



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 08:40 AM GMT

PDB ID : 3FHQ  
Title : Structure of endo-beta-N-acetylglucosaminidase A  
Authors : Jie, Y.; Li, L.; Shaw, N.; Li, Y.; Song, J.; Zhang, W.; Xia, C.; Zhang, R.;  
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Deposited on : 2008-12-10  
Resolution : 2.45 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

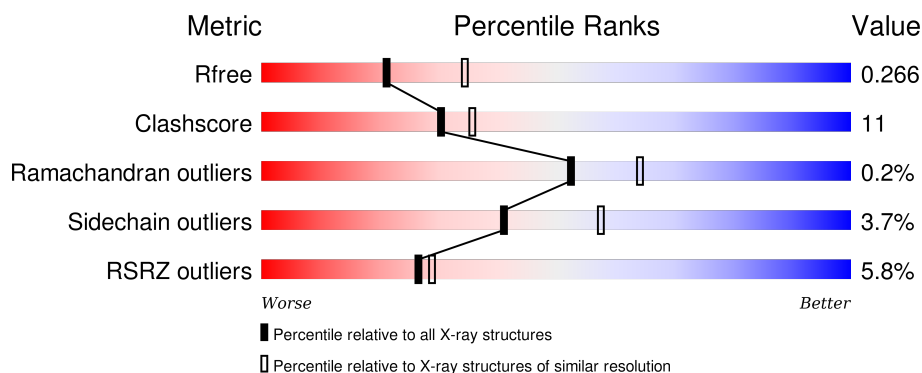
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.45 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	4776 (2.50-2.42)
Clashscore	102246	1030 (2.48-2.44)
Ramachandran outliers	100387	1024 (2.48-2.44)
Sidechain outliers	100360	1024 (2.48-2.44)
RSRZ outliers	91569	4787 (2.50-2.42)

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	621	<div> <div>4%</div> <div>77%</div> <div>18%</div> <div>• •</div> </div>
1	B	621	<div> <div>6%</div> <div>77%</div> <div>18%</div> <div>• •</div> </div>
1	D	621	<div> <div>4%</div> <div>76%</div> <div>18%</div> <div>• •</div> </div>
1	F	621	<div> <div>8%</div> <div>75%</div> <div>19%</div> <div>• •</div> </div>

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 20045 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 Endo-beta-N-acetylglucosaminidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	601	Total	C	N	O	S	0	0	0
			4781	3031	801	938	11			
1	B	599	Total	C	N	O	S	0	0	0
			4757	3017	797	932	11			
1	D	597	Total	C	N	O	S	0	0	0
			4746	3011	793	931	11			
1	F	596	Total	C	N	O	S	0	0	0
			4736	3003	793	929	11			

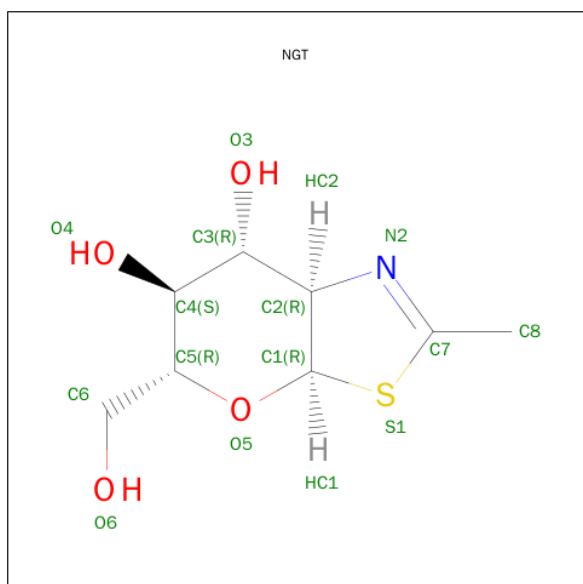
There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	43	ASP	ASN	engineered	UNP Q9ZB22
A	455	ASP	GLY	engineered	UNP Q9ZB22
A	518	THR	ILE	engineered	UNP Q9ZB22
A	583	ILE	LEU	engineered	UNP Q9ZB22
B	43	ASP	ASN	engineered	UNP Q9ZB22
B	455	ASP	GLY	engineered	UNP Q9ZB22
B	518	THR	ILE	engineered	UNP Q9ZB22
B	583	ILE	LEU	engineered	UNP Q9ZB22
D	43	ASP	ASN	engineered	UNP Q9ZB22
D	455	ASP	GLY	engineered	UNP Q9ZB22
D	518	THR	ILE	engineered	UNP Q9ZB22
D	583	ILE	LEU	engineered	UNP Q9ZB22
F	43	ASP	ASN	engineered	UNP Q9ZB22
F	455	ASP	GLY	engineered	UNP Q9ZB22
F	518	THR	ILE	engineered	UNP Q9ZB22
F	583	ILE	LEU	engineered	UNP Q9ZB22

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

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	3	Total	C	O	0	0
			33	18	15		
2	B	3	Total	C	O	0	0
			33	18	15		
2	D	3	Total	C	O	0	0
			33	18	15		
2	F	3	Total	C	O	0	0
			33	18	15		

- Molecule 3 is 3AR,5R,6S,7R,7AR-5-HYDROXYMETHYL-2-METHYL-5,6,7,7A-TETRAHYDRO-3AH-PYRANO[3,2-D]THIAZOLE-6,7-DIOL (three-letter code: NGT) (formula: C<sub>8</sub>H<sub>13</sub>NO<sub>4</sub>S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	S	0	0
			14	8	1	4	1		
3	B	1	Total	C	N	O	S	0	0
			14	8	1	4	1		
3	D	1	Total	C	N	O	S	0	0
			14	8	1	4	1		
3	F	1	Total	C	N	O	S	0	0
			14	8	1	4	1		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	244	Total	O	0	0
			244	244		

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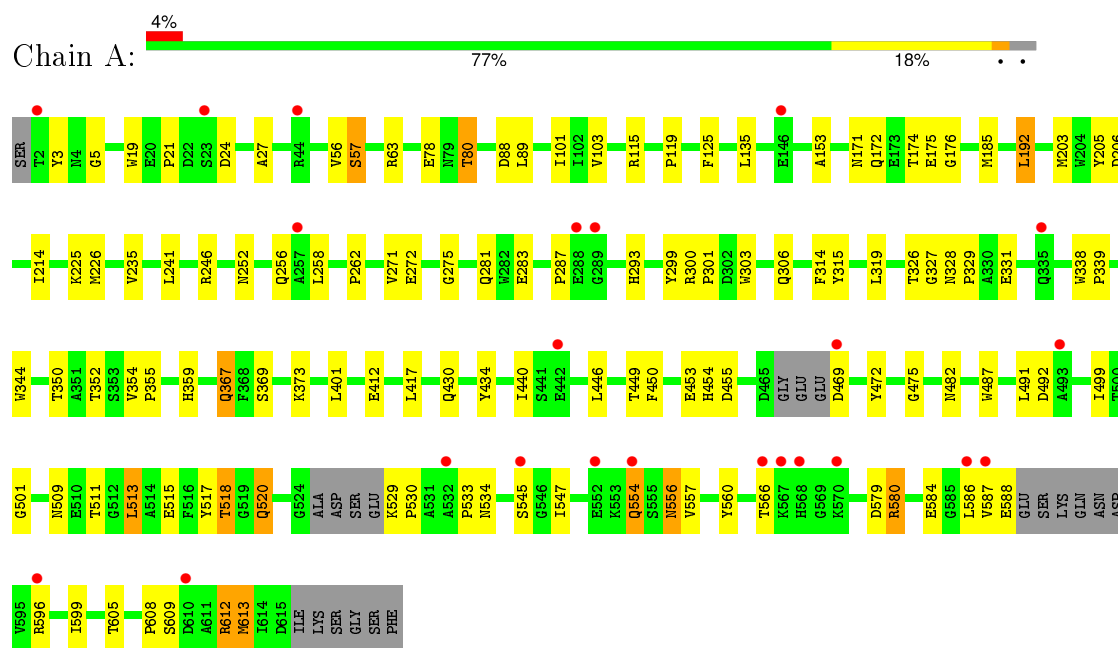
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	182	Total 182	O 182	0	0
4	D	236	Total 236	O 236	0	0
4	F	175	Total 175	O 175	0	0

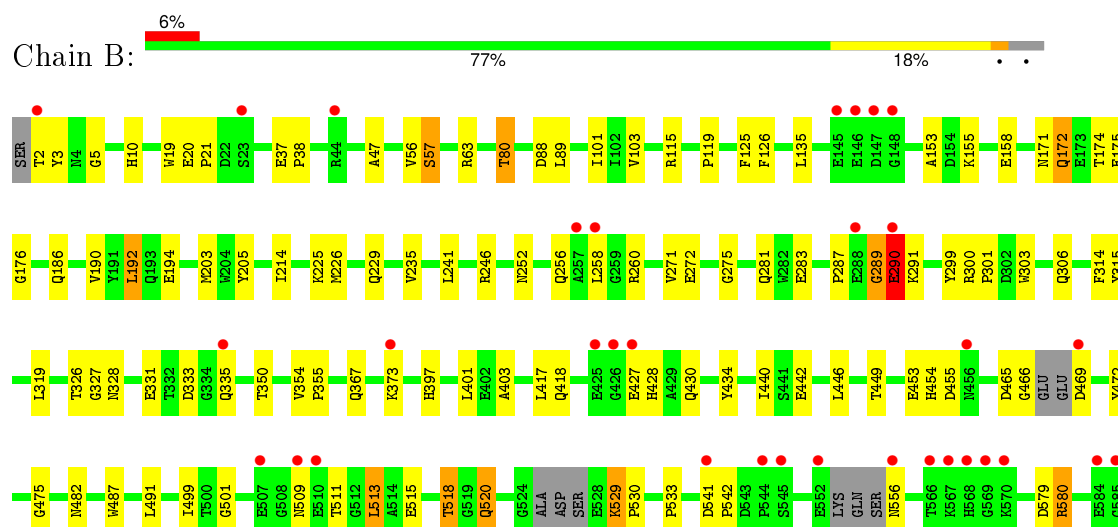
### 3 Residue-property plots

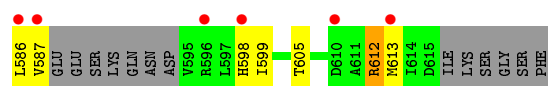
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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: Endo-beta-N-acetylglucosaminidase

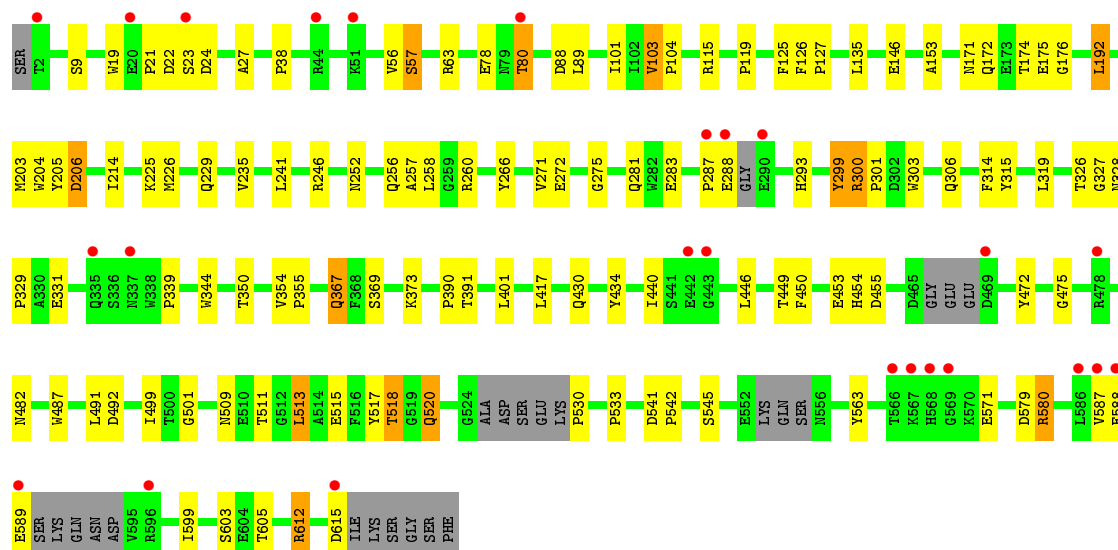
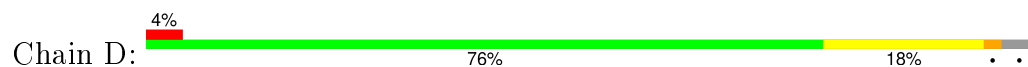


#### • Molecule 1: Endo-beta-N-acetylglucosaminidase

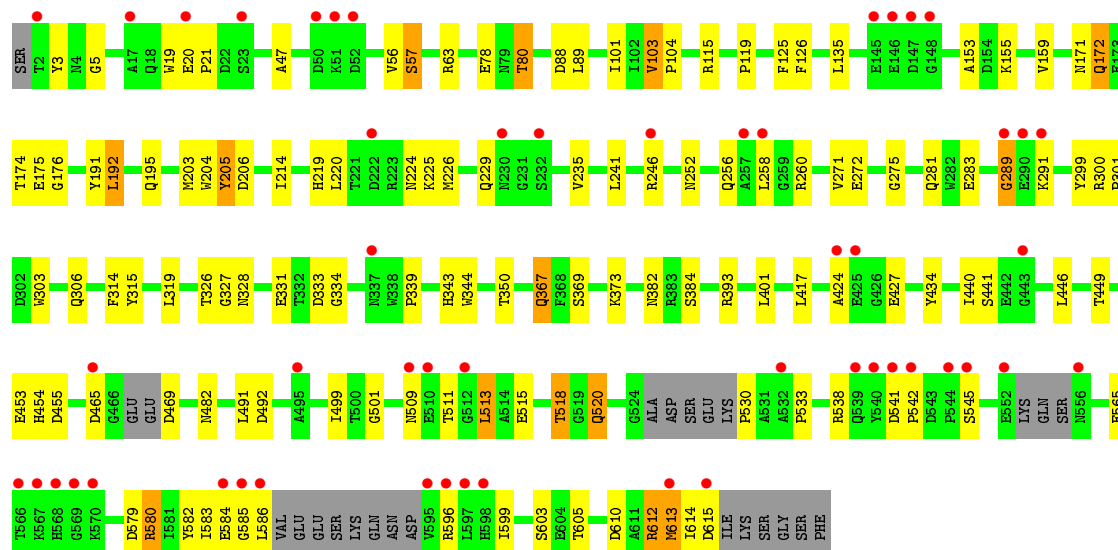
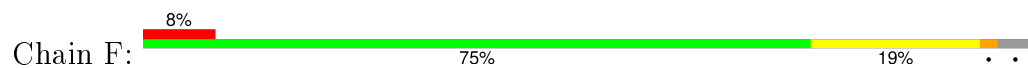




● Molecule 1: Endo-beta-N-acetylglucosaminidase



● Molecule 1: Endo-beta-N-acetylglucosaminidase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	78.33Å 79.27Å 117.04Å 80.51° 83.84° 64.33°	Depositor
Resolution (Å)	35.41 – 2.45 35.41 – 2.45	Depositor EDS
% Data completeness (in resolution range)	94.2 (35.41-2.45) 91.0 (35.41-2.45)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.46 (at 2.45Å)	Xtriage
Refinement program	PHENIX (phenix.refine)	Depositor
R, $R_{free}$	0.221 , 0.264 0.235 , 0.266	Depositor DCC
$R_{free}$ test set	4331 reflections (5.28%)	DCC
Wilson B-factor (Å <sup>2</sup> )	36.4	Xtriage
Anisotropy	0.216	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 43.3	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.34$	Xtriage
Outliers	0 of 86302 reflections	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	20045	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.43% 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 [i](#)

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

Bond lengths and bond angles in the following residue types are not validated in this section: NGT, BMA, 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	0.55	0/4927	0.61	0/6718
1	B	0.54	0/4902	0.60	2/6684 (0.0%)
1	D	0.56	2/4890 (0.0%)	0.61	1/6667 (0.0%)
1	F	0.51	0/4881	0.60	2/6655 (0.0%)
All	All	0.54	2/19600 (0.0%)	0.61	5/26724 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	299	TYR	CD2-CE2	-5.54	1.31	1.39
1	D	299	TYR	CD1-CE1	-5.26	1.31	1.39

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	300	ARG	N-CA-C	5.42	125.64	111.00
1	F	610	ASP	CB-CG-OD2	5.20	122.98	118.30
1	B	469	ASP	CB-CG-OD2	5.13	122.92	118.30
1	F	205	TYR	CB-CA-C	5.11	120.63	110.40
1	B	289	GLY	N-CA-C	-5.07	100.43	113.10

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

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	4781	0	4392	102	0
1	B	4757	0	4363	105	0
1	D	4746	0	4347	99	0
1	F	4736	0	4341	110	0
2	A	33	0	27	1	0
2	B	33	0	27	2	0
2	D	33	0	27	2	0
2	F	33	0	27	1	0
3	A	14	0	12	1	0
3	B	14	0	12	1	0
3	D	14	0	12	1	0
3	F	14	0	12	1	0
4	A	244	0	0	9	0
4	B	182	0	0	7	0
4	D	236	0	0	12	0
4	F	175	0	0	5	0
All	All	20045	0	17599	404	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 11.

All (404) 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:A:547:ILE:CD1	1:A:586:LEU:HD13	1.55	1.36
1:D:588:GLU:O	1:D:589:GLU:HB2	1.45	1.16
1:D:545:SER:HA	1:D:587:VAL:HB	1.28	1.13
1:A:547:ILE:HD13	1:A:586:LEU:HD13	1.23	1.10
1:A:547:ILE:HD11	1:A:586:LEU:HD13	1.30	1.05
1:F:56:VAL:HG12	1:F:89:LEU:HB3	1.39	1.01
1:A:56:VAL:HG12	1:A:89:LEU:HB3	1.45	0.99
1:B:56:VAL:HG12	1:B:89:LEU:HB3	1.41	0.99
1:A:554:GLN:HG3	1:A:557:VAL:HG21	1.43	0.98
1:F:596:ARG:HD2	1:F:613:MET:CE	1.93	0.98
1:B:511:THR:HG22	1:B:513:LEU:H	1.26	0.98
1:F:511:THR:HG22	1:F:513:LEU:H	1.23	0.97
1:A:511:THR:HG22	1:A:513:LEU:H	1.29	0.96
1:A:587:VAL:O	1:A:588:GLU:HG3	1.64	0.96
1:D:56:VAL:HG12	1:D:89:LEU:HB3	1.48	0.95
1:D:511:THR:HG22	1:D:513:LEU:H	1.30	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:586:LEU:O	1:B:587:VAL:HG23	1.68	0.94
1:B:335:GLN:NE2	1:F:326:THR:OG1	2.02	0.93
1:F:596:ARG:HG2	1:F:615:ASP:OD1	1.75	0.87
1:A:545:SER:HA	1:A:587:VAL:HB	1.56	0.87
1:A:115:ARG:O	1:A:350:THR:HG21	1.77	0.83
1:A:547:ILE:HD13	1:A:586:LEU:CD1	2.07	0.83
1:F:115:ARG:O	1:F:350:THR:HG21	1.80	0.82
1:D:115:ARG:O	1:D:350:THR:HG21	1.79	0.82
1:A:554:GLN:HG3	1:A:557:VAL:CG2	2.11	0.81
1:A:587:VAL:O	1:A:588:GLU:CB	2.30	0.80
1:A:587:VAL:O	1:A:588:GLU:CG	2.29	0.79
1:B:586:LEU:O	1:B:587:VAL:CG2	2.30	0.79
1:D:390:PRO:HB3	4:D:832:HOH:O	1.84	0.78
1:B:19:TRP:CH2	1:B:21:PRO:HG3	2.19	0.77
1:B:397:HIS:CE1	1:F:289:GLY:HA2	2.19	0.77
1:D:272:GLU:OE1	2:D:622:BMA:O2	2.01	0.76
1:B:20:GLU:OE1	1:B:20:GLU:HA	1.85	0.76
1:F:579:ASP:OD1	1:F:580:ARG:HG2	1.86	0.75
1:A:547:ILE:CD1	1:A:586:LEU:CD1	2.51	0.75
1:F:57:SER:OG	1:F:301:PRO:HG2	1.87	0.74
1:F:596:ARG:HD2	1:F:613:MET:HE2	1.70	0.73
1:A:587:VAL:O	1:A:588:GLU:HB2	1.89	0.72
1:B:115:ARG:O	1:B:350:THR:HG21	1.90	0.72
1:F:271:VAL:HG22	1:F:299:TYR:O	1.90	0.72
1:A:579:ASP:OD1	1:A:580:ARG:HG2	1.90	0.71
1:F:565:GLU:OE1	1:F:596:ARG:NE	2.23	0.70
1:B:579:ASP:OD1	1:B:580:ARG:HG2	1.90	0.70
1:F:533:PRO:O	1:F:612:ARG:HD2	1.90	0.70
1:D:272:GLU:HG2	2:D:624:MAN:O4	1.90	0.70
1:A:547:ILE:HD11	1:A:586:LEU:CD1	2.14	0.70
1:D:545:SER:CA	1:D:587:VAL:HB	2.17	0.70
1:B:586:LEU:O	1:B:587:VAL:CB	2.38	0.70
1:D:579:ASP:OD1	1:D:580:ARG:HG2	1.91	0.70
1:F:509:ASN:OD1	1:F:511:THR:HB	1.91	0.70
1:B:417:LEU:HB3	1:B:518:THR:HG23	1.74	0.70
1:B:57:SER:OG	1:B:301:PRO:HG2	1.91	0.69
1:D:80:THR:HG21	4:D:838:HOH:O	1.92	0.69
1:B:511:THR:HG22	1:B:513:LEU:N	2.05	0.69
1:B:533:PRO:O	1:B:612:ARG:HD2	1.92	0.69
1:F:596:ARG:CD	1:F:613:MET:CE	2.71	0.69
1:F:63:ARG:NH1	1:F:306:GLN:HG2	2.08	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:533:PRO:O	1:A:612:ARG:HD2	1.93	0.68
1:B:63:ARG:NH1	1:B:306:GLN:HG2	2.07	0.68
1:D:9:SER:OG	4:D:692:HOH:O	1.97	0.68
1:B:190:VAL:O	1:B:194:GLU:HG3	1.94	0.68
1:A:63:ARG:NH1	1:A:306:GLN:HG2	2.09	0.68
1:F:538:ARG:HG3	4:F:798:HOH:O	1.93	0.68
2:B:624:MAN:O6	4:B:676:HOH:O	1.76	0.67
1:B:509:ASN:OD1	1:B:511:THR:HB	1.95	0.67
1:F:511:THR:HG22	1:F:513:LEU:N	2.03	0.67
1:D:509:ASN:OD1	1:D:511:THR:HB	1.95	0.67
1:F:291:LYS:HB2	4:F:668:HOH:O	1.95	0.67
1:D:533:PRO:O	1:D:612:ARG:HD2	1.93	0.67
1:D:511:THR:HG22	1:D:513:LEU:N	2.07	0.66
1:B:449:THR:OG1	1:B:520:GLN:HG2	1.96	0.66
1:A:556:ASN:N	1:A:556:ASN:OD1	2.29	0.65
1:F:417:LEU:HB3	1:F:518:THR:HG23	1.79	0.65
1:F:449:THR:OG1	1:F:520:GLN:HG2	1.96	0.65
1:A:57:SER:OG	1:A:301:PRO:HG2	1.97	0.64
1:D:63:ARG:NH1	1:D:306:GLN:HG2	2.12	0.64
1:A:511:THR:HG22	1:A:513:LEU:N	2.07	0.64
1:A:509:ASN:OD1	1:A:511:THR:HB	1.97	0.64
1:D:57:SER:OG	1:D:301:PRO:HG2	1.96	0.64
1:F:596:ARG:CG	1:F:613:MET:HE1	2.28	0.63
1:B:586:LEU:C	1:B:587:VAL:HG23	2.19	0.63
1:A:326:THR:HB	4:A:679:HOH:O	1.98	0.63
1:B:175:GLU:HG3	1:B:214:ILE:HD12	1.81	0.63
1:D:326:THR:HG21	1:D:331:GLU:O	1.99	0.63
1:B:56:VAL:HG11	1:B:203:MET:HE1	1.82	0.62
1:F:582:TYR:CE2	1:F:584:GLU:HG3	2.35	0.62
1:F:175:GLU:HG3	1:F:214:ILE:HD12	1.82	0.62
1:D:417:LEU:HB3	1:D:518:THR:HG23	1.80	0.62
1:D:588:GLU:O	1:D:589:GLU:CB	2.29	0.62
1:B:511:THR:CG2	1:B:513:LEU:HB2	2.30	0.62
1:A:326:THR:HG21	1:A:331:GLU:O	2.00	0.61
1:D:146:GLU:HG3	4:D:820:HOH:O	1.98	0.61
4:A:829:HOH:O	1:B:556:ASN:HB2	1.99	0.61
1:F:326:THR:HG21	1:F:331:GLU:O	1.99	0.61
1:A:271:VAL:HG22	1:A:299:TYR:O	2.00	0.61
1:F:511:THR:CG2	1:F:513:LEU:HB2	2.31	0.61
1:A:326:THR:CG2	1:A:328:ASN:HB3	2.31	0.61
1:B:586:LEU:O	1:B:587:VAL:HB	2.01	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:56:VAL:HG11	1:F:203:MET:HE1	1.83	0.60
1:D:326:THR:CG2	1:D:328:ASN:HB3	2.31	0.60
1:A:256:GLN:HG2	1:B:442:GLU:OE1	2.01	0.60
1:B:287:PRO:HG2	1:B:291:LYS:O	2.01	0.60
1:D:449:THR:OG1	1:D:520:GLN:HG2	2.01	0.60
1:D:326:THR:HB	4:D:661:HOH:O	2.02	0.60
1:D:19:TRP:CH2	1:D:21:PRO:HG3	2.37	0.59
1:F:465:ASP:HB3	4:F:633:HOH:O	2.02	0.59
1:A:175:GLU:HG3	1:A:214:ILE:HD12	1.84	0.59
1:D:326:THR:HG22	1:D:328:ASN:N	2.18	0.59
1:A:449:THR:OG1	1:A:520:GLN:HG2	2.03	0.59
1:F:596:ARG:HG2	1:F:613:MET:HE1	1.85	0.59
1:D:440:ILE:HD11	1:D:499:ILE:HG13	1.85	0.59
1:F:174:THR:C	1:F:214:ILE:HD11	2.23	0.59
1:D:487:TRP:CE2	4:D:792:HOH:O	2.56	0.58
1:D:175:GLU:HG3	1:D:214:ILE:HD12	1.86	0.58
1:B:326:THR:CG2	1:B:328:ASN:HB3	2.33	0.58
1:A:417:LEU:HB3	1:A:518:THR:HG23	1.84	0.58
1:B:287:PRO:O	1:B:289:GLY:O	2.21	0.58
1:B:271:VAL:HG22	1:B:299:TYR:O	2.03	0.58
1:A:566:THR:HG22	4:A:877:HOH:O	2.04	0.58
1:B:80:THR:HG21	4:B:629:HOH:O	2.02	0.58
1:A:262:PRO:HD3	1:B:442:GLU:OE1	2.04	0.57
1:B:326:THR:HG22	1:B:328:ASN:N	2.18	0.57
1:A:554:GLN:HG2	1:A:560:TYR:OH	2.04	0.57
1:A:319:LEU:HD21	1:A:327:GLY:HA2	1.86	0.57
1:A:511:THR:CG2	1:A:513:LEU:HB2	2.34	0.57
1:B:326:THR:HG21	1:B:331:GLU:O	2.05	0.57
1:F:205:TYR:OH	3:F:625:NGT:HC1	2.05	0.57
1:D:511:THR:CG2	1:D:513:LEU:HB2	2.35	0.56
1:B:3:TYR:CZ	1:B:5:GLY:HA3	2.40	0.56
1:F:565:GLU:OE1	1:F:596:ARG:NH2	2.38	0.56
1:A:19:TRP:CH2	1:A:21:PRO:HG3	2.40	0.56
1:D:56:VAL:HG11	1:D:203:MET:HE1	1.86	0.56
1:F:326:THR:CG2	1:F:328:ASN:HB3	2.35	0.56
1:D:319:LEU:HD21	1:D:327:GLY:HA2	1.88	0.56
1:B:319:LEU:HD21	1:B:327:GLY:HA2	1.87	0.56
1:A:80:THR:HG21	4:A:626:HOH:O	2.05	0.56
1:F:219:HIS:HE1	4:F:710:HOH:O	1.88	0.56
1:A:352:THR:HB	4:A:781:HOH:O	2.06	0.56
1:B:427:GLU:CG	1:B:428:HIS:N	2.69	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:174:THR:C	1:B:214:ILE:HD11	2.27	0.56
1:D:174:THR:C	1:D:214:ILE:HD11	2.25	0.56
1:F:135:LEU:HD11	1:F:176:GLY:O	2.06	0.56
1:B:135:LEU:HD11	1:B:176:GLY:O	2.06	0.56
1:F:272:GLU:OE1	2:F:622:BMA:O2	2.16	0.55
1:D:24:ASP:HB3	1:D:27:ALA:HB2	1.88	0.55
1:D:205:TYR:OH	3:D:625:NGT:HC1	2.06	0.55
1:F:326:THR:HG22	1:F:328:ASN:N	2.22	0.55
1:D:204:TRP:CD1	1:D:205:TYR:O	2.60	0.55
1:B:272:GLU:OE1	2:B:622:BMA:O2	2.20	0.55
1:D:283:GLU:H	1:D:283:GLU:CD	2.10	0.55
1:A:326:THR:HG22	1:A:328:ASN:N	2.21	0.55
1:A:174:THR:C	1:A:214:ILE:HD11	2.26	0.55
1:A:440:ILE:HD11	1:A:499:ILE:HG13	1.89	0.55
1:D:612:ARG:HD3	4:D:836:HOH:O	2.07	0.55
1:D:293:HIS:HE1	4:D:708:HOH:O	1.90	0.54
1:F:319:LEU:HD21	1:F:327:GLY:HA2	1.89	0.54
1:A:56:VAL:HG11	1:A:203:MET:HE1	1.88	0.54
1:B:440:ILE:HD11	1:B:499:ILE:HG13	1.88	0.54
1:A:326:THR:HG22	1:A:328:ASN:HB3	1.89	0.54
1:D:22:ASP:HB2	4:D:856:HOH:O	2.07	0.54
1:B:333:ASP:OD1	1:F:333:ASP:CG	2.46	0.54
1:B:283:GLU:H	1:B:283:GLU:CD	2.11	0.54
1:D:271:VAL:HG22	1:D:299:TYR:O	2.07	0.54
1:F:204:TRP:CD1	1:F:205:TYR:O	2.62	0.53
1:B:101:ILE:HB	1:B:125:PHE:O	2.08	0.53
1:F:605:THR:O	1:F:605:THR:HG22	2.09	0.53
1:F:204:TRP:NE1	1:F:205:TYR:O	2.41	0.53
1:A:63:ARG:NH1	4:A:788:HOH:O	2.41	0.53
1:F:283:GLU:H	1:F:283:GLU:CD	2.11	0.53
1:A:283:GLU:CD	1:A:283:GLU:H	2.11	0.53
1:F:153:ALA:HB1	1:F:192:LEU:HD13	1.91	0.53
1:A:272:GLU:OE1	2:A:622:BMA:O2	2.18	0.53
1:D:204:TRP:NE1	1:D:205:TYR:O	2.42	0.52
1:B:613:MET:HG3	4:B:695:HOH:O	2.09	0.52
1:F:440:ILE:HD11	1:F:499:ILE:HG13	1.90	0.52
1:F:56:VAL:HG12	1:F:89:LEU:CB	2.26	0.52
1:F:545:SER:O	1:F:585:GLY:HA2	2.10	0.52
1:D:326:THR:HG22	1:D:328:ASN:HB3	1.90	0.52
1:F:613:MET:O	1:F:614:ILE:HD13	2.10	0.52
1:A:605:THR:O	1:A:605:THR:HG22	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:289:GLY:O	1:B:290:GLU:O	2.28	0.52
1:A:533:PRO:HG2	1:A:599:ILE:HG22	1.92	0.52
1:D:367:GLN:OE1	1:D:369:SER:OG	2.20	0.52
1:A:153:ALA:HB1	1:A:192:LEU:HD13	1.92	0.52
1:B:205:TYR:OH	3:B:625:NGT:HC1	2.09	0.52
1:D:38:PRO:HD2	4:D:758:HOH:O	2.10	0.52
1:F:424:ALA:O	1:F:427:GLU:HB3	2.10	0.52
1:B:434:TYR:O	1:B:501:GLY:HA2	2.10	0.52
1:F:101:ILE:HB	1:F:125:PHE:O	2.10	0.52
1:B:80:THR:OG1	1:B:80:THR:O	2.28	0.51
1:A:534:ASN:ND2	4:A:907:HOH:O	2.42	0.51
1:F:326:THR:HG22	1:F:328:ASN:HB3	1.93	0.51
1:F:3:TYR:CZ	1:F:5:GLY:HA3	2.44	0.51
1:D:153:ALA:HB1	1:D:192:LEU:HD13	1.91	0.51
1:B:225:LYS:HB2	1:B:258:LEU:HD11	1.93	0.51
1:A:80:THR:OG1	1:A:80:THR:O	2.29	0.51
1:F:174:THR:O	1:F:214:ILE:HD11	2.11	0.51
1:D:605:THR:O	1:D:605:THR:HG22	2.11	0.51
1:F:334:GLY:HA3	1:F:343:HIS:CE1	2.45	0.51
1:A:300:ARG:N	1:A:301:PRO:HD3	2.25	0.51
1:D:80:THR:OG1	1:D:80:THR:O	2.29	0.51
1:B:599:ILE:N	1:B:599:ILE:HD12	2.25	0.51
1:A:275:GLY:HA3	1:A:303:TRP:CD2	2.46	0.51
1:A:367:GLN:OE1	1:A:369:SER:OG	2.19	0.51
1:F:583:ILE:HG21	1:F:586:LEU:HD22	1.92	0.51
1:D:135:LEU:HD11	1:D:176:GLY:O	2.11	0.51
1:F:565:GLU:OE1	1:F:596:ARG:CZ	2.59	0.50
1:B:335:GLN:OE1	1:F:333:ASP:CB	2.60	0.50
1:B:605:THR:HG22	1:B:605:THR:O	2.11	0.50
1:A:135:LEU:HD11	1:A:176:GLY:O	2.12	0.50
1:B:229:GLN:OE1	1:B:260:ARG:HD3	2.11	0.50
1:F:541:ASP:HB2	1:F:542:PRO:HD3	1.92	0.50
1:F:300:ARG:N	1:F:301:PRO:HD3	2.26	0.50
1:F:596:ARG:CD	1:F:613:MET:HE1	2.41	0.50
1:D:487:TRP:NE1	4:D:792:HOH:O	2.34	0.50
1:D:580:ARG:HH11	1:D:580:ARG:HG2	1.77	0.50
1:D:326:THR:HG22	1:D:328:ASN:H	1.76	0.50
1:B:326:THR:HG22	1:B:328:ASN:HB3	1.93	0.50
1:B:275:GLY:HA3	1:B:303:TRP:CD2	2.47	0.50
1:F:191:TYR:CZ	1:F:195:GLN:HG3	2.47	0.50
1:A:596:ARG:HD3	1:A:613:MET:CE	2.42	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:246:ARG:HE	1:D:281:GLN:HG3	1.77	0.50
1:F:229:GLN:OE1	1:F:260:ARG:HD3	2.12	0.50
1:B:246:ARG:HD3	4:B:913:HOH:O	2.12	0.49
1:A:446:LEU:HG	1:A:491:LEU:HD11	1.94	0.49
1:A:287:PRO:HG3	1:A:293:HIS:CE1	2.47	0.49
1:F:80:THR:O	1:F:80:THR:OG1	2.28	0.49
1:F:393:ARG:HD2	4:F:695:HOH:O	2.12	0.49
1:B:153:ALA:HB1	1:B:192:LEU:HD13	1.94	0.49
1:D:275:GLY:HA3	1:D:303:TRP:CD2	2.48	0.49
1:D:446:LEU:HG	1:D:491:LEU:HD11	1.95	0.48
1:B:454:HIS:O	1:B:455:ASP:HB2	2.12	0.48
1:F:275:GLY:HA3	1:F:303:TRP:CD2	2.48	0.48
1:A:529:LYS:HE3	1:A:609:SER:HA	1.94	0.48
1:B:56:VAL:HG12	1:B:89:LEU:CB	2.29	0.48
1:B:88:ASP:O	1:B:119:PRO:HD2	2.13	0.48
1:B:446:LEU:HG	1:B:491:LEU:HD11	1.94	0.48
1:F:599:ILE:N	1:F:599:ILE:HD12	2.27	0.48
1:B:300:ARG:NH2	4:B:889:HOH:O	2.42	0.48
1:B:289:GLY:C	1:B:290:GLU:O	2.50	0.48
1:F:175:GLU:HG3	1:F:214:ILE:CD1	2.44	0.48
1:A:252:ASN:O	1:A:256:GLN:HG3	2.14	0.48
1:F:225:LYS:HB2	1:F:258:LEU:HD11	1.94	0.48
1:B:453:GLU:HB2	1:B:515:GLU:HB3	1.95	0.48
1:B:520:GLN:O	1:B:520:GLN:HG3	2.11	0.48
1:F:80:THR:HG23	1:F:315:TYR:HE1	1.78	0.48
1:A:580:ARG:HG2	1:A:580:ARG:HH11	1.78	0.47
1:B:246:ARG:HE	1:B:281:GLN:HG3	1.79	0.47
1:D:300:ARG:N	1:D:301:PRO:HD3	2.29	0.47
1:A:434:TYR:O	1:A:501:GLY:HA2	2.14	0.47
1:B:511:THR:HG22	1:B:513:LEU:HB2	1.96	0.47
1:A:246:ARG:HE	1:A:281:GLN:HG3	1.79	0.47
1:B:20:GLU:OE1	1:B:158:GLU:OE2	2.32	0.47
1:D:434:TYR:O	1:D:501:GLY:HA2	2.14	0.47
1:B:326:THR:HG22	1:B:328:ASN:H	1.78	0.47
1:D:56:VAL:HG11	1:D:203:MET:CE	2.44	0.47
1:F:19:TRP:CZ3	1:F:21:PRO:HD3	2.49	0.47
1:D:225:LYS:HB2	1:D:258:LEU:HD11	1.96	0.47
1:F:226:MET:O	1:F:235:VAL:HG21	2.14	0.47
1:B:397:HIS:ND1	1:F:289:GLY:CA	2.78	0.47
1:B:291:LYS:HB3	4:B:767:HOH:O	2.15	0.47
1:B:541:ASP:HB2	1:B:542:PRO:HD3	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:88:ASP:O	1:A:119:PRO:HD2	2.15	0.46
1:F:434:TYR:O	1:F:501:GLY:HA2	2.14	0.46
1:B:335:GLN:OE1	1:F:333:ASP:HB3	2.15	0.46
1:B:300:ARG:N	1:B:301:PRO:HD3	2.29	0.46
1:D:533:PRO:HG2	1:D:599:ILE:HG22	1.97	0.46
1:F:580:ARG:HG2	1:F:580:ARG:HH11	1.80	0.46
1:D:252:ASN:O	1:D:256:GLN:HG3	2.15	0.46
1:F:246:ARG:HE	1:F:281:GLN:HG3	1.80	0.46
1:A:101:ILE:HB	1:A:125:PHE:O	2.15	0.46
1:D:257:ALA:O	1:F:441:SER:HB2	2.16	0.46
1:A:225:LYS:HB2	1:A:258:LEU:HD11	1.96	0.46
1:D:80:THR:HG23	1:D:314:PHE:HE2	1.81	0.46
1:D:587:VAL:HG12	1:D:587:VAL:O	2.15	0.46
1:D:454:HIS:CD2	1:D:513:LEU:HB3	2.50	0.46
1:B:63:ARG:HH12	1:B:306:GLN:HG2	1.81	0.46
1:B:80:THR:HG23	1:B:315:TYR:HE1	1.81	0.46
1:D:101:ILE:HB	1:D:125:PHE:O	2.16	0.46
1:A:175:GLU:HG3	1:A:214:ILE:CD1	2.45	0.45
1:D:287:PRO:HG3	1:D:293:HIS:NE2	2.31	0.45
1:A:354:VAL:HG13	1:A:355:PRO:HA	1.98	0.45
1:A:373:LYS:HE2	1:A:482:ASN:ND2	2.31	0.45
1:F:367:GLN:OE1	1:F:369:SER:OG	2.21	0.45
1:B:47:ALA:HB1	1:F:47:ALA:CB	2.46	0.45
1:A:430:GLN:HG2	1:A:472:TYR:CE2	2.52	0.45
1:F:454:HIS:O	1:F:455:ASP:HB2	2.16	0.45
1:A:80:THR:HG23	1:A:315:TYR:HE1	1.81	0.45
1:F:565:GLU:CD	1:F:596:ARG:HE	2.18	0.45
1:B:19:TRP:O	1:B:155:LYS:NZ	2.37	0.45
1:D:339:PRO:HG2	1:D:344:TRP:CH2	2.52	0.45
1:A:3:TYR:CZ	1:A:5:GLY:HA3	2.52	0.45
1:D:391:THR:HA	4:D:657:HOH:O	2.16	0.45
1:A:599:ILE:N	1:A:599:ILE:HD12	2.32	0.45
1:F:103:VAL:HA	1:F:104:PRO:HD3	1.78	0.45
1:A:175:GLU:HA	1:A:214:ILE:HD12	1.99	0.45
1:D:80:THR:HG23	1:D:315:TYR:HE1	1.82	0.44
1:A:80:THR:HG23	1:A:314:PHE:HE2	1.82	0.44
1:A:454:HIS:O	1:A:455:ASP:HB2	2.16	0.44
1:D:56:VAL:HG13	1:D:266:TYR:CE1	2.52	0.44
1:F:533:PRO:HG2	1:F:599:ILE:HG22	1.99	0.44
1:D:9:SER:O	1:D:104:PRO:HD2	2.18	0.44
1:D:599:ILE:N	1:D:599:ILE:HD12	2.32	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:175:GLU:HA	1:D:214:ILE:HD12	2.00	0.44
1:F:88:ASP:O	1:F:119:PRO:HD2	2.17	0.44
1:F:511:THR:HG22	1:F:513:LEU:HB2	1.99	0.44
1:F:454:HIS:CD2	1:F:513:LEU:HB3	2.52	0.44
1:F:175:GLU:HA	1:F:214:ILE:HD12	1.98	0.44
1:F:20:GLU:HA	1:F:21:PRO:HD2	1.84	0.44
1:F:520:GLN:O	1:F:520:GLN:HG3	2.13	0.44
1:B:430:GLN:HG2	1:B:472:TYR:CE2	2.53	0.44
1:A:56:VAL:HG11	1:A:203:MET:CE	2.47	0.44
1:A:205:TYR:OH	3:A:625:NGT:HC1	2.17	0.44
1:B:454:HIS:CD2	1:B:513:LEU:HB3	2.52	0.44
1:A:454:HIS:CD2	1:A:513:LEU:HB3	2.52	0.44
1:D:175:GLU:HG3	1:D:214:ILE:CD1	2.48	0.44
1:D:354:VAL:HG13	1:D:355:PRO:HA	1.98	0.44
1:D:454:HIS:O	1:D:455:ASP:HB2	2.17	0.44
1:F:326:THR:HG22	1:F:328:ASN:H	1.82	0.44
1:B:47:ALA:CB	1:F:47:ALA:CB	2.96	0.44
1:D:430:GLN:HG2	1:D:472:TYR:CE2	2.53	0.44
1:D:206:ASP:CG	1:D:206:ASP:O	2.56	0.44
1:F:334:GLY:CA	1:F:343:HIS:CE1	3.01	0.43
1:A:554:GLN:H	1:A:554:GLN:HG2	1.46	0.43
1:A:326:THR:HG22	1:A:328:ASN:CB	2.48	0.43
1:F:252:ASN:O	1:F:256:GLN:HG3	2.18	0.43
1:B:226:MET:O	1:B:235:VAL:HG21	2.17	0.43
1:D:373:LYS:HE2	1:D:482:ASN:ND2	2.33	0.43
1:D:78:GLU:O	1:D:80:THR:HG22	2.18	0.43
1:D:475:GLY:HA3	1:D:487:TRP:CE3	2.53	0.43
1:F:446:LEU:HG	1:F:491:LEU:HD11	1.99	0.43
1:B:335:GLN:CD	1:F:333:ASP:HB2	2.38	0.43
1:A:326:THR:HG22	1:A:328:ASN:H	1.83	0.43
1:B:613:MET:CG	4:B:695:HOH:O	2.65	0.43
1:D:453:GLU:HB2	1:D:515:GLU:HB3	2.00	0.43
1:B:465:ASP:HA	1:B:466:GLY:HA2	1.62	0.43
1:B:475:GLY:HA3	1:B:487:TRP:CE3	2.54	0.43
1:F:80:THR:HG23	1:F:314:PHE:HE2	1.84	0.43
1:B:56:VAL:HG11	1:B:203:MET:CE	2.48	0.43
1:A:24:ASP:HB3	1:A:27:ALA:HB2	2.00	0.43
1:B:126:PHE:HB2	1:B:172:GLN:HA	2.00	0.43
1:B:373:LYS:HE2	1:B:482:ASN:ND2	2.33	0.43
1:B:175:GLU:HG3	1:B:214:ILE:CD1	2.46	0.43
1:F:582:TYR:OH	1:F:584:GLU:HG2	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:37:GLU:HA	1:B:38:PRO:HD3	1.83	0.43
1:A:339:PRO:HG2	1:A:344:TRP:CH2	2.54	0.43
1:F:56:VAL:HG11	1:F:203:MET:CE	2.48	0.43
1:B:175:GLU:HA	1:B:214:ILE:HD12	2.00	0.43
1:A:78:GLU:O	1:A:80:THR:HG22	2.19	0.43
1:A:192:LEU:HA	1:A:192:LEU:HD12	1.87	0.43
1:A:453:GLU:HB2	1:A:515:GLU:HB3	2.00	0.43
1:B:354:VAL:HG13	1:B:355:PRO:HA	2.00	0.43
1:B:427:GLU:HG3	1:B:428:HIS:H	1.83	0.43
1:B:529:LYS:HA	1:B:530:PRO:HD3	1.80	0.43
1:D:563:TYR:HA	1:D:571:GLU:O	2.19	0.43
1:D:229:GLN:OE1	1:D:260:ARG:HD3	2.18	0.42
1:F:339:PRO:HG2	1:F:344:TRP:CH2	2.53	0.42
1:B:397:HIS:CE1	1:F:289:GLY:CA	2.98	0.42
1:D:520:GLN:HG3	1:D:520:GLN:O	2.16	0.42
1:F:582:TYR:OH	1:F:584:GLU:CG	2.68	0.42
1:A:469:ASP:N	4:A:652:HOH:O	2.52	0.42
1:D:226:MET:O	1:D:235:VAL:HG21	2.20	0.42
1:D:80:THR:CG2	1:D:314:PHE:HE2	2.32	0.42
1:D:326:THR:HG22	1:D:328:ASN:CB	2.49	0.42
1:A:596:ARG:HB3	1:A:613:MET:HE2	2.01	0.42
1:D:587:VAL:CG1	1:D:587:VAL:O	2.68	0.42
1:A:328:ASN:HA	1:A:329:PRO:HD2	1.89	0.42
1:D:88:ASP:O	1:D:119:PRO:HD2	2.20	0.42
1:F:382:ASN:OD1	1:F:384:SER:HB2	2.19	0.42
1:F:155:LYS:O	1:F:159:VAL:HG23	2.20	0.41
1:D:511:THR:HG22	1:D:513:LEU:HB2	2.02	0.41
1:A:80:THR:CG2	1:A:314:PHE:HE2	2.33	0.41
1:B:598:HIS:CE1	1:B:613:MET:HG2	2.56	0.41
1:F:220:LEU:HD12	1:F:224:ASN:OD1	2.20	0.41
1:A:450:PHE:HA	1:A:517:TYR:O	2.20	0.41
1:D:541:ASP:HB2	1:D:542:PRO:HD3	2.01	0.41
1:B:533:PRO:HG2	1:B:599:ILE:HG22	2.02	0.41
1:D:328:ASN:HA	1:D:329:PRO:HD2	1.90	0.41
1:F:80:THR:CG2	1:F:314:PHE:HE2	2.34	0.41
1:B:252:ASN:O	1:B:256:GLN:HG3	2.19	0.41
1:F:126:PHE:HB2	1:F:172:GLN:HA	2.03	0.41
1:A:511:THR:HG22	1:A:513:LEU:HB2	2.01	0.41
1:A:520:GLN:HG3	1:A:520:GLN:O	2.18	0.41
1:F:530:PRO:HG3	1:F:603:SER:HB3	2.02	0.41
1:D:103:VAL:HA	1:D:104:PRO:HD3	1.79	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:78:GLU:O	1:F:80:THR:HG22	2.20	0.41
1:A:475:GLY:HA3	1:A:487:TRP:CE3	2.56	0.41
1:B:135:LEU:HD11	1:B:176:GLY:C	2.41	0.41
1:A:185:MET:O	1:A:185:MET:HE2	2.21	0.41
1:A:359:HIS:CD2	1:A:412:GLU:HB2	2.56	0.41
1:F:373:LYS:HE2	1:F:482:ASN:ND2	2.36	0.41
1:A:338:TRP:O	4:A:649:HOH:O	2.21	0.41
1:F:453:GLU:HB2	1:F:515:GLU:HB3	2.03	0.41
1:B:186:GLN:O	1:B:190:VAL:HG23	2.21	0.40
1:B:80:THR:HG23	1:B:314:PHE:HE2	1.86	0.40
1:A:530:PRO:O	1:A:609:SER:HB2	2.22	0.40
1:B:403:ALA:HA	1:B:418:GLN:O	2.21	0.40
1:D:63:ARG:HH12	1:D:306:GLN:HG2	1.85	0.40
1:B:427:GLU:HG2	1:B:428:HIS:N	2.36	0.40
1:D:126:PHE:HA	1:D:127:PRO:HD3	1.91	0.40
1:D:450:PHE:HA	1:D:517:TYR:O	2.22	0.40
1:A:63:ARG:HH12	1:A:306:GLN:HG2	1.83	0.40
1:D:530:PRO:HG3	1:D:603:SER:HB3	2.02	0.40
1:A:226:MET:O	1:A:235:VAL:HG21	2.22	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	593/621 (96%)	570 (96%)	23 (4%)	0	100	100
1	B	589/621 (95%)	566 (96%)	21 (4%)	2 (0%)	46	57
1	D	585/621 (94%)	565 (97%)	19 (3%)	1 (0%)	52	64
1	F	586/621 (94%)	562 (96%)	22 (4%)	2 (0%)	46	57
All	All	2353/2484 (95%)	2263 (96%)	85 (4%)	5 (0%)	52	64

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	290	GLU
1	B	10	HIS
1	F	206	ASP
1	D	206	ASP
1	F	289	GLY

### 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	498/515 (97%)	477 (96%)	21 (4%)	36	51
1	B	494/515 (96%)	477 (97%)	17 (3%)	44	61
1	D	493/515 (96%)	475 (96%)	18 (4%)	41	57
1	F	492/515 (96%)	475 (96%)	17 (4%)	43	60
All	All	1977/2060 (96%)	1904 (96%)	73 (4%)	41	57

All (73) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	57	SER
1	A	80	THR
1	A	103	VAL
1	A	171	ASN
1	A	172	GLN
1	A	192	LEU
1	A	206	ASP
1	A	241	LEU
1	A	367	GLN
1	A	401	LEU
1	A	492	ASP
1	A	513	LEU
1	A	518	THR
1	A	520	GLN
1	A	554	GLN

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Mol	Chain	Res	Type
1	A	556	ASN
1	A	580	ARG
1	A	584	GLU
1	A	608	PRO
1	A	612	ARG
1	A	613	MET
1	B	2	THR
1	B	57	SER
1	B	80	THR
1	B	103	VAL
1	B	171	ASN
1	B	172	GLN
1	B	192	LEU
1	B	241	LEU
1	B	290	GLU
1	B	367	GLN
1	B	401	LEU
1	B	513	LEU
1	B	518	THR
1	B	520	GLN
1	B	529	LYS
1	B	580	ARG
1	B	612	ARG
1	D	23	SER
1	D	57	SER
1	D	80	THR
1	D	103	VAL
1	D	171	ASN
1	D	172	GLN
1	D	192	LEU
1	D	241	LEU
1	D	288	GLU
1	D	367	GLN
1	D	401	LEU
1	D	492	ASP
1	D	513	LEU
1	D	518	THR
1	D	520	GLN
1	D	580	ARG
1	D	612	ARG
1	D	615	ASP
1	F	57	SER

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Mol	Chain	Res	Type
1	F	80	THR
1	F	103	VAL
1	F	171	ASN
1	F	172	GLN
1	F	192	LEU
1	F	241	LEU
1	F	367	GLN
1	F	401	LEU
1	F	469	ASP
1	F	492	ASP
1	F	513	LEU
1	F	518	THR
1	F	520	GLN
1	F	580	ARG
1	F	612	ARG
1	F	613	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	428	HIS
1	B	335	GLN
1	D	48	ASN
1	D	250	GLN
1	D	293	HIS
1	D	539	GLN
1	F	48	ASN
1	F	171	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 ⓘ

12 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	BMA	A	622	3,2	11,11,12	1.19	1 (9%)	14,15,17	1.93	4 (28%)
2	MAN	A	623	2	11,11,12	1.04	1 (9%)	14,15,17	2.42	6 (42%)
2	MAN	A	624	2	11,11,12	1.80	2 (18%)	14,15,17	2.30	7 (50%)
2	BMA	B	622	3,2	11,11,12	1.19	1 (9%)	14,15,17	1.93	4 (28%)
2	MAN	B	623	2	11,11,12	1.04	1 (9%)	14,15,17	2.42	6 (42%)
2	MAN	B	624	2	11,11,12	1.80	2 (18%)	14,15,17	2.30	7 (50%)
2	BMA	D	622	3,2	11,11,12	1.19	1 (9%)	14,15,17	1.92	4 (28%)
2	MAN	D	623	2	11,11,12	1.05	1 (9%)	14,15,17	2.42	6 (42%)
2	MAN	D	624	2	11,11,12	1.81	2 (18%)	14,15,17	2.30	7 (50%)
2	BMA	F	622	3,2	11,11,12	1.19	1 (9%)	14,15,17	1.93	4 (28%)
2	MAN	F	623	2	11,11,12	1.03	1 (9%)	14,15,17	2.41	6 (42%)
2	MAN	F	624	2	11,11,12	1.81	2 (18%)	14,15,17	2.30	7 (50%)

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	BMA	A	622	3,2	-	0/2/19/22	0/1/1/1
2	MAN	A	623	2	-	0/2/19/22	0/1/1/1
2	MAN	A	624	2	-	0/2/19/22	0/1/1/1
2	BMA	B	622	3,2	-	0/2/19/22	0/1/1/1
2	MAN	B	623	2	-	0/2/19/22	0/1/1/1
2	MAN	B	624	2	-	0/2/19/22	0/1/1/1
2	BMA	D	622	3,2	-	0/2/19/22	0/1/1/1
2	MAN	D	623	2	-	0/2/19/22	0/1/1/1
2	MAN	D	624	2	-	0/2/19/22	0/1/1/1
2	BMA	F	622	3,2	-	0/2/19/22	0/1/1/1
2	MAN	F	623	2	-	0/2/19/22	0/1/1/1
2	MAN	F	624	2	-	0/2/19/22	0/1/1/1



All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	624	MAN	O3-C3	-2.62	1.36	1.43
2	A	624	MAN	O3-C3	-2.60	1.36	1.43
2	B	624	MAN	O3-C3	-2.60	1.36	1.43
2	F	624	MAN	O3-C3	-2.59	1.36	1.43
2	D	623	MAN	O2-C2	-2.44	1.37	1.43
2	A	623	MAN	O2-C2	-2.42	1.37	1.43
2	B	623	MAN	O2-C2	-2.41	1.37	1.43
2	F	623	MAN	O2-C2	-2.40	1.38	1.43
2	F	622	BMA	C1-C2	2.85	1.59	1.52
2	B	622	BMA	C1-C2	2.87	1.59	1.52
2	A	622	BMA	C1-C2	2.88	1.59	1.52
2	D	622	BMA	C1-C2	2.90	1.59	1.52
2	D	624	MAN	C2-C3	4.32	1.58	1.52
2	A	624	MAN	C2-C3	4.32	1.58	1.52
2	F	624	MAN	C2-C3	4.34	1.58	1.52
2	B	624	MAN	C2-C3	4.34	1.58	1.52

All (68) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	623	MAN	C1-C2-C3	-2.85	106.17	109.54
2	D	624	MAN	O5-C1-C2	-2.84	106.25	110.86
2	A	624	MAN	O5-C1-C2	-2.82	106.28	110.86
2	D	623	MAN	C1-C2-C3	-2.81	106.21	109.54
2	F	624	MAN	O5-C1-C2	-2.81	106.30	110.86
2	A	623	MAN	C1-C2-C3	-2.81	106.22	109.54
2	B	624	MAN	O5-C1-C2	-2.80	106.31	110.86
2	F	623	MAN	C1-C2-C3	-2.76	106.27	109.54
2	A	622	BMA	O5-C1-C2	-2.03	107.57	110.86
2	B	622	BMA	O5-C1-C2	-2.02	107.57	110.86
2	F	622	BMA	O5-C1-C2	-2.02	107.58	110.86
2	D	622	BMA	O5-C1-C2	-2.01	107.60	110.86
2	D	624	MAN	C2-C3-C4	2.12	114.64	111.04
2	F	624	MAN	C2-C3-C4	2.13	114.65	111.04
2	B	624	MAN	C2-C3-C4	2.13	114.65	111.04
2	A	624	MAN	C2-C3-C4	2.13	114.66	111.04
2	A	623	MAN	O4-C4-C5	2.23	115.14	109.24
2	B	623	MAN	O4-C4-C5	2.23	115.14	109.24
2	F	623	MAN	O4-C4-C5	2.23	115.15	109.24
2	F	624	MAN	C1-O5-C5	2.23	115.08	112.25
2	D	623	MAN	O4-C4-C5	2.24	115.19	109.24
2	B	624	MAN	C1-O5-C5	2.25	115.10	112.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	624	MAN	C1-O5-C5	2.27	115.13	112.25
2	D	624	MAN	C1-O5-C5	2.27	115.13	112.25
2	D	622	BMA	O4-C4-C5	2.61	116.16	109.24
2	F	624	MAN	O5-C5-C6	2.62	113.02	107.35
2	A	622	BMA	O4-C4-C5	2.63	116.20	109.24
2	D	624	MAN	O5-C5-C6	2.64	113.06	107.35
2	A	624	MAN	O5-C5-C6	2.64	113.06	107.35
2	B	622	BMA	O4-C4-C5	2.64	116.24	109.24
2	B	624	MAN	O5-C5-C6	2.65	113.09	107.35
2	F	622	BMA	O4-C4-C5	2.65	116.27	109.24
2	D	623	MAN	O2-C2-C1	2.73	114.69	109.21
2	B	623	MAN	O2-C2-C1	2.74	114.70	109.21
2	A	623	MAN	O2-C2-C1	2.74	114.71	109.21
2	F	623	MAN	O2-C2-C1	2.75	114.73	109.21
2	D	622	BMA	O2-C2-C3	2.76	115.68	110.12
2	F	622	BMA	O2-C2-C3	2.78	115.70	110.12
2	A	622	BMA	O2-C2-C3	2.78	115.71	110.12
2	B	622	BMA	O2-C2-C3	2.78	115.71	110.12
2	D	623	MAN	C1-O5-C5	3.15	116.25	112.25
2	F	623	MAN	C1-O5-C5	3.15	116.25	112.25
2	A	623	MAN	C1-O5-C5	3.16	116.25	112.25
2	B	623	MAN	C1-O5-C5	3.16	116.25	112.25
2	F	624	MAN	O3-C3-C4	3.21	117.58	110.34
2	A	624	MAN	O3-C3-C4	3.22	117.59	110.34
2	D	624	MAN	O3-C3-C4	3.22	117.59	110.34
2	B	624	MAN	O3-C3-C4	3.24	117.63	110.34
2	B	624	MAN	O2-C2-C3	3.50	117.15	110.12
2	A	624	MAN	O2-C2-C3	3.50	117.16	110.12
2	F	624	MAN	O2-C2-C3	3.50	117.17	110.12
2	D	624	MAN	O2-C2-C3	3.52	117.21	110.12
2	B	624	MAN	O3-C3-C2	3.93	117.10	110.00
2	D	624	MAN	O3-C3-C2	3.93	117.10	110.00
2	A	624	MAN	O3-C3-C2	3.94	117.11	110.00
2	F	624	MAN	O3-C3-C2	3.96	117.15	110.00
2	D	623	MAN	O3-C3-C2	4.26	117.69	110.00
2	A	623	MAN	O3-C3-C2	4.27	117.70	110.00
2	B	623	MAN	O3-C3-C2	4.27	117.71	110.00
2	F	623	MAN	O3-C3-C2	4.28	117.73	110.00
2	F	623	MAN	O2-C2-C3	4.29	118.75	110.12
2	A	623	MAN	O2-C2-C3	4.30	118.78	110.12
2	B	623	MAN	O2-C2-C3	4.33	118.82	110.12
2	D	623	MAN	O2-C2-C3	4.33	118.83	110.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	622	BMA	O2-C2-C1	4.53	118.28	109.21
2	D	622	BMA	O2-C2-C1	4.53	118.29	109.21
2	A	622	BMA	O2-C2-C1	4.54	118.31	109.21
2	F	622	BMA	O2-C2-C1	4.55	118.34	109.21

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

6 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	622	BMA	1	0
2	B	622	BMA	1	0
2	B	624	MAN	1	0
2	D	622	BMA	1	0
2	D	624	MAN	1	0
2	F	622	BMA	1	0

## 5.6 Ligand geometry ⓘ

4 ligands 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	NGT	A	625	2	13,15,15	2.84	1 (7%)	11,22,22	1.04	0
3	NGT	B	625	2	13,15,15	2.87	1 (7%)	11,22,22	1.05	0
3	NGT	D	625	2	13,15,15	2.86	1 (7%)	11,22,22	1.04	0
3	NGT	F	625	2	13,15,15	2.83	1 (7%)	11,22,22	1.04	0

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	NGT	A	625	2	-	0/2/30/30	0/2/2/2
3	NGT	B	625	2	-	0/2/30/30	0/2/2/2
3	NGT	D	625	2	-	0/2/30/30	0/2/2/2
3	NGT	F	625	2	-	0/2/30/30	0/2/2/2

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	625	NGT	C7-S1	-10.21	1.68	1.77
3	D	625	NGT	C7-S1	-10.21	1.68	1.77
3	A	625	NGT	C7-S1	-10.13	1.68	1.77
3	F	625	NGT	C7-S1	-10.08	1.68	1.77

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	625	NGT	1	0
3	B	625	NGT	1	0
3	D	625	NGT	1	0
3	F	625	NGT	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	601/621 (96%)	0.27	23 (3%)	44	48	20, 31, 52, 75	0
1	B	599/621 (96%)	0.43	39 (6%)	22	24	20, 36, 57, 89	0
1	D	597/621 (96%)	0.24	25 (4%)	40	43	21, 33, 51, 74	0
1	F	596/621 (95%)	0.59	52 (8%)	13	13	20, 39, 60, 81	0
All	All	2393/2484 (96%)	0.38	139 (5%)	26	29	20, 34, 56, 89	0

All (139) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	568	HIS	7.1
1	F	510	GLU	6.9
1	F	257	ALA	6.3
1	F	596	ARG	6.3
1	A	586	LEU	6.1
1	A	568	HIS	6.1
1	A	567	LYS	5.8
1	F	568	HIS	5.8
1	B	335	GLN	5.5
1	F	567	LYS	5.4
1	B	587	VAL	5.3
1	F	569	GLY	5.2
1	A	335	GLN	5.2
1	F	148	GLY	5.1
1	B	596	ARG	5.1
1	A	596	ARG	5.0
1	B	257	ALA	5.0
1	F	585	GLY	4.9
1	D	288	GLU	4.8
1	B	567	LYS	4.8
1	D	567	LYS	4.8

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Mol	Chain	Res	Type	RSRZ
1	D	44	ARG	4.8
1	A	566	THR	4.7
1	D	335	GLN	4.5
1	B	146	GLU	4.4
1	F	290	GLU	4.4
1	F	556	ASN	4.4
1	F	552	GLU	4.3
1	D	596	ARG	4.3
1	F	2	THR	4.3
1	F	289	GLY	4.3
1	A	23	SER	4.3
1	F	545	SER	4.2
1	B	2	THR	4.1
1	B	290	GLU	4.1
1	F	51	LYS	4.0
1	A	288	GLU	4.0
1	B	456	ASN	3.9
1	B	510	GLU	3.9
1	A	587	VAL	3.8
1	F	425	GLU	3.8
1	B	568	HIS	3.7
1	F	50	ASP	3.7
1	F	544	PRO	3.6
1	B	148	GLY	3.6
1	D	566	THR	3.6
1	B	541	ASP	3.6
1	B	552	GLU	3.4
1	B	425	GLU	3.4
1	F	246	ARG	3.4
1	B	23	SER	3.4
1	A	44	ARG	3.3
1	D	615	ASP	3.3
1	D	290	GLU	3.3
1	D	23	SER	3.2
1	A	493	ALA	3.2
1	F	424	ALA	3.2
1	F	509	ASN	3.2
1	B	544	PRO	3.1
1	F	566	THR	3.1
1	F	23	SER	3.1
1	A	552	GLU	3.1
1	F	613	MET	3.1

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Mol	Chain	Res	Type	RSRZ
1	D	2	THR	3.1
1	B	586	LEU	3.1
1	A	289	GLY	3.1
1	A	2	THR	3.0
1	F	20	GLU	3.0
1	B	569	GLY	2.9
1	F	541	ASP	2.9
1	F	539	GLN	2.9
1	B	556	ASN	2.9
1	B	545	SER	2.8
1	B	584	GLU	2.8
1	D	478	ARG	2.8
1	A	554	GLN	2.8
1	D	51	LYS	2.8
1	B	426	GLY	2.8
1	F	230	ASN	2.8
1	D	569	GLY	2.7
1	F	615	ASP	2.7
1	B	469	ASP	2.7
1	F	595	VAL	2.7
1	F	17	ALA	2.6
1	F	146	GLU	2.6
1	F	542	PRO	2.6
1	F	443	GLY	2.6
1	B	570	LYS	2.6
1	B	598	HIS	2.6
1	F	147	ASP	2.5
1	B	145	GLU	2.5
1	F	532	ALA	2.5
1	D	588	GLU	2.5
1	F	145	GLU	2.5
1	F	258	LEU	2.5
1	A	469	ASP	2.5
1	A	146	GLU	2.5
1	F	598	HIS	2.5
1	A	570	LYS	2.5
1	F	495	ALA	2.5
1	D	442	GLU	2.5
1	F	570	LYS	2.4
1	F	465	ASP	2.4
1	B	566	THR	2.4
1	D	337	ASN	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	585	GLY	2.4
1	D	587	VAL	2.4
1	F	232	SER	2.4
1	D	586	LEU	2.3
1	B	613	MET	2.3
1	F	584	GLU	2.3
1	F	512	GLY	2.3
1	F	586	LEU	2.3
1	A	442	GLU	2.3
1	A	532	ALA	2.3
1	B	610	ASP	2.3
1	F	52	ASP	2.2
1	A	545	SER	2.2
1	F	337	ASN	2.2
1	D	469	ASP	2.2
1	D	443	GLY	2.1
1	B	373	LYS	2.1
1	A	610	ASP	2.1
1	F	597	LEU	2.1
1	B	288	GLU	2.1
1	B	507	GLU	2.1
1	F	540	TYR	2.1
1	B	258	LEU	2.1
1	D	80	THR	2.1
1	F	291	LYS	2.1
1	B	147	ASP	2.1
1	B	509	ASN	2.1
1	D	20	GLU	2.1
1	D	589	GLU	2.1
1	D	287	PRO	2.1
1	B	44	ARG	2.0
1	A	257	ALA	2.0
1	B	427	GLU	2.0
1	F	222	ASP	2.0

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

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
2	MAN	A	624	11/12	0.88	0.20	-	20,20,20,20	0
2	BMA	D	622	11/12	0.86	0.14	-	20,20,20,20	0
2	MAN	D	624	11/12	0.85	0.18	-	20,20,20,20	0
2	MAN	D	623	11/12	0.87	0.18	-	20,20,20,20	0
2	BMA	A	622	11/12	0.91	0.14	-	20,20,20,20	0
2	MAN	F	624	11/12	0.87	0.21	-	20,20,20,20	0
2	MAN	F	623	11/12	0.85	0.21	-	20,20,20,20	0
2	MAN	B	623	11/12	0.81	0.22	-	20,20,20,20	0
2	BMA	B	622	11/12	0.87	0.12	-	20,20,20,20	0
2	MAN	A	623	11/12	0.88	0.16	-	20,20,20,20	0
2	BMA	F	622	11/12	0.91	0.14	-	20,20,20,20	0
2	MAN	B	624	11/12	0.80	0.20	-	20,20,20,20	0

### 6.4 Ligands [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	NGT	F	625	14/14	0.92	0.14	-1.00	20,20,20,20	0
3	NGT	A	625	14/14	0.93	0.13	-1.31	20,20,20,20	0
3	NGT	D	625	14/14	0.93	0.13	-1.51	20,20,20,20	0
3	NGT	B	625	14/14	0.91	0.14	-1.68	20,20,20,20	0

### 6.5 Other polymers [i](#)

There are no such residues in this entry.