



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 08:55 AM UTC

PDB ID : 3OBA / pdb_00003oba
Title : Structure of the beta-galactosidase from Kluyveromyces lactis
Authors : Fernandez-Leiro, R.; Pereira-Rodriguez, A.; Becerra, M.; Gonzalez-Siso, I.;
Cerdan, M.E.; Sanz-Aparicio, J.
Deposited on : 2010-08-06
Resolution : 2.75 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

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

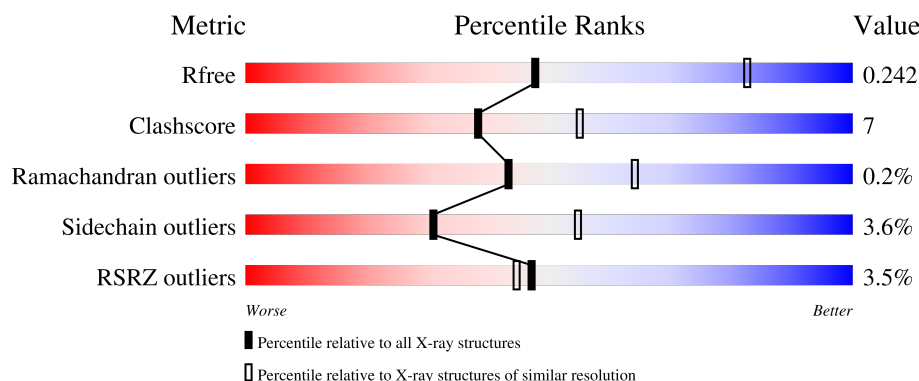
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.75 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}	180053	1009 (2.76-2.76)
Clashscore	190562	1044 (2.76-2.76)
Ramachandran outliers	187476	1024 (2.76-2.76)
Sidechain outliers	187428	1024 (2.76-2.76)
RSRZ outliers	180081	1009 (2.76-2.76)

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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. 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	1032	0% 85% 13% ..
1	B	1032	3% 84% 13% ..
1	C	1032	5% 84% 14% ..
1	D	1032	5% 84% 14% ..

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	GOL	B	1027	-	-	X	-
3	GOL	C	1026	-	-	X	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 35030 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 Beta-galactosidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1024	Total	C	N	O	S	0	0	0
			8325	5335	1388	1587	15			
1	C	1024	Total	C	N	O	S	0	0	0
			8325	5335	1388	1587	15			
1	D	1024	Total	C	N	O	S	0	0	0
			8325	5335	1388	1587	15			
1	B	1024	Total	C	N	O	S	0	0	0
			8325	5335	1388	1587	15			

There are 32 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-6	ASP	-	expression tag	UNP P00723
A	-5	TYR	-	expression tag	UNP P00723
A	-4	LYS	-	expression tag	UNP P00723
A	-3	ASP	-	expression tag	UNP P00723
A	-2	ASP	-	expression tag	UNP P00723
A	-1	ASP	-	expression tag	UNP P00723
A	0	ASP	-	expression tag	UNP P00723
A	1	LYS	-	expression tag	UNP P00723
C	-6	ASP	-	expression tag	UNP P00723
C	-5	TYR	-	expression tag	UNP P00723
C	-4	LYS	-	expression tag	UNP P00723
C	-3	ASP	-	expression tag	UNP P00723
C	-2	ASP	-	expression tag	UNP P00723
C	-1	ASP	-	expression tag	UNP P00723
C	0	ASP	-	expression tag	UNP P00723
C	1	LYS	-	expression tag	UNP P00723
D	-6	ASP	-	expression tag	UNP P00723
D	-5	TYR	-	expression tag	UNP P00723
D	-4	LYS	-	expression tag	UNP P00723
D	-3	ASP	-	expression tag	UNP P00723
D	-2	ASP	-	expression tag	UNP P00723

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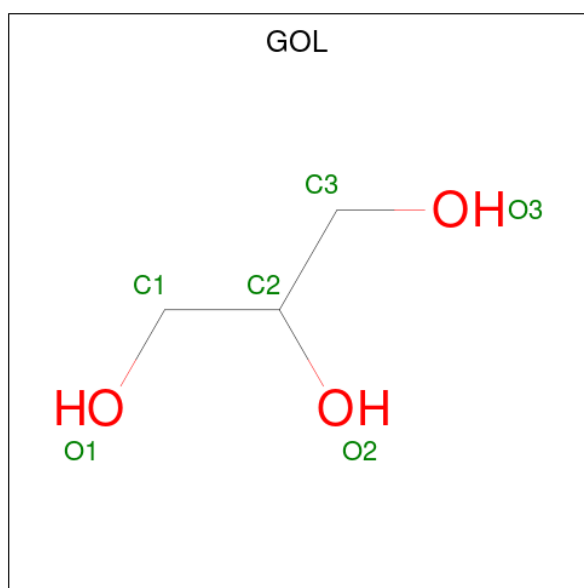
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Chain	Residue	Modelled	Actual	Comment	Reference
D	-1	ASP	-	expression tag	UNP P00723
D	0	ASP	-	expression tag	UNP P00723
D	1	LYS	-	expression tag	UNP P00723
B	-6	ASP	-	expression tag	UNP P00723
B	-5	TYR	-	expression tag	UNP P00723
B	-4	LYS	-	expression tag	UNP P00723
B	-3	ASP	-	expression tag	UNP P00723
B	-2	ASP	-	expression tag	UNP P00723
B	-1	ASP	-	expression tag	UNP P00723
B	0	ASP	-	expression tag	UNP P00723
B	1	LYS	-	expression tag	UNP P00723

- Molecule 2 is MANGANESE (III) ION (CCD ID: MN3) (formula: Mn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Mn 1 1	0	0
2	C	1	Total Mn 1 1	0	0
2	D	1	Total Mn 1 1	0	0
2	B	1	Total Mn 1 1	0	0

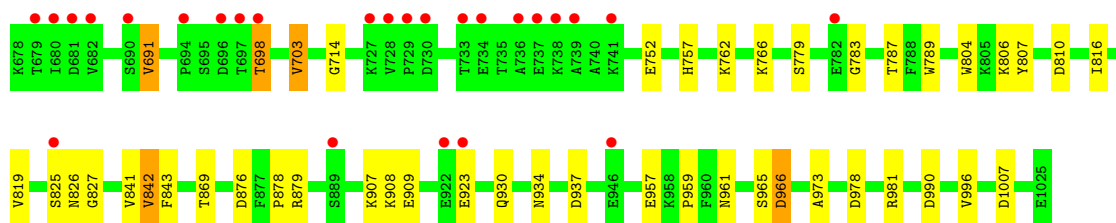
- Molecule 3 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



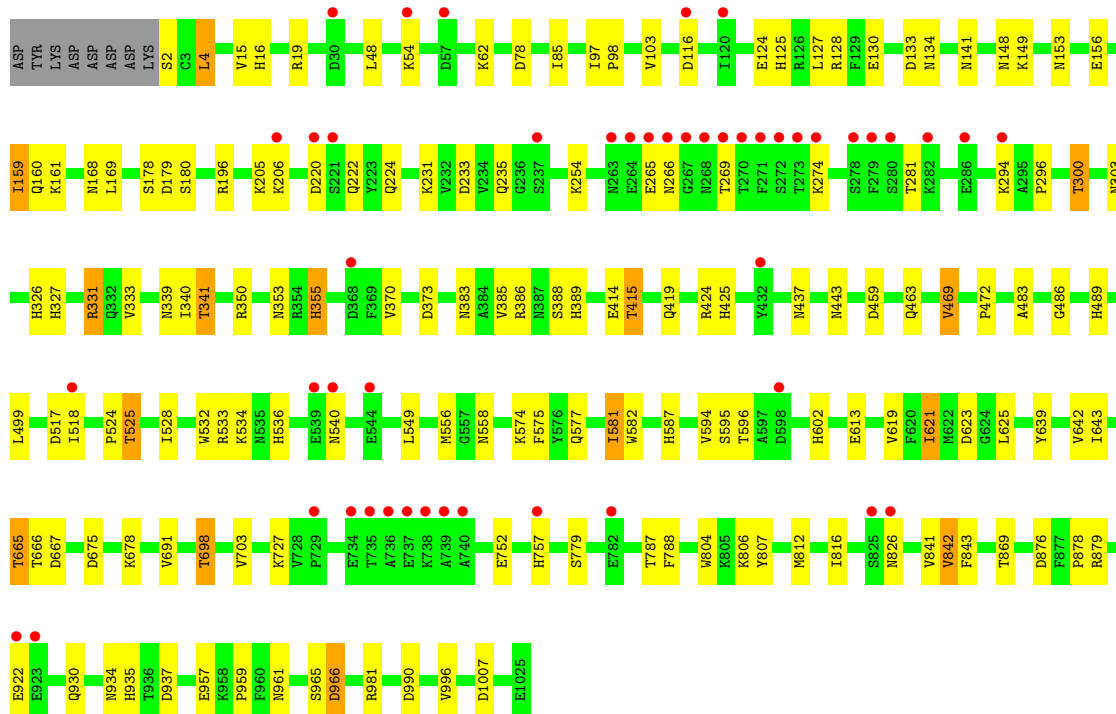
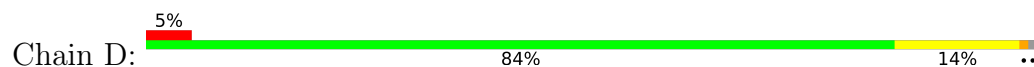
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 6 3 3	0	0
3	A	1	Total C O 6 3 3	0	0
3	C	1	Total C O 6 3 3	0	0
3	C	1	Total C O 6 3 3	0	0
3	C	1	Total C O 6 3 3	0	0
3	C	1	Total C O 6 3 3	0	0
3	D	1	Total C O 6 3 3	0	0
3	D	1	Total C O 6 3 3	0	0
3	B	1	Total C O 6 3 3	0	0
3	B	1	Total C O 6 3 3	0	0

- Molecule 4 is water.

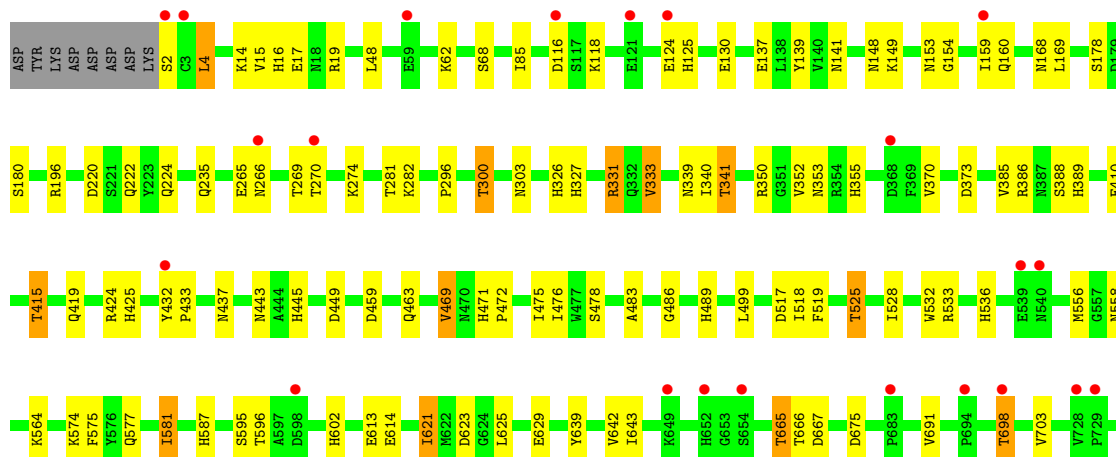
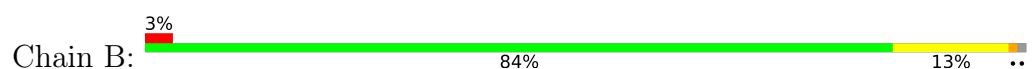
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	426	Total O 426 426	0	0
4	C	436	Total O 436 436	0	0
4	D	396	Total O 396 396	0	0
4	B	408	Total O 408 408	0	0

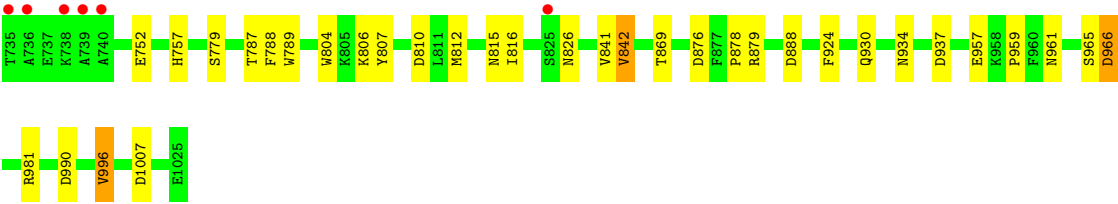


• Molecule 1: Beta-galactosidase



• Molecule 1: Beta-galactosidase





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	140.03Å 153.34Å 216.16Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	62.57 – 2.75 62.57 – 2.75	Depositor EDS
% Data completeness (in resolution range)	99.9 (62.57-2.75) 99.9 (62.57-2.75)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	0.17	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.22 (at 2.77Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.207 , 0.243 0.206 , 0.242	Depositor DCC
R_{free} test set	6092 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	24.0	Xtriage
Anisotropy	0.109	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 24.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	35030	wwPDB-VP
Average B, all atoms (Å ²)	19.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.99% 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: GOL, MN3

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.50	2/8561 (0.0%)	0.79	5/11614 (0.0%)
1	B	0.48	0/8561	0.78	2/11614 (0.0%)
1	C	0.48	0/8561	0.79	5/11614 (0.0%)
1	D	0.49	0/8561	0.78	4/11614 (0.0%)
All	All	0.49	2/34244 (0.0%)	0.78	16/46456 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	349	PHE	C-O	-8.42	1.13	1.24
1	A	348	LEU	C-N	-7.35	1.23	1.33

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	966	ASP	N-CA-C	-6.88	105.83	114.56
1	A	966	ASP	N-CA-C	-6.60	106.17	114.56
1	C	966	ASP	N-CA-C	-6.05	106.88	114.56
1	D	966	ASP	N-CA-C	-5.82	107.17	114.56
1	B	469	VAL	CB-CA-C	-5.70	103.73	112.05
1	C	469	VAL	CB-CA-C	-5.60	103.87	112.05
1	C	469	VAL	N-CA-C	5.52	118.78	111.17
1	D	966	ASP	N-CA-CB	-5.47	103.72	111.00
1	A	469	VAL	CB-CA-C	-5.44	104.10	112.05
1	C	966	ASP	N-CA-CB	-5.23	104.05	111.00
1	A	843	PHE	N-CA-C	5.21	118.21	110.14
1	A	966	ASP	N-CA-CB	-5.13	104.17	111.00
1	D	469	VAL	CB-CA-C	-5.11	104.59	112.05
1	C	843	PHE	N-CA-C	5.10	118.05	110.14
1	A	469	VAL	N-CA-C	5.04	118.12	111.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	843	PHE	N-CA-C	5.00	117.76	109.85

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	8325	0	7972	103	0
1	B	8325	0	7972	114	0
1	C	8325	0	7972	131	0
1	D	8325	0	7972	126	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	12	0	16	0	0
3	B	12	0	14	4	0
3	C	24	0	32	11	0
3	D	12	0	16	0	0
4	A	426	0	0	13	0
4	B	408	0	0	17	0
4	C	436	0	0	28	0
4	D	396	0	0	27	0
All	All	35030	0	31966	451	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 7.

All (451) 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:C:356:ASP:O	3:C:1026:GOL:H11	1.36	1.26
1:B:265:GLU:HB3	1:B:266:ASN:HB2	1.30	1.09
1:A:265:GLU:HB3	1:A:266:ASN:HB2	1.35	1.05

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:265:GLU:HB3	1:C:266:ASN:HB2	1.34	1.04
1:D:265:GLU:HB3	1:D:266:ASN:HB2	1.37	1.04
1:C:340:ILE:H	1:C:577:GLN:HE22	1.07	1.00
1:D:665:THR:HG22	1:D:667:ASP:H	1.27	1.00
1:A:340:ILE:H	1:A:577:GLN:HE22	1.10	1.00
1:C:665:THR:HG22	1:C:667:ASP:H	1.28	0.98
1:B:665:THR:HG22	1:B:667:ASP:H	1.28	0.98
1:A:665:THR:HG22	1:A:667:ASP:H	1.28	0.94
1:B:14:LYS:HE2	4:B:1186:HOH:O	1.68	0.94
1:B:340:ILE:H	1:B:577:GLN:HE22	1.05	0.94
1:D:103:VAL:HB	3:B:1027:GOL:H32	1.50	0.93
1:D:340:ILE:H	1:D:577:GLN:HE22	1.11	0.91
1:A:116:ASP:HB2	1:B:270:THR:HG21	1.53	0.90
1:C:221:SER:HB2	4:C:1048:HOH:O	1.74	0.87
1:D:254:LYS:HE3	4:D:1065:HOH:O	1.76	0.84
1:C:356:ASP:O	3:C:1026:GOL:C1	2.25	0.82
1:C:19:ARG:HH11	1:C:148:ASN:ND2	1.76	0.82
1:A:581:ILE:HD11	1:A:625:LEU:HG	1.63	0.81
1:B:19:ARG:HH11	1:B:148:ASN:ND2	1.79	0.80
1:D:19:ARG:HH11	1:D:148:ASN:ND2	1.78	0.80
1:D:62:LYS:HE3	4:D:1605:HOH:O	1.81	0.79
1:A:19:ARG:HH11	1:A:148:ASN:ND2	1.82	0.78
1:B:340:ILE:N	1:B:577:GLN:HE22	1.81	0.77
1:D:54:LYS:HD2	4:D:1064:HOH:O	1.85	0.76
1:A:116:ASP:HB2	1:B:270:THR:CG2	2.15	0.76
1:D:581:ILE:HD11	1:D:625:LEU:HG	1.68	0.75
1:A:525:THR:HB	1:A:528:ILE:HD12	1.67	0.75
1:A:787:THR:OG1	1:A:879:ARG:NH2	2.20	0.75
1:C:879:ARG:NH1	1:C:990:ASP:OD1	2.20	0.74
1:C:787:THR:OG1	1:C:879:ARG:NH2	2.20	0.74
1:A:879:ARG:NH1	1:A:990:ASP:OD1	2.21	0.74
1:D:787:THR:OG1	1:D:879:ARG:NH2	2.20	0.74
1:A:340:ILE:N	1:A:577:GLN:HE22	1.86	0.73
1:D:525:THR:HG21	4:D:1069:HOH:O	1.87	0.73
1:B:525:THR:HB	1:B:528:ILE:HD12	1.70	0.73
1:D:340:ILE:N	1:D:577:GLN:HE22	1.86	0.73
1:C:581:ILE:HD11	1:C:625:LEU:HG	1.70	0.72
1:B:787:THR:OG1	1:B:879:ARG:NH2	2.23	0.72
1:B:581:ILE:HD11	1:B:625:LEU:HG	1.70	0.72
1:C:525:THR:HB	1:C:528:ILE:HD12	1.72	0.71
1:D:879:ARG:NH1	1:D:990:ASP:OD1	2.25	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:536:HIS:HE1	4:C:1082:HOH:O	1.74	0.70
1:B:300:THR:HG22	1:B:303:ASN:H	1.55	0.69
1:C:691:VAL:HB	4:C:1347:HOH:O	1.92	0.69
1:C:340:ILE:N	1:C:577:GLN:HE22	1.84	0.69
1:D:533:ARG:HG3	1:D:575:PHE:CD2	2.28	0.69
1:C:153:ASN:HB3	1:C:463:GLN:HG2	1.74	0.69
1:C:594:VAL:HG22	4:C:1136:HOH:O	1.92	0.69
1:A:265:GLU:CB	1:A:266:ASN:HB2	2.18	0.69
1:A:300:THR:HG22	1:A:303:ASN:H	1.58	0.69
1:D:153:ASN:HB3	1:D:463:GLN:HG2	1.74	0.69
1:B:265:GLU:CB	1:B:266:ASN:HB2	2.15	0.69
1:C:533:ARG:HG3	1:C:575:PHE:CD2	2.28	0.69
1:A:14:LYS:HE3	4:A:1295:HOH:O	1.91	0.69
1:C:265:GLU:CB	1:C:266:ASN:HB2	2.18	0.69
1:D:265:GLU:CB	1:D:266:ASN:HB2	2.20	0.68
1:C:281:THR:HG22	4:C:1296:HOH:O	1.92	0.68
1:D:300:THR:HG22	1:D:303:ASN:H	1.57	0.68
1:D:274:LYS:HA	4:D:1186:HOH:O	1.93	0.68
1:A:153:ASN:HB3	1:A:463:GLN:HG2	1.75	0.68
1:C:281:THR:CG2	4:C:1296:HOH:O	2.42	0.68
1:A:533:ARG:HG3	1:A:575:PHE:CD2	2.28	0.68
1:B:153:ASN:HB3	1:B:463:GLN:HG2	1.76	0.68
1:C:300:THR:HG22	1:C:303:ASN:H	1.59	0.67
1:D:525:THR:HB	1:D:528:ILE:HD12	1.75	0.67
1:B:533:ARG:HG3	1:B:575:PHE:CD2	2.30	0.67
1:D:54:LYS:CD	4:D:1064:HOH:O	2.41	0.67
1:D:265:GLU:HG3	4:D:1116:HOH:O	1.94	0.66
1:A:270:THR:HG21	1:B:116:ASP:HB2	1.78	0.66
1:B:341:THR:HG22	4:B:1045:HOH:O	1.95	0.66
1:C:594:VAL:HG21	4:B:1209:HOH:O	1.96	0.65
1:B:879:ARG:NH1	1:B:990:ASP:OD1	2.30	0.65
1:C:189:TRP:HD1	3:C:1026:GOL:H32	1.60	0.64
1:D:415:THR:HB	1:D:483:ALA:HA	1.78	0.64
1:D:540:ASN:HA	4:D:1159:HOH:O	1.97	0.64
1:D:525:THR:HG22	1:D:528:ILE:H	1.62	0.64
1:D:161:LYS:HE2	4:D:1089:HOH:O	1.98	0.64
1:D:4:LEU:HD13	1:B:816:ILE:HG22	1.79	0.63
1:A:178:SER:OG	1:A:180:SER:HB3	1.99	0.63
1:A:675:ASP:OD2	1:A:698:THR:HB	1.99	0.63
1:C:909:GLU:H	3:C:1028:GOL:H11	1.63	0.63
1:A:415:THR:HB	1:A:483:ALA:HA	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:530:GLU:HG2	4:A:1241:HOH:O	1.99	0.63
1:A:539:GLU:HA	4:A:1640:HOH:O	1.97	0.63
1:B:340:ILE:H	1:B:577:GLN:NE2	1.89	0.63
1:B:564:LYS:HE3	4:B:1452:HOH:O	1.99	0.63
1:A:525:THR:HG21	4:A:1396:HOH:O	1.97	0.62
1:C:415:THR:HB	1:C:483:ALA:HA	1.80	0.61
1:C:558:ASN:H	1:C:930:GLN:NE2	1.97	0.61
1:B:675:ASP:OD2	1:B:698:THR:HB	2.01	0.61
1:A:286:GLU:HG2	4:A:1272:HOH:O	2.00	0.61
1:D:341:THR:HG22	4:D:1198:HOH:O	2.00	0.61
1:A:331:ARG:HG2	1:A:331:ARG:HH11	1.66	0.61
1:B:558:ASN:H	1:B:930:GLN:NE2	1.99	0.61
1:C:934:ASN:HD21	1:C:961:ASN:HB3	1.66	0.60
1:A:19:ARG:NH2	1:A:459:ASP:OD1	2.34	0.60
1:A:19:ARG:HD3	1:A:148:ASN:HD22	1.67	0.60
1:A:525:THR:HG22	1:A:528:ILE:H	1.66	0.60
1:A:712:LYS:HD2	4:A:1175:HOH:O	2.01	0.60
1:B:339:ASN:HD21	1:B:574:LYS:HG2	1.66	0.60
1:B:415:THR:HB	1:B:483:ALA:HA	1.83	0.60
1:B:19:ARG:NH2	1:B:459:ASP:OD1	2.33	0.60
1:B:614:GLU:HG2	4:B:1297:HOH:O	1.99	0.60
1:D:934:ASN:HD21	1:D:961:ASN:HB3	1.67	0.60
1:D:103:VAL:CB	3:B:1027:GOL:H32	2.27	0.60
1:D:339:ASN:HD21	1:D:574:LYS:HG2	1.66	0.59
1:C:19:ARG:HD3	1:C:148:ASN:HD22	1.67	0.59
1:C:339:ASN:HD21	1:C:574:LYS:HG2	1.67	0.59
1:C:581:ILE:HG22	4:C:1421:HOH:O	2.02	0.59
1:B:525:THR:HG22	1:B:528:ILE:H	1.68	0.59
1:D:816:ILE:HG22	1:B:4:LEU:HD13	1.84	0.59
1:C:19:ARG:NH2	1:C:459:ASP:OD1	2.34	0.59
1:A:934:ASN:HD21	1:A:961:ASN:HB3	1.67	0.59
1:D:178:SER:OG	1:D:180:SER:HB3	2.03	0.59
1:D:331:ARG:HH11	1:D:331:ARG:HG2	1.67	0.59
1:B:581:ILE:HG12	1:B:625:LEU:HD11	1.84	0.59
1:C:415:THR:HG21	4:C:1069:HOH:O	2.03	0.58
1:D:665:THR:CG2	1:D:666:THR:N	2.66	0.58
1:D:19:ARG:NH2	1:D:459:ASP:OD1	2.35	0.58
1:A:755:GLY:HA2	1:D:78:ASP:OD1	2.03	0.58
1:C:525:THR:HG22	1:C:528:ILE:H	1.67	0.58
1:C:581:ILE:HG12	1:C:625:LEU:HD11	1.85	0.58
1:B:934:ASN:HD21	1:B:961:ASN:HB3	1.66	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:815:ASN:OD1	3:B:1027:GOL:O3	2.20	0.58
1:A:339:ASN:HD21	1:A:574:LYS:HG2	1.69	0.58
1:D:141:ASN:HD21	1:D:168:ASN:HA	1.68	0.58
1:A:270:THR:CG2	1:B:116:ASP:HB2	2.34	0.58
1:A:558:ASN:H	1:A:930:GLN:NE2	2.01	0.58
1:C:189:TRP:CD1	3:C:1026:GOL:H32	2.39	0.57
1:C:675:ASP:OD2	1:C:698:THR:HB	2.04	0.57
1:D:675:ASP:OD2	1:D:698:THR:HB	2.05	0.57
1:B:274:LYS:NZ	4:B:1060:HOH:O	2.32	0.57
1:A:740:ALA:HB3	4:A:1335:HOH:O	2.04	0.57
1:C:331:ARG:HG2	1:C:331:ARG:HH11	1.70	0.57
1:B:752:GLU:HG2	1:B:757:HIS:HD2	1.69	0.57
1:B:178:SER:OG	1:B:180:SER:HB3	2.05	0.56
1:C:141:ASN:HD21	1:C:168:ASN:HA	1.69	0.56
1:A:752:GLU:HG2	1:A:757:HIS:HD2	1.70	0.56
1:A:879:ARG:HH11	1:A:990:ASP:CG	2.14	0.56
1:A:19:ARG:HD3	1:A:148:ASN:ND2	2.20	0.56
1:A:966:ASP:HB3	1:A:981:ARG:HH11	1.70	0.56
1:C:19:ARG:HD3	1:C:148:ASN:ND2	2.21	0.56
1:D:806:LYS:HD3	1:B:424:ARG:HB3	1.88	0.56
1:A:966:ASP:HB3	1:A:981:ARG:NH1	2.21	0.56
1:D:807:TYR:OH	1:B:425:HIS:HD2	1.89	0.56
1:D:807:TYR:OH	1:B:425:HIS:CD2	2.59	0.56
1:C:908:LYS:H	3:C:1028:GOL:C1	2.19	0.55
1:D:19:ARG:HD3	1:D:148:ASN:HD22	1.71	0.55
1:C:178:SER:OG	1:C:180:SER:HB3	2.07	0.55
1:D:581:ILE:HG12	1:D:625:LEU:HD11	1.89	0.55
1:B:639:TYR:O	1:B:643:ILE:HG12	2.06	0.55
1:C:752:GLU:HG2	1:C:757:HIS:HD2	1.71	0.55
1:D:558:ASN:H	1:D:930:GLN:NE2	2.05	0.55
1:A:665:THR:CG2	1:A:666:THR:N	2.70	0.55
1:C:966:ASP:HB3	1:C:981:ARG:HH11	1.71	0.55
1:C:433:PRO:HD3	4:C:1084:HOH:O	2.06	0.55
1:D:639:TYR:O	1:D:643:ILE:HG12	2.07	0.55
1:C:556:MET:HA	1:C:623:ASP:HA	1.89	0.55
1:B:141:ASN:HD21	1:B:168:ASN:HA	1.72	0.54
1:C:966:ASP:HB3	1:C:981:ARG:NH1	2.22	0.54
1:C:879:ARG:HH11	1:C:990:ASP:CG	2.16	0.54
1:A:581:ILE:HG12	1:A:625:LEU:HD11	1.90	0.54
1:B:331:ARG:HG2	1:B:331:ARG:HH11	1.71	0.54
1:B:966:ASP:HB3	1:B:981:ARG:HH11	1.71	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:19:ARG:HD3	1:B:148:ASN:HD22	1.72	0.54
1:B:556:MET:HA	1:B:623:ASP:HA	1.90	0.53
1:A:141:ASN:HD21	1:A:168:ASN:HA	1.72	0.53
1:C:265:GLU:HG3	4:C:1203:HOH:O	2.08	0.53
1:B:62:LYS:HE3	4:B:1094:HOH:O	2.07	0.53
1:D:141:ASN:ND2	1:D:169:LEU:H	2.07	0.53
1:B:966:ASP:HB3	1:B:981:ARG:NH1	2.24	0.53
1:A:425:HIS:CD2	1:C:807:TYR:OH	2.62	0.53
1:D:556:MET:HA	1:D:623:ASP:HA	1.91	0.53
1:D:752:GLU:HG2	1:D:757:HIS:HD2	1.74	0.52
1:C:141:ASN:ND2	1:C:169:LEU:H	2.08	0.52
1:B:665:THR:CG2	1:B:666:THR:N	2.72	0.52
1:C:639:TYR:O	1:C:643:ILE:HG12	2.10	0.52
1:C:657:ILE:HB	4:C:1347:HOH:O	2.10	0.52
1:C:665:THR:CG2	1:C:666:THR:N	2.71	0.52
1:D:879:ARG:HH11	1:D:990:ASP:CG	2.17	0.52
1:C:907:LYS:HA	3:C:1028:GOL:H12	1.92	0.52
1:A:149:LYS:NZ	1:A:179:ASP:OD1	2.43	0.52
1:C:19:ARG:HH11	1:C:148:ASN:HD21	1.56	0.52
1:D:922:GLU:HG2	4:D:1083:HOH:O	2.09	0.52
1:C:340:ILE:H	1:C:577:GLN:NE2	1.91	0.51
1:A:130:GLU:HB2	1:A:196:ARG:HB3	1.92	0.51
1:A:141:ASN:ND2	1:A:169:LEU:H	2.08	0.51
1:C:592:GLU:HG2	4:C:1105:HOH:O	2.10	0.51
1:D:19:ARG:HH11	1:D:148:ASN:HD21	1.58	0.51
1:B:19:ARG:HD3	1:B:148:ASN:ND2	2.25	0.51
1:B:996:VAL:HA	4:B:1138:HOH:O	2.10	0.51
1:A:556:MET:HA	1:A:623:ASP:HA	1.92	0.51
1:D:424:ARG:HB3	1:B:806:LYS:HD3	1.91	0.51
1:C:553:GLY:HA3	4:C:1421:HOH:O	2.09	0.51
1:C:130:GLU:HB2	1:C:196:ARG:HB3	1.92	0.51
1:C:923:GLU:HB2	4:C:1129:HOH:O	2.09	0.51
1:A:424:ARG:HB3	1:C:806:LYS:HD3	1.93	0.51
1:D:19:ARG:HD3	1:D:148:ASN:ND2	2.25	0.50
1:D:153:ASN:CB	1:D:463:GLN:HG2	2.41	0.50
1:D:206:LYS:HG2	4:D:1086:HOH:O	2.11	0.50
1:A:419:GLN:NE2	1:A:443:ASN:HD22	2.08	0.50
1:A:752:GLU:HG2	1:A:757:HIS:CD2	2.46	0.50
1:D:665:THR:HG22	1:D:667:ASP:N	2.11	0.50
1:B:888:ASP:HB2	4:B:1077:HOH:O	2.10	0.50
1:D:125:HIS:HD2	1:D:160:GLN:OE1	1.95	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:966:ASP:HB3	1:D:981:ARG:NH1	2.26	0.50
1:D:4:LEU:HD13	1:B:816:ILE:CG2	2.42	0.50
1:B:141:ASN:ND2	1:B:169:LEU:H	2.09	0.50
1:C:783:GLY:HA2	3:C:1029:GOL:H12	1.93	0.50
1:C:415:THR:O	1:C:415:THR:CG2	2.60	0.50
1:C:581:ILE:CG2	4:C:1421:HOH:O	2.58	0.50
1:B:804:TRP:CE3	1:B:878:PRO:HG3	2.47	0.50
1:D:130:GLU:HB2	1:D:196:ARG:HB3	1.93	0.50
1:C:532:TRP:O	1:C:536:HIS:HD2	1.95	0.49
1:D:85:ILE:HG23	1:D:613:GLU:HG2	1.93	0.49
1:D:804:TRP:CE3	1:D:878:PRO:HG3	2.47	0.49
1:B:125:HIS:HD2	1:B:160:GLN:OE1	1.96	0.49
1:A:937:ASP:HA	1:A:959:PRO:HB2	1.95	0.49
1:C:206:LYS:HB2	4:C:1276:HOH:O	2.12	0.49
1:C:341:THR:HG22	4:C:1135:HOH:O	2.13	0.49
1:D:532:TRP:O	1:D:536:HIS:HD2	1.95	0.49
1:B:532:TRP:O	1:B:536:HIS:HD2	1.96	0.49
1:C:153:ASN:CB	1:C:463:GLN:HG2	2.41	0.49
1:C:189:TRP:HB2	3:C:1026:GOL:H31	1.94	0.49
4:A:1130:HOH:O	1:D:594:VAL:HG21	2.12	0.49
1:C:752:GLU:HG2	1:C:757:HIS:CD2	2.48	0.49
1:B:341:THR:CG2	4:B:1045:HOH:O	2.57	0.49
1:A:220:ASP:OD2	1:A:222:GLN:HG2	2.12	0.49
1:C:429:GLU:HG2	4:C:1066:HOH:O	2.12	0.49
1:D:103:VAL:HG21	3:B:1027:GOL:H12	1.95	0.49
1:D:841:VAL:O	1:D:842:VAL:HB	2.13	0.49
1:C:266:ASN:HB3	1:C:269:THR:OG1	2.13	0.48
1:A:331:ARG:HG2	1:A:331:ARG:NH1	2.28	0.48
1:D:966:ASP:HB3	1:D:981:ARG:HH11	1.77	0.48
1:B:536:HIS:HE1	4:B:1048:HOH:O	1.96	0.48
1:D:816:ILE:CG2	1:B:4:LEU:HD13	2.44	0.48
1:C:149:LYS:NZ	1:C:179:ASP:OD1	2.43	0.48
1:A:532:TRP:O	1:A:536:HIS:HD2	1.96	0.48
1:D:965:SER:OG	1:D:966:ASP:N	2.45	0.48
1:B:282:LYS:HD2	4:B:1533:HOH:O	2.13	0.48
1:A:257:ASP:OD2	1:B:68:SER:HB2	2.13	0.48
1:D:665:THR:HG22	1:D:666:THR:N	2.28	0.48
1:D:678:LYS:HB2	4:D:1091:HOH:O	2.13	0.48
1:A:90:GLN:HB2	1:C:842:VAL:HG22	1.95	0.48
1:D:341:THR:CG2	4:D:1198:HOH:O	2.60	0.48
1:D:752:GLU:HG2	1:D:757:HIS:CD2	2.49	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:425:HIS:HD2	1:C:807:TYR:OH	1.97	0.48
1:D:419:GLN:NE2	1:D:443:ASN:HD22	2.11	0.48
1:B:153:ASN:CB	1:B:463:GLN:HG2	2.43	0.48
1:B:752:GLU:HG2	1:B:757:HIS:CD2	2.47	0.48
1:A:125:HIS:HD2	1:A:160:GLN:OE1	1.97	0.48
1:C:595:SER:HB2	1:C:602:HIS:HD2	1.79	0.47
1:B:130:GLU:HB2	1:B:196:ARG:HB3	1.95	0.47
1:A:341:THR:HG22	4:A:1029:HOH:O	2.14	0.47
1:C:224:GLN:O	1:C:296:PRO:HD2	2.15	0.47
1:D:536:HIS:HE1	4:D:1054:HOH:O	1.97	0.47
1:B:220:ASP:OD2	1:B:222:GLN:HG2	2.13	0.47
1:C:804:TRP:CE3	1:C:878:PRO:HG3	2.49	0.47
1:D:353:ASN:OD1	1:D:386:ARG:HD3	2.14	0.47
1:A:415:THR:O	1:A:415:THR:CG2	2.62	0.47
1:A:415:THR:HG21	4:A:1216:HOH:O	2.14	0.47
1:A:804:TRP:CE3	1:A:878:PRO:HG3	2.50	0.47
1:A:807:TYR:OH	1:C:425:HIS:CD2	2.67	0.47
1:D:388:SER:HA	1:D:389:HIS:HA	1.74	0.47
1:B:517:ASP:O	1:B:518:ILE:HD13	2.14	0.47
1:C:766:LYS:HE2	4:C:1204:HOH:O	2.14	0.47
1:A:153:ASN:CB	1:A:463:GLN:HG2	2.43	0.47
1:A:419:GLN:HE22	1:A:443:ASN:HD22	1.63	0.46
1:A:353:ASN:OD1	1:A:386:ARG:HD3	2.15	0.46
1:B:937:ASP:HA	1:B:959:PRO:HB2	1.96	0.46
1:D:414:GLU:OE2	4:D:1686:HOH:O	2.21	0.46
1:D:224:GLN:O	1:D:296:PRO:HD2	2.15	0.46
1:D:326:HIS:CG	1:D:327:HIS:H	2.34	0.46
1:B:353:ASN:OD1	1:B:386:ARG:HD3	2.15	0.46
1:B:587:HIS:HB2	1:B:621:ILE:HD12	1.97	0.46
1:B:352:VAL:HG12	1:B:581:ILE:HG13	1.97	0.46
1:A:388:SER:HA	1:A:389:HIS:HA	1.75	0.46
1:A:841:VAL:O	1:A:842:VAL:HB	2.15	0.46
1:C:85:ILE:HG23	1:C:613:GLU:HG2	1.97	0.46
1:D:231:LYS:HE2	4:D:1068:HOH:O	2.15	0.46
1:D:19:ARG:HH11	1:D:148:ASN:HD22	1.62	0.46
1:A:639:TYR:O	1:A:643:ILE:HG12	2.15	0.46
1:C:19:ARG:HH11	1:C:148:ASN:HD22	1.62	0.46
1:C:326:HIS:CG	1:C:327:HIS:H	2.34	0.46
1:C:937:ASP:HA	1:C:959:PRO:HB2	1.98	0.46
1:D:937:ASP:HA	1:D:959:PRO:HB2	1.98	0.46
1:B:415:THR:O	1:B:415:THR:CG2	2.63	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:85:ILE:HG23	1:A:613:GLU:HG2	1.97	0.45
1:A:517:ASP:O	1:A:518:ILE:HD13	2.16	0.45
1:B:19:ARG:HH11	1:B:148:ASN:HD21	1.60	0.45
1:C:17:GLU:HG3	4:C:1246:HOH:O	2.16	0.45
1:C:965:SER:OG	1:C:966:ASP:N	2.47	0.45
1:C:220:ASP:OD2	1:C:222:GLN:HG2	2.16	0.45
1:D:331:ARG:HG2	1:D:331:ARG:NH1	2.30	0.45
1:D:340:ILE:H	1:D:577:GLN:NE2	1.95	0.45
1:D:425:HIS:CD2	1:B:807:TYR:OH	2.70	0.45
1:D:595:SER:HB2	1:D:602:HIS:HD2	1.81	0.45
1:A:4:LEU:HD13	1:C:816:ILE:HG22	1.98	0.45
1:C:388:SER:HA	1:C:389:HIS:HA	1.75	0.45
1:C:841:VAL:O	1:C:842:VAL:HB	2.16	0.45
1:D:355:HIS:HE1	4:D:1689:HOH:O	1.99	0.45
1:C:125:HIS:HD2	1:C:160:GLN:OE1	1.99	0.45
1:C:189:TRP:HB2	3:C:1026:GOL:C3	2.47	0.45
1:D:149:LYS:NZ	1:D:179:ASP:OD1	2.48	0.45
1:D:233:ASP:HB2	4:D:1068:HOH:O	2.17	0.45
1:A:629:GLU:HG3	4:A:1037:HOH:O	2.17	0.45
1:C:934:ASN:ND2	4:C:1047:HOH:O	2.49	0.45
1:D:340:ILE:HG12	1:D:518:ILE:HD11	1.98	0.45
1:D:149:LYS:HD3	1:D:180:SER:HB2	1.99	0.45
1:D:350:ARG:HD3	1:D:643:ILE:O	2.17	0.45
1:C:331:ARG:HG2	1:C:331:ARG:NH1	2.32	0.45
1:C:340:ILE:HG12	1:C:518:ILE:HD11	1.99	0.45
1:D:205:LYS:HB3	4:D:1184:HOH:O	2.17	0.45
1:B:533:ARG:NH2	4:B:1263:HOH:O	2.50	0.45
1:C:463:GLN:NE2	4:C:1090:HOH:O	2.50	0.44
1:A:340:ILE:HG12	1:A:518:ILE:HD11	1.99	0.44
1:B:153:ASN:CG	1:B:463:GLN:HG2	2.43	0.44
1:C:647:HIS:HE1	4:C:1289:HOH:O	2.01	0.44
1:D:16:HIS:CD2	1:D:19:ARG:H	2.36	0.44
1:C:97:ILE:HA	1:C:98:PRO:HA	1.85	0.44
1:D:266:ASN:HB3	1:D:269:THR:OG1	2.18	0.44
1:D:556:MET:CE	1:D:619:VAL:HG13	2.47	0.44
1:B:118:LYS:HE2	4:B:1602:HOH:O	2.16	0.44
1:B:410:GLU:HG3	1:B:478:SER:HB3	1.99	0.44
1:C:153:ASN:CG	1:C:463:GLN:HG2	2.42	0.44
1:D:153:ASN:CG	1:D:463:GLN:HG2	2.43	0.44
1:A:127:LEU:HG	1:A:159:ILE:HG13	1.99	0.44
1:C:353:ASN:OD1	1:C:386:ARG:HD3	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:300:THR:HG22	1:B:303:ASN:N	2.29	0.44
1:B:85:ILE:HG23	1:B:613:GLU:HG2	1.99	0.43
1:B:475:ILE:HG13	1:B:476:ILE:HG13	1.99	0.43
1:A:149:LYS:HD3	1:A:180:SER:HB2	1.99	0.43
1:A:350:ARG:HD3	1:A:643:ILE:O	2.18	0.43
1:D:116:ASP:HB2	4:D:1330:HOH:O	2.18	0.43
1:B:266:ASN:HB3	1:B:269:THR:OG1	2.18	0.43
1:A:159:ILE:HD13	1:A:159:ILE:HA	1.86	0.43
1:C:581:ILE:HD12	1:C:582:TRP:C	2.43	0.43
1:A:581:ILE:HD11	1:A:625:LEU:CG	2.43	0.43
1:A:757:HIS:HB3	4:A:1370:HOH:O	2.17	0.43
1:C:355:HIS:HE1	4:C:1680:HOH:O	2.01	0.43
1:C:415:THR:HB	1:C:483:ALA:CA	2.48	0.43
1:C:415:THR:O	1:C:415:THR:HG23	2.19	0.43
1:B:266:ASN:CG	4:B:1056:HOH:O	2.61	0.43
1:B:595:SER:HB2	1:B:602:HIS:HD2	1.83	0.43
1:D:415:THR:O	1:D:415:THR:CG2	2.66	0.43
1:B:486:GLY:H	1:B:489:HIS:HD2	1.66	0.43
1:A:595:SER:HB2	1:A:602:HIS:HD2	1.84	0.43
1:C:419:GLN:NE2	1:C:443:ASN:HD22	2.17	0.43
1:B:340:ILE:HG12	1:B:518:ILE:HD11	2.01	0.43
1:B:388:SER:HA	1:B:389:HIS:HA	1.77	0.43
1:C:410:GLU:HG3	1:C:478:SER:HB3	2.01	0.43
1:C:470:ASN:HB2	4:C:1076:HOH:O	2.19	0.43
1:D:127:LEU:HG	1:D:159:ILE:HG13	2.00	0.43
1:A:326:HIS:CG	1:A:327:HIS:H	2.36	0.43
1:C:762:LYS:HG2	1:C:819:VAL:HG11	2.00	0.43
1:D:300:THR:HG22	1:D:303:ASN:N	2.30	0.43
1:D:425:HIS:HD2	1:B:807:TYR:OH	2.00	0.43
1:D:581:ILE:HD12	1:D:582:TRP:C	2.43	0.43
1:A:340:ILE:H	1:A:577:GLN:NE2	1.94	0.42
1:D:587:HIS:HB2	1:D:621:ILE:HD12	2.01	0.42
1:B:924:PHE:HA	4:B:1167:HOH:O	2.18	0.42
1:C:542:LYS:HD2	4:C:1576:HOH:O	2.19	0.42
1:C:825:SER:O	1:C:827:GLY:N	2.52	0.42
1:D:486:GLY:H	1:D:489:HIS:HD2	1.67	0.42
1:A:153:ASN:CG	1:A:463:GLN:HG2	2.45	0.42
1:A:224:GLN:O	1:A:296:PRO:HD2	2.19	0.42
1:B:471:HIS:HA	1:B:472:PRO:HD2	1.91	0.42
1:A:471:HIS:HA	1:A:472:PRO:HD2	1.92	0.42
1:C:352:VAL:HG12	1:C:581:ILE:HG13	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:383:ASN:OD1	1:C:383:ASN:C	2.62	0.42
1:B:326:HIS:CG	1:B:327:HIS:H	2.37	0.42
1:A:4:LEU:HD13	1:C:816:ILE:CG2	2.50	0.42
1:A:762:LYS:HG2	1:A:819:VAL:HG11	2.00	0.42
1:C:300:THR:HB	4:C:1223:HOH:O	2.18	0.42
1:B:331:ARG:HG2	1:B:331:ARG:NH1	2.34	0.42
1:B:419:GLN:NE2	1:B:443:ASN:HD22	2.18	0.42
1:C:789:TRP:CE3	1:C:810:ASP:HB3	2.54	0.42
1:D:524:PRO:HG3	1:D:549:LEU:HD22	2.01	0.42
1:B:841:VAL:O	1:B:842:VAL:HB	2.19	0.42
1:A:587:HIS:HB2	1:A:621:ILE:HD12	2.02	0.42
1:A:825:SER:O	1:A:827:GLY:N	2.53	0.42
1:C:149:LYS:HD3	1:C:180:SER:HB2	2.01	0.42
1:C:595:SER:HB2	1:C:602:HIS:CD2	2.54	0.42
1:C:703:VAL:HG13	1:C:714:GLY:HA2	2.02	0.42
1:D:419:GLN:HE22	1:D:443:ASN:HD22	1.66	0.42
1:B:16:HIS:CD2	1:B:19:ARG:H	2.38	0.42
1:B:788:PHE:CE2	1:B:812:MET:HG2	2.55	0.42
1:B:965:SER:OG	1:B:966:ASP:N	2.43	0.42
1:B:14:LYS:NZ	1:B:17:GLU:OE1	2.53	0.42
1:B:224:GLN:O	1:B:296:PRO:HD2	2.19	0.42
1:B:789:TRP:CE3	1:B:810:ASP:HB3	2.55	0.42
1:B:879:ARG:NH1	1:B:990:ASP:CG	2.78	0.42
1:C:973:ALA:HB1	1:C:978:ASP:HB2	2.02	0.42
1:A:128:ARG:HB2	1:A:156:GLU:HG2	2.02	0.41
1:A:582:TRP:HA	1:A:583:GLU:HA	1.85	0.41
1:C:783:GLY:O	3:C:1029:GOL:H11	2.20	0.41
1:D:595:SER:HB2	1:D:602:HIS:CD2	2.55	0.41
1:B:137:GLU:HG3	1:B:139:TYR:HE1	1.84	0.41
1:C:333:VAL:HA	1:C:341:THR:O	2.20	0.41
1:C:445:HIS:HA	1:C:449:ASP:HB3	2.01	0.41
1:D:254:LYS:HA	4:D:1312:HOH:O	2.19	0.41
1:D:383:ASN:OD1	1:D:383:ASN:C	2.62	0.41
1:B:595:SER:HB2	1:B:602:HIS:CD2	2.56	0.41
1:D:220:ASP:OD2	1:D:222:GLN:HG2	2.21	0.41
1:A:266:ASN:HB3	1:A:269:THR:OG1	2.20	0.41
1:C:486:GLY:H	1:C:489:HIS:HD2	1.69	0.41
1:D:331:ARG:HE	1:D:472:PRO:HA	1.86	0.41
1:D:534:LYS:HE2	4:D:1490:HOH:O	2.21	0.41
1:C:154:GLY:O	1:C:463:GLN:NE2	2.53	0.41
1:C:524:PRO:HG3	1:C:549:LEU:HD22	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:582:TRP:HA	1:C:583:GLU:HA	1.89	0.41
1:D:54:LYS:HD3	4:D:1064:HOH:O	2.16	0.41
1:A:415:THR:HB	1:A:483:ALA:CA	2.50	0.41
1:C:127:LEU:HG	1:C:159:ILE:HG13	2.02	0.41
1:D:97:ILE:HA	1:D:98:PRO:HA	1.86	0.41
1:B:154:GLY:O	1:B:463:GLN:NE2	2.54	0.41
1:A:524:PRO:HG3	1:A:549:LEU:HD22	2.03	0.41
1:B:518:ILE:HG22	1:B:519:PHE:O	2.21	0.41
1:D:415:THR:HB	1:D:483:ALA:CA	2.47	0.41
1:D:788:PHE:CE2	1:D:812:MET:HG2	2.56	0.41
1:D:370:VAL:O	1:D:373:ASP:HB2	2.21	0.41
1:B:804:TRP:CD2	1:B:878:PRO:HG3	2.56	0.41
1:A:149:LYS:NZ	1:A:179:ASP:OD2	2.52	0.40
1:A:525:THR:HG23	1:A:527:GLU:OE1	2.21	0.40
1:D:517:ASP:O	1:D:518:ILE:HD13	2.21	0.40
1:B:149:LYS:HD3	1:B:180:SER:HB2	2.03	0.40
1:A:595:SER:HB2	1:A:602:HIS:CD2	2.56	0.40
1:C:587:HIS:HB2	1:C:621:ILE:HD12	2.03	0.40
1:D:133:ASP:HA	1:D:134:ASN:HA	1.92	0.40
1:D:294:LYS:HB2	4:D:1515:HOH:O	2.22	0.40
1:D:727:LYS:HB2	4:D:1246:HOH:O	2.20	0.40
1:B:331:ARG:NH1	1:B:333:VAL:HG12	2.36	0.40
1:B:370:VAL:O	1:B:373:ASP:HB2	2.21	0.40
1:A:19:ARG:HH11	1:A:148:ASN:HD21	1.64	0.40
1:A:112:THR:HA	1:A:168:ASN:O	2.20	0.40
1:B:350:ARG:HD3	1:B:643:ILE:O	2.21	0.40
1:B:445:HIS:HA	1:B:449:ASP:HB3	2.03	0.40
1:B:629:GLU:HG3	4:B:1067:HOH:O	2.20	0.40
1:A:86:TYR:CD2	1:A:621:ILE:HG12	2.57	0.40
1:C:295:ALA:HB2	4:C:1288:HOH:O	2.21	0.40
1:C:518:ILE:HG22	1:C:519:PHE:O	2.21	0.40
1:D:935:HIS:HE1	4:D:1203:HOH:O	2.03	0.40
1:A:498:GLN:HB3	4:A:1094:HOH:O	2.21	0.40
1:C:115:LEU:HD23	1:C:115:LEU:HA	1.98	0.40
1:D:128:ARG:HB2	1:D:156:GLU:HG2	2.04	0.40
1:D:804:TRP:CD2	1:D:878:PRO:HG3	2.56	0.40
1:B:432:TYR:HA	1:B:433:PRO:HD3	1.98	0.40
1:B:879:ARG:HH11	1:B:990:ASP:CG	2.29	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	1022/1032 (99%)	978 (96%)	42 (4%)	2 (0%)	43	64
1	B	1022/1032 (99%)	976 (96%)	44 (4%)	2 (0%)	43	64
1	C	1022/1032 (99%)	973 (95%)	47 (5%)	2 (0%)	43	64
1	D	1022/1032 (99%)	974 (95%)	46 (4%)	2 (0%)	43	64
All	All	4088/4128 (99%)	3901 (95%)	179 (4%)	8 (0%)	43	64

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	826	ASN
1	A	842	VAL
1	C	826	ASN
1	C	842	VAL
1	D	826	ASN
1	D	842	VAL
1	B	826	ASN
1	B	842	VAL

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	905/913 (99%)	873 (96%)	32 (4%)	32	56
1	B	905/913 (99%)	872 (96%)	33 (4%)	31	55

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	905/913 (99%)	872 (96%)	33 (4%)	31	55
1	D	905/913 (99%)	872 (96%)	33 (4%)	31	55
All	All	3620/3652 (99%)	3489 (96%)	131 (4%)	31	55

All (131) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	SER
1	A	4	LEU
1	A	15	VAL
1	A	48	LEU
1	A	124	GLU
1	A	235	GLN
1	A	281	THR
1	A	300	THR
1	A	331	ARG
1	A	333	VAL
1	A	341	THR
1	A	355	HIS
1	A	385	VAL
1	A	415	THR
1	A	437	ASN
1	A	469	VAL
1	A	499	LEU
1	A	525	THR
1	A	581	ILE
1	A	596	THR
1	A	621	ILE
1	A	642	VAL
1	A	665	THR
1	A	691	VAL
1	A	698	THR
1	A	703	VAL
1	A	779	SER
1	A	869	THR
1	A	876	ASP
1	A	957	GLU
1	A	996	VAL
1	A	1007	ASP
1	C	2	SER
1	C	4	LEU

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Mol	Chain	Res	Type
1	C	15	VAL
1	C	48	LEU
1	C	124	GLU
1	C	159	ILE
1	C	235	GLN
1	C	281	THR
1	C	300	THR
1	C	331	ARG
1	C	333	VAL
1	C	341	THR
1	C	355	HIS
1	C	385	VAL
1	C	415	THR
1	C	437	ASN
1	C	469	VAL
1	C	499	LEU
1	C	525	THR
1	C	581	ILE
1	C	596	THR
1	C	621	ILE
1	C	642	VAL
1	C	665	THR
1	C	691	VAL
1	C	698	THR
1	C	703	VAL
1	C	779	SER
1	C	869	THR
1	C	876	ASP
1	C	957	GLU
1	C	996	VAL
1	C	1007	ASP
1	D	2	SER
1	D	4	LEU
1	D	15	VAL
1	D	48	LEU
1	D	124	GLU
1	D	159	ILE
1	D	235	GLN
1	D	281	THR
1	D	300	THR
1	D	331	ARG
1	D	333	VAL

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Mol	Chain	Res	Type
1	D	341	THR
1	D	355	HIS
1	D	385	VAL
1	D	415	THR
1	D	437	ASN
1	D	469	VAL
1	D	499	LEU
1	D	525	THR
1	D	581	ILE
1	D	596	THR
1	D	621	ILE
1	D	642	VAL
1	D	665	THR
1	D	691	VAL
1	D	698	THR
1	D	703	VAL
1	D	779	SER
1	D	869	THR
1	D	876	ASP
1	D	957	GLU
1	D	996	VAL
1	D	1007	ASP
1	B	2	SER
1	B	4	LEU
1	B	15	VAL
1	B	48	LEU
1	B	124	GLU
1	B	159	ILE
1	B	235	GLN
1	B	281	THR
1	B	300	THR
1	B	331	ARG
1	B	333	VAL
1	B	341	THR
1	B	355	HIS
1	B	385	VAL
1	B	415	THR
1	B	437	ASN
1	B	469	VAL
1	B	499	LEU
1	B	525	THR
1	B	581	ILE

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Mol	Chain	Res	Type
1	B	596	THR
1	B	621	ILE
1	B	642	VAL
1	B	665	THR
1	B	691	VAL
1	B	698	THR
1	B	703	VAL
1	B	779	SER
1	B	869	THR
1	B	876	ASP
1	B	957	GLU
1	B	996	VAL
1	B	1007	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (111) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	16	HIS
1	A	18	ASN
1	A	29	GLN
1	A	125	HIS
1	A	134	ASN
1	A	141	ASN
1	A	148	ASN
1	A	188	GLN
1	A	208	HIS
1	A	235	GLN
1	A	284	ASN
1	A	339	ASN
1	A	355	HIS
1	A	387	ASN
1	A	419	GLN
1	A	425	HIS
1	A	427	ASN
1	A	443	ASN
1	A	489	HIS
1	A	536	HIS
1	A	567	GLN
1	A	577	GLN
1	A	647	HIS
1	A	652	HIS
1	A	930	GLN

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Mol	Chain	Res	Type
1	A	932	ASN
1	A	934	ASN
1	A	935	HIS
1	C	16	HIS
1	C	18	ASN
1	C	29	GLN
1	C	125	HIS
1	C	141	ASN
1	C	148	ASN
1	C	188	GLN
1	C	208	HIS
1	C	235	GLN
1	C	284	ASN
1	C	339	ASN
1	C	355	HIS
1	C	419	GLN
1	C	425	HIS
1	C	427	ASN
1	C	463	GLN
1	C	489	HIS
1	C	512	ASN
1	C	536	HIS
1	C	577	GLN
1	C	647	HIS
1	C	757	HIS
1	C	861	ASN
1	C	930	GLN
1	C	932	ASN
1	C	934	ASN
1	C	1014	GLN
1	D	16	HIS
1	D	29	GLN
1	D	125	HIS
1	D	141	ASN
1	D	148	ASN
1	D	208	HIS
1	D	235	GLN
1	D	263	ASN
1	D	284	ASN
1	D	339	ASN
1	D	355	HIS
1	D	387	ASN

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Mol	Chain	Res	Type
1	D	419	GLN
1	D	425	HIS
1	D	443	ASN
1	D	489	HIS
1	D	536	HIS
1	D	567	GLN
1	D	577	GLN
1	D	647	HIS
1	D	715	HIS
1	D	757	HIS
1	D	861	ASN
1	D	930	GLN
1	D	934	ASN
1	D	935	HIS
1	D	955	GLN
1	D	1014	GLN
1	B	16	HIS
1	B	29	GLN
1	B	125	HIS
1	B	141	ASN
1	B	148	ASN
1	B	188	GLN
1	B	208	HIS
1	B	235	GLN
1	B	268	ASN
1	B	284	ASN
1	B	339	ASN
1	B	355	HIS
1	B	387	ASN
1	B	419	GLN
1	B	425	HIS
1	B	443	ASN
1	B	489	HIS
1	B	512	ASN
1	B	536	HIS
1	B	577	GLN
1	B	647	HIS
1	B	861	ASN
1	B	930	GLN
1	B	932	ASN
1	B	934	ASN
1	B	935	HIS

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Mol	Chain	Res	Type
1	B	955	GLN
1	B	1014	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 14 ligands modelled in this entry, 4 are monoatomic - leaving 10 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	GOL	C	1028	-	5,5,5	0.44	0	5,5,5	0.31	0
3	GOL	A	1026	-	5,5,5	0.48	0	5,5,5	0.11	0
3	GOL	D	1026	-	5,5,5	0.46	0	5,5,5	0.30	0
3	GOL	B	1026	-	5,5,5	0.42	0	5,5,5	0.51	0
3	GOL	A	1027	-	5,5,5	0.44	0	5,5,5	0.40	0
3	GOL	C	1026	-	5,5,5	0.37	0	5,5,5	0.60	0
3	GOL	B	1027	-	5,5,5	1.38	1 (20%)	5,5,5	0.94	0
3	GOL	D	1027	-	5,5,5	0.40	0	5,5,5	0.51	0
3	GOL	C	1029	-	5,5,5	0.42	0	5,5,5	0.42	0
3	GOL	C	1027	-	5,5,5	0.41	0	5,5,5	0.34	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	GOL	C	1028	-	-	4/4/4/4	-
3	GOL	A	1026	-	-	2/4/4/4	-
3	GOL	D	1026	-	-	2/4/4/4	-
3	GOL	B	1026	-	-	2/4/4/4	-
3	GOL	A	1027	-	-	2/4/4/4	-
3	GOL	C	1026	-	-	2/4/4/4	-
3	GOL	B	1027	-	-	3/4/4/4	-
3	GOL	D	1027	-	-	2/4/4/4	-
3	GOL	C	1029	-	-	2/4/4/4	-
3	GOL	C	1027	-	-	2/4/4/4	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1027	GOL	O2-C2	-2.46	1.36	1.43

There are no bond angle outliers.

There are no chirality outliers.

All (23) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1026	GOL	C1-C2-C3-O3
3	C	1026	GOL	C1-C2-C3-O3
3	C	1026	GOL	O2-C2-C3-O3
3	C	1027	GOL	C1-C2-C3-O3
3	C	1027	GOL	O2-C2-C3-O3
3	C	1028	GOL	O1-C1-C2-C3
3	C	1028	GOL	C1-C2-C3-O3
3	D	1027	GOL	C1-C2-C3-O3
3	B	1026	GOL	O1-C1-C2-O2
3	B	1026	GOL	O1-C1-C2-C3
3	B	1027	GOL	C1-C2-C3-O3
3	D	1027	GOL	O2-C2-C3-O3
3	A	1027	GOL	C1-C2-C3-O3
3	C	1029	GOL	O1-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
3	A	1026	GOL	O2-C2-C3-O3
3	C	1028	GOL	O1-C1-C2-O2
3	C	1028	GOL	O2-C2-C3-O3
3	B	1027	GOL	O2-C2-C3-O3
3	B	1027	GOL	O1-C1-C2-O2
3	C	1029	GOL	O1-C1-C2-O2
3	D	1026	GOL	C1-C2-C3-O3
3	A	1027	GOL	O2-C2-C3-O3
3	D	1026	GOL	O1-C1-C2-O2

There are no ring outliers.

4 monomers are involved in 15 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	1028	GOL	3	0
3	C	1026	GOL	6	0
3	B	1027	GOL	4	0
3	C	1029	GOL	2	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, 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	1024/1032 (99%)	-0.06	10 (0%)	79	79	8, 17, 37, 62	0
1	B	1024/1032 (99%)	0.05	28 (2%)	56	54	8, 17, 37, 62	0
1	C	1024/1032 (99%)	0.16	56 (5%)	30	30	8, 17, 37, 62	0
1	D	1024/1032 (99%)	0.12	48 (4%)	36	36	8, 17, 37, 62	0
All	All	4096/4128 (99%)	0.07	142 (3%)	47	44	8, 17, 37, 62	0

All (142) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	270	THR	8.9
1	D	266	ASN	8.8
1	D	267	GLY	8.4
1	D	273	THR	8.3
1	D	271	PHE	7.7
1	C	270	THR	7.6
1	D	272	SER	7.4
1	C	272	SER	7.3
1	C	273	THR	7.1
1	C	268	ASN	7.1
1	C	267	GLY	6.6
1	C	266	ASN	6.4
1	D	268	ASN	6.2
1	C	271	PHE	6.2
1	D	269	THR	5.8
1	C	269	THR	5.4
1	B	652	HIS	5.1
1	C	729	PRO	4.8
1	D	736	ALA	4.8
1	D	220	ASP	4.8
1	D	738	LYS	4.2

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Mol	Chain	Res	Type	RSRZ
1	D	739	ALA	4.2
1	B	266	ASN	4.2
1	C	739	ALA	4.1
1	D	737	GLU	4.0
1	B	739	ALA	3.9
1	C	737	GLU	3.9
1	D	265	GLU	3.8
1	A	266	ASN	3.8
1	C	265	GLU	3.8
1	C	825	SER	3.7
1	B	729	PRO	3.6
1	D	206	LYS	3.5
1	D	368	ASP	3.5
1	C	923	GLU	3.4
1	D	221	SER	3.4
1	C	738	LYS	3.3
1	C	206	LYS	3.3
1	C	274	LYS	3.3
1	C	922	GLU	3.3
1	B	728	VAL	3.3
1	C	728	VAL	3.2
1	D	116	ASP	3.2
1	B	539	GLU	3.2
1	B	121	GLU	3.2
1	C	121	GLU	3.2
1	D	740	ALA	3.1
1	B	736	ALA	3.1
1	A	540	ASN	3.1
1	D	274	LYS	3.1
1	D	729	PRO	3.0
1	A	739	ALA	3.0
1	C	696	ASP	2.9
1	C	654	SER	2.9
1	C	277	ILE	2.9
1	C	279	PHE	2.9
1	C	782	GLU	2.9
1	C	540	ASN	2.9
1	C	677	GLY	2.9
1	D	30	ASP	2.8
1	C	116	ASP	2.8
1	B	683	PRO	2.8
1	C	736	ALA	2.8

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Mol	Chain	Res	Type	RSRZ
1	C	264	GLU	2.8
1	C	730	ASP	2.8
1	C	698	THR	2.8
1	D	598	ASP	2.7
1	B	270	THR	2.7
1	C	679	THR	2.7
1	D	57	ASP	2.7
1	C	237	SER	2.7
1	C	276	PHE	2.7
1	D	922	GLU	2.7
1	B	654	SER	2.7
1	B	540	ASN	2.6
1	B	598	ASP	2.6
1	C	680	ILE	2.6
1	C	681	ASP	2.6
1	C	652	HIS	2.6
1	B	124	GLU	2.6
1	C	682	VAL	2.6
1	B	694	PRO	2.6
1	A	742	ILE	2.5
1	D	432	TYR	2.5
1	D	294	LYS	2.5
1	C	694	PRO	2.5
1	C	29	GLN	2.5
1	D	264	GLU	2.5
1	D	237	SER	2.4
1	C	289	PHE	2.4
1	D	279	PHE	2.4
1	C	697	THR	2.4
1	B	3	CYS	2.4
1	C	248	GLU	2.4
1	C	734	GLU	2.4
1	C	263	ASN	2.4
1	D	282	LYS	2.4
1	A	732	VAL	2.4
1	C	247	TYR	2.3
1	B	698	THR	2.3
1	C	741	LYS	2.3
1	D	263	ASN	2.3
1	B	740	ALA	2.3
1	B	738	LYS	2.3
1	B	432	TYR	2.3

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Mol	Chain	Res	Type	RSRZ
1	C	592	GLU	2.3
1	D	286	GLU	2.3
1	B	368	ASP	2.3
1	D	54	LYS	2.2
1	D	735	THR	2.2
1	A	220	ASP	2.2
1	D	757	HIS	2.2
1	C	733	THR	2.2
1	B	735	THR	2.2
1	D	280	SER	2.2
1	D	825	SER	2.2
1	D	120	ILE	2.2
1	A	124	GLU	2.1
1	C	946	GLU	2.1
1	C	889	SER	2.1
1	D	278	SER	2.1
1	B	825	SER	2.1
1	A	539	GLU	2.1
1	A	598	ASP	2.1
1	D	544	GLU	2.1
1	D	734	GLU	2.1
1	C	727	LYS	2.1
1	C	432	TYR	2.1
1	B	159	ILE	2.1
1	A	116	ASP	2.1
1	B	116	ASP	2.1
1	B	2	SER	2.1
1	D	539	GLU	2.1
1	B	649	LYS	2.1
1	C	281	THR	2.1
1	D	540	ASN	2.1
1	D	782	GLU	2.0
1	D	923	GLU	2.0
1	B	59	GLU	2.0
1	C	690	SER	2.0
1	D	518	ILE	2.0
1	D	826	ASN	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](#)

There are no oligosaccharides in this entry.

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. 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	B-factors($\text{\AA}^2$)	Q<0.9
3	GOL	D	1026	6/6	0.75	0.25	49,50,51,51	0
3	GOL	C	1026	6/6	0.85	0.20	25,26,29,30	0
3	GOL	B	1027	6/6	0.89	0.11	12,15,16,18	0
3	GOL	A	1026	6/6	0.90	0.13	29,29,30,30	0
3	GOL	C	1028	6/6	0.92	0.13	17,19,19,19	0
3	GOL	B	1026	6/6	0.94	0.08	22,23,23,24	0
3	GOL	C	1029	6/6	0.94	0.08	10,10,11,11	0
3	GOL	C	1027	6/6	0.95	0.08	16,16,16,18	0
3	GOL	A	1027	6/6	0.96	0.08	21,22,22,23	0
3	GOL	D	1027	6/6	0.97	0.05	10,11,12,14	0
2	MN3	C	2001	1/1	0.99	0.03	8,8,8,8	0
2	MN3	D	2001	1/1	0.99	0.04	11,11,11,11	0
2	MN3	A	2001	1/1	1.00	0.03	8,8,8,8	0
2	MN3	B	2001	1/1	1.00	0.03	8,8,8,8	0

6.5 Other polymers [i](#)

There are no such residues in this entry.