



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2017 – 03:51 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.;
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 X-ray Structure 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/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : trunk28620
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
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) : recalc28949

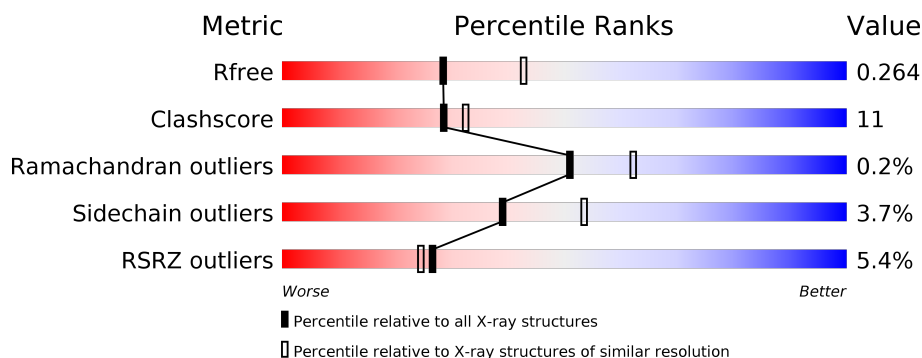
1 Overall quality at a glance

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}	100719	1119 (2.48-2.44)
Clashscore	112137	1193 (2.48-2.44)
Ramachandran outliers	110173	1185 (2.48-2.44)
Sidechain outliers	110143	1185 (2.48-2.44)
RSRZ outliers	101464	1126 (2.48-2.44)

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. 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> <div></div> <div>77%</div> <div>18%</div> <div>• •</div> </div> </div>
1	B	621	<div> <div>6%</div> <div> <div></div> <div>77%</div> <div>18%</div> <div>• •</div> </div> </div>
1	D	621	<div> <div>3%</div> <div> <div></div> <div>76%</div> <div>18%</div> <div>• •</div> </div> </div>
1	F	621	<div> <div>8%</div> <div> <div></div> <div>75%</div> <div>19%</div> <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			

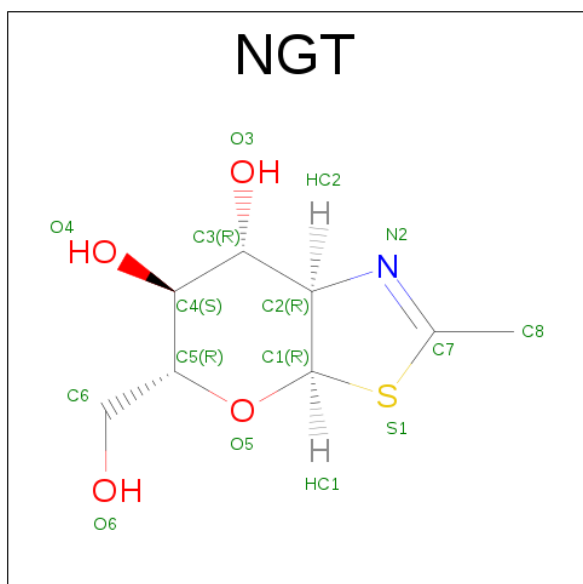
There are 16 discrepancies between the modelled and reference sequences:

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: 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		

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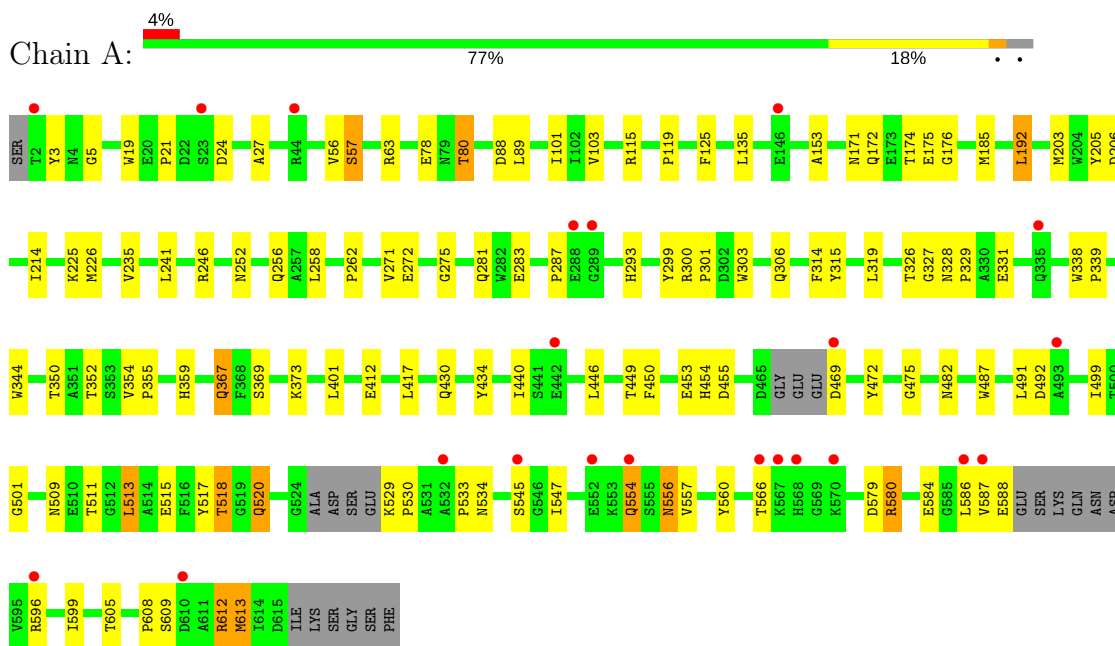
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	182	Total 182	O 182	0	0
4	D	236	Total 236	O 236	0	0
4	F	175	Total 175	O 175	0	0

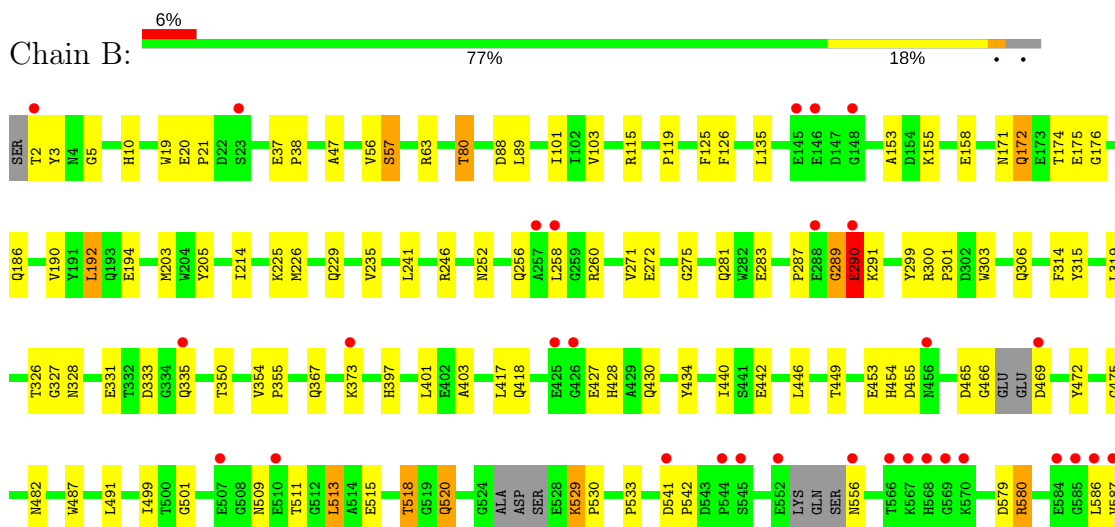
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes 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

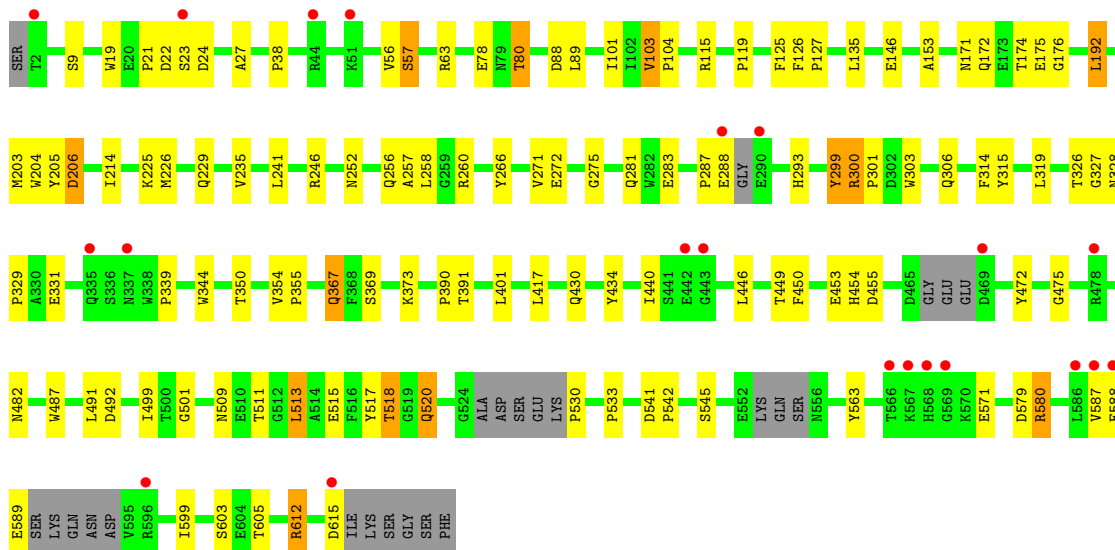
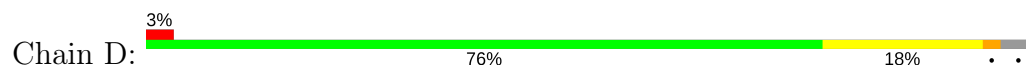


• Molecule 1: Endo-beta-N-acetylglucosaminidase

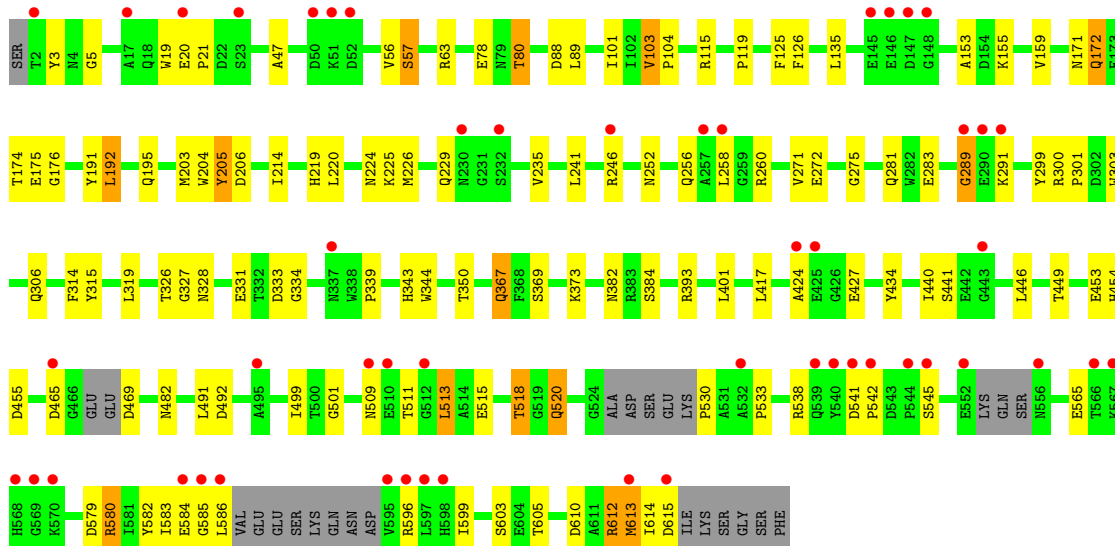
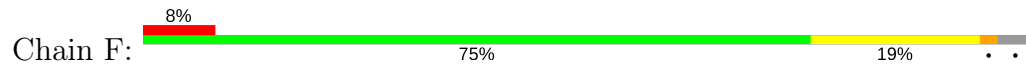




● Molecule 1: Endo-beta-N-acetylglucosaminidase



● Molecule 1: Endo-beta-N-acetylglucosaminidase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, 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) 91.0 (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 0.229 , 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)	0.37 , 43.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	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.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 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: 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

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: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:F:565:GLU:OE1	1:F:596:ARG:NE	2.23	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:D:533:PRO:O	1:D:612:ARG:HD2	1.93	0.67
1:F:291:LYS:HB2	4:F:668:HOH:O	1.95	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:B:586:LEU:C	1:B:587:VAL:HG23	2.19	0.63
1:F:596:ARG:CG	1:F:613:MET:HE1	2.28	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:175:GLU:HG3	1:F:214:ILE:HD12	1.82	0.62
1:F:582:TYR:CE2	1:F:584:GLU:HG3	2.35	0.62
1:D:417:LEU:HB3	1:D:518:THR:HG23	1.80	0.62
1:B:511:THR:CG2	1:B:513:LEU:HB2	2.30	0.62
1:D:588:GLU:O	1:D:589:GLU:CB	2.29	0.62
1:A:326:THR:HG21	1:A:331:GLU:O	2.00	0.61
4:A:829:HOH:O	1:B:556:ASN:HB2	1.99	0.61
1:D:146:GLU:HG3	4:D:820:HOH:O	1.98	0.61
1:A:271:VAL:HG22	1:A:299:TYR:O	2.00	0.61
1:F:326:THR:HG21	1:F:331:GLU:O	1.99	0.61
1:A:326:THR:CG2	1:A:328:ASN:HB3	2.31	0.61
1:F:511:THR:CG2	1:F:513:LEU:HB2	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:A:175:GLU:HG3	1:A:214:ILE:HD12	1.84	0.59
1:F:465:ASP:HB3	4:F:633:HOH:O	2.02	0.59
1:A:449:THR:OG1	1:A:520:GLN:HG2	2.03	0.59
1:D:326:THR:HG22	1:D:328:ASN:N	2.18	0.59
1:D:440:ILE:HD11	1:D:499:ILE:HG13	1.85	0.59
1:F:596:ARG:HG2	1:F:613:MET:HE1	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:A:566:THR:HG22	4:A:877:HOH:O	2.04	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: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:B:3:TYR:CZ	1:B:5:GLY:HA3	2.40	0.56
1:D:511:THR:CG2	1:D:513:LEU:HB2	2.35	0.56
1:A:19:TRP:CH2	1:A:21:PRO:HG3	2.40	0.56
1:F:565:GLU:OE1	1:F:596:ARG:NH2	2.38	0.56
1:B:319:LEU:HD21	1:B:327:GLY:HA2	1.87	0.56
1:D:56:VAL:HG11	1:D:203:MET:HE1	1.86	0.56
1:D:319:LEU:HD21	1:D:327:GLY:HA2	1.88	0.56
1:F:326:THR:CG2	1:F:328:ASN:HB3	2.35	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:B:135:LEU:HD11	1:B:176:GLY:O	2.06	0.56
1:F:135:LEU:HD11	1:F: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:B:272:GLU:OE1	2:B:622:BMA:O2	2.20	0.55
1:D:204:TRP:CD1	1:D:205:TYR:O	2.60	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:B:101:ILE:HB	1:B:125:PHE:O	2.08	0.53
1:F:204:TRP:CD1	1:F:205:TYR:O	2.62	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:283:GLU:CD	1:A:283:GLU:H	2.11	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:272:GLU:OE1	2:A:622:BMA:O2	2.18	0.53
1:F:153:ALA:HB1	1:F:192:LEU:HD13	1.91	0.53
1:B:613:MET:HG3	4:B:695:HOH:O	2.09	0.52
1:D:204:TRP:NE1	1:D:205:TYR:O	2.42	0.52
1:F:440:ILE:HD11	1:F:499:ILE:HG13	1.90	0.52
1:F:545:SER:O	1:F:585:GLY:HA2	2.10	0.52
1:F:56:VAL:HG12	1:F:89:LEU:CB	2.26	0.52
1:D:326:THR:HG22	1:D:328:ASN:HB3	1.90	0.52
1:A:605:THR:O	1:A:605:THR:HG22	2.09	0.52
1:F:613:MET:O	1:F:614:ILE:HD13	2.10	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:D:153:ALA:HB1	1:D:192:LEU:HD13	1.91	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: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:D:605:THR:O	1:D:605:THR:HG22	2.11	0.51
1:F:174:THR:O	1:F:214:ILE:HD11	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:A:275:GLY:HA3	1:A:303:TRP:CD2	2.46	0.51
1:B:599:ILE:N	1:B:599:ILE:HD12	2.25	0.51
1:D:80:THR:OG1	1:D:80:THR:O	2.29	0.51
1:A:367:GLN:OE1	1:A:369:SER:OG	2.19	0.51
1:D:135:LEU:HD11	1:D:176:GLY:O	2.11	0.51
1:F:583:ILE:HG21	1:F:586:LEU:HD22	1.92	0.51
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:F:565:GLU:OE1	1:F:596:ARG:CZ	2.59	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:D:487:TRP:NE1	4:D:792:HOH:O	2.34	0.50
1:F:596:ARG:CD	1:F:613:MET:HE1	2.41	0.50
1:D:326:THR:HG22	1:D:328:ASN:H	1.76	0.50
1:D:580:ARG:HH11	1:D:580:ARG:HG2	1.77	0.50
1:B:275:GLY:HA3	1:B:303:TRP:CD2	2.47	0.50
1:B:326:THR:HG22	1:B:328:ASN:HB3	1.93	0.50
1:A:596:ARG:HD3	1:A:613:MET:CE	2.42	0.50
1:F:191:TYR:CZ	1:F:195:GLN:HG3	2.47	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:A:446:LEU:HG	1:A:491:LEU:HD11	1.94	0.49
1:B:246:ARG:HD3	4:B:913:HOH:O	2.12	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:A:529:LYS:HE3	1:A:609:SER:HA	1.94	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:B:446:LEU:HG	1:B:491:LEU:HD11	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:289:GLY:C	1:B:290:GLU:O	2.50	0.48
1:B:300:ARG:NH2	4:B:889:HOH:O	2.42	0.48
1:F:599:ILE:HD12	1:F:599:ILE:N	2.27	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:A:434:TYR:O	1:A:501:GLY:HA2	2.14	0.47
1:D:300:ARG:N	1:D:301:PRO:HD3	2.29	0.47
1:A:246:ARG:HE	1:A:281:GLN:HG3	1.79	0.47
1:B:511:THR:HG22	1:B:513:LEU:HB2	1.96	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:291:LYS:HB3	4:B:767:HOH:O	2.15	0.47
1:B:397:HIS:ND1	1:F:289:GLY:CA	2.78	0.47
1:A:88:ASP:O	1:A:119:PRO:HD2	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:541:ASP:HB2	1:B:542:PRO:HD3	1.96	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: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:F:580:ARG:HG2	1:F:580:ARG:HH11	1.80	0.46
1:A:101:ILE:HB	1:A:125:PHE:O	2.15	0.46
1:A:225:LYS:HB2	1:A:258:LEU:HD11	1.96	0.46
1:D:257:ALA:O	1:F:441:SER:HB2	2.16	0.46
1:D:80:THR:HG23	1:D:314:PHE:HE2	1.81	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:454:HIS:CD2	1:D:513:LEU:HB3	2.50	0.46
1:D:587:VAL:HG12	1:D:587:VAL:O	2.15	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:A:80:THR:HG23	1:A:315:TYR:HE1	1.81	0.45
1:F:454:HIS:O	1:F:455:ASP:HB2	2.16	0.45
1:F:565:GLU:CD	1:F:596:ARG:HE	2.18	0.45
1:A:3:TYR:CZ	1:A:5:GLY:HA3	2.52	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: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:A:80:THR:HG23	1:A:314:PHE:HE2	1.82	0.44
1:D:80:THR:HG23	1:D:315:TYR:HE1	1.82	0.44
1:A:454:HIS:O	1:A:455:ASP:HB2	2.16	0.44
1:D:9:SER:O	1:D:104:PRO:HD2	2.18	0.44
1:D:175:GLU:HA	1:D:214:ILE:HD12	2.00	0.44
1:D:56:VAL:HG13	1:D:266:TYR:CE1	2.52	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:F:533:PRO:HG2	1:F:599:ILE:HG22	1.99	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: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:454:HIS:CD2	1:F:513:LEU:HB3	2.52	0.44
1:B:430:GLN:HG2	1:B:472:TYR:CE2	2.53	0.44
1:F:520:GLN:O	1:F:520:GLN:HG3	2.13	0.44
1:A:205:TYR:OH	3:A:625:NGT:HC1	2.17	0.44
1:A:56:VAL:HG11	1:A:203:MET:CE	2.47	0.44
1:A:454:HIS:CD2	1:A:513:LEU:HB3	2.52	0.44
1:B:454:HIS:CD2	1:B: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:206:ASP:CG	1:D:206:ASP:O	2.56	0.44
1:D:430:GLN:HG2	1:D:472:TYR:CE2	2.53	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:F:334:GLY:CA	1:F:343:HIS:CE1	3.01	0.43
1:A:326:THR:HG22	1:A:328:ASN:CB	2.48	0.43
1:A:554:GLN:H	1:A:554:GLN:HG2	1.46	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:F:252:ASN:O	1:F:256:GLN:HG3	2.18	0.43
1:D:475:GLY:HA3	1:D:487:TRP:CE3	2.53	0.43
1:D:78:GLU:O	1:D:80:THR:HG22	2.18	0.43
1:F:446:LEU:HG	1:F:491:LEU:HD11	1.99	0.43
1:A:326:THR:HG22	1:A:328:ASN:H	1.83	0.43
1:B:335:GLN:CD	1:F:333:ASP:HB2	2.38	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: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:F:80:THR:HG23	1:F:314:PHE:HE2	1.84	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:56:VAL:HG11	1:B:203:MET:CE	2.48	0.43
1:B:373:LYS:HE2	1:B:482:ASN:ND2	2.33	0.43
1:A:339:PRO:HG2	1:A:344:TRP:CH2	2.54	0.43
1:B:175:GLU:HG3	1:B:214:ILE:CD1	2.46	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:F:582:TYR:OH	1:F:584:GLU:HG2	2.18	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:A:78:GLU:O	1:A:80:THR:HG22	2.19	0.43
1:B:175:GLU:HA	1:B:214:ILE:HD12	2.00	0.43
1:B:354:VAL:HG13	1:B:355:PRO:HA	2.00	0.43
1:F:56:VAL:HG11	1:F:203:MET:CE	2.48	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:A:469:ASP:N	4:A:652:HOH:O	2.52	0.42
1:F:582:TYR:OH	1:F:584:GLU:CG	2.68	0.42
1:D:226:MET:O	1:D:235:VAL:HG21	2.20	0.42
1:D:326:THR:HG22	1:D:328:ASN:CB	2.49	0.42
1:D:80:THR:CG2	1:D:314:PHE:HE2	2.32	0.42
1:A:596:ARG:HB3	1:A:613:MET:HE2	2.01	0.42
1:A:328:ASN:HA	1:A:329:PRO:HD2	1.89	0.42
1:D:587:VAL:CG1	1:D:587:VAL:O	2.68	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: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:D:511:THR:HG22	1:D:513:LEU:HB2	2.02	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:252:ASN:O	1:B:256:GLN:HG3	2.19	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:126:PHE:HB2	1:F:172:GLN:HA	2.03	0.41
1:F:80:THR:CG2	1:F:314:PHE:HE2	2.34	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:A:475:GLY:HA3	1:A:487:TRP:CE3	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:185:MET:O	1:A:185:MET:HE2	2.21	0.41
1:B:135:LEU:HD11	1:B:176:GLY:C	2.41	0.41
1:A:338:TRP:O	4:A:649:HOH:O	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: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: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:63:ARG:HH12	1:D:306:GLN:HG2	1.85	0.40
1:D:450:PHE:HA	1:D:517:TYR:O	2.22	0.40
1:A:226:MET:O	1:A:235:VAL:HG21	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

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%)	44	55
1	D	585/621 (94%)	565 (97%)	19 (3%)	1 (0%)	51	62
1	F	586/621 (94%)	562 (96%)	22 (4%)	2 (0%)	44	55
All	All	2353/2484 (95%)	2263 (96%)	85 (4%)	5 (0%)	51	62

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%)	34	47
1	B	494/515 (96%)	477 (97%)	17 (3%)	42	57
1	D	493/515 (96%)	475 (96%)	18 (4%)	39	53
1	F	492/515 (96%)	475 (96%)	17 (4%)	41	56
All	All	1977/2060 (96%)	1904 (96%)	73 (4%)	39	53

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	1.21	1 (9%)	13,15,17	1.92	4 (30%)
2	MAN	A	623	2	11,11,12	1.07	1 (9%)	13,15,17	2.44	6 (46%)
2	MAN	A	624	2	11,11,12	1.84	2 (18%)	13,15,17	2.29	6 (46%)
2	BMA	B	622	3,2	11,11,12	1.22	1 (9%)	13,15,17	1.92	4 (30%)
2	MAN	B	623	2	11,11,12	1.07	1 (9%)	13,15,17	2.44	6 (46%)
2	MAN	B	624	2	11,11,12	1.84	2 (18%)	13,15,17	2.29	6 (46%)
2	BMA	D	622	3,2	11,11,12	1.21	1 (9%)	13,15,17	1.91	4 (30%)
2	MAN	D	623	2	11,11,12	1.07	1 (9%)	13,15,17	2.44	6 (46%)
2	MAN	D	624	2	11,11,12	1.85	2 (18%)	13,15,17	2.29	6 (46%)
2	BMA	F	622	3,2	11,11,12	1.21	1 (9%)	13,15,17	1.92	4 (30%)
2	MAN	F	623	2	11,11,12	1.06	1 (9%)	13,15,17	2.44	6 (46%)
2	MAN	F	624	2	11,11,12	1.85	2 (18%)	13,15,17	2.29	6 (46%)

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	-2.73	1.36	1.43
2	A	624	MAN	O3-C3	-2.70	1.36	1.43
2	B	624	MAN	O3-C3	-2.70	1.36	1.43
2	F	624	MAN	O3-C3	-2.70	1.36	1.43
2	D	623	MAN	O2-C2	-2.49	1.37	1.43
2	A	623	MAN	O2-C2	-2.48	1.37	1.43
2	B	623	MAN	O2-C2	-2.47	1.37	1.43
2	F	623	MAN	O2-C2	-2.45	1.38	1.43
2	F	622	BMA	C1-C2	2.88	1.59	1.52
2	B	622	BMA	C1-C2	2.90	1.59	1.52
2	A	622	BMA	C1-C2	2.91	1.59	1.52
2	D	622	BMA	C1-C2	2.93	1.59	1.52
2	D	624	MAN	C2-C3	4.39	1.58	1.52
2	A	624	MAN	C2-C3	4.39	1.58	1.52
2	F	624	MAN	C2-C3	4.40	1.58	1.52
2	B	624	MAN	C2-C3	4.41	1.58	1.52

All (64) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	624	MAN	O5-C1-C2	-2.90	106.25	110.79
2	A	624	MAN	O5-C1-C2	-2.88	106.28	110.79
2	F	624	MAN	O5-C1-C2	-2.87	106.30	110.79
2	B	624	MAN	O5-C1-C2	-2.86	106.31	110.79
2	B	623	MAN	C1-C2-C3	-2.75	106.17	109.65
2	D	623	MAN	C1-C2-C3	-2.71	106.21	109.65
2	A	623	MAN	C1-C2-C3	-2.71	106.22	109.65
2	F	623	MAN	C1-C2-C3	-2.67	106.27	109.65
2	A	622	BMA	O5-C1-C2	-2.05	107.57	110.79
2	B	622	BMA	O5-C1-C2	-2.05	107.57	110.79
2	F	622	BMA	O5-C1-C2	-2.05	107.58	110.79
2	D	622	BMA	O5-C1-C2	-2.03	107.60	110.79
2	F	624	MAN	C1-O5-C5	2.12	115.08	112.17
2	B	624	MAN	C1-O5-C5	2.13	115.10	112.17
2	A	624	MAN	C1-O5-C5	2.15	115.13	112.17
2	D	624	MAN	C1-O5-C5	2.15	115.13	112.17
2	D	624	MAN	C2-C3-C4	2.16	114.64	110.88
2	F	624	MAN	C2-C3-C4	2.17	114.65	110.88
2	B	624	MAN	C2-C3-C4	2.17	114.65	110.88
2	A	624	MAN	C2-C3-C4	2.17	114.66	110.88
2	A	623	MAN	O4-C4-C5	2.32	115.14	109.28
2	B	623	MAN	O4-C4-C5	2.33	115.14	109.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	623	MAN	O4-C4-C5	2.33	115.15	109.28
2	D	623	MAN	O4-C4-C5	2.34	115.19	109.28
2	D	623	MAN	O2-C2-C1	2.71	114.69	109.18
2	B	623	MAN	O2-C2-C1	2.72	114.70	109.18
2	A	623	MAN	O2-C2-C1	2.72	114.71	109.18
2	F	623	MAN	O2-C2-C1	2.73	114.73	109.18
2	D	622	BMA	O4-C4-C5	2.73	116.16	109.28
2	A	622	BMA	O4-C4-C5	2.74	116.20	109.28
2	B	622	BMA	O4-C4-C5	2.76	116.24	109.28
2	F	622	BMA	O4-C4-C5	2.77	116.27	109.28
2	D	622	BMA	O2-C2-C3	2.80	115.68	110.17
2	F	622	BMA	O2-C2-C3	2.81	115.70	110.17
2	A	622	BMA	O2-C2-C3	2.82	115.71	110.17
2	B	622	BMA	O2-C2-C3	2.82	115.71	110.17
2	D	623	MAN	C1-O5-C5	2.96	116.25	112.17
2	F	623	MAN	C1-O5-C5	2.96	116.25	112.17
2	A	623	MAN	C1-O5-C5	2.97	116.25	112.17
2	B	623	MAN	C1-O5-C5	2.97	116.25	112.17
2	F	624	MAN	O3-C3-C4	3.32	117.58	110.36
2	A	624	MAN	O3-C3-C4	3.32	117.59	110.36
2	D	624	MAN	O3-C3-C4	3.32	117.59	110.36
2	B	624	MAN	O3-C3-C4	3.34	117.63	110.36
2	B	624	MAN	O2-C2-C3	3.55	117.15	110.17
2	A	624	MAN	O2-C2-C3	3.56	117.16	110.17
2	F	624	MAN	O2-C2-C3	3.56	117.17	110.17
2	D	624	MAN	O2-C2-C3	3.58	117.21	110.17
2	B	624	MAN	O3-C3-C2	3.89	117.10	110.02
2	D	624	MAN	O3-C3-C2	3.89	117.10	110.02
2	A	624	MAN	O3-C3-C2	3.90	117.11	110.02
2	F	624	MAN	O3-C3-C2	3.91	117.15	110.02
2	D	623	MAN	O3-C3-C2	4.21	117.69	110.02
2	A	623	MAN	O3-C3-C2	4.22	117.70	110.02
2	B	623	MAN	O3-C3-C2	4.22	117.71	110.02
2	F	623	MAN	O3-C3-C2	4.23	117.73	110.02
2	F	623	MAN	O2-C2-C3	4.37	118.75	110.17
2	A	623	MAN	O2-C2-C3	4.38	118.78	110.17
2	B	623	MAN	O2-C2-C3	4.40	118.82	110.17
2	D	623	MAN	O2-C2-C3	4.40	118.83	110.17
2	B	622	BMA	O2-C2-C1	4.48	118.28	109.18
2	D	622	BMA	O2-C2-C1	4.48	118.29	109.18
2	A	622	BMA	O2-C2-C1	4.49	118.31	109.18
2	F	622	BMA	O2-C2-C1	4.50	118.34	109.18

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 [i](#)

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	1.52	1 (9%)
3	NGT	B	625	2	13,15,15	2.87	1 (7%)	11,22,22	1.53	1 (9%)
3	NGT	D	625	2	13,15,15	2.86	1 (7%)	11,22,22	1.52	1 (9%)
3	NGT	F	625	2	13,15,15	2.83	1 (7%)	11,22,22	1.51	1 (9%)

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

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	625	NGT	C8-C7-S1	3.85	124.76	118.96
3	D	625	NGT	C8-C7-S1	3.87	124.79	118.96
3	A	625	NGT	C8-C7-S1	3.89	124.81	118.96
3	B	625	NGT	C8-C7-S1	3.91	124.84	118.96

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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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%)	0.21	22 (3%)	42 39	20, 31, 52, 75	0
1	B	599/621 (96%)	0.37	35 (5%)	24 22	20, 36, 57, 89	0
1	D	597/621 (96%)	0.19	21 (3%)	44 41	21, 33, 51, 74	0
1	F	596/621 (95%)	0.52	51 (8%)	11 9	20, 39, 60, 81	0
All	All	2393/2484 (96%)	0.32	129 (5%)	26 24	20, 34, 56, 89	0

All (129) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	568	HIS	6.9
1	F	510	GLU	6.7
1	F	596	ARG	6.1
1	F	257	ALA	6.1
1	A	568	HIS	5.9
1	A	586	LEU	5.9
1	A	567	LYS	5.6
1	F	568	HIS	5.6
1	B	335	GLN	5.3
1	F	567	LYS	5.2
1	B	587	VAL	5.1
1	A	335	GLN	5.0
1	F	569	GLY	5.0
1	F	148	GLY	4.9
1	B	596	ARG	4.9
1	A	596	ARG	4.8
1	B	257	ALA	4.7
1	F	585	GLY	4.7
1	D	288	GLU	4.7
1	B	567	LYS	4.6
1	D	567	LYS	4.6

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Mol	Chain	Res	Type	RSRZ
1	D	44	ARG	4.6
1	A	566	THR	4.4
1	D	335	GLN	4.3
1	B	146	GLU	4.3
1	F	290	GLU	4.3
1	F	556	ASN	4.2
1	F	552	GLU	4.2
1	D	596	ARG	4.1
1	A	23	SER	4.1
1	F	2	THR	4.1
1	F	289	GLY	4.1
1	F	545	SER	4.0
1	B	2	THR	3.9
1	B	290	GLU	3.9
1	F	51	LYS	3.8
1	A	288	GLU	3.8
1	B	456	ASN	3.8
1	B	510	GLU	3.7
1	F	425	GLU	3.6
1	A	587	VAL	3.6
1	B	568	HIS	3.6
1	F	50	ASP	3.5
1	F	544	PRO	3.5
1	D	566	THR	3.4
1	B	148	GLY	3.4
1	B	541	ASP	3.4
1	B	552	GLU	3.3
1	B	425	GLU	3.2
1	F	246	ARG	3.2
1	B	23	SER	3.2
1	A	44	ARG	3.2
1	D	615	ASP	3.1
1	D	23	SER	3.1
1	D	290	GLU	3.1
1	A	493	ALA	3.1
1	F	509	ASN	3.0
1	F	424	ALA	3.0
1	A	552	GLU	3.0
1	F	23	SER	3.0
1	B	586	LEU	3.0
1	D	2	THR	3.0
1	F	566	THR	3.0

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Mol	Chain	Res	Type	RSRZ
1	B	544	PRO	3.0
1	F	613	MET	2.9
1	A	289	GLY	2.9
1	A	2	THR	2.9
1	F	20	GLU	2.8
1	B	569	GLY	2.8
1	F	539	GLN	2.7
1	B	584	GLU	2.7
1	B	556	ASN	2.7
1	D	478	ARG	2.7
1	B	545	SER	2.7
1	F	541	ASP	2.7
1	D	51	LYS	2.7
1	A	554	GLN	2.7
1	F	230	ASN	2.6
1	B	426	GLY	2.6
1	D	569	GLY	2.6
1	F	615	ASP	2.6
1	B	469	ASP	2.6
1	F	146	GLU	2.5
1	F	595	VAL	2.5
1	B	570	LYS	2.5
1	F	17	ALA	2.5
1	F	542	PRO	2.5
1	B	598	HIS	2.5
1	F	443	GLY	2.4
1	B	145	GLU	2.4
1	A	146	GLU	2.4
1	D	588	GLU	2.4
1	F	145	GLU	2.4
1	F	147	ASP	2.4
1	F	532	ALA	2.4
1	F	258	LEU	2.4
1	A	570	LYS	2.4
1	F	598	HIS	2.4
1	A	469	ASP	2.4
1	D	442	GLU	2.4
1	F	570	LYS	2.3
1	F	495	ALA	2.3
1	D	337	ASN	2.3
1	F	465	ASP	2.3
1	B	566	THR	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	585	GLY	2.3
1	F	232	SER	2.3
1	D	587	VAL	2.2
1	D	586	LEU	2.2
1	F	584	GLU	2.2
1	F	586	LEU	2.2
1	A	442	GLU	2.2
1	B	613	MET	2.2
1	F	512	GLY	2.2
1	A	532	ALA	2.1
1	A	545	SER	2.1
1	B	610	ASP	2.1
1	F	337	ASN	2.1
1	F	52	ASP	2.1
1	B	373	LYS	2.1
1	D	469	ASP	2.0
1	B	288	GLU	2.0
1	B	507	GLU	2.0
1	D	443	GLY	2.0
1	F	540	TYR	2.0
1	A	610	ASP	2.0
1	F	291	LYS	2.0
1	B	258	LEU	2.0
1	F	597	LEU	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, 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	RSCC	RSR	LLDF	B-factors(Å ²)	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

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
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, 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	RSCC	RSR	LLDF	B-factors(\AA^2)	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.