



Full wwPDB X-ray Structure Validation Report

Feb 26, 2014 – 09:34 PM GMT

PDB ID : 3FHQ
Title : Structure of endo-beta-N-acetylglucosaminidaseA
Authors : Jie, Y.; Li, L.; Shaw, N.; Li, Y.; Song, J.; Zhang, W.; Xia, C.; Zhang, R.;
Joachimiak, A.; Zhang, H.-C.; Wang, L.-X.; Wang, P.; Liu, Z.-J.
Deposited on : 2008-12-10
Resolution : 2.45 Å(reported)

This is a full wwPDB validation report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

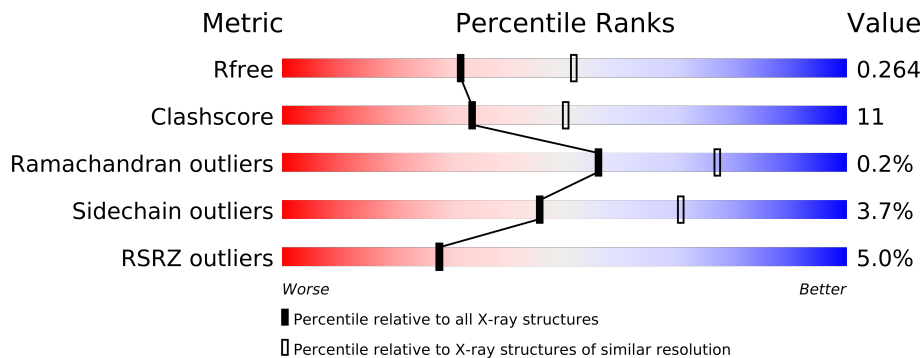
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

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}	66092	3566 (2.50-2.42)
Clashscore	79885	4471 (2.50-2.42)
Ramachandran outliers	78287	4383 (2.50-2.42)
Sidechain outliers	78261	4385 (2.50-2.42)
RSRZ outliers	66119	3568 (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 ≥ 3 , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	621	
1	B	621	
1	D	621	
1	F	621	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 20045 atoms, of which 0 are hydrogen and 0 are deuterium.

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

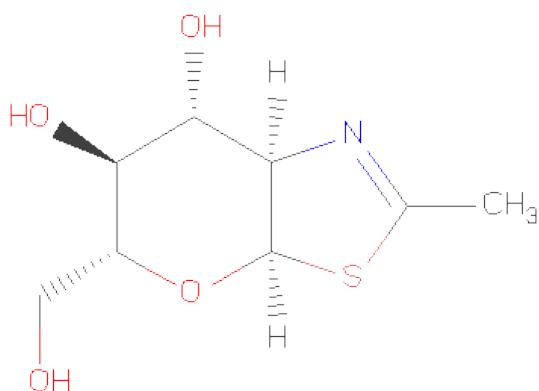
- Molecule 2 is a polymer of unknown type called SUGAR (3-MER).

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

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 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: C₈H₁₃NO₄S).



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.

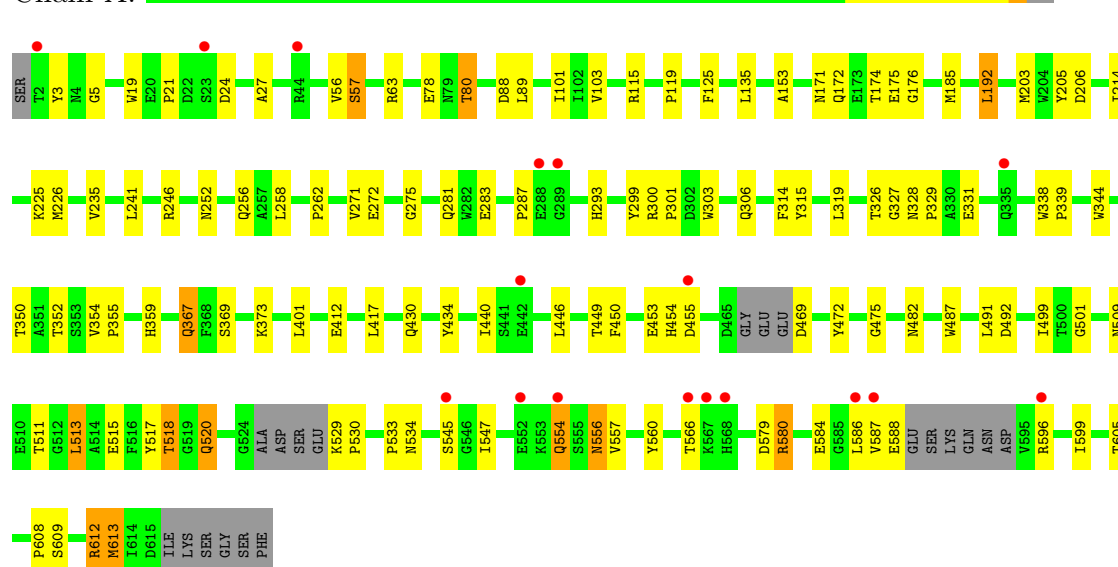
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	244	Total	O	0	0
			244	244		
4	B	182	Total	O	0	0
			182	182		
4	D	236	Total	O	0	0
			236	236		
4	F	175	Total	O	0	0
			175	175		

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.

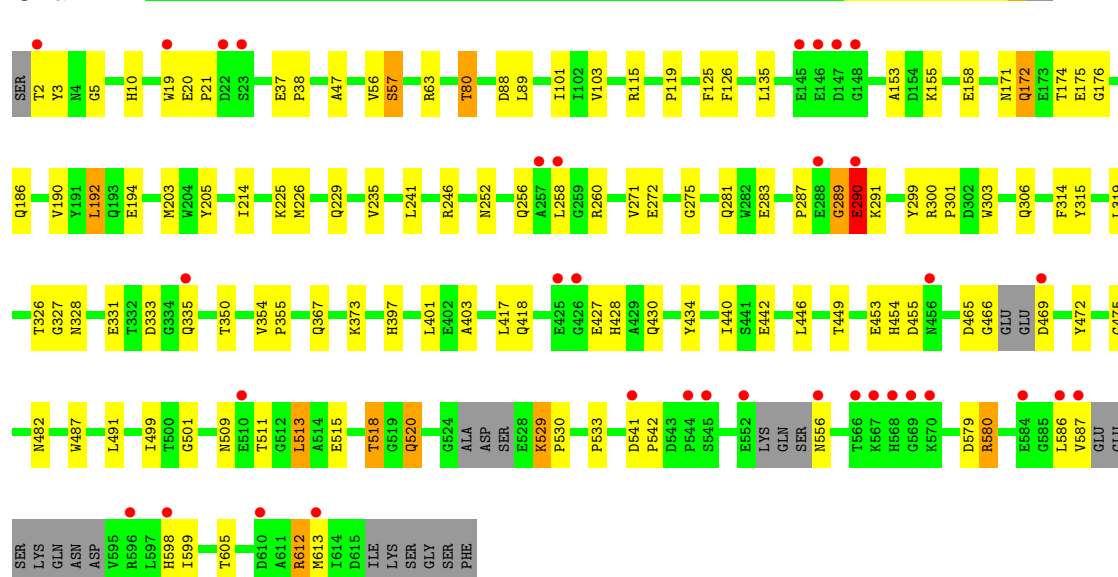
• Molecule 1: Endo-beta-N-acetylglucosaminidase

Chain A:



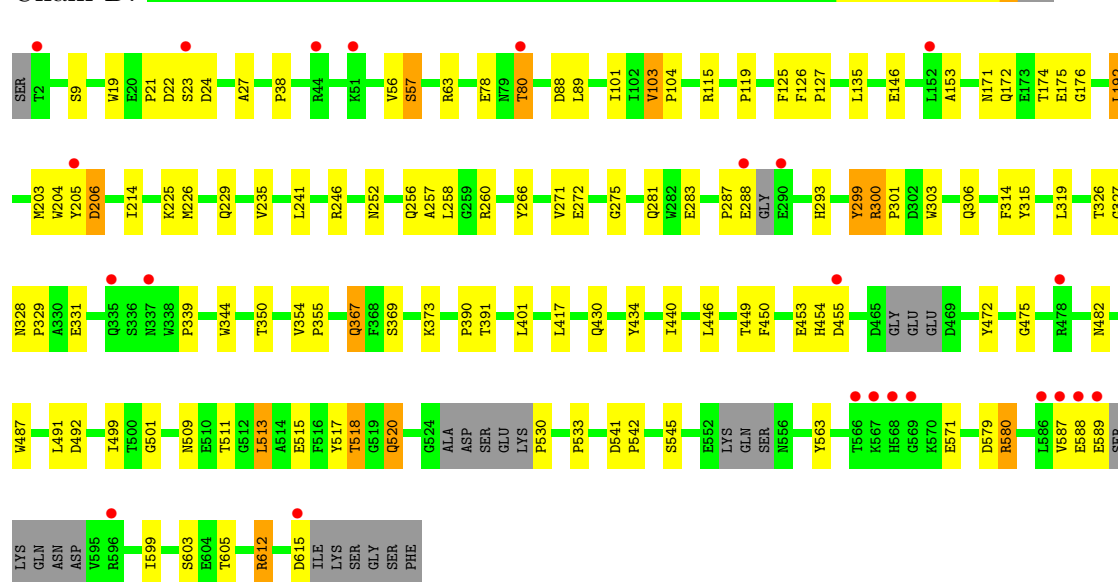
• Molecule 1: Endo-beta-N-acetylglucosaminidase

Chain B:



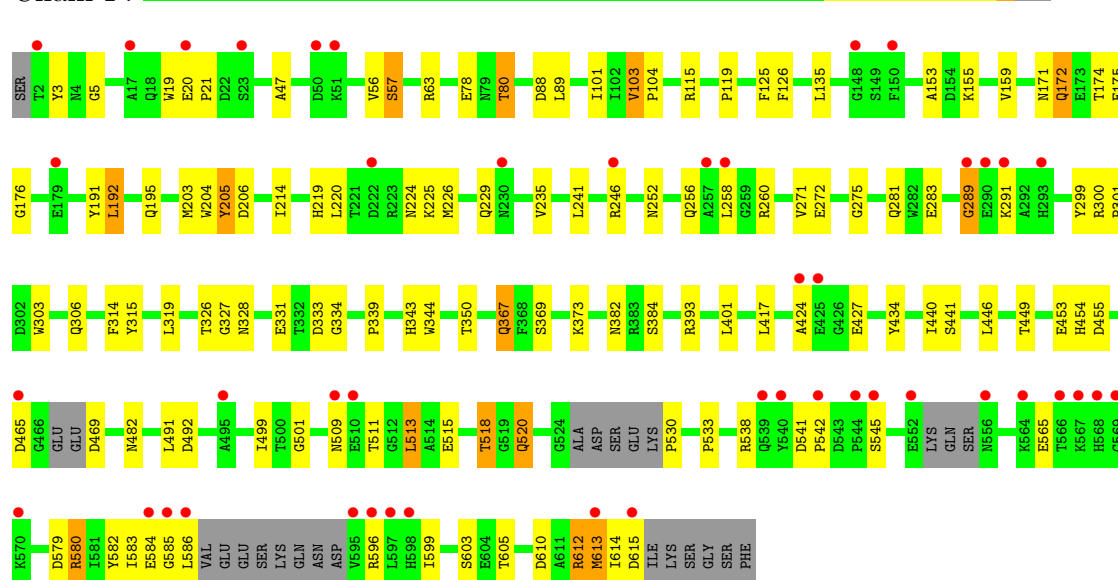
• Molecule 1: Endo-beta-N-acetylglucosaminidase

Chain D:



• Molecule 1: Endo-beta-N-acetylglucosaminidase

Chain F:



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	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) 94.2 (35.41-2.45)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.46 (at 2.45Å)	Xtriage
Refinement program	PHENIX (phenix.refine)	Depositor
R, R_{free}	0.221 , 0.264 0.230 , 0.264	Depositor DCC
R_{free} test set	4331 reflections (5.02%)	DCC
Wilson B-factor (Å ²)	36.4	Xtriage
Anisotropy	0.216	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 30.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	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 ²)	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.*

¹Intensities estimated from amplitudes.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit,

and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

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

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 11.

All (404) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(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
1:A:533:PRO:O	1:A:612:ARG:HD2	1.93	0.68

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
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

5.3.1 Protein backbone ⓘ

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%)	50	70
1	D	585/621 (94%)	565 (97%)	19 (3%)	1 (0%)	56	77
1	F	586/621 (94%)	562 (96%)	22 (4%)	2 (0%)	50	70
All	All	2353/2484 (95%)	2263 (96%)	85 (4%)	5 (0%)	56	77

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%)	40	64
1	B	494/515 (96%)	477 (97%)	17 (3%)	49	74
1	D	493/515 (96%)	475 (96%)	18 (4%)	45	70
1	F	492/515 (96%)	475 (96%)	17 (4%)	48	72
All	All	1977/2060 (96%)	1904 (96%)	73 (4%)	45	70

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
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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
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
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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
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 chains 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	10,11,12	0.83	0	11,15,17	1.89	3 (27%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	MAN	A	623	2	10,11,12	1.14	1 (10%)	11,15,17	2.42	4 (36%)
2	MAN	A	624	2	10,11,12	1.52	3 (30%)	11,15,17	2.85	5 (45%)
2	BMA	B	622	3,2	10,11,12	0.83	0	11,15,17	1.88	3 (27%)
2	MAN	B	623	2	10,11,12	1.14	1 (10%)	11,15,17	2.43	4 (36%)
2	MAN	B	624	2	10,11,12	1.52	3 (30%)	11,15,17	2.86	5 (45%)
2	BMA	D	622	3,2	10,11,12	0.82	0	11,15,17	1.88	3 (27%)
2	MAN	D	623	2	10,11,12	1.15	1 (10%)	11,15,17	2.42	4 (36%)
2	MAN	D	624	2	10,11,12	1.53	3 (30%)	11,15,17	2.85	5 (45%)
2	BMA	F	622	3,2	10,11,12	0.83	0	11,15,17	1.90	3 (27%)
2	MAN	F	623	2	10,11,12	1.13	1 (10%)	11,15,17	2.43	4 (36%)
2	MAN	F	624	2	10,11,12	1.52	3 (30%)	11,15,17	2.84	5 (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	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	623	MAN	O2-C2	-2.65	1.37	1.43
2	A	623	MAN	O2-C2	-2.63	1.37	1.43
2	B	623	MAN	O2-C2	-2.62	1.37	1.43
2	F	623	MAN	O2-C2	-2.60	1.38	1.43
2	D	624	MAN	O3-C3	-2.60	1.36	1.43
2	A	624	MAN	O3-C3	-2.57	1.36	1.43

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	624	MAN	O3-C3	-2.57	1.36	1.43
2	F	624	MAN	O3-C3	-2.57	1.36	1.43
2	B	624	MAN	C3-C2	2.53	1.58	1.52
2	F	624	MAN	C3-C2	2.53	1.58	1.52
2	A	624	MAN	C3-C2	2.52	1.58	1.52
2	D	624	MAN	C3-C2	2.52	1.58	1.52
2	F	624	MAN	O2-C2	-2.11	1.39	1.43
2	D	624	MAN	O2-C2	-2.11	1.39	1.43
2	A	624	MAN	O2-C2	-2.10	1.39	1.43
2	B	624	MAN	O2-C2	-2.06	1.39	1.43

All (48) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	624	MAN	O5-C5-C6	5.82	113.09	106.98
2	A	624	MAN	O5-C5-C6	5.80	113.06	106.98
2	D	624	MAN	O5-C5-C6	5.79	113.06	106.98
2	F	624	MAN	O5-C5-C6	5.75	113.02	106.98
2	F	622	BMA	O5-C5-C6	4.33	111.52	106.98
2	A	622	BMA	O5-C5-C6	4.27	111.47	106.98
2	B	622	BMA	O5-C5-C6	4.26	111.45	106.98
2	F	623	MAN	O3-C3-C2	4.26	117.73	109.94
2	D	622	BMA	O5-C5-C6	4.25	111.44	106.98
2	B	623	MAN	O3-C3-C2	4.25	117.71	109.94
2	A	623	MAN	O3-C3-C2	4.25	117.70	109.94
2	D	623	MAN	O3-C3-C2	4.24	117.69	109.94
2	B	623	MAN	O5-C5-C6	4.17	111.36	106.98
2	F	623	MAN	O5-C5-C6	4.14	111.32	106.98
2	A	623	MAN	O5-C5-C6	4.12	111.31	106.98
2	D	623	MAN	O5-C5-C6	4.12	111.30	106.98
2	D	623	MAN	O2-C2-C3	4.01	118.83	110.18
2	B	623	MAN	O2-C2-C3	4.01	118.82	110.18
2	A	623	MAN	O2-C2-C3	3.99	118.78	110.18
2	F	623	MAN	O2-C2-C3	3.97	118.75	110.18
2	F	624	MAN	O3-C3-C2	3.94	117.15	109.94
2	A	624	MAN	O3-C3-C2	3.92	117.11	109.94
2	D	624	MAN	O3-C3-C2	3.92	117.10	109.94
2	B	624	MAN	O3-C3-C2	3.91	117.10	109.94
2	D	624	MAN	O2-C2-C3	3.26	117.21	110.18
2	B	624	MAN	O3-C3-C4	3.24	117.63	110.35
2	F	624	MAN	O2-C2-C3	3.24	117.17	110.18
2	A	624	MAN	O2-C2-C3	3.24	117.16	110.18

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	624	MAN	O2-C2-C3	3.23	117.15	110.18
2	D	624	MAN	O3-C3-C4	3.23	117.59	110.35
2	A	624	MAN	O3-C3-C4	3.23	117.59	110.35
2	F	624	MAN	O3-C3-C4	3.22	117.58	110.35
2	A	624	MAN	C4-C3-C2	3.10	114.66	110.50
2	F	624	MAN	C4-C3-C2	3.09	114.65	110.50
2	B	624	MAN	C4-C3-C2	3.09	114.65	110.50
2	D	624	MAN	C4-C3-C2	3.08	114.64	110.50
2	F	622	BMA	O4-C4-C5	2.65	116.27	109.28
2	B	622	BMA	O4-C4-C5	2.64	116.24	109.28
2	A	622	BMA	O4-C4-C5	2.62	116.20	109.28
2	D	622	BMA	O4-C4-C5	2.61	116.16	109.28
2	B	622	BMA	O2-C2-C3	2.57	115.71	110.18
2	A	622	BMA	O2-C2-C3	2.56	115.71	110.18
2	F	622	BMA	O2-C2-C3	2.56	115.70	110.18
2	D	622	BMA	O2-C2-C3	2.55	115.68	110.18
2	D	623	MAN	O4-C4-C5	2.24	115.19	109.28
2	F	623	MAN	O4-C4-C5	2.23	115.15	109.28
2	B	623	MAN	O4-C4-C5	2.22	115.14	109.28
2	A	623	MAN	O4-C4-C5	2.22	115.14	109.28

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

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	15,15,15	2.73	2 (13%)	22,22,22	2.42	3 (13%)
3	NGT	B	625	2	15,15,15	2.76	2 (13%)	22,22,22	2.43	3 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	NGT	D	625	2	15,15,15	2.75	2 (13%)	22,22,22	2.41	3 (13%)
3	NGT	F	625	2	15,15,15	2.72	2 (13%)	22,22,22	2.40	3 (13%)

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

All (8) 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
3	B	625	NGT	C1-S1	-2.59	1.77	1.83
3	A	625	NGT	C1-S1	-2.57	1.77	1.83
3	D	625	NGT	C1-S1	-2.56	1.77	1.83
3	F	625	NGT	C1-S1	-2.55	1.77	1.83

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	625	NGT	C8-C7-N2	-8.64	119.81	124.31
3	A	625	NGT	C8-C7-N2	-8.61	119.83	124.31
3	D	625	NGT	C8-C7-N2	-8.60	119.84	124.31
3	F	625	NGT	C8-C7-N2	-8.52	119.87	124.31
3	B	625	NGT	S1-C7-N2	-4.68	115.31	117.91
3	A	625	NGT	S1-C7-N2	-4.66	115.33	117.91
3	F	625	NGT	S1-C7-N2	-4.65	115.33	117.91
3	D	625	NGT	S1-C7-N2	-4.63	115.34	117.91
3	B	625	NGT	C8-C7-S1	3.91	124.84	118.96
3	A	625	NGT	C8-C7-S1	3.89	124.81	118.96
3	D	625	NGT	C8-C7-S1	3.87	124.79	118.96
3	F	625	NGT	C8-C7-S1	3.85	124.76	118.96

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

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, 95th 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 ²)	Q<0.9
1	A	601/621 (96%)	0.22	17 (2%)	50	52	20, 31, 52, 75	0
1	B	599/621 (96%)	0.37	35 (5%)	22	22	20, 36, 57, 89	0
1	D	597/621 (96%)	0.22	23 (3%)	37	38	21, 33, 51, 74	0
1	F	596/621 (95%)	0.54	46 (7%)	13	12	20, 39, 60, 81	0
All	All	2393/2484 (96%)	0.34	121 (5%)	28	27	20, 34, 56, 89	0

All (121) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	568	HIS	6.6
1	A	586	LEU	6.1
1	F	596	ARG	5.6
1	F	510	GLU	5.4
1	F	567	LYS	5.3
1	B	335	GLN	5.3
1	F	568	HIS	5.1
1	B	587	VAL	5.1
1	A	567	LYS	4.9
1	A	596	ARG	4.9
1	D	567	LYS	4.9
1	B	596	ARG	4.9
1	B	567	LYS	4.6
1	F	257	ALA	4.6
1	D	288	GLU	4.6
1	F	290	GLU	4.6
1	A	335	GLN	4.5
1	A	568	HIS	4.5
1	F	545	SER	4.3
1	F	552	GLU	4.3
1	D	596	ARG	4.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	F	569	GLY	4.2
1	D	44	ARG	4.1
1	D	335	GLN	4.1
1	F	585	GLY	4.0
1	B	290	GLU	3.9
1	F	51	LYS	3.8
1	D	566	THR	3.7
1	F	556	ASN	3.7
1	A	23	SER	3.6
1	B	148	GLY	3.5
1	B	425	GLU	3.5
1	A	288	GLU	3.4
1	F	148	GLY	3.4
1	D	290	GLU	3.4
1	B	23	SER	3.4
1	A	566	THR	3.4
1	F	289	GLY	3.4
1	B	146	GLU	3.4
1	F	2	THR	3.3
1	A	587	VAL	3.3
1	F	425	GLU	3.2
1	B	586	LEU	3.2
1	F	613	MET	3.2
1	B	510	GLU	3.2
1	B	257	ALA	3.2
1	F	50	ASP	3.2
1	F	246	ARG	3.2
1	D	615	ASP	3.1
1	B	568	HIS	3.1
1	F	570	LYS	3.1
1	B	2	THR	3.1
1	B	570	LYS	3.0
1	F	23	SER	3.0
1	A	44	ARG	3.0
1	F	566	THR	3.0
1	B	584	GLU	3.0
1	B	426	GLY	2.9
1	F	230	ASN	2.9
1	F	20	GLU	2.9
1	B	456	ASN	2.9
1	F	509	ASN	2.9
1	F	544	PRO	2.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	556	ASN	2.8
1	B	258	LEU	2.8
1	A	442	GLU	2.8
1	F	595	VAL	2.8
1	B	552	GLU	2.7
1	B	541	ASP	2.7
1	A	289	GLY	2.7
1	A	554	GLN	2.7
1	F	615	ASP	2.6
1	F	258	LEU	2.6
1	B	598	HIS	2.6
1	F	465	ASP	2.6
1	F	542	PRO	2.5
1	B	545	SER	2.5
1	D	586	LEU	2.5
1	F	586	LEU	2.5
1	B	19	TRP	2.5
1	D	23	SER	2.5
1	F	564	LYS	2.5
1	F	598	HIS	2.4
1	D	2	THR	2.4
1	D	152	LEU	2.4
1	F	179	GLU	2.4
1	A	545	SER	2.4
1	D	337	ASN	2.4
1	A	552	GLU	2.4
1	F	584	GLU	2.4
1	F	539	GLN	2.4
1	A	2	THR	2.4
1	B	469	ASP	2.3
1	D	51	LYS	2.3
1	D	587	VAL	2.3
1	B	569	GLY	2.3
1	F	17	ALA	2.3
1	F	424	ALA	2.3
1	F	291	LYS	2.2
1	D	455	ASP	2.2
1	B	288	GLU	2.2
1	D	588	GLU	2.2
1	D	589	GLU	2.2
1	F	222	ASP	2.2
1	B	544	PRO	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	566	THR	2.2
1	F	597	LEU	2.2
1	B	613	MET	2.2
1	B	145	GLU	2.2
1	F	540	TYR	2.1
1	B	22	ASP	2.1
1	B	147	ASP	2.1
1	D	80	THR	2.1
1	D	569	GLY	2.1
1	F	150	PHE	2.1
1	D	478	ARG	2.0
1	F	495	ALA	2.0
1	B	610	ASP	2.0
1	F	293	HIS	2.0
1	D	205	TYR	2.0
1	A	455	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 ⓘ

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, 95th 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	RSR	LLDF	B-factors(Å ²)	Q<0.9
2	MAN	D	624	11/12	0.17	3.57	20,20,20,20	0
2	MAN	B	624	11/12	0.20	3.46	20,20,20,20	0
2	MAN	F	624	11/12	0.20	2.69	20,20,20,20	0
2	MAN	A	624	11/12	0.22	2.54	20,20,20,20	0
2	MAN	B	623	11/12	0.21	1.97	20,20,20,20	0
2	MAN	D	623	11/12	0.17	1.58	20,20,20,20	0
2	MAN	F	623	11/12	0.22	1.27	20,20,20,20	0
2	MAN	A	623	11/12	0.16	1.05	20,20,20,20	0
2	BMA	D	622	11/12	0.13	-0.45	20,20,20,20	0
2	BMA	A	622	11/12	0.12	-0.71	20,20,20,20	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
2	BMA	F	622	11/12	0.13	-1.25	20,20,20,20	0
2	BMA	B	622	11/12	0.12	-3.90	20,20,20,20	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, 95th 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	RSR	LLDF	B-factors(\AA^2)	Q<0.9
3	NGT	F	625	14/14	0.14	-0.86	20,20,20,20	0
3	NGT	D	625	14/14	0.13	-1.13	20,20,20,20	0
3	NGT	B	625	14/14	0.14	-1.21	20,20,20,20	0
3	NGT	A	625	14/14	0.13	-1.32	20,20,20,20	0

6.5 Other polymers

There are no such residues in this entry.