



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 04:18 PM UTC

PDB ID : 3OB8 / pdb_00003ob8
Title : Structure of the beta-galactosidase from Kluyveromyces lactis in complex with galactose
Authors : Fernandez-Leiro, R.; Pereira-Rodriguez, A.; Becerra, M.; Gonzalez-Siso, I.; Cerdan, M.E.; Sanz-Aparicio, J.
Deposited on : 2010-08-06
Resolution : 2.80 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

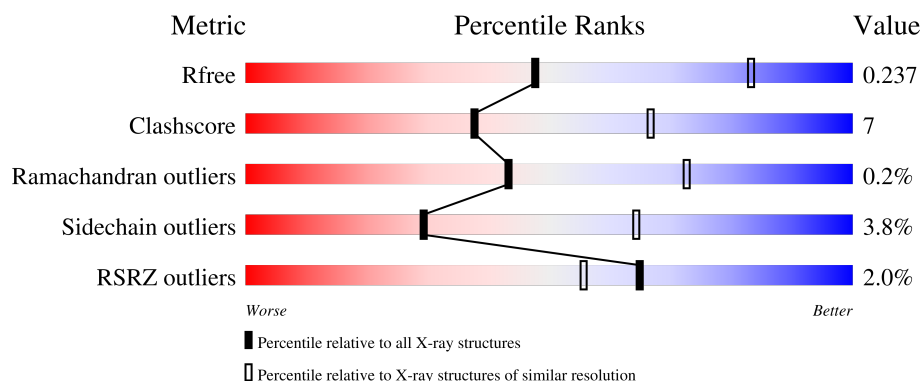
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

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	2% 84% 14% ..
1	C	1032	3% 84% 14% ..
1	D	1032	2% 84% 14% ..

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 34419 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	B	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	C	1024	Total	C	N	O	S	0	0	0
			8325	5335	1388	1587	15			

There are 32 discrepancies between the modelled and reference sequences:

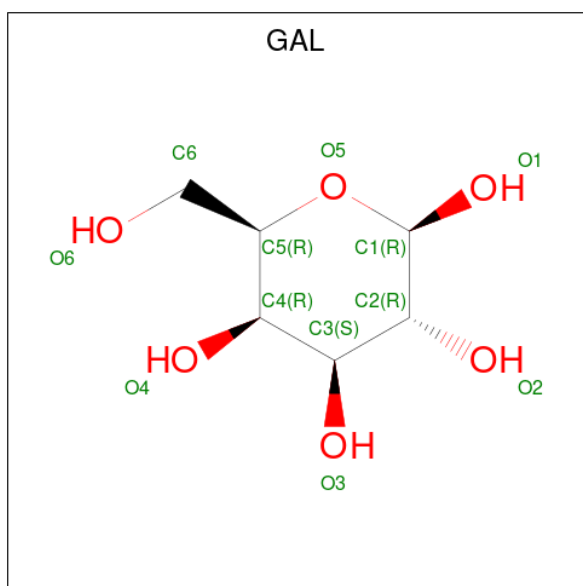
Chain	Residue	Modelled	Actual	Comment	Reference
A	-6	ASP	-	expression tag	UNP P00723
A	-5	TYR	-	expression tag	UNP P00723
A	-4	LYS	-	expression tag	UNP P00723
A	-3	ASP	-	expression tag	UNP P00723
A	-2	ASP	-	expression tag	UNP P00723
A	-1	ASP	-	expression tag	UNP P00723
A	0	ASP	-	expression tag	UNP P00723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

- Molecule 2 is beta-D-galactopyranose (CCD ID: GAL) (formula: C₆H₁₂O₆).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			12	6	6		
2	B	1	Total	C	O	0	0
			12	6	6		
2	D	1	Total	C	O	0	0
			12	6	6		
2	C	1	Total	C	O	0	0
			12	6	6		

- Molecule 3 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

- Molecule 4 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	4	Total Na 4 4	0	0
4	B	4	Total Na 4 4	0	0
4	D	4	Total Na 4 4	0	0
4	C	4	Total Na 4 4	0	0

- Molecule 5 is MANGANESE (II) ION (CCD ID: MN) (formula: Mn).

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

- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	231	Total O 231 231	0	0
6	B	293	Total O 293 293	0	0
6	D	253	Total O 253 253	0	0

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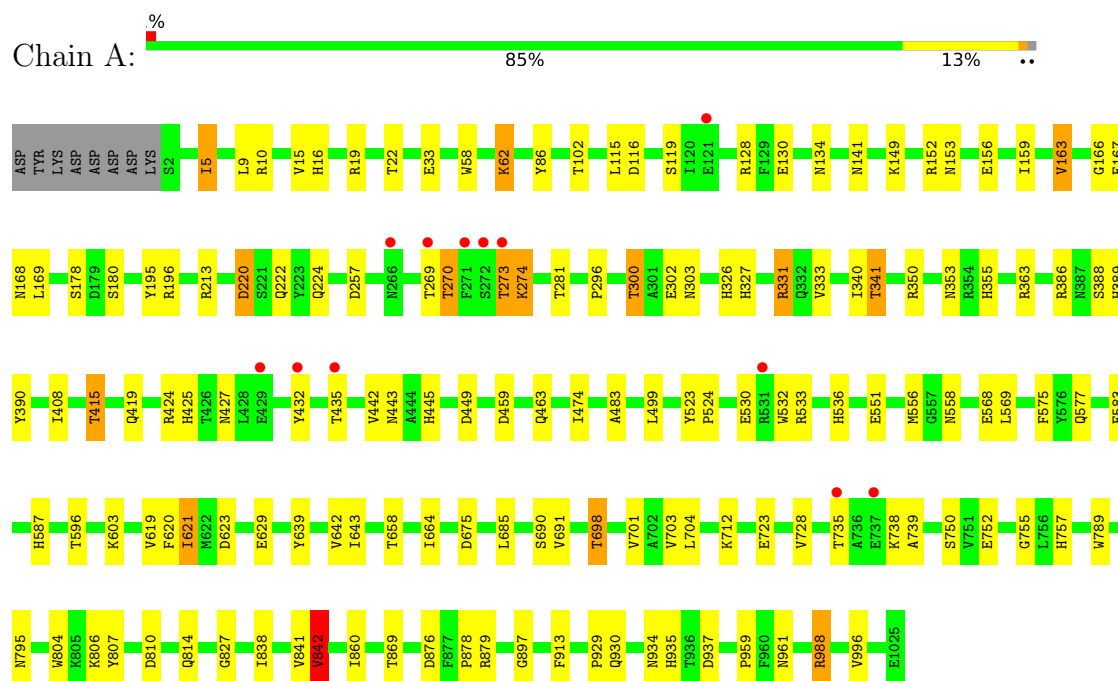
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	C	270	Total	O	0	0
			270	270		

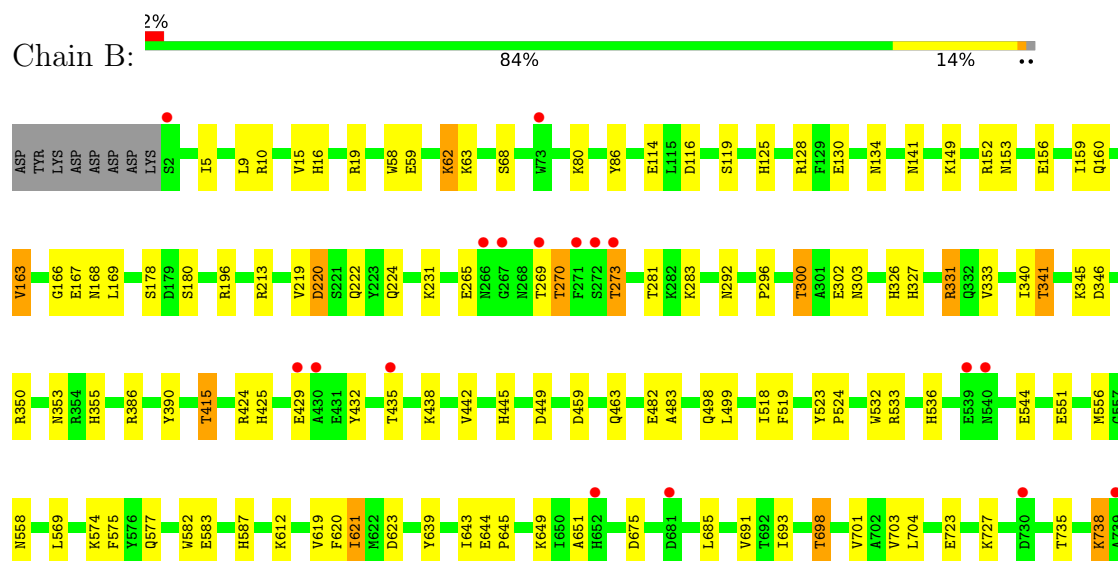
3 Residue-property plots [i](#)

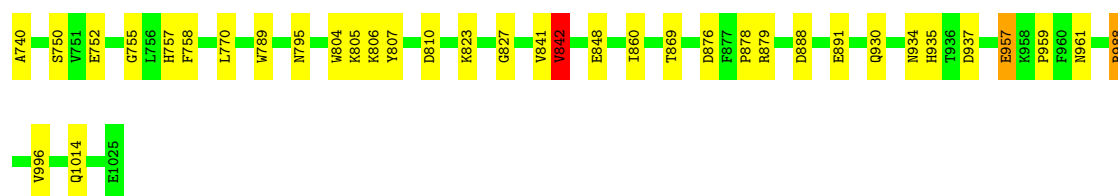
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Beta-galactosidase

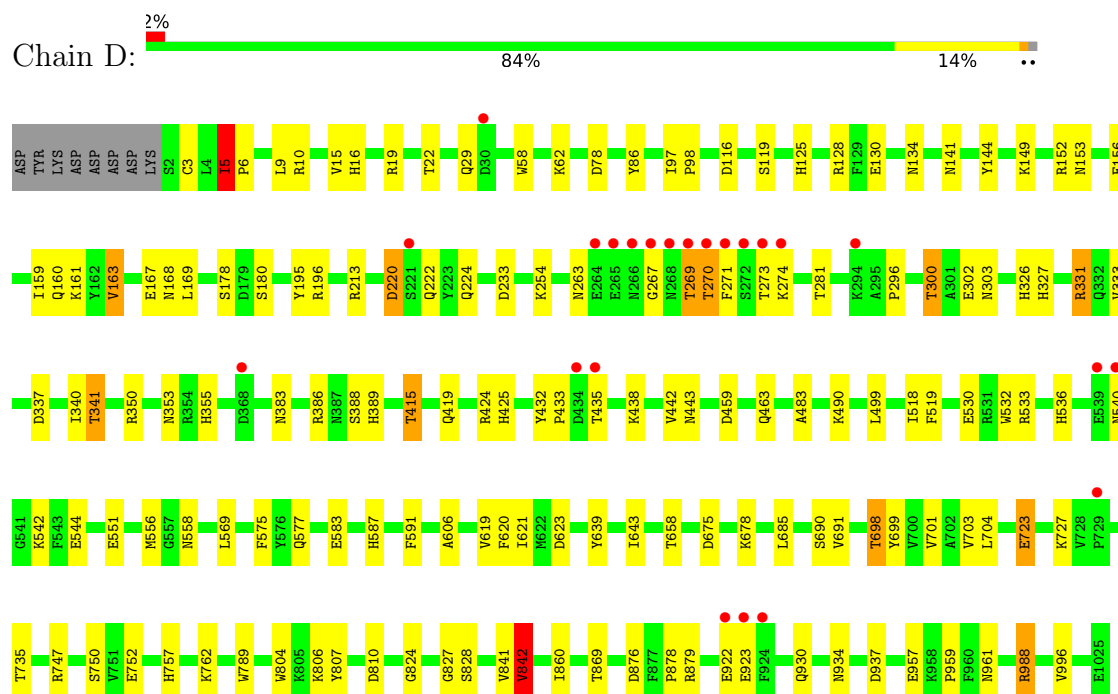


• Molecule 1: Beta-galactosidase

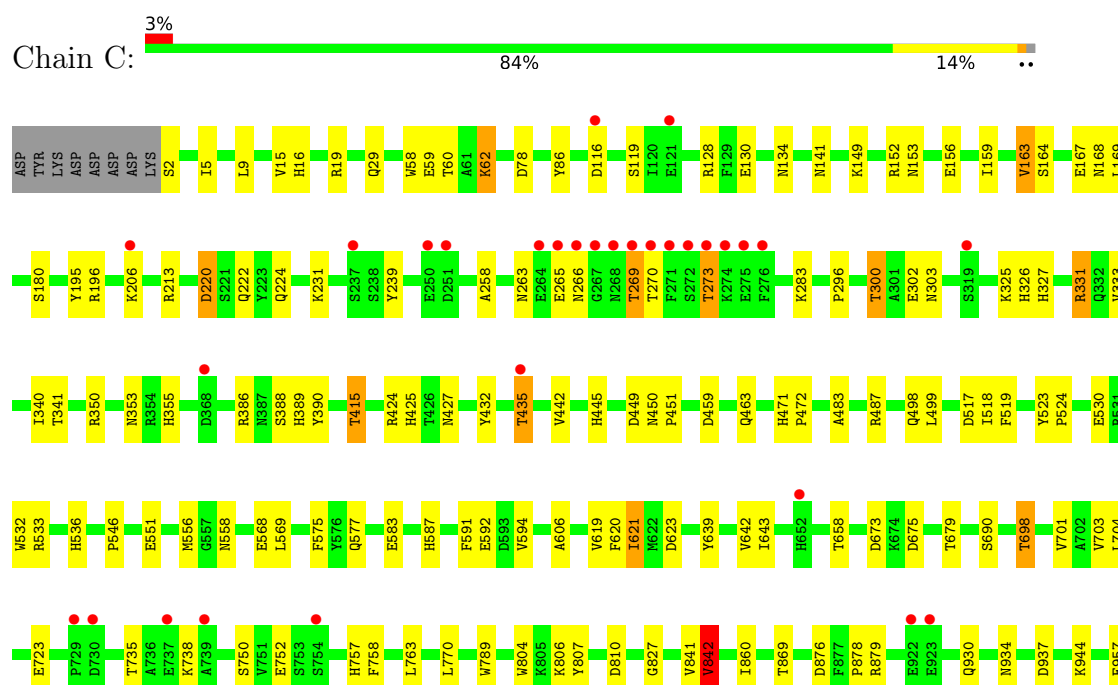




• Molecule 1: Beta-galactosidase



• Molecule 1: Beta-galactosidase



Y958	P959	P960	N961	R988	Y996	N1017	E1025
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4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	140.38Å 153.45Å 217.17Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.30 – 2.80 49.30 – 2.80	Depositor EDS
% Data completeness (in resolution range)	99.9 (49.30-2.80) 99.9 (49.30-2.80)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	0.10	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.35 (at 2.81Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.214 , 0.246 0.210 , 0.237	Depositor DCC
R_{free} test set	5800 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	38.7	Xtriage
Anisotropy	0.064	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 29.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	34419	wwPDB-VP
Average B, all atoms (Å ²)	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.14% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: MN, MG, NA, GAL

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	0/8561	0.80	0/11614
1	B	0.57	1/8561 (0.0%)	0.80	0/11614
1	C	0.56	0/8561	0.79	0/11614
1	D	0.56	0/8561	0.79	1/11614 (0.0%)
All	All	0.56	1/34244 (0.0%)	0.80	1/46456 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	345	LYS	C-O	-5.40	1.17	1.24

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	5	ILE	CB-CA-C	5.14	115.12	110.13

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	8325	0	7972	120	0
1	B	8325	0	7972	128	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	8325	0	7972	115	1
1	D	8325	0	7972	122	1
2	A	12	0	12	1	0
2	B	12	0	12	1	0
2	C	12	0	11	1	0
2	D	12	0	11	1	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	A	4	0	0	0	0
4	B	4	0	0	0	0
4	C	4	0	0	0	0
4	D	4	0	0	0	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
5	C	1	0	0	0	0
5	D	1	0	0	0	0
6	A	231	0	0	19	0
6	B	293	0	0	34	0
6	C	270	0	0	28	0
6	D	253	0	0	32	0
All	All	34419	0	31934	455	1

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 (455) 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:587:HIS:HB2	1:C:621:ILE:HG13	1.28	1.11
1:D:587:HIS:HB2	1:D:621:ILE:HG13	1.27	1.09
1:B:587:HIS:HB2	1:B:621:ILE:HG13	1.29	1.07
1:A:587:HIS:HB2	1:A:621:ILE:HG13	1.29	1.06
1:B:841:VAL:O	1:B:842:VAL:HG13	1.56	1.06
1:C:841:VAL:O	1:C:842:VAL:HG13	1.56	1.05
1:D:841:VAL:O	1:D:842:VAL:HG13	1.56	1.05
1:A:841:VAL:O	1:A:842:VAL:HG13	1.56	1.04
1:C:164:SER:HB2	6:C:1127:HOH:O	1.56	1.03
1:D:691:VAL:HB	6:D:1141:HOH:O	1.56	1.02
1:A:712:LYS:HD2	6:A:1074:HOH:O	1.61	1.00

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:340:ILE:H	1:A:577:GLN:HE22	1.13	0.96
1:D:340:ILE:H	1:D:577:GLN:HE22	1.07	0.93
1:D:540:ASN:HA	6:D:1079:HOH:O	1.68	0.92
1:C:340:ILE:H	1:C:577:GLN:HE22	1.07	0.92
1:D:438:LYS:HG3	6:D:1271:HOH:O	1.72	0.89
1:D:270:THR:HG21	6:D:1200:HOH:O	1.71	0.88
1:B:340:ILE:H	1:B:577:GLN:HE22	1.12	0.88
1:B:612:LYS:HE2	6:B:1204:HOH:O	1.73	0.86
1:D:29:GLN:HG3	6:D:1032:HOH:O	1.75	0.85
1:B:544:GLU:HG2	6:B:1130:HOH:O	1.75	0.85
1:D:841:VAL:C	1:D:842:VAL:CG1	2.51	0.84
1:A:841:VAL:C	1:A:842:VAL:CG1	2.51	0.83
1:C:841:VAL:C	1:C:842:VAL:CG1	2.51	0.83
1:A:596:THR:HG21	6:A:1086:HOH:O	1.78	0.83
6:A:1181:HOH:O	1:B:114:GLU:HG3	1.80	0.82
1:B:841:VAL:C	1:B:842:VAL:CG1	2.51	0.82
1:D:271:PHE:HB3	6:D:1185:HOH:O	1.80	0.81
1:B:283:LYS:HE2	6:B:1238:HOH:O	1.79	0.80
1:A:153:ASN:HB3	1:A:463:GLN:HG2	1.64	0.80
1:C:841:VAL:O	1:C:842:VAL:CG1	2.30	0.79
1:A:841:VAL:O	1:A:842:VAL:CG1	2.30	0.79
1:B:649:LYS:HE2	6:B:1162:HOH:O	1.81	0.79
1:D:490:LYS:HE3	6:D:1203:HOH:O	1.80	0.79
1:B:841:VAL:O	1:B:842:VAL:CG1	2.30	0.78
1:B:498:GLN:HG2	6:B:1099:HOH:O	1.82	0.78
1:B:740:ALA:HB3	6:B:1194:HOH:O	1.83	0.78
1:C:592:GLU:HG2	6:C:1199:HOH:O	1.82	0.77
1:D:841:VAL:O	1:D:842:VAL:CG1	2.30	0.77
1:B:153:ASN:HB3	1:B:463:GLN:HG2	1.68	0.76
1:D:153:ASN:HB3	1:D:463:GLN:HG2	1.66	0.76
1:B:957:GLU:HB3	6:B:1132:HOH:O	1.86	0.76
1:C:153:ASN:HB3	1:C:463:GLN:HG2	1.67	0.76
1:D:340:ILE:N	1:D:577:GLN:HE22	1.84	0.74
1:B:752:GLU:HG2	1:B:757:HIS:CD2	2.23	0.74
1:B:340:ILE:N	1:B:577:GLN:HE22	1.86	0.74
1:A:752:GLU:HG2	1:A:757:HIS:CD2	2.24	0.73
1:B:80:LYS:HE3	6:B:1272:HOH:O	1.89	0.73
1:B:848:GLU:HG3	6:B:1128:HOH:O	1.88	0.72
1:B:341:THR:HG22	6:B:1127:HOH:O	1.89	0.71
1:C:340:ILE:N	1:C:577:GLN:HE22	1.84	0.71
1:B:425:HIS:HE1	6:B:1093:HOH:O	1.73	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:346:ASP:OD1	1:B:346:ASP:O	2.09	0.70
1:B:934:ASN:HD21	1:B:961:ASN:HB3	1.56	0.70
1:A:340:ILE:N	1:A:577:GLN:HE22	1.87	0.70
1:D:536:HIS:HE1	6:D:1124:HOH:O	1.75	0.70
1:C:752:GLU:HG2	1:C:757:HIS:CD2	2.27	0.70
1:B:58:TRP:O	1:B:62:LYS:HB2	1.92	0.69
1:B:231:LYS:HE2	6:B:1116:HOH:O	1.90	0.69
1:C:265:GLU:HG2	6:C:1172:HOH:O	1.91	0.69
1:D:752:GLU:HG2	1:D:757:HIS:CD2	2.28	0.68
1:C:415:THR:HG21	6:C:1249:HOH:O	1.92	0.68
1:C:679:THR:HG21	6:C:1228:HOH:O	1.92	0.68
1:D:271:PHE:HZ	6:D:1226:HOH:O	1.77	0.68
1:B:842:VAL:CG2	1:B:842:VAL:O	2.42	0.68
1:A:934:ASN:HD21	1:A:961:ASN:HB3	1.58	0.67
1:D:841:VAL:C	1:D:842:VAL:HG12	2.19	0.67
1:B:551:GLU:OE1	2:B:2001:GAL:H1	1.94	0.67
1:C:58:TRP:O	1:C:62:LYS:HB2	1.94	0.67
1:C:934:ASN:HD21	1:C:961:ASN:HB3	1.58	0.67
1:A:842:VAL:O	1:A:842:VAL:CG2	2.42	0.67
1:D:934:ASN:HD21	1:D:961:ASN:HB3	1.60	0.67
1:D:841:VAL:C	1:D:842:VAL:HG13	2.18	0.67
1:B:438:LYS:HB2	6:B:1282:HOH:O	1.93	0.67
1:A:58:TRP:O	1:A:62:LYS:HB2	1.94	0.67
1:C:842:VAL:CG2	1:C:842:VAL:O	2.42	0.66
1:D:213:ARG:NH2	1:D:499:LEU:O	2.29	0.66
1:D:842:VAL:O	1:D:842:VAL:CG2	2.42	0.66
1:C:60:THR:HG23	6:C:1132:HOH:O	1.94	0.66
1:C:220:ASP:OD2	1:C:222:GLN:HG2	1.95	0.66
1:B:888:ASP:HB3	6:B:1273:HOH:O	1.96	0.66
1:A:116:ASP:H	1:B:270:THR:HG21	1.61	0.66
1:A:116:ASP:HB2	1:B:270:THR:HG21	1.77	0.66
1:A:841:VAL:C	1:A:842:VAL:HG12	2.19	0.66
1:A:755:GLY:HA2	1:D:78:ASP:OD1	1.96	0.66
1:C:841:VAL:C	1:C:842:VAL:HG12	2.19	0.65
1:B:841:VAL:C	1:B:842:VAL:HG12	2.19	0.65
1:A:116:ASP:HB2	1:B:270:THR:CG2	2.27	0.65
1:B:213:ARG:NH2	1:B:499:LEU:O	2.30	0.64
1:A:213:ARG:NH2	1:A:499:LEU:O	2.30	0.64
1:C:533:ARG:HG3	1:C:575:PHE:CD2	2.32	0.64
1:C:587:HIS:CB	1:C:621:ILE:HG13	2.18	0.64
1:A:568:GLU:HG3	6:A:1202:HOH:O	1.97	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:267:GLY:HA2	6:D:1208:HOH:O	1.97	0.64
1:C:675:ASP:OD2	1:C:698:THR:HB	1.98	0.64
1:C:213:ARG:NH2	1:C:499:LEU:O	2.31	0.63
1:D:58:TRP:O	1:D:62:LYS:HB2	1.98	0.63
1:C:558:ASN:H	1:C:930:GLN:NE2	1.97	0.63
1:B:842:VAL:O	1:B:842:VAL:HG23	1.99	0.63
1:D:116:ASP:HB2	6:D:1090:HOH:O	1.99	0.63
1:D:587:HIS:CB	1:D:621:ILE:HG13	2.17	0.63
1:C:1017:ASN:HB3	6:C:1138:HOH:O	1.98	0.62
1:B:587:HIS:CB	1:B:621:ILE:HG13	2.18	0.62
1:A:842:VAL:O	1:A:842:VAL:HG23	1.99	0.62
1:B:533:ARG:HG3	1:B:575:PHE:CD2	2.34	0.62
1:D:533:ARG:HG3	1:D:575:PHE:CD2	2.35	0.62
1:C:842:VAL:O	1:C:842:VAL:HG23	1.99	0.62
1:D:220:ASP:OD2	1:D:222:GLN:HG2	1.99	0.62
1:D:842:VAL:O	1:D:842:VAL:HG23	1.99	0.62
1:D:639:TYR:O	1:D:643:ILE:HG12	2.00	0.62
1:A:533:ARG:HG3	1:A:575:PHE:CD2	2.35	0.62
1:B:639:TYR:O	1:B:643:ILE:HG12	2.01	0.61
1:A:220:ASP:OD2	1:A:222:GLN:HG2	2.00	0.61
1:A:273:THR:HG21	1:B:166:GLY:HA2	1.82	0.61
1:B:220:ASP:OD2	1:B:222:GLN:HG2	2.00	0.61
1:D:341:THR:HG22	6:D:1137:HOH:O	2.00	0.61
1:A:664:ILE:HA	6:A:1219:HOH:O	1.99	0.61
1:C:29:GLN:HB2	6:C:1264:HOH:O	2.00	0.61
1:C:331:ARG:C	1:C:331:ARG:HD3	2.26	0.60
1:C:639:TYR:O	1:C:643:ILE:HG12	2.01	0.60
1:A:587:HIS:CB	1:A:621:ILE:HG13	2.19	0.60
1:C:283:LYS:HE2	6:C:1107:HOH:O	2.01	0.60
1:B:823:LYS:HE2	6:B:1172:HOH:O	2.01	0.60
1:C:415:THR:HB	1:C:483:ALA:HA	1.84	0.60
1:D:415:THR:HB	1:D:483:ALA:HA	1.84	0.59
1:B:424:ARG:O	1:D:806:LYS:HE2	2.02	0.59
1:C:340:ILE:H	1:C:577:GLN:NE2	1.90	0.59
1:A:300:THR:HG22	1:A:302:GLU:H	1.68	0.59
1:B:425:HIS:HD2	1:D:807:TYR:OH	1.86	0.59
1:D:331:ARG:HD3	1:D:331:ARG:C	2.27	0.58
1:B:59:GLU:CB	6:B:1182:HOH:O	2.50	0.58
1:B:675:ASP:OD2	1:B:698:THR:HB	2.03	0.58
1:D:340:ILE:H	1:D:577:GLN:NE2	1.90	0.58
1:D:556:MET:HA	1:D:623:ASP:HA	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:340:ILE:H	1:A:577:GLN:NE2	1.94	0.57
1:A:415:THR:HB	1:A:483:ALA:HA	1.85	0.57
1:A:424:ARG:O	1:C:806:LYS:HE2	2.05	0.57
1:A:675:ASP:OD2	1:A:698:THR:HB	2.04	0.57
1:D:153:ASN:CB	1:D:463:GLN:HG2	2.33	0.57
1:C:141:ASN:ND2	1:C:169:LEU:H	2.03	0.57
1:D:551:GLU:OE1	2:D:2001:GAL:H1	2.05	0.57
1:A:728:VAL:HG23	6:A:1079:HOH:O	2.04	0.56
1:C:239:TYR:HE2	6:C:1290:HOH:O	1.87	0.56
1:A:274:LYS:HD3	6:A:1245:HOH:O	2.04	0.56
1:C:300:THR:HG22	1:C:302:GLU:H	1.70	0.56
1:C:757:HIS:HB3	6:C:1045:HOH:O	2.05	0.56
1:B:331:ARG:HD3	1:B:331:ARG:C	2.30	0.56
1:C:263:ASN:HA	6:C:1073:HOH:O	2.05	0.56
1:C:463:GLN:NE2	6:C:1244:HOH:O	2.39	0.56
1:A:331:ARG:HD3	1:A:331:ARG:C	2.31	0.56
1:D:128:ARG:HB2	1:D:156:GLU:HG2	1.87	0.56
1:A:806:LYS:HE2	1:C:424:ARG:O	2.05	0.56
1:B:556:MET:HA	1:B:623:ASP:HA	1.87	0.56
1:B:651:ALA:HA	6:B:1149:HOH:O	2.06	0.56
1:A:556:MET:HA	1:A:623:ASP:HA	1.89	0.55
1:A:739:ALA:HB1	6:A:1143:HOH:O	2.06	0.55
1:D:29:GLN:HB3	6:D:1028:HOH:O	2.05	0.55
1:B:300:THR:HG22	1:B:302:GLU:H	1.72	0.55
1:B:219:VAL:HG12	6:B:1098:HOH:O	2.06	0.55
1:D:300:THR:HG22	1:D:303:ASN:H	1.71	0.55
1:D:675:ASP:OD2	1:D:698:THR:HB	2.07	0.55
1:A:153:ASN:CB	1:A:463:GLN:HG2	2.35	0.55
1:C:355:HIS:HE1	6:C:1065:HOH:O	1.88	0.55
1:C:556:MET:HA	1:C:623:ASP:HA	1.87	0.55
1:B:727:LYS:HE3	6:B:1124:HOH:O	2.06	0.54
1:B:86:TYR:CE1	1:B:621:ILE:HD13	2.42	0.54
1:D:350:ARG:HD3	1:D:643:ILE:O	2.06	0.54
1:B:340:ILE:H	1:B:577:GLN:NE2	1.93	0.54
1:B:415:THR:HB	1:B:483:ALA:HA	1.90	0.54
1:D:141:ASN:ND2	1:D:169:LEU:H	2.05	0.54
1:D:263:ASN:HA	6:D:1123:HOH:O	2.07	0.54
1:B:346:ASP:OD2	1:B:574:LYS:HE2	2.07	0.54
1:A:804:TRP:CE3	1:A:878:PRO:HG3	2.43	0.53
1:D:558:ASN:H	1:D:930:GLN:NE2	2.06	0.53
1:A:341:THR:HG22	6:A:1126:HOH:O	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:153:ASN:CB	1:B:463:GLN:HG2	2.37	0.53
1:A:270:THR:HG21	1:B:116:ASP:H	1.72	0.53
1:B:128:ARG:HB2	1:B:156:GLU:HG2	1.91	0.53
1:B:353:ASN:OD1	1:B:386:ARG:HD3	2.08	0.53
1:C:153:ASN:CB	1:C:463:GLN:HG2	2.36	0.53
1:A:300:THR:HG22	1:A:303:ASN:H	1.73	0.53
1:A:300:THR:HG22	1:A:302:GLU:N	2.24	0.53
1:C:415:THR:O	1:C:415:THR:CG2	2.56	0.53
1:D:415:THR:O	1:D:415:THR:CG2	2.57	0.53
1:D:161:LYS:HE2	6:D:1263:HOH:O	2.09	0.53
1:D:300:THR:HG22	1:D:302:GLU:N	2.24	0.53
1:B:738:LYS:HE3	6:B:1047:HOH:O	2.09	0.53
1:B:152:ARG:HD2	1:B:152:ARG:N	2.25	0.52
1:D:300:THR:HG22	1:D:302:GLU:H	1.73	0.52
1:B:558:ASN:H	1:B:930:GLN:NE2	2.07	0.52
1:B:300:THR:HG22	1:B:303:ASN:H	1.73	0.52
1:C:331:ARG:HD3	1:C:331:ARG:O	2.09	0.52
6:B:1207:HOH:O	1:C:594:VAL:HG21	2.09	0.52
1:D:141:ASN:HD21	1:D:168:ASN:HA	1.75	0.52
1:B:63:LYS:HE3	6:B:1095:HOH:O	2.09	0.52
1:C:128:ARG:HB2	1:C:156:GLU:HG2	1.91	0.52
1:C:141:ASN:HD21	1:C:168:ASN:HA	1.74	0.52
1:A:415:THR:CG2	1:A:415:THR:O	2.59	0.51
1:D:337:ASP:HB3	6:D:1199:HOH:O	2.10	0.51
1:D:583:GLU:OE1	1:D:587:HIS:NE2	2.36	0.51
1:C:532:TRP:O	1:C:536:HIS:HD2	1.94	0.51
1:C:944:LYS:HE2	6:C:1150:HOH:O	2.09	0.51
1:B:806:LYS:HE2	1:D:424:ARG:O	2.11	0.51
1:B:19:ARG:NH2	1:B:459:ASP:OD1	2.42	0.51
1:D:270:THR:CG2	6:D:1200:HOH:O	2.43	0.51
1:C:130:GLU:HB2	1:C:196:ARG:HB3	1.92	0.51
1:A:16:HIS:CD2	1:A:19:ARG:H	2.29	0.51
1:B:415:THR:O	1:B:415:THR:CG2	2.58	0.51
1:B:425:HIS:CD2	1:D:807:TYR:OH	2.63	0.51
1:A:128:ARG:HB2	1:A:156:GLU:HG2	1.91	0.51
1:A:432:TYR:HB2	1:A:435:THR:HG22	1.92	0.51
1:B:935:HIS:HE1	6:B:1101:HOH:O	1.94	0.51
1:B:752:GLU:HG2	1:B:757:HIS:HD2	1.74	0.51
1:D:544:GLU:HG3	6:D:1193:HOH:O	2.10	0.51
1:B:130:GLU:HB2	1:B:196:ARG:HB3	1.92	0.51
1:B:300:THR:HG22	1:B:302:GLU:N	2.25	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:789:TRP:CE3	1:C:810:ASP:HB3	2.46	0.50
1:C:152:ARG:HD2	1:C:152:ARG:N	2.27	0.50
1:A:130:GLU:HB2	1:A:196:ARG:HB3	1.94	0.50
1:A:752:GLU:HG2	1:A:757:HIS:HD2	1.76	0.50
1:B:804:TRP:CE3	1:B:878:PRO:HG3	2.46	0.50
1:A:558:ASN:H	1:A:930:GLN:NE2	2.09	0.50
1:D:331:ARG:HD3	1:D:331:ARG:O	2.12	0.50
1:C:353:ASN:OD1	1:C:386:ARG:HD3	2.11	0.50
1:C:350:ARG:HD3	1:C:643:ILE:O	2.12	0.50
1:B:789:TRP:CE3	1:B:810:ASP:HB3	2.47	0.49
1:D:130:GLU:HB2	1:D:196:ARG:HB3	1.93	0.49
1:C:224:GLN:O	1:C:296:PRO:HD2	2.12	0.49
1:B:141:ASN:HD21	1:B:168:ASN:HA	1.76	0.49
1:B:265:GLU:HB2	6:B:1190:HOH:O	2.12	0.49
1:D:152:ARG:HD2	1:D:152:ARG:N	2.27	0.49
1:C:879:ARG:NE	1:C:988:ARG:HD3	2.28	0.49
1:A:270:THR:CG2	1:B:116:ASP:HB2	2.43	0.49
1:B:59:GLU:HB2	6:B:1182:HOH:O	2.12	0.49
1:D:153:ASN:CG	1:D:463:GLN:HG2	2.38	0.49
1:D:922:GLU:HB2	6:D:1172:HOH:O	2.13	0.49
1:A:929:PRO:HA	6:A:1246:HOH:O	2.13	0.49
1:B:149:LYS:HD3	1:B:180:SER:HB2	1.95	0.49
1:D:3:CYS:HA	6:D:1230:HOH:O	2.12	0.49
1:D:86:TYR:CE1	1:D:621:ILE:HD13	2.48	0.49
1:D:269:THR:HG22	6:D:1156:HOH:O	2.13	0.49
1:A:806:LYS:HE3	1:C:427:ASN:ND2	2.28	0.49
1:B:141:ASN:ND2	1:B:169:LEU:H	2.11	0.49
1:A:935:HIS:HE1	6:A:1121:HOH:O	1.96	0.48
1:B:879:ARG:NE	1:B:988:ARG:HD3	2.28	0.48
1:B:891:GLU:CD	6:B:1135:HOH:O	2.56	0.48
1:D:159:ILE:HG22	1:D:163:VAL:HG23	1.95	0.48
1:D:353:ASN:OD1	1:D:386:ARG:HD3	2.13	0.48
1:C:331:ARG:C	1:C:331:ARG:CD	2.86	0.48
1:B:429:GLU:HG2	6:B:1262:HOH:O	2.11	0.48
1:A:141:ASN:HD21	1:A:168:ASN:HA	1.79	0.48
1:D:727:LYS:HE3	6:D:1076:HOH:O	2.13	0.48
1:C:432:TYR:HB2	1:C:435:THR:HG22	1.95	0.48
1:A:435:THR:HG23	6:A:1078:HOH:O	2.13	0.48
1:A:639:TYR:O	1:A:643:ILE:HG12	2.12	0.48
1:B:5:ILE:HG13	1:B:10:ARG:HD3	1.96	0.48
1:D:923:GLU:HB2	6:D:1064:HOH:O	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:16:HIS:CD2	1:B:19:ARG:H	2.31	0.48
1:B:224:GLN:O	1:B:296:PRO:HD2	2.13	0.48
1:D:331:ARG:C	1:D:331:ARG:CD	2.86	0.48
1:D:432:TYR:HB2	1:D:435:THR:HG22	1.94	0.48
1:A:141:ASN:ND2	1:A:169:LEU:H	2.11	0.48
1:C:300:THR:HG22	1:C:302:GLU:N	2.28	0.48
1:D:879:ARG:NE	1:D:988:ARG:HD3	2.28	0.48
1:A:551:GLU:OE1	2:A:2001:GAL:H1	2.14	0.47
1:B:432:TYR:HB2	1:B:435:THR:HG22	1.95	0.47
1:B:532:TRP:O	1:B:536:HIS:HD2	1.97	0.47
1:A:270:THR:HG21	1:B:116:ASP:HB2	1.97	0.47
1:D:224:GLN:O	1:D:296:PRO:HD2	2.14	0.47
1:D:518:ILE:HG22	1:D:519:PHE:O	2.14	0.47
1:A:603:LYS:HE2	6:A:1067:HOH:O	2.13	0.47
1:A:19:ARG:NH2	1:A:459:ASP:OD1	2.48	0.47
1:A:350:ARG:HD3	1:A:643:ILE:O	2.15	0.47
1:A:879:ARG:NE	1:A:988:ARG:HD3	2.29	0.47
1:D:532:TRP:O	1:D:536:HIS:HD2	1.96	0.47
1:D:698:THR:HG22	6:D:1051:HOH:O	2.14	0.47
1:D:789:TRP:CE3	1:D:810:ASP:HB3	2.50	0.47
1:A:22:THR:OG1	1:A:463:GLN:NE2	2.48	0.47
1:B:805:LYS:HE2	6:B:1250:HOH:O	2.14	0.47
1:B:350:ARG:HD3	1:B:643:ILE:O	2.15	0.47
1:C:789:TRP:CD2	1:C:810:ASP:HB3	2.50	0.47
1:A:152:ARG:HD2	1:A:152:ARG:N	2.30	0.46
1:A:326:HIS:CG	1:A:327:HIS:H	2.33	0.46
1:B:435:THR:HG23	6:B:1072:HOH:O	2.13	0.46
1:C:265:GLU:HB2	6:C:1084:HOH:O	2.14	0.46
1:C:206:LYS:HD2	6:C:1087:HOH:O	2.15	0.46
1:C:300:THR:HG22	1:C:303:ASN:H	1.80	0.46
1:A:86:TYR:CE1	1:A:621:ILE:HD13	2.50	0.46
1:A:353:ASN:OD1	1:A:386:ARG:HD3	2.15	0.46
1:B:841:VAL:C	1:B:842:VAL:HG13	2.18	0.46
1:D:16:HIS:CD2	1:D:19:ARG:H	2.33	0.46
1:C:86:TYR:CE1	1:C:621:ILE:HD13	2.51	0.46
1:A:789:TRP:CE3	1:A:810:ASP:HB3	2.51	0.46
1:A:937:ASP:HA	1:A:959:PRO:HB2	1.96	0.46
1:B:807:TYR:OH	1:D:425:HIS:HD2	1.97	0.46
1:D:19:ARG:NH2	1:D:459:ASP:OD1	2.48	0.46
1:D:149:LYS:HD3	1:D:180:SER:HB2	1.97	0.46
1:A:149:LYS:HD3	1:A:180:SER:HB2	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:804:TRP:CE3	1:D:878:PRO:HG3	2.50	0.46
1:C:116:ASP:HB3	1:C:119:SER:H	1.80	0.46
1:A:427:ASN:ND2	1:C:806:LYS:HE3	2.30	0.46
1:B:758:PHE:HD1	1:B:770:LEU:HD13	1.81	0.46
1:D:937:ASP:HA	1:D:959:PRO:HB2	1.97	0.46
1:B:879:ARG:HE	1:B:988:ARG:HD3	1.81	0.46
1:D:530:GLU:HG2	6:D:1219:HOH:O	2.16	0.46
1:A:178:SER:OG	1:A:180:SER:HB3	2.16	0.45
1:B:755:GLY:N	1:C:78:ASP:OD2	2.37	0.45
1:B:937:ASP:HA	1:B:959:PRO:HB2	1.98	0.45
1:C:16:HIS:CD2	1:C:19:ARG:H	2.34	0.45
1:C:220:ASP:HB3	6:C:1041:HOH:O	2.16	0.45
1:D:22:THR:OG1	1:D:463:GLN:NE2	2.50	0.45
1:D:233:ASP:HB2	6:D:1122:HOH:O	2.16	0.45
1:D:326:HIS:CG	1:D:327:HIS:H	2.34	0.45
1:C:265:GLU:HG3	6:C:1067:HOH:O	2.17	0.45
1:C:879:ARG:HE	1:C:988:ARG:HD3	1.81	0.45
1:B:116:ASP:HB3	1:B:119:SER:H	1.81	0.45
1:A:300:THR:CG2	1:A:302:GLU:H	2.29	0.45
1:A:755:GLY:HA2	1:D:78:ASP:CG	2.42	0.45
1:A:804:TRP:CD2	1:A:878:PRO:HG3	2.52	0.45
1:C:326:HIS:CG	1:C:327:HIS:H	2.35	0.45
1:C:530:GLU:OE2	1:C:533:ARG:NH1	2.50	0.45
1:C:804:TRP:CE3	1:C:878:PRO:HG3	2.52	0.45
1:A:735:THR:HB	1:A:827:GLY:HA3	1.98	0.45
1:D:415:THR:O	1:D:415:THR:HG23	2.17	0.45
1:A:629:GLU:HG3	6:A:1071:HOH:O	2.16	0.44
1:B:292:ASN:HB2	6:B:1283:HOH:O	2.17	0.44
1:B:1014:GLN:HB2	6:B:1026:HOH:O	2.17	0.44
1:C:415:THR:O	1:C:415:THR:HG23	2.17	0.44
1:A:102:THR:HG22	1:C:763:LEU:HD12	1.99	0.44
1:D:125:HIS:HD2	1:D:160:GLN:OE1	2.00	0.44
1:D:699:TYR:HB2	6:D:1051:HOH:O	2.17	0.44
1:C:735:THR:HB	1:C:827:GLY:HA3	1.99	0.44
1:A:658:THR:HG23	1:A:690:SER:HB3	1.99	0.44
1:B:789:TRP:CD2	1:B:810:ASP:HB3	2.51	0.44
1:A:425:HIS:CD2	1:C:807:TYR:OH	2.71	0.44
1:B:153:ASN:CG	1:B:463:GLN:HG2	2.43	0.44
1:D:723:GLU:HG3	6:D:1142:HOH:O	2.17	0.44
1:C:153:ASN:CG	1:C:463:GLN:HG2	2.43	0.44
1:A:116:ASP:HB3	1:A:119:SER:H	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:879:ARG:HE	1:A:988:ARG:HD3	1.83	0.44
1:A:159:ILE:HG22	1:A:163:VAL:HG23	1.99	0.44
1:B:685:LEU:HD21	1:B:691:VAL:HG23	1.99	0.44
1:D:735:THR:HB	1:D:827:GLY:HA3	2.00	0.44
1:A:806:LYS:HE3	1:C:427:ASN:HD21	1.83	0.44
1:A:738:LYS:HA	6:A:1110:HOH:O	2.18	0.44
1:A:532:TRP:O	1:A:536:HIS:HD2	2.01	0.43
1:B:755:GLY:HA2	1:C:78:ASP:OD1	2.17	0.43
1:C:19:ARG:NH2	1:C:459:ASP:OD1	2.48	0.43
1:D:5:ILE:HG13	1:D:10:ARG:HD3	2.00	0.43
1:D:178:SER:OG	1:D:180:SER:HB3	2.18	0.43
1:C:518:ILE:HG22	1:C:519:PHE:O	2.18	0.43
1:C:937:ASP:HA	1:C:959:PRO:HB2	1.99	0.43
1:D:583:GLU:OE2	1:D:623:ASP:OD1	2.34	0.43
1:D:685:LEU:HD21	1:D:691:VAL:HG23	2.00	0.43
1:C:355:HIS:HD2	1:C:390:TYR:OH	2.02	0.43
1:A:355:HIS:HD2	1:A:390:TYR:OH	2.02	0.43
1:A:386:ARG:HG3	1:A:408:ILE:HB	2.01	0.43
1:D:116:ASP:HB3	1:D:119:SER:H	1.83	0.43
1:D:879:ARG:HE	1:D:988:ARG:HD3	1.84	0.43
1:B:326:HIS:CG	1:B:327:HIS:H	2.36	0.43
1:A:5:ILE:HG13	1:A:10:ARG:HD3	2.00	0.43
1:A:388:SER:HA	1:A:389:HIS:HA	1.78	0.43
1:A:814:GLN:HG3	1:A:838:ILE:HG12	1.99	0.43
1:C:591:PHE:CD2	1:C:606:ALA:HB2	2.53	0.43
1:B:583:GLU:OE2	1:B:623:ASP:OD1	2.36	0.43
1:C:498:GLN:HG2	6:C:1170:HOH:O	2.18	0.43
1:B:300:THR:CG2	1:B:302:GLU:H	2.32	0.43
1:B:355:HIS:HD2	1:B:390:TYR:OH	2.02	0.43
1:B:621:ILE:HD12	1:B:621:ILE:HA	1.94	0.43
1:D:678:LYS:HD3	6:D:1136:HOH:O	2.19	0.43
1:A:33:GLU:HA	1:B:265:GLU:OE1	2.19	0.42
1:B:178:SER:OG	1:B:180:SER:HB3	2.18	0.42
1:B:735:THR:HB	1:B:827:GLY:HA3	2.00	0.42
1:A:415:THR:O	1:A:415:THR:HG23	2.19	0.42
1:D:97:ILE:HA	1:D:98:PRO:HA	1.84	0.42
1:D:300:THR:CG2	1:D:302:GLU:H	2.32	0.42
1:D:355:HIS:HE1	6:D:1087:HOH:O	2.02	0.42
1:A:224:GLN:O	1:A:296:PRO:HD2	2.20	0.42
1:A:166:GLY:HA2	1:B:273:THR:HG21	2.01	0.42
1:A:363:ARG:HD3	6:A:1030:HOH:O	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:583:GLU:OE1	1:A:587:HIS:NE2	2.38	0.42
1:A:795:ASN:HB3	6:A:1049:HOH:O	2.19	0.42
1:B:415:THR:O	1:B:415:THR:HG23	2.19	0.42
1:B:445:HIS:HA	1:B:449:ASP:HB3	2.01	0.42
1:A:331:ARG:C	1:A:331:ARG:CD	2.91	0.42
1:A:755:GLY:N	1:D:78:ASP:OD2	2.45	0.42
1:A:152:ARG:HG3	1:A:195:TYR:OH	2.19	0.42
1:B:482:GLU:HA	6:B:1078:HOH:O	2.19	0.42
1:D:419:GLN:NE2	1:D:443:ASN:HB2	2.35	0.42
1:D:658:THR:HG23	1:D:690:SER:HB3	2.00	0.42
1:C:149:LYS:HD3	1:C:180:SER:HB2	2.01	0.42
1:D:254:LYS:HG2	6:D:1153:HOH:O	2.19	0.42
1:D:542:LYS:HD3	6:D:1052:HOH:O	2.20	0.42
1:C:152:ARG:HG3	1:C:195:TYR:OH	2.20	0.42
1:C:673:ASP:OD1	1:C:673:ASP:C	2.63	0.42
1:A:530:GLU:OE2	1:A:533:ARG:NH1	2.53	0.42
1:D:388:SER:HA	1:D:389:HIS:HA	1.80	0.42
1:D:747:ARG:O	1:D:762:LYS:HB2	2.20	0.42
1:D:789:TRP:CD2	1:D:810:ASP:HB3	2.55	0.42
1:C:388:SER:HA	1:C:389:HIS:HA	1.79	0.42
1:C:546:PRO:CB	1:C:577:GLN:HE21	2.33	0.42
1:D:591:PHE:CD2	1:D:606:ALA:HB2	2.55	0.42
1:C:258:ALA:HB3	6:C:1237:HOH:O	2.20	0.42
1:C:551:GLU:OE1	2:C:2001:GAL:H1	2.19	0.42
1:A:115:LEU:HD23	1:A:115:LEU:HA	1.94	0.41
1:C:568:GLU:HG2	6:C:1074:HOH:O	2.19	0.41
1:A:355:HIS:HE1	6:A:1235:HOH:O	2.02	0.41
1:B:582:TRP:CD1	1:B:583:GLU:HB2	2.55	0.41
1:B:807:TYR:OH	1:D:425:HIS:CD2	2.73	0.41
1:A:153:ASN:CG	1:A:463:GLN:HG2	2.44	0.41
1:D:432:TYR:HA	1:D:433:PRO:HD3	1.95	0.41
1:C:269:THR:HG21	6:C:1084:HOH:O	2.19	0.41
1:D:383:ASN:OD1	1:D:383:ASN:C	2.63	0.41
1:C:583:GLU:OE2	1:C:623:ASP:OD1	2.38	0.41
1:C:231:LYS:HG2	6:C:1047:HOH:O	2.20	0.41
1:C:517:ASP:O	1:C:518:ILE:HD13	2.20	0.41
1:C:758:PHE:HD1	1:C:770:LEU:HD13	1.85	0.41
1:B:125:HIS:HD2	1:B:160:GLN:OE1	2.04	0.41
1:B:159:ILE:HG22	1:B:163:VAL:HG23	2.01	0.41
1:C:487:ARG:HB2	6:C:1211:HOH:O	2.20	0.41
1:D:5:ILE:HA	1:D:6:PRO:HD3	1.96	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:257:ASP:OD2	1:B:68:SER:HB2	2.21	0.41
1:C:450:ASN:HA	1:C:451:PRO:HD3	1.95	0.41
1:C:498:GLN:HG3	6:C:1062:HOH:O	2.21	0.41
1:A:425:HIS:HD2	1:C:807:TYR:OH	2.02	0.41
1:A:523:TYR:N	1:A:524:PRO:HD3	2.36	0.41
1:B:523:TYR:N	1:B:524:PRO:HD3	2.36	0.41
1:D:824:GLY:HA3	1:D:828:SER:O	2.20	0.41
1:C:159:ILE:HG22	1:C:163:VAL:HG23	2.02	0.41
1:C:266:ASN:CG	1:C:325:LYS:HD2	2.46	0.41
1:C:658:THR:HG23	1:C:690:SER:HB3	2.02	0.41
1:A:897:GLY:O	1:A:913:PHE:HA	2.20	0.41
1:B:644:GLU:HA	1:B:645:PRO:HD3	1.99	0.41
1:C:59:GLU:HB2	6:C:1206:HOH:O	2.20	0.41
1:A:331:ARG:NH2	1:A:474:ILE:O	2.54	0.40
1:A:583:GLU:OE2	1:A:623:ASP:OD1	2.39	0.40
1:A:685:LEU:HD21	1:A:691:VAL:HG23	2.02	0.40
1:A:755:GLY:HA3	6:A:1169:HOH:O	2.21	0.40
1:A:789:TRP:CD2	1:A:810:ASP:HB3	2.55	0.40
1:C:445:HIS:HA	1:C:449:ASP:HB3	2.03	0.40
1:C:471:HIS:HA	1:C:472:PRO:HD2	1.95	0.40
1:A:419:GLN:NE2	1:A:443:ASN:HB2	2.36	0.40
1:B:331:ARG:C	1:B:331:ARG:CD	2.93	0.40
1:B:518:ILE:HG22	1:B:519:PHE:O	2.21	0.40
1:B:795:ASN:HB3	6:B:1110:HOH:O	2.21	0.40
1:B:59:GLU:HG3	6:B:1182:HOH:O	2.21	0.40
1:C:220:ASP:CB	6:C:1041:HOH:O	2.70	0.40
1:C:523:TYR:N	1:C:524:PRO:HD3	2.37	0.40
1:A:807:TYR:OH	1:C:425:HIS:CD2	2.74	0.40
1:B:691:VAL:HG12	1:B:693:ILE:HG13	2.03	0.40
1:D:5:ILE:O	1:D:10:ARG:NH1	2.52	0.40
1:D:152:ARG:HG3	1:D:195:TYR:OH	2.22	0.40
1:D:419:GLN:HE22	1:D:443:ASN:HB2	1.87	0.40
1:A:350:ARG:HG2	1:A:643:ILE:HB	2.03	0.40
1:A:445:HIS:HA	1:A:449:ASP:HB3	2.03	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:144:TYR:O	1:C:273:THR:OG1[3_545]	1.80	0.40

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%)	971 (95%)	48 (5%)	3 (0%)	36	66
1	B	1022/1032 (99%)	971 (95%)	49 (5%)	2 (0%)	43	72
1	C	1022/1032 (99%)	973 (95%)	47 (5%)	2 (0%)	43	72
1	D	1022/1032 (99%)	971 (95%)	49 (5%)	2 (0%)	43	72
All	All	4088/4128 (99%)	3886 (95%)	193 (5%)	9 (0%)	43	72

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	842	VAL
1	B	842	VAL
1	D	842	VAL
1	C	842	VAL
1	A	62	LYS
1	A	274	LYS
1	D	274	LYS
1	C	62	LYS
1	B	62	LYS

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%)	871 (96%)	34 (4%)	29	64
1	B	905/913 (99%)	871 (96%)	34 (4%)	29	64

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	905/913 (99%)	868 (96%)	37 (4%)	27	62
1	D	905/913 (99%)	872 (96%)	33 (4%)	31	66
All	All	3620/3652 (99%)	3482 (96%)	138 (4%)	29	64

All (138) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	ILE
1	A	9	LEU
1	A	15	VAL
1	A	134	ASN
1	A	163	VAL
1	A	167	GLU
1	A	220	ASP
1	A	269	THR
1	A	270	THR
1	A	273	THR
1	A	281	THR
1	A	300	THR
1	A	331	ARG
1	A	333	VAL
1	A	341	THR
1	A	415	THR
1	A	442	VAL
1	A	569	LEU
1	A	619	VAL
1	A	620	PHE
1	A	621	ILE
1	A	642	VAL
1	A	698	THR
1	A	701	VAL
1	A	703	VAL
1	A	704	LEU
1	A	723	GLU
1	A	750	SER
1	A	842	VAL
1	A	860	ILE
1	A	869	THR
1	A	876	ASP
1	A	988	ARG
1	A	996	VAL

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Mol	Chain	Res	Type
1	B	9	LEU
1	B	15	VAL
1	B	134	ASN
1	B	163	VAL
1	B	167	GLU
1	B	220	ASP
1	B	269	THR
1	B	270	THR
1	B	273	THR
1	B	281	THR
1	B	300	THR
1	B	331	ARG
1	B	333	VAL
1	B	341	THR
1	B	415	THR
1	B	442	VAL
1	B	569	LEU
1	B	619	VAL
1	B	620	PHE
1	B	621	ILE
1	B	698	THR
1	B	701	VAL
1	B	703	VAL
1	B	704	LEU
1	B	723	GLU
1	B	738	LYS
1	B	750	SER
1	B	842	VAL
1	B	860	ILE
1	B	869	THR
1	B	876	ASP
1	B	957	GLU
1	B	988	ARG
1	B	996	VAL
1	D	5	ILE
1	D	9	LEU
1	D	15	VAL
1	D	134	ASN
1	D	163	VAL
1	D	167	GLU
1	D	220	ASP
1	D	269	THR

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Mol	Chain	Res	Type
1	D	270	THR
1	D	273	THR
1	D	281	THR
1	D	300	THR
1	D	331	ARG
1	D	333	VAL
1	D	341	THR
1	D	415	THR
1	D	442	VAL
1	D	569	LEU
1	D	619	VAL
1	D	620	PHE
1	D	698	THR
1	D	701	VAL
1	D	703	VAL
1	D	704	LEU
1	D	723	GLU
1	D	750	SER
1	D	842	VAL
1	D	860	ILE
1	D	869	THR
1	D	876	ASP
1	D	957	GLU
1	D	988	ARG
1	D	996	VAL
1	C	2	SER
1	C	5	ILE
1	C	9	LEU
1	C	15	VAL
1	C	134	ASN
1	C	163	VAL
1	C	167	GLU
1	C	220	ASP
1	C	269	THR
1	C	270	THR
1	C	273	THR
1	C	300	THR
1	C	331	ARG
1	C	333	VAL
1	C	341	THR
1	C	415	THR
1	C	435	THR

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Mol	Chain	Res	Type
1	C	442	VAL
1	C	569	LEU
1	C	619	VAL
1	C	620	PHE
1	C	621	ILE
1	C	642	VAL
1	C	698	THR
1	C	701	VAL
1	C	703	VAL
1	C	704	LEU
1	C	723	GLU
1	C	738	LYS
1	C	750	SER
1	C	842	VAL
1	C	860	ILE
1	C	869	THR
1	C	876	ASP
1	C	957	GLU
1	C	988	ARG
1	C	996	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (101) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	16	HIS
1	A	29	GLN
1	A	99	ASN
1	A	125	HIS
1	A	141	ASN
1	A	243	ASN
1	A	339	ASN
1	A	355	HIS
1	A	419	GLN
1	A	423	ASN
1	A	425	HIS
1	A	427	ASN
1	A	463	GLN
1	A	512	ASN
1	A	567	GLN
1	A	577	GLN
1	A	757	HIS
1	A	808	ASN

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Mol	Chain	Res	Type
1	A	930	GLN
1	A	932	ASN
1	A	934	ASN
1	A	935	HIS
1	A	955	GLN
1	B	16	HIS
1	B	29	GLN
1	B	99	ASN
1	B	125	HIS
1	B	141	ASN
1	B	243	ASN
1	B	339	ASN
1	B	355	HIS
1	B	387	ASN
1	B	392	ASN
1	B	419	GLN
1	B	423	ASN
1	B	425	HIS
1	B	463	GLN
1	B	489	HIS
1	B	498	GLN
1	B	567	GLN
1	B	577	GLN
1	B	647	HIS
1	B	930	GLN
1	B	932	ASN
1	B	934	ASN
1	B	935	HIS
1	B	955	GLN
1	D	16	HIS
1	D	29	GLN
1	D	99	ASN
1	D	125	HIS
1	D	134	ASN
1	D	141	ASN
1	D	188	GLN
1	D	243	ASN
1	D	263	ASN
1	D	266	ASN
1	D	339	ASN
1	D	355	HIS
1	D	387	ASN

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Mol	Chain	Res	Type
1	D	392	ASN
1	D	419	GLN
1	D	423	ASN
1	D	425	HIS
1	D	463	GLN
1	D	489	HIS
1	D	536	HIS
1	D	567	GLN
1	D	577	GLN
1	D	757	HIS
1	D	930	GLN
1	D	932	ASN
1	D	934	ASN
1	D	935	HIS
1	C	16	HIS
1	C	29	GLN
1	C	99	ASN
1	C	125	HIS
1	C	134	ASN
1	C	141	ASN
1	C	188	GLN
1	C	263	ASN
1	C	339	ASN
1	C	355	HIS
1	C	387	ASN
1	C	392	ASN
1	C	419	GLN
1	C	423	ASN
1	C	425	HIS
1	C	427	ASN
1	C	463	GLN
1	C	489	HIS
1	C	498	GLN
1	C	577	GLN
1	C	647	HIS
1	C	757	HIS
1	C	930	GLN
1	C	932	ASN
1	C	934	ASN
1	C	935	HIS
1	C	955	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 28 ligands modelled in this entry, 24 are monoatomic - leaving 4 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
2	GAL	D	2001	4	12,12,12	0.47	0	17,17,17	1.03	1 (5%)
2	GAL	C	2001	4	12,12,12	0.53	0	17,17,17	1.24	1 (5%)
2	GAL	B	2001	4	12,12,12	0.55	0	17,17,17	0.62	0
2	GAL	A	2001	4	12,12,12	0.55	0	17,17,17	0.97	1 (5%)

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	GAL	D	2001	4	-	2/2/22/22	0/1/1/1
2	GAL	C	2001	4	-	1/2/22/22	0/1/1/1
2	GAL	B	2001	4	-	2/2/22/22	0/1/1/1
2	GAL	A	2001	4	-	2/2/22/22	0/1/1/1

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
2	C	2001	GAL	C1-O5-C5	3.11	119.67	113.65
2	D	2001	GAL	C1-O5-C5	2.45	118.40	113.65
2	A	2001	GAL	C1-O5-C5	2.40	118.30	113.65

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	2001	GAL	O5-C5-C6-O6
2	A	2001	GAL	O5-C5-C6-O6
2	D	2001	GAL	O5-C5-C6-O6
2	B	2001	GAL	C4-C5-C6-O6
2	A	2001	GAL	C4-C5-C6-O6
2	C	2001	GAL	O5-C5-C6-O6
2	D	2001	GAL	C4-C5-C6-O6

There are no ring outliers.

4 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	2001	GAL	1	0
2	C	2001	GAL	1	0
2	B	2001	GAL	1	0
2	A	2001	GAL	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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%)	-0.15	12 (1%) 76 68	28, 34, 42, 50	0
1	B	1024/1032 (99%)	-0.08	17 (1%) 69 60	28, 34, 42, 50	0
1	C	1024/1032 (99%)	0.04	30 (2%) 53 43	28, 34, 42, 50	0
1	D	1024/1032 (99%)	-0.02	23 (2%) 62 52	28, 34, 42, 50	0
All	All	4096/4128 (99%)	-0.05	82 (2%) 65 56	28, 34, 42, 50	0

All (82) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	272	SER	8.0
1	C	270	THR	8.0
1	D	273	THR	7.2
1	C	269	THR	6.7
1	D	269	THR	6.6
1	D	271	PHE	6.4
1	C	266	ASN	6.0
1	D	270	THR	5.9
1	C	267	GLY	5.7
1	C	271	PHE	5.7
1	C	268	ASN	5.4
1	C	272	SER	5.3
1	C	923	GLU	4.9
1	D	267	GLY	4.9
1	D	266	ASN	4.6
1	C	273	THR	4.3
1	C	264	GLU	4.1
1	D	922	GLU	4.1
1	A	271	PHE	4.1
1	B	266	ASN	4.0
1	B	652	HIS	4.0

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Mol	Chain	Res	Type	RSRZ
1	D	268	ASN	3.9
1	A	272	SER	3.9
1	D	923	GLU	3.9
1	D	221	SER	3.9
1	C	250	GLU	3.5
1	B	739	ALA	3.4
1	A	273	THR	3.4
1	A	266	ASN	3.3
1	B	272	SER	3.3
1	C	754	SER	3.1
1	C	276	PHE	3.0
1	C	922	GLU	3.0
1	B	271	PHE	3.0
1	C	730	ASP	2.9
1	D	30	ASP	2.9
1	D	368	ASP	2.9
1	B	267	GLY	2.8
1	B	269	THR	2.8
1	B	539	GLU	2.7
1	C	116	ASP	2.7
1	C	265	GLU	2.7
1	B	430	ALA	2.6
1	C	739	ALA	2.6
1	B	730	ASP	2.6
1	A	531	ARG	2.5
1	C	206	LYS	2.5
1	C	275	GLU	2.5
1	A	269	THR	2.5
1	B	2	SER	2.4
1	D	539	GLU	2.4
1	B	273	THR	2.4
1	C	368	ASP	2.4
1	B	429	GLU	2.4
1	D	265	GLU	2.4
1	C	319	SER	2.4
1	D	540	ASN	2.4
1	D	274	LYS	2.4
1	B	435	THR	2.3
1	C	435	THR	2.3
1	C	737	GLU	2.3
1	D	435	THR	2.3
1	C	121	GLU	2.3

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Mol	Chain	Res	Type	RSRZ
1	D	434	ASP	2.3
1	B	681	ASP	2.2
1	C	274	LYS	2.2
1	D	294	LYS	2.2
1	D	729	PRO	2.2
1	C	729	PRO	2.2
1	C	237	SER	2.1
1	C	652	HIS	2.1
1	D	924	PHE	2.1
1	B	540	ASN	2.1
1	A	435	THR	2.1
1	B	73	TRP	2.1
1	A	737	GLU	2.1
1	A	121	GLU	2.0
1	D	264	GLU	2.0
1	A	735	THR	2.0
1	A	429	GLU	2.0
1	C	251	ASP	2.0
1	A	432	TYR	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](#)

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(Å ²)	Q<0.9
4	NA	D	3006	1/1	0.77	0.11	36,36,36,36	0
4	NA	C	3006	1/1	0.86	0.10	33,33,33,33	0
2	GAL	C	2001	12/12	0.89	0.11	39,45,45,46	0
2	GAL	B	2001	12/12	0.90	0.09	35,38,39,41	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	GAL	A	2001	12/12	0.91	0.09	39,41,42,42	0
3	MG	A	3001	1/1	0.91	0.18	22,22,22,22	0
4	NA	B	3006	1/1	0.92	0.05	19,19,19,19	0
2	GAL	D	2001	12/12	0.92	0.09	41,44,45,45	0
3	MG	B	3001	1/1	0.92	0.18	30,30,30,30	0
3	MG	C	3001	1/1	0.93	0.07	38,38,38,38	0
4	NA	C	3004	1/1	0.94	0.10	13,13,13,13	0
4	NA	D	3003	1/1	0.96	0.12	20,20,20,20	0
4	NA	D	3002	1/1	0.96	0.07	9,9,9,9	0
4	NA	B	3003	1/1	0.97	0.06	13,13,13,13	0
4	NA	B	3004	1/1	0.97	0.09	5,5,5,5	0
4	NA	A	3003	1/1	0.97	0.07	19,19,19,19	0
4	NA	A	3006	1/1	0.97	0.03	22,22,22,22	0
4	NA	C	3003	1/1	0.98	0.05	18,18,18,18	0
4	NA	B	3002	1/1	0.99	0.08	2,2,2,2	0
4	NA	C	3002	1/1	0.99	0.06	11,11,11,11	0
3	MG	D	3001	1/1	0.99	0.03	23,23,23,23	0
4	NA	A	3002	1/1	0.99	0.03	2,2,2,2	0
4	NA	D	3004	1/1	0.99	0.07	5,5,5,5	0
5	MN	A	3005	1/1	0.99	0.02	24,24,24,24	0
5	MN	B	3005	1/1	0.99	0.02	30,30,30,30	0
5	MN	D	3005	1/1	0.99	0.02	25,25,25,25	0
5	MN	C	3005	1/1	0.99	0.02	30,30,30,30	0
4	NA	A	3004	1/1	1.00	0.03	2,2,2,2	0

6.5 Other polymers [i](#)

There are no such residues in this entry.