2	B	900	HDD	C3C-C4C-NC	2.97	113.05	109.21
2	C	900	HDD	CMB-C2B-C3B	2.97	130.90	125.09
2	D	900	HDD	CMC-C2C-C3C	3.31	131.56	125.09
2	D	900	HDD	CAA-C2A-C1A	3.47	130.77	127.01
2	B	900	HDD	O1D-CGD-O2D	3.48	124.11	120.80
2	D	900	HDD	C3C-C4C-NC	3.52	113.76	109.21
2	C	900	HDD	O1D-CGD-O2D	3.53	124.16	120.80
2	C	900	HDD	CAA-C2A-C1A	3.54	130.85	127.01
2	C	900	HDD	C3C-C4C-NC	3.58	113.83	109.21
2	A	900	HDD	C3C-C4C-NC	3.75	114.06	109.21
2	C	900	HDD	CMC-C2C-C3C	4.13	133.17	125.09
4	B	905	NAG	C1-O5-C5	5.84	119.66	112.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 16 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	900	HDD	3	0
2	B	900	HDD	7	0
2	C	900	HDD	3	0
2	D	900	HDD	3	0

## 5.7 Other polymers

There are no such residues in this entry.

## 5.8 Polymer linkage issues

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	669/717 (93%)	-0.35	8 (1%) 81 81	19, 42, 74, 122	0
1	B	671/717 (93%)	-0.05	25 (3%) 45 45	24, 54, 88, 127	0
1	C	670/717 (93%)	-0.20	13 (1%) 70 70	24, 46, 84, 119	0
1	D	669/717 (93%)	-0.31	6 (0%) 85 86	22, 44, 78, 118	0
All	All	2679/2868 (93%)	-0.23	52 (1%) 70 70	19, 46, 83, 127	0

All (52) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	698	SER	6.9
1	A	670	SER	5.5
1	B	302	ALA	5.4
1	B	611	ASP	4.9
1	A	672	GLU	4.8
1	A	621	ALA	4.8
1	B	517	GLY	3.7
1	B	654	GLU	3.6
1	B	676	MET	3.5
1	B	27	GLU	3.4
1	B	618	ALA	3.4
1	B	534	ALA	3.3
1	D	421	SER	3.3
1	D	178	ARG	3.1
1	B	304	GLY	3.1
1	B	565	ASP	3.1
1	D	672	GLU	3.0
1	B	655	VAL	3.0
1	B	299	GLN	3.0
1	C	661	VAL	2.9
1	A	653	SER	2.8

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Mol	Chain	Res	Type	RSRZ
1	B	662	PRO	2.8
1	C	677	PHE	2.7
1	D	676	MET	2.7
1	C	685	LEU	2.7
1	B	649	GLY	2.6
1	C	671	GLU	2.6
1	A	650	GLY	2.6
1	A	647	VAL	2.5
1	C	681	PHE	2.5
1	B	561	SER	2.4
1	B	647	VAL	2.4
1	C	654	GLU	2.4
1	B	664	ASP	2.3
1	A	618	ALA	2.2
1	C	676	MET	2.2
1	C	664	ASP	2.2
1	B	303	PHE	2.2
1	B	668	VAL	2.2
1	D	653	SER	2.2
1	C	409	ARG	2.2
1	C	672	GLU	2.2
1	B	566	GLN	2.1
1	B	560	GLU	2.1
1	B	614	ALA	2.1
1	C	647	VAL	2.1
1	C	673	SER	2.1
1	B	620	THR	2.0
1	B	305	PHE	2.0
1	A	671	GLU	2.0
1	C	318	TYR	2.0
1	D	565	ASP	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(Å <sup>2</sup> )	Q<0.9
3	NAG	A	903	14/15	0.93	0.21	0.37	54,63,72,81	0
3	NAG	B	903	14/15	0.95	0.20	0.30	65,71,81,84	0
3	NAG	D	903	14/15	0.91	0.14	0.05	51,62,66,67	0
3	NAG	C	903	14/15	0.91	0.16	-0.88	54,62,70,71	0
3	NAG	A	905	14/15	0.90	0.22	-	67,76,83,84	0
3	NAG	D	904	14/15	0.93	0.27	-	53,57,63,69	0
3	NAG	B	904	14/15	0.94	0.32	-	63,75,81,83	0
3	NAG	A	901	14/15	0.95	0.16	-	44,50,56,67	0
3	NAG	D	906	14/15	0.71	0.33	-	75,90,94,96	0
3	NAG	A	906	14/15	0.65	0.38	-	70,89,95,96	0
3	NAG	C	902	14/15	0.65	0.20	-	59,92,103,103	0
3	NAG	A	902	14/15	0.90	0.17	-	56,70,75,77	0
3	NAG	B	902	14/15	0.85	0.42	-	77,101,106,106	0
3	NAG	D	901	14/15	0.94	0.16	-	45,53,63,64	0
3	NAG	C	901	14/15	0.94	0.13	-	62,65,71,83	0
3	NAG	D	905	14/15	0.84	0.20	-	62,72,81,88	0
3	NAG	D	902	14/15	0.93	0.23	-	68,72,80,84	0
3	NAG	B	901	14/15	0.88	0.25	-	65,82,85,88	0
3	NAG	C	904	14/15	0.90	0.23	-	65,69,78,80	0
3	NAG	A	904	14/15	0.73	0.22	-	68,87,100,108	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(Å <sup>2</sup> )	Q<0.9
2	HDD	D	900	44/44	0.98	0.20	0.83	29,38,44,45	0
2	HDD	B	900	44/44	0.97	0.19	0.69	36,46,55,58	0
2	HDD	A	900	44/44	0.97	0.18	0.55	25,38,44,49	0
2	HDD	C	900	44/44	0.97	0.16	0.18	30,40,50,55	0
4	NAG	B	905	14/15	0.92	0.31	-	86,94,99,100	0
5	CA	B	910	1/1	0.97	0.22	-	37,37,37,37	1

## 6.5 Other polymers

There are no such residues in this entry.