



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 07:24 PM UTC

PDB ID : 8J9F / pdb_00008j9f
Title : Structure of STG-hydrolyzing beta-glucosidase 1 (PSTG1)
Authors : Yanai, T.; Imaizumi, R.; Takahashi, Y.; Katsumura, E.; Yamamoto, M.;
Nakayama, T.; Yamashita, S.; Takeshita, K.; Sakai, N.; Matsuura, H.
Deposited on : 2023-05-03
Resolution : 2.85 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

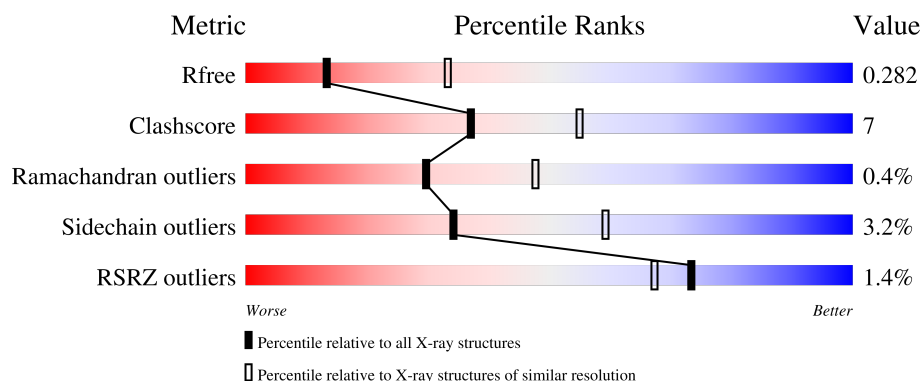
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.85 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	1407 (2.88-2.84)
Clashscore	190562	1446 (2.88-2.84)
Ramachandran outliers	187476	1406 (2.88-2.84)
Sidechain outliers	187428	1407 (2.88-2.84)
RSRZ outliers	180081	1408 (2.88-2.84)

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	780	0% 78% 16% • •
1	B	780	2% 77% 18% • 5%
1	C	780	0% 77% 17% • •
1	D	780	2% 78% 17% • •

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 23612 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-glucosidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	745	Total	C	N	O	S	0	0	0
			5765	3651	983	1107	24			
1	B	744	Total	C	N	O	S	0	0	0
			5756	3647	981	1103	25			
1	C	749	Total	C	N	O	S	0	0	0
			5795	3667	989	1114	25			
1	D	749	Total	C	N	O	S	0	0	0
			5787	3662	987	1113	25			

There are 108 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-26	MET	-	initiating methionine	UNP D6RVX0
A	-25	ASN	-	expression tag	UNP D6RVX0
A	-24	HIS	-	expression tag	UNP D6RVX0
A	-23	LYS	-	expression tag	UNP D6RVX0
A	-22	VAL	-	expression tag	UNP D6RVX0
A	-21	HIS	-	expression tag	UNP D6RVX0
A	-20	HIS	-	expression tag	UNP D6RVX0
A	-19	HIS	-	expression tag	UNP D6RVX0
A	-18	HIS	-	expression tag	UNP D6RVX0
A	-17	HIS	-	expression tag	UNP D6RVX0
A	-16	HIS	-	expression tag	UNP D6RVX0
A	-15	ILE	-	expression tag	UNP D6RVX0
A	-14	GLU	-	expression tag	UNP D6RVX0
A	-13	GLY	-	expression tag	UNP D6RVX0
A	-12	ARG	-	expression tag	UNP D6RVX0
A	-11	HIS	-	expression tag	UNP D6RVX0
A	-10	MET	-	expression tag	UNP D6RVX0
A	-9	GLU	-	expression tag	UNP D6RVX0
A	-8	LEU	-	expression tag	UNP D6RVX0
A	-7	GLY	-	expression tag	UNP D6RVX0
A	-6	THR	-	expression tag	UNP D6RVX0

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
A	-5	LEU	-	expression tag	UNP D6RVX0
A	-4	GLU	-	expression tag	UNP D6RVX0
A	-3	GLY	-	expression tag	UNP D6RVX0
A	-2	SER	-	expression tag	UNP D6RVX0
A	-1	GLU	-	expression tag	UNP D6RVX0
A	0	PHE	-	expression tag	UNP D6RVX0
B	-26	MET	-	initiating methionine	UNP D6RVX0
B	-25	ASN	-	expression tag	UNP D6RVX0
B	-24	HIS	-	expression tag	UNP D6RVX0
B	-23	LYS	-	expression tag	UNP D6RVX0
B	-22	VAL	-	expression tag	UNP D6RVX0
B	-21	HIS	-	expression tag	UNP D6RVX0
B	-20	HIS	-	expression tag	UNP D6RVX0
B	-19	HIS	-	expression tag	UNP D6RVX0
B	-18	HIS	-	expression tag	UNP D6RVX0
B	-17	HIS	-	expression tag	UNP D6RVX0
B	-16	HIS	-	expression tag	UNP D6RVX0
B	-15	ILE	-	expression tag	UNP D6RVX0
B	-14	GLU	-	expression tag	UNP D6RVX0
B	-13	GLY	-	expression tag	UNP D6RVX0
B	-12	ARG	-	expression tag	UNP D6RVX0
B	-11	HIS	-	expression tag	UNP D6RVX0
B	-10	MET	-	expression tag	UNP D6RVX0
B	-9	GLU	-	expression tag	UNP D6RVX0
B	-8	LEU	-	expression tag	UNP D6RVX0
B	-7	GLY	-	expression tag	UNP D6RVX0
B	-6	THR	-	expression tag	UNP D6RVX0
B	-5	LEU	-	expression tag	UNP D6RVX0
B	-4	GLU	-	expression tag	UNP D6RVX0
B	-3	GLY	-	expression tag	UNP D6RVX0
B	-2	SER	-	expression tag	UNP D6RVX0
B	-1	GLU	-	expression tag	UNP D6RVX0
B	0	PHE	-	expression tag	UNP D6RVX0
C	-26	MET	-	initiating methionine	UNP D6RVX0
C	-25	ASN	-	expression tag	UNP D6RVX0
C	-24	HIS	-	expression tag	UNP D6RVX0
C	-23	LYS	-	expression tag	UNP D6RVX0
C	-22	VAL	-	expression tag	UNP D6RVX0
C	-21	HIS	-	expression tag	UNP D6RVX0
C	-20	HIS	-	expression tag	UNP D6RVX0
C	-19	HIS	-	expression tag	UNP D6RVX0
C	-18	HIS	-	expression tag	UNP D6RVX0

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
C	-17	HIS	-	expression tag	UNP D6RVX0
C	-16	HIS	-	expression tag	UNP D6RVX0
C	-15	ILE	-	expression tag	UNP D6RVX0
C	-14	GLU	-	expression tag	UNP D6RVX0
C	-13	GLY	-	expression tag	UNP D6RVX0
C	-12	ARG	-	expression tag	UNP D6RVX0
C	-11	HIS	-	expression tag	UNP D6RVX0
C	-10	MET	-	expression tag	UNP D6RVX0
C	-9	GLU	-	expression tag	UNP D6RVX0
C	-8	LEU	-	expression tag	UNP D6RVX0
C	-7	GLY	-	expression tag	UNP D6RVX0
C	-6	THR	-	expression tag	UNP D6RVX0
C	-5	LEU	-	expression tag	UNP D6RVX0
C	-4	GLU	-	expression tag	UNP D6RVX0
C	-3	GLY	-	expression tag	UNP D6RVX0
C	-2	SER	-	expression tag	UNP D6RVX0
C	-1	GLU	-	expression tag	UNP D6RVX0
C	0	PHE	-	expression tag	UNP D6RVX0
D	-26	MET	-	initiating methionine	UNP D6RVX0
D	-25	ASN	-	expression tag	UNP D6RVX0
D	-24	HIS	-	expression tag	UNP D6RVX0
D	-23	LYS	-	expression tag	UNP D6RVX0
D	-22	VAL	-	expression tag	UNP D6RVX0
D	-21	HIS	-	expression tag	UNP D6RVX0
D	-20	HIS	-	expression tag	UNP D6RVX0
D	-19	HIS	-	expression tag	UNP D6RVX0
D	-18	HIS	-	expression tag	UNP D6RVX0
D	-17	HIS	-	expression tag	UNP D6RVX0
D	-16	HIS	-	expression tag	UNP D6RVX0
D	-15	ILE	-	expression tag	UNP D6RVX0
D	-14	GLU	-	expression tag	UNP D6RVX0
D	-13	GLY	-	expression tag	UNP D6RVX0
D	-12	ARG	-	expression tag	UNP D6RVX0
D	-11	HIS	-	expression tag	UNP D6RVX0
D	-10	MET	-	expression tag	UNP D6RVX0
D	-9	GLU	-	expression tag	UNP D6RVX0
D	-8	LEU	-	expression tag	UNP D6RVX0
D	-7	GLY	-	expression tag	UNP D6RVX0
D	-6	THR	-	expression tag	UNP D6RVX0
D	-5	LEU	-	expression tag	UNP D6RVX0
D	-4	GLU	-	expression tag	UNP D6RVX0
D	-3	GLY	-	expression tag	UNP D6RVX0

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
D	-2	SER	-	expression tag	UNP D6RVX0
D	-1	GLU	-	expression tag	UNP D6RVX0
D	0	PHE	-	expression tag	UNP D6RVX0

- Molecule 2 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



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

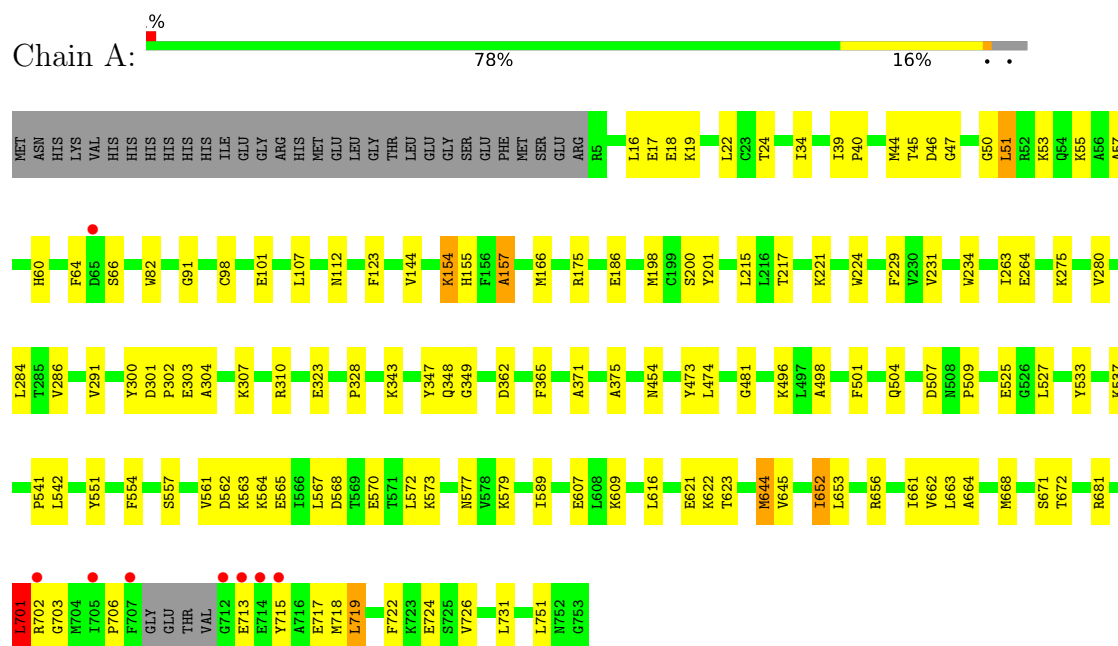
- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	109	Total O 109 109	0	0
3	B	136	Total O 136 136	0	0
3	C	109	Total O 109 109	0	0
3	D	137	Total O 137 137	0	0

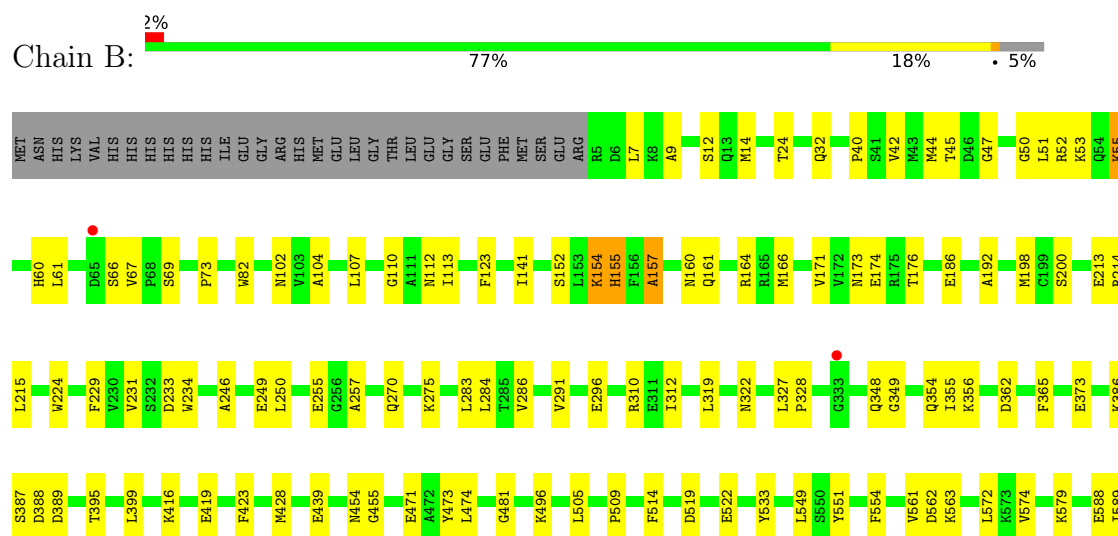
3 Residue-property plots [i](#)

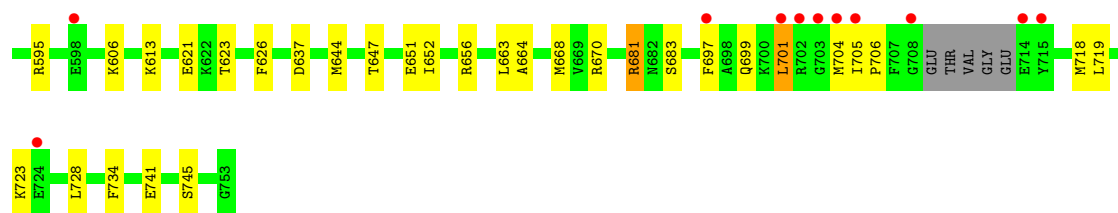
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

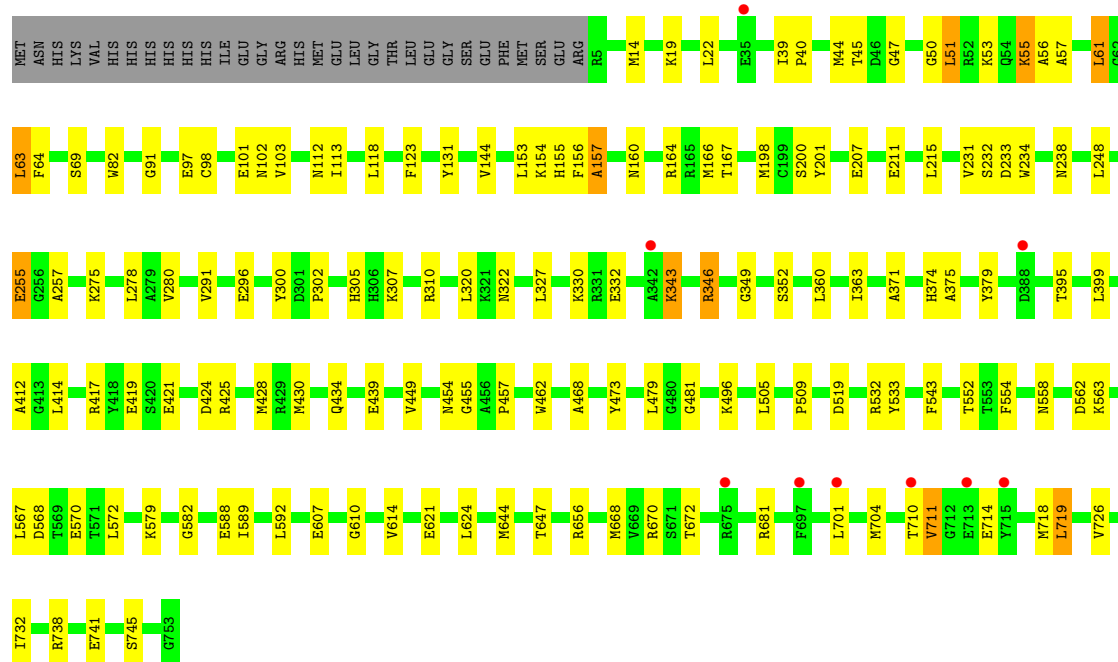
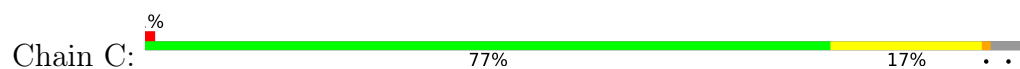


• Molecule 1: Beta-glucosidase

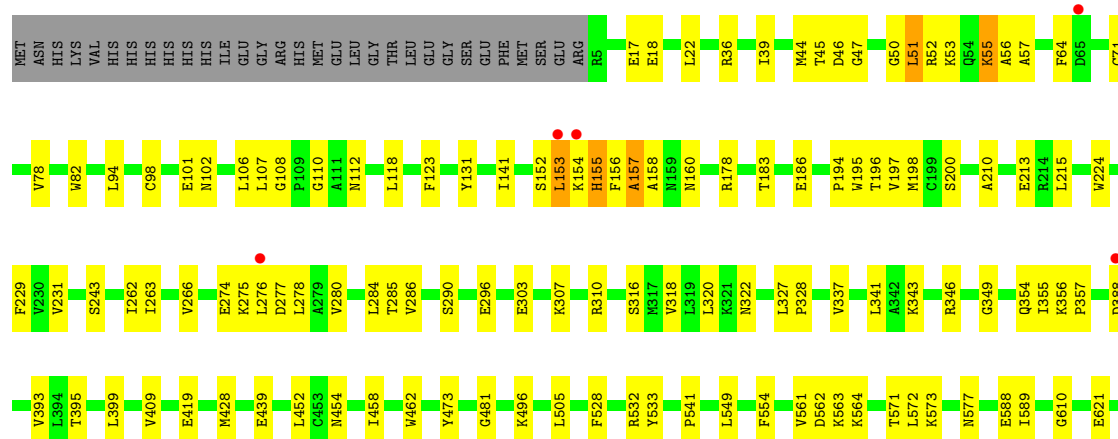
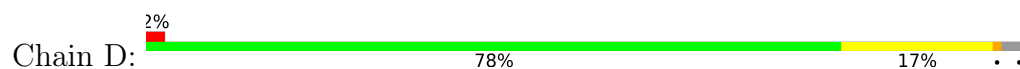


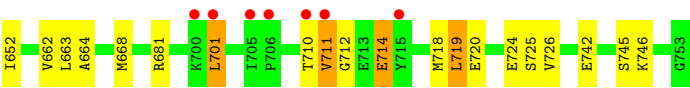


• Molecule 1: Beta-glucosidase



• Molecule 1: Beta-glucosidase





4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	65.30Å 113.25Å 158.66Å 71.47° 82.68° 79.83°	Depositor
Resolution (Å)	47.60 – 2.85 47.60 – 2.85	Depositor EDS
% Data completeness (in resolution range)	99.7 (47.60-2.85) 99.7 (47.60-2.85)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.64 (at 2.86Å)	Xtriage
Refinement program	REFMAC 5.8.0405, PHENIX 1.20.1-4487	Depositor
R, R_{free}	0.232 , 0.282 0.232 , 0.282	Depositor DCC
R_{free} test set	5067 reflections (5.13%)	wwPDB-VP
Wilson B-factor (Å ²)	23.2	Xtriage
Anisotropy	0.087	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 46.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.25$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.86	EDS
Total number of atoms	23612	wwPDB-VP
Average B, all atoms (Å ²)	20.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 10.32% 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

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	0.48	0/5876	0.69	2/7947 (0.0%)
1	B	0.48	0/5867	0.69	2/7934 (0.0%)
1	C	0.46	0/5906	0.67	6/7988 (0.1%)
1	D	0.47	0/5898	0.68	2/7978 (0.0%)
All	All	0.47	0/23547	0.68	12/31847 (0.0%)

There are no bond length outliers.

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	154	LYS	CA-C-N	6.37	133.70	121.54
1	B	154	LYS	C-N-CA	6.37	133.70	121.54
1	C	558	ASN	CB-CA-C	-5.87	104.30	111.82
1	C	154	LYS	CA-C-N	5.53	132.11	121.54
1	C	154	LYS	C-N-CA	5.53	132.11	121.54
1	A	154	LYS	CA-C-N	5.46	131.97	121.54
1	A	154	LYS	C-N-CA	5.46	131.97	121.54
1	C	346	ARG	CA-CB-CG	-5.46	103.17	114.10
1	C	156	PHE	CA-C-N	5.12	131.32	121.54
1	C	156	PHE	C-N-CA	5.12	131.32	121.54
1	D	156	PHE	CA-C-N	5.08	131.25	121.54
1	D	156	PHE	C-N-CA	5.08	131.25	121.54

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	5765	0	5716	82	0
1	B	5756	0	5713	87	0
1	C	5795	0	5743	81	0
1	D	5787	0	5737	86	0
2	A	6	0	8	1	0
2	B	6	0	8	1	0
2	D	6	0	8	0	0
3	A	109	0	0	9	0
3	B	136	0	0	8	0
3	C	109	0	0	6	0
3	D	137	0	0	8	0
All	All	23612	0	22933	328	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 (328) 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:D:110:GLY:HA2	1:D:154:LYS:HB2	1.50	0.93
1:C:496:LYS:HD2	1:C:589:ILE:HB	1.64	0.80
1:A:82:TRP:HB2	1:A:589:ILE:HD13	1.69	0.75
1:B:554:PHE:O	1:B:656:ARG:NH2	2.21	0.73
1:A:701:LEU:O	1:A:703:GLY:N	2.21	0.72
1:A:701:LEU:C	1:A:703:GLY:H	1.98	0.71
1:D:110:GLY:CA	1:D:154:LYS:HB2	2.19	0.71
1:B:496:LYS:HD2	1:B:589:ILE:HB	1.73	0.70
1:D:82:TRP:HB2	1:D:589:ILE:HD13	1.72	0.70
1:D:496:LYS:HD2	1:D:589:ILE:HB	1.74	0.70
1:A:554:PHE:O	1:A:656:ARG:NH2	2.26	0.69
1:C:82:TRP:HB2	1:C:589:ILE:HD13	1.76	0.68
1:B:270:GLN:NE2	1:D:213:GLU:OE2	2.27	0.67
1:B:113:ILE:O	1:B:160:ASN:ND2	2.29	0.66
1:D:108:GLY:HA2	1:D:154:LYS:HG3	1.78	0.66
1:A:16:LEU:N	3:A:901:HOH:O	2.24	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:323:GLU:HG2	3:A:999:HOH:O	1.96	0.65
1:C:567:LEU:HD12	1:C:570:GLU:OE2	1.97	0.64
1:D:47:GLY:HA3	1:D:50:GLY:O	1.98	0.63
1:B:328:PRO:HB3	1:B:551:TYR:CE2	2.33	0.63
1:C:22:LEU:HD12	1:C:280:VAL:HG13	1.79	0.63
1:C:55:LYS:H	1:C:55:LYS:HD2	1.63	0.62
1:D:710:THR:O	1:D:712:GLY:N	2.32	0.62
1:A:57:ALA:HB1	1:A:64:PHE:HD2	1.65	0.61
1:D:195:TRP:HZ3	1:D:290:SER:HB3	1.64	0.61
1:D:346:ARG:HH22	1:D:419:GLU:HB2	1.66	0.61
1:D:57:ALA:HA	3:D:905:HOH:O	2.00	0.61
1:B:310:ARG:CZ	1:B:481:GLY:HA3	2.30	0.61
1:C:112:ASN:OD1	1:C:155:HIS:HB2	2.00	0.61
1:C:310:ARG:HD2	3:C:839:HOH:O	2.02	0.60
1:C:47:GLY:HA3	1:C:50:GLY:O	2.02	0.60
1:B:102:ASN:HB2	3:B:1000:HOH:O	2.02	0.60
1:A:40:PRO:HG3	1:A:291:VAL:HG21	1.84	0.59
1:B:663:LEU:HA	3:B:1001:HOH:O	2.01	0.59
1:C:425:ARG:NH2	1:C:457:PRO:O	2.29	0.59
1:A:47:GLY:HA3	1:A:50:GLY:O	2.02	0.59
1:B:47:GLY:HA3	1:B:50:GLY:O	2.03	0.59
1:B:55:LYS:HE3	1:B:67:VAL:HG22	1.85	0.59
1:B:697:PHE:CE2	1:B:701:LEU:HD13	2.38	0.58
1:A:662:VAL:HG23	1:A:663:LEU:HG	1.84	0.58
1:C:568:ASP:OD2	1:C:672:THR:N	2.35	0.57
1:A:362:ASP:HB3	1:A:365:PHE:HB3	1.86	0.57
1:B:112:ASN:OD1	1:B:155:HIS:HB2	2.05	0.57
1:D:55:LYS:H	1:D:55:LYS:HD2	1.69	0.57
1:D:742:GLU:HG3	1:D:746:LYS:HE2	1.86	0.57
1:D:152:SER:HA	1:D:196:THR:O	2.05	0.57
1:C:47:GLY:HA2	3:C:845:HOH:O	2.04	0.56
1:D:57:ALA:HB1	1:D:64:PHE:HD2	1.70	0.56
1:A:572:LEU:HD12	1:A:573:LYS:H	1.69	0.56
1:C:113:ILE:O	1:C:160:ASN:ND2	2.37	0.56
1:C:562:ASP:OD1	1:C:563:LYS:N	2.38	0.56
1:D:44:MET:HE2	1:D:107:LEU:HD21	1.88	0.56
1:C:352:SER:OG	1:C:421:GLU:OE1	2.23	0.56
1:D:18:GLU:OE1	1:D:36:ARG:NH1	2.39	0.55
1:D:153:LEU:HG	1:D:197:VAL:HG22	1.88	0.55
1:B:110:GLY:HA2	1:B:154:LYS:HG2	1.88	0.55
1:D:562:ASP:OD1	1:D:563:LYS:N	2.39	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:14:MET:HE1	1:B:284:LEU:HD11	1.88	0.55
1:A:264:GLU:HG2	3:A:979:HOH:O	2.07	0.55
1:B:157:ALA:HB3	1:B:200:SER:OG	2.06	0.55
1:A:454:ASN:O	1:A:473:TYR:HA	2.06	0.54
1:B:171:VAL:HB	1:B:522:GLU:HA	1.89	0.54
1:C:614:VAL:HB	1:C:624:LEU:HD21	1.89	0.54
1:A:229:PHE:HE2	1:A:286:VAL:HB	1.72	0.54
1:C:704:MET:HG2	1:C:738:ARG:NH2	2.23	0.54
1:D:153:LEU:HB2	1:D:197:VAL:HG22	1.90	0.54
1:B:123:PHE:CE2	1:B:349:GLY:HA3	2.42	0.54
1:B:509:PRO:HB3	1:B:533:TYR:CD1	2.43	0.53
1:A:310:ARG:CZ	1:A:481:GLY:HA3	2.39	0.53
1:B:32:GLN:NE2	3:B:903:HOH:O	2.33	0.53
1:A:644:MET:HE2	1:A:645:VAL:H	1.74	0.53
1:A:17:GLU:HG3	1:A:263:ILE:HD13	1.91	0.53
1:D:55:LYS:HG2	1:D:56:ALA:H	1.73	0.52
1:B:419:GLU:OE2	1:B:455:GLY:N	2.40	0.52
1:A:51:LEU:HD11	1:A:98:CYS:SG	2.50	0.52
1:A:568:ASP:OD2	1:A:672:THR:N	2.39	0.52
1:A:701:LEU:HD21	1:A:731:LEU:HD13	1.92	0.52
1:B:40:PRO:HG3	1:B:291:VAL:HG21	1.90	0.52
1:B:47:GLY:HA2	3:B:968:HOH:O	2.09	0.52
1:C:395:THR:O	1:C:399:LEU:HG	2.10	0.52
1:D:112:ASN:OD1	1:D:155:HIS:HB2	2.10	0.52
1:C:61:LEU:HG	1:D:718:MET:CE	2.40	0.52
1:D:17:GLU:HG3	1:D:263:ILE:HD13	1.92	0.52
1:D:577:ASN:HB3	1:D:621:GLU:OE2	2.09	0.52
1:B:681:ARG:NH1	1:B:741:GLU:OE2	2.43	0.52
1:D:318:VAL:HG23	3:D:987:HOH:O	2.09	0.51
1:B:60:HIS:O	2:B:801:GOL:H32	2.11	0.51
1:D:22:LEU:HD12	1:D:280:VAL:HG13	1.91	0.51
1:C:91:GLY:O	1:C:144:VAL:HA	2.11	0.51
1:C:346:ARG:HH22	1:C:419:GLU:HB2	1.76	0.51
1:B:174:GLU:OE1	1:B:214:ARG:NH2	2.43	0.51
1:A:123:PHE:CE2	1:A:349:GLY:HA3	2.45	0.51
1:C:55:LYS:HG2	1:C:56:ALA:H	1.76	0.51
1:C:496:LYS:HE2	1:C:656:ARG:O	2.10	0.51
1:B:387:SER:HG	1:B:389:ASP:H	1.57	0.51
1:C:44:MET:HE1	1:C:231:VAL:HG21	1.93	0.50
1:A:328:PRO:HB3	1:A:551:TYR:CE2	2.46	0.50
1:C:211:GLU:OE1	1:C:238:ASN:HB3	2.12	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:561:VAL:HB	1:D:572:LEU:HD11	1.94	0.50
1:B:637:ASP:OD2	1:B:644:MET:HE2	2.10	0.50
1:C:310:ARG:CZ	1:C:481:GLY:HA3	2.41	0.50
1:A:509:PRO:HB3	1:A:533:TYR:CD2	2.47	0.50
1:B:213:GLU:HG3	1:B:246:ALA:HA	1.93	0.50
1:C:198:MET:HA	1:C:231:VAL:O	2.11	0.50
1:B:683:SER:O	1:B:728:LEU:HG	2.12	0.49
1:A:557:SER:O	1:A:577:ASN:HB2	2.11	0.49
1:B:257:ALA:HB2	3:B:1017:HOH:O	2.11	0.49
1:A:371:ALA:HB1	1:A:375:ALA:HB3	1.94	0.49
1:B:44:MET:HE2	1:B:107:LEU:HD21	1.94	0.49
1:A:46:ASP:HA	1:A:107:LEU:HB2	1.95	0.49
1:A:579:LYS:HG3	1:A:621:GLU:HB2	1.94	0.49
1:C:123:PHE:CE2	1:C:349:GLY:HA3	2.47	0.49
1:A:186:GLU:HG3	1:A:224:TRP:CE2	2.47	0.49
1:A:198:MET:HA	1:A:231:VAL:O	2.12	0.49
1:D:310:ARG:CZ	1:D:481:GLY:HA3	2.42	0.48
1:D:462:TRP:H	1:D:462:TRP:CD1	2.31	0.48
1:B:395:THR:O	1:B:399:LEU:HG	2.12	0.48
1:D:662:VAL:HG23	1:D:663:LEU:HG	1.93	0.48
1:A:44:MET:HE2	1:A:107:LEU:HD21	1.95	0.48
1:B:387:SER:OG	1:B:388:ASP:N	2.46	0.48
1:C:51:LEU:HD11	1:C:98:CYS:SG	2.53	0.48
1:D:356:LYS:HD2	1:D:357:PRO:HD2	1.96	0.48
1:D:341:LEU:HD22	3:D:914:HOH:O	2.12	0.48
1:A:722:PHE:O	1:A:726:VAL:HG23	2.14	0.48
1:B:73:PRO:HG2	1:B:312:ILE:HG22	1.95	0.48
1:C:40:PRO:HG3	1:C:291:VAL:HG21	1.96	0.48
1:D:141:ILE:HD13	1:D:194:PRO:HB3	1.95	0.48
1:A:718:MET:HE2	1:B:61:LEU:HD13	1.94	0.48
1:C:419:GLU:OE2	1:C:455:GLY:N	2.36	0.48
1:D:554:PHE:CZ	1:D:588:GLU:HB2	2.49	0.48
1:A:562:ASP:OD1	1:A:563:LYS:N	2.47	0.48
1:B:428:MET:HG3	1:B:505:LEU:HD13	1.96	0.48
1:C:462:TRP:CD1	1:C:462:TRP:H	2.31	0.48
1:C:53:LYS:HD2	1:C:101:GLU:HB3	1.96	0.47
1:B:561:VAL:HB	1:B:572:LEU:HD11	1.95	0.47
1:D:178:ARG:O	1:D:183:THR:OG1	2.25	0.47
1:A:154:LYS:HD2	1:A:155:HIS:NE2	2.29	0.47
1:A:607:GLU:O	1:A:609:LYS:HG2	2.14	0.47
1:B:322:ASN:ND2	1:B:327:LEU:HB2	2.29	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:91:GLY:O	1:A:144:VAL:HA	2.14	0.47
1:A:496:LYS:HD2	1:A:589:ILE:HB	1.95	0.47
1:A:652:ILE:O	1:A:664:ALA:HA	2.15	0.47
1:B:355:ILE:HD11	3:B:968:HOH:O	2.15	0.47
1:A:572:LEU:HD12	1:A:573:LYS:N	2.29	0.47
1:B:595:ARG:HD3	1:B:651:GLU:OE1	2.15	0.47
1:D:454:ASN:O	1:D:473:TYR:HA	2.14	0.47
1:C:63:LEU:HD21	1:D:719:LEU:HG	1.97	0.47
1:C:371:ALA:HB1	1:C:375:ALA:HB3	1.97	0.47
1:C:275:LYS:HA	1:C:275:LYS:HD3	1.66	0.46
1:D:718:MET:HE3	1:D:718:MET:HB2	1.72	0.46
1:A:53:LYS:HD2	1:A:101:GLU:HB3	1.97	0.46
1:A:19:LYS:HG2	1:A:280:VAL:HG21	1.96	0.46
1:B:647:THR:HG23	1:B:670:ARG:HA	1.96	0.46
1:D:53:LYS:HD2	1:D:101:GLU:HB3	1.97	0.46
1:D:276:LEU:O	1:D:280:VAL:HG23	2.14	0.46
1:D:337:VAL:HA	1:D:409:VAL:O	2.15	0.46
1:A:715:TYR:OH	1:B:354:GLN:NE2	2.47	0.46
1:B:164:ARG:NE	1:B:519:ASP:OD1	2.41	0.46
1:D:395:THR:O	1:D:399:LEU:HG	2.16	0.46
1:C:19:LYS:HG2	1:C:280:VAL:HG21	1.98	0.46
1:C:61:LEU:HG	1:D:718:MET:HE2	1.96	0.46
1:C:509:PRO:HB3	1:C:533:TYR:CD2	2.50	0.46
1:A:112:ASN:OD1	1:A:155:HIS:HB2	2.16	0.46
1:C:343:LYS:HD3	1:C:379:TYR:CZ	2.51	0.46
1:A:18:GLU:HB3	1:A:34:ILE:HD13	1.97	0.46
1:B:668:MET:HB3	1:B:668:MET:HE3	1.57	0.46
1:C:255:GLU:OE2	1:C:257:ALA:HB3	2.16	0.46
1:A:175:ARG:NH2	1:A:527:LEU:HD11	2.31	0.46
1:B:198:MET:HA	1:B:231:VAL:O	2.16	0.46
1:D:274:GLU:HA	1:D:277:ASP:HB2	1.98	0.46
1:B:141:ILE:HB	1:B:192:ALA:HB1	1.99	0.45
1:D:322:ASN:ND2	1:D:327:LEU:HB2	2.31	0.45
1:C:167:THR:HB	1:C:519:ASP:OD2	2.16	0.45
1:A:577:ASN:OD1	1:A:623:THR:OG1	2.35	0.45
1:B:52:ARG:HG3	1:B:354:GLN:O	2.16	0.45
1:B:161:GLN:HB3	1:B:514:PHE:HE1	1.82	0.45
1:B:186:GLU:HG3	1:B:224:TRP:CE2	2.52	0.45
1:D:356:LYS:HD2	1:D:357:PRO:CD	2.46	0.45
1:B:229:PHE:HE2	1:B:286:VAL:HB	1.82	0.45
1:D:123:PHE:CE2	1:D:349:GLY:HA3	2.51	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:39:ILE:HD13	1:D:284:LEU:HD21	1.99	0.45
1:A:60:HIS:O	2:A:801:GOL:H32	2.15	0.45
1:B:699:GLN:C	1:B:701:LEU:H	2.25	0.45
1:C:51:LEU:HD21	1:C:103:VAL:HG21	1.98	0.45
1:D:46:ASP:HA	1:D:107:LEU:HB2	1.98	0.45
1:A:616:LEU:HD23	1:A:622:LYS:HE3	1.99	0.45
1:C:454:ASN:O	1:C:473:TYR:HA	2.18	0.45
1:C:554:PHE:CE2	1:C:588:GLU:HB2	2.52	0.44
1:D:102:ASN:HB2	3:D:1004:HOH:O	2.16	0.44
1:A:565:GLU:HG2	3:A:976:HOH:O	2.17	0.44
1:D:198:MET:HA	1:D:231:VAL:O	2.18	0.44
1:D:572:LEU:HD12	1:D:573:LYS:H	1.82	0.44
1:D:701:LEU:HD13	1:D:701:LEU:HA	1.75	0.44
1:B:319:LEU:HD23	1:B:549:LEU:HB2	2.00	0.44
1:D:720:GLU:HG3	1:D:724:GLU:OE2	2.18	0.44
1:A:300:TYR:O	1:A:302:PRO:HD3	2.17	0.44
1:A:541:PRO:HA	3:A:944:HOH:O	2.16	0.44
1:A:653:LEU:HD22	1:A:661:ILE:HG21	1.98	0.44
1:B:255:GLU:OE1	1:B:257:ALA:HB3	2.17	0.44
1:C:44:MET:HE2	1:C:234:TRP:HH2	1.82	0.44
1:C:417:ARG:NH1	3:C:810:HOH:O	2.44	0.44
1:B:562:ASP:OD1	1:B:563:LYS:N	2.50	0.44
1:B:579:LYS:HB2	1:B:621:GLU:HB2	2.00	0.44
1:D:210:ALA:O	1:D:243:SER:OG	2.33	0.44
1:D:52:ARG:HG3	1:D:354:GLN:O	2.18	0.44
1:D:262:ILE:O	1:D:266:VAL:HG23	2.18	0.44
1:A:537:LYS:HB3	3:A:936:HOH:O	2.17	0.44
1:A:719:LEU:HD23	1:A:719:LEU:HA	1.82	0.44
1:C:157:ALA:HB3	1:C:200:SER:OG	2.17	0.44
1:A:561:VAL:HB	1:A:572:LEU:HD11	2.00	0.43
1:B:454:ASN:O	1:B:473:TYR:HA	2.17	0.43
1:C:102:ASN:HB2	3:C:898:HOH:O	2.17	0.43
1:C:232:SER:HB3	1:C:248:LEU:HD11	2.00	0.43
1:C:552:THR:OG1	1:C:582:GLY:HA3	2.18	0.43
1:D:131:TYR:CE2	1:D:610:GLY:HA2	2.53	0.43
1:A:347:TYR:CE1	1:A:348:GLN:HG2	2.53	0.43
1:C:505:LEU:HB2	3:C:879:HOH:O	2.17	0.43
1:A:157:ALA:HB3	1:A:200:SER:OG	2.19	0.43
1:D:274:GLU:O	1:D:278:LEU:HD13	2.19	0.43
1:B:123:PHE:CZ	1:B:349:GLY:HA3	2.54	0.43
1:B:362:ASP:HB3	1:B:365:PHE:HB3	2.00	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:705:ILE:CD1	1:B:723:LYS:HG2	2.48	0.43
1:A:496:LYS:HE2	1:A:656:ARG:O	2.18	0.43
1:B:24:THR:HB	3:B:1009:HOH:O	2.19	0.43
1:A:504:GLN:HG2	1:A:507:ASP:OD2	2.19	0.43
1:C:233:ASP:OD1	1:C:234:TRP:N	2.44	0.43
1:C:320:LEU:HD22	1:C:543:PHE:CD1	2.53	0.43
1:C:711:VAL:HG21	1:C:719:LEU:HD12	2.00	0.43
1:B:249:GLU:HB3	1:B:283:LEU:HD21	2.00	0.43
1:D:532:ARG:NH1	3:D:908:HOH:O	2.42	0.43
1:B:275:LYS:HA	1:B:275:LYS:HD3	1.87	0.43
1:C:300:TYR:O	1:C:302:PRO:HD3	2.17	0.43
1:A:47:GLY:HA2	3:A:973:HOH:O	2.18	0.43
1:B:574:VAL:HB	1:B:626:PHE:HB2	2.01	0.43
1:C:164:ARG:NE	1:C:519:ASP:OD1	2.48	0.43
1:C:166:MET:HA	1:C:201:TYR:HB3	2.01	0.43
1:B:373:GLU:OE1	3:B:901:HOH:O	2.21	0.43
1:B:428:MET:HE2	1:B:428:MET:HB3	1.78	0.43
1:D:318:VAL:HG12	1:D:320:LEU:HG	2.01	0.43
1:D:652:ILE:O	1:D:664:ALA:HA	2.19	0.43
1:B:231:VAL:HG23	1:B:250:LEU:HB3	2.01	0.42
1:B:705:ILE:HD13	1:B:723:LYS:HG2	2.01	0.42
1:C:97:GLU:OE2	1:C:305:HIS:ND1	2.39	0.42
1:A:22:LEU:HD12	1:A:280:VAL:HG13	2.01	0.42
1:D:528:PHE:O	1:D:533:TYR:HB2	2.18	0.42
1:D:714:GLU:H	1:D:714:GLU:HG3	1.53	0.42
1:A:498:ALA:HB3	3:A:992:HOH:O	2.20	0.42
1:B:110:GLY:CA	1:B:154:LYS:HG2	2.49	0.42
1:D:158:ALA:HB1	1:D:160:ASN:OD1	2.18	0.42
1:D:186:GLU:HG3	1:D:224:TRP:CE2	2.54	0.42
1:D:328:PRO:HD2	3:D:980:HOH:O	2.19	0.42
1:A:567:LEU:HD12	1:A:570:GLU:OE2	2.19	0.42
1:B:233:ASP:OD1	1:B:234:TRP:N	2.48	0.42
1:B:706:PRO:HD3	1:B:734:PHE:O	2.20	0.42
1:C:57:ALA:HB1	1:C:64:PHE:HD2	1.85	0.42
1:A:304:ALA:O	1:A:307:LYS:HB2	2.19	0.42
1:A:668:MET:HE3	1:A:668:MET:HB3	1.82	0.42
1:C:668:MET:HE3	1:C:668:MET:HB3	1.72	0.42
1:D:71:CYS:HB2	1:D:355:ILE:HB	2.02	0.42
1:A:166:MET:HE2	1:A:166:MET:HB3	1.95	0.42
1:A:301:ASP:OD1	1:A:303:GLU:HB3	2.20	0.42
1:A:717:GLU:HB3	1:B:423:PHE:CE2	2.55	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:118:LEU:O	1:C:424:ASP:HB3	2.20	0.42
1:C:363:ILE:HD11	1:C:479:LEU:HD11	2.00	0.42
1:C:532:ARG:NH2	1:C:607:GLU:HG2	2.34	0.42
1:D:229:PHE:HE2	1:D:286:VAL:HB	1.84	0.42
1:D:310:ARG:HD2	3:D:946:HOH:O	2.20	0.42
1:D:668:MET:HE3	1:D:668:MET:HB3	1.82	0.42
1:B:82:TRP:HB2	1:B:589:ILE:HD13	2.00	0.42
1:D:541:PRO:HA	3:D:906:HOH:O	2.19	0.42
1:B:7:LEU:HD23	1:B:7:LEU:HA	1.80	0.41
1:C:330:LYS:HD3	1:C:332:GLU:OE2	2.20	0.41
1:C:732:ILE:HD13	1:C:741:GLU:HG2	2.02	0.41
1:D:94:LEU:HD13	1:D:106:LEU:HD21	2.02	0.41
1:B:42:VAL:HB	1:B:104:ALA:CB	2.51	0.41
1:B:348:GLN:C	1:B:474:LEU:HD13	2.45	0.41
1:A:751:LEU:HD23	1:A:751:LEU:HA	1.82	0.41
1:B:166:MET:HE2	1:B:166:MET:HB3	1.78	0.41
1:C:322:ASN:ND2	1:C:327:LEU:HB2	2.35	0.41
1:C:718:MET:HE3	1:C:718:MET:HB2	1.90	0.41
1:D:452:LEU:HD13	1:D:458:ILE:HD11	2.01	0.41
1:A:525:GLU:CD	1:A:525:GLU:H	2.28	0.41
1:A:701:LEU:C	1:A:703:GLY:N	2.65	0.41
1:C:55:LYS:HG2	3:C:812:HOH:O	2.19	0.41
1:A:501:PHE:O	1:A:542:LEU:HB3	2.20	0.41
1:B:652:ILE:O	1:B:664:ALA:HA	2.21	0.41
1:C:579:LYS:HG3	1:C:621:GLU:HB2	2.01	0.41
1:D:51:LEU:HD11	1:D:98:CYS:SG	2.61	0.41
1:D:303:GLU:OE2	1:D:303:GLU:HA	2.08	0.41
1:A:217:THR:HA	1:A:221:LYS:HB2	2.02	0.41
1:B:55:LYS:H	1:B:55:LYS:HG2	1.34	0.41
1:C:131:TYR:CE2	1:C:610:GLY:HA2	2.55	0.41
1:A:24:THR:HB	3:A:984:HOH:O	2.20	0.41
1:A:166:MET:HA	1:A:201:TYR:HB3	2.01	0.41
1:B:53:LYS:O	1:B:66:SER:HB2	2.21	0.41
1:C:332:GLU:HA	1:C:374:HIS:O	2.21	0.41
1:C:421:GLU:O	1:D:718:MET:HE3	2.21	0.41
1:D:78:VAL:HA	1:D:316:SER:OG	2.21	0.41
1:A:44:MET:HE2	1:A:234:TRP:HH2	1.85	0.41
1:A:348:GLN:C	1:A:474:LEU:HD13	2.46	0.41
1:B:9:ALA:O	1:B:12:SER:OG	2.35	0.41
1:D:153:LEU:HD22	1:D:153:LEU:HA	1.91	0.41
1:B:588:GLU:O	1:B:613:LYS:HA	2.21	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:718:MET:HE3	1:B:718:MET:HB2	1.96	0.40
1:C:428:MET:HE2	1:C:428:MET:HB3	1.73	0.40
1:A:303:GLU:OE1	1:A:303:GLU:HA	2.21	0.40
1:B:173:ASN:ND2	1:B:176:THR:H	2.19	0.40
1:C:14:MET:HE3	1:C:39:ILE:CD1	2.51	0.40
1:C:449:VAL:HG22	1:C:468:ALA:HB3	2.04	0.40
1:C:592:LEU:C	1:C:592:LEU:HD23	2.47	0.40
1:C:647:THR:HG23	1:C:670:ARG:HA	2.02	0.40
1:D:118:LEU:HD11	1:D:505:LEU:HD21	2.03	0.40
1:D:452:LEU:HD11	1:D:462:TRP:HH2	1.86	0.40
1:A:568:ASP:OD2	1:A:671:SER:HA	2.21	0.40
1:B:496:LYS:HE2	1:B:656:ARG:O	2.21	0.40
1:B:549:LEU:HA	1:B:549:LEU:HD23	1.88	0.40
1:C:430:MET:HB3	1:C:430:MET:HE2	1.80	0.40
1:C:554:PHE:CZ	1:C:588:GLU:HB2	2.56	0.40
1:D:157:ALA:HB3	1:D:200:SER:OG	2.21	0.40
1:A:39:ILE:HD13	1:A:284:LEU:HD21	2.03	0.40
1:A:53:LYS:O	1:A:66:SER:HB2	2.21	0.40
1:C:346:ARG:HD2	1:C:414:LEU:O	2.21	0.40
1:B:386:LYS:HD3	1:B:386:LYS:HA	1.92	0.40
1:B:454:ASN:OD1	1:B:471:GLU:OE2	2.39	0.40
1:C:412:ALA:HB1	1:C:434:GLN:OE1	2.22	0.40
1:D:55:LYS:H	1:D:55:LYS:CD	2.31	0.40
1:D:428:MET:HE2	1:D:428:MET:HB3	1.92	0.40
1:D:549:LEU:HA	1:D:549:LEU:HD23	1.88	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	741/780 (95%)	710 (96%)	26 (4%)	5 (1%)	18 35

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	740/780 (95%)	712 (96%)	26 (4%)	2 (0%)	36	54
1	C	747/780 (96%)	719 (96%)	27 (4%)	1 (0%)	48	68
1	D	747/780 (96%)	722 (97%)	22 (3%)	3 (0%)	30	48
All	All	2975/3120 (95%)	2863 (96%)	101 (3%)	11 (0%)	30	48

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	157	ALA
1	A	702	ARG
1	B	157	ALA
1	C	157	ALA
1	D	155	HIS
1	D	157	ALA
1	D	711	VAL
1	A	701	LEU
1	A	706	PRO
1	A	713	GLU
1	B	155	HIS

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	611/648 (94%)	598 (98%)	13 (2%)	47	70
1	B	610/648 (94%)	593 (97%)	17 (3%)	38	62
1	C	614/648 (95%)	588 (96%)	26 (4%)	26	51
1	D	613/648 (95%)	590 (96%)	23 (4%)	29	54
All	All	2448/2592 (94%)	2369 (97%)	79 (3%)	34	59

All (79) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	45	THR
1	A	51	LEU
1	A	55	LYS
1	A	215	LEU
1	A	275	LYS
1	A	343	LYS
1	A	564	LYS
1	A	644	MET
1	A	652	ILE
1	A	681	ARG
1	A	701	LEU
1	A	719	LEU
1	A	724	GLU
1	B	45	THR
1	B	51	LEU
1	B	55	LYS
1	B	69	SER
1	B	152	SER
1	B	215	LEU
1	B	296	GLU
1	B	356	LYS
1	B	416	LYS
1	B	439	GLU
1	B	606	LYS
1	B	623	THR
1	B	681	ARG
1	B	701	LEU
1	B	704	MET
1	B	719	LEU
1	B	745	SER
1	C	45	THR
1	C	51	LEU
1	C	55	LYS
1	C	61	LEU
1	C	63	LEU
1	C	69	SER
1	C	153	LEU
1	C	207	GLU
1	C	215	LEU
1	C	255	GLU
1	C	278	LEU
1	C	296	GLU
1	C	307	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	343	LYS
1	C	360	LEU
1	C	439	GLU
1	C	572	LEU
1	C	644	MET
1	C	681	ARG
1	C	701	LEU
1	C	710	THR
1	C	711	VAL
1	C	714	GLU
1	C	719	LEU
1	C	726	VAL
1	C	745	SER
1	D	45	THR
1	D	51	LEU
1	D	55	LYS
1	D	153	LEU
1	D	215	LEU
1	D	275	LYS
1	D	285	THR
1	D	296	GLU
1	D	307	LYS
1	D	343	LYS
1	D	388	ASP
1	D	393	VAL
1	D	439	GLU
1	D	564	LYS
1	D	571	THR
1	D	681	ARG
1	D	701	LEU
1	D	711	VAL
1	D	714	GLU
1	D	719	LEU
1	D	725	SER
1	D	726	VAL
1	D	745	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	147	GLN
1	A	161	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	293	GLN
1	A	294	HIS
1	A	513	ASN
1	A	538	GLN
1	B	147	GLN
1	B	270	GLN
1	B	293	GLN
1	B	354	GLN
1	B	400	GLN
1	C	381	GLN
1	C	513	ASN
1	D	102	ASN
1	D	238	ASN
1	D	270	GLN
1	D	513	ASN
1	D	538	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](#)

3 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
2	GOL	A	801	-	5,5,5	2.14	2 (40%)	5,5,5	0.73	0
2	GOL	D	801	-	5,5,5	1.42	1 (20%)	5,5,5	0.80	0
2	GOL	B	801	-	5,5,5	1.78	1 (20%)	5,5,5	1.07	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
2	GOL	A	801	-	-	2/4/4/4	-
2	GOL	D	801	-	-	2/4/4/4	-
2	GOL	B	801	-	-	4/4/4/4	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	801	GOL	C1-C2	4.07	1.67	1.51
2	B	801	GOL	C1-C2	3.40	1.64	1.51
2	D	801	GOL	C3-C2	2.54	1.61	1.51
2	A	801	GOL	C3-C2	2.17	1.60	1.51

There are no bond angle outliers.

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	801	GOL	O2-C2-C3-O3
2	A	801	GOL	C1-C2-C3-O3
2	B	801	GOL	O1-C1-C2-C3
2	B	801	GOL	C1-C2-C3-O3
2	D	801	GOL	O1-C1-C2-C3
2	D	801	GOL	O1-C1-C2-O2
2	B	801	GOL	O2-C2-C3-O3
2	B	801	GOL	O1-C1-C2-O2

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	801	GOL	1	0
2	B	801	GOL	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	745/780 (95%)	-0.06	8 (1%) 78 73	7, 17, 42, 84	0
1	B	744/780 (95%)	-0.03	13 (1%) 69 63	8, 16, 43, 74	0
1	C	749/780 (96%)	0.01	9 (1%) 76 71	9, 18, 46, 91	0
1	D	749/780 (96%)	-0.05	12 (1%) 70 64	7, 16, 42, 85	0
All	All	2987/3120 (95%)	-0.03	42 (1%) 73 67	7, 17, 44, 91	0

All (42) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	714	GLU	5.3
1	C	710	THR	4.9
1	D	715	TYR	4.1
1	D	711	VAL	4.0
1	A	715	TYR	3.5
1	B	714	GLU	3.5
1	B	702	ARG	3.4
1	B	715	TYR	3.2
1	D	705	ILE	2.9
1	C	35	GLU	2.7
1	B	708	GLY	2.7
1	A	707	PHE	2.7
1	D	388	ASP	2.7
1	A	712	GLY	2.6
1	D	706	PRO	2.6
1	C	715	TYR	2.6
1	B	701	LEU	2.5
1	C	697	PHE	2.4
1	D	710	THR	2.4
1	D	153	LEU	2.4
1	A	702	ARG	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	713	GLU	2.4
1	B	704	MET	2.4
1	D	154	LYS	2.3
1	B	697	PHE	2.3
1	C	713	GLU	2.3
1	C	701	LEU	2.3
1	B	703	GLY	2.3
1	B	705	ILE	2.2
1	D	65	ASP	2.2
1	B	65	ASP	2.1
1	A	65	ASP	2.1
1	B	333	GLY	2.1
1	D	276	LEU	2.1
1	C	675	ARG	2.1
1	B	724	GLU	2.1
1	D	701	LEU	2.0
1	C	388	ASP	2.0
1	B	598	GLU	2.0
1	D	700	LYS	2.0
1	A	705	ILE	2.0
1	C	342	ALA	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($\text{\AA}^2$)	Q<0.9
2	GOL	A	801	6/6	0.83	0.17	17,18,19,19	0
2	GOL	B	801	6/6	0.86	0.16	13,14,14,14	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	GOL	D	801	6/6	0.88	0.15	14,15,15,15	0

6.5 Other polymers [i](#)

There are no such residues in this entry.