



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 18, 2026 – 01:48 PM UTC

PDB ID : 3ABZ / pdb_00003abz
Title : Crystal structure of Se-Met labeled Beta-glucosidase from Kluyveromyces marxianus
Authors : Yoshida, E.; Hidaka, M.; Fushinobu, S.; Katayama, T.; Kumagai, H.
Deposited on : 2009-12-25
Resolution : 2.15 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

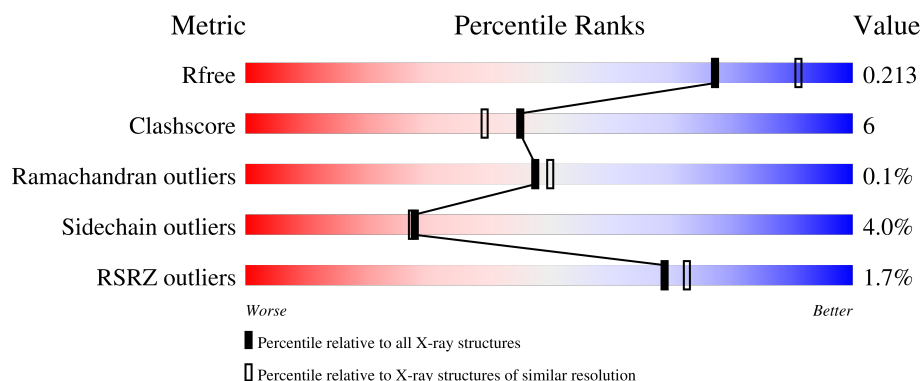
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.15 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	2057 (2.16-2.16)
Clashscore	190562	2159 (2.16-2.16)
Ramachandran outliers	187476	2134 (2.16-2.16)
Sidechain outliers	187428	2133 (2.16-2.16)
RSRZ outliers	180081	2059 (2.16-2.16)

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	845	% 87% 12% .
1	B	845	4% 80% 13% .
1	C	845	% 84% 13% ..
1	D	845	% 85% 12% ..

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
2	GOL	A	5002	-	-	X	-
2	GOL	B	5006	-	-	X	-

2 Entry composition [i](#)

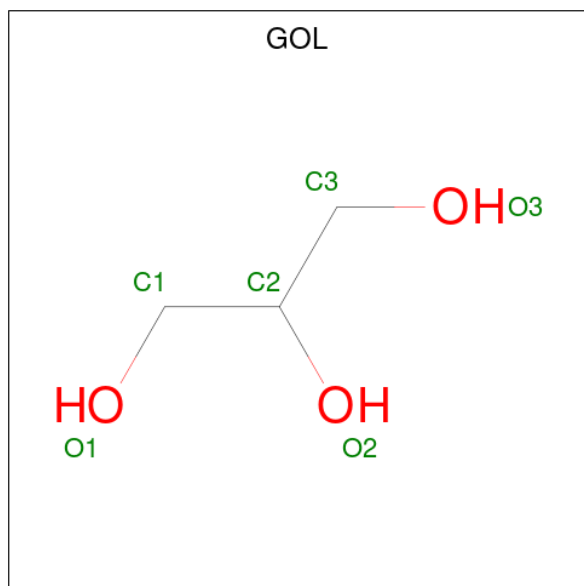
There are 3 unique types of molecules in this entry. The entry contains 29154 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 I.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	844	Total	C	N	O	S	Se	0	0	0
			6606	4197	1110	1284	5	10			
1	B	810	Total	C	N	O	S	Se	0	0	0
			6351	4040	1065	1232	4	10			
1	C	836	Total	C	N	O	S	Se	0	0	0
			6550	4161	1102	1272	5	10			
1	D	833	Total	C	N	O	S	Se	0	0	0
			6521	4146	1096	1264	5	10			

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



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

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

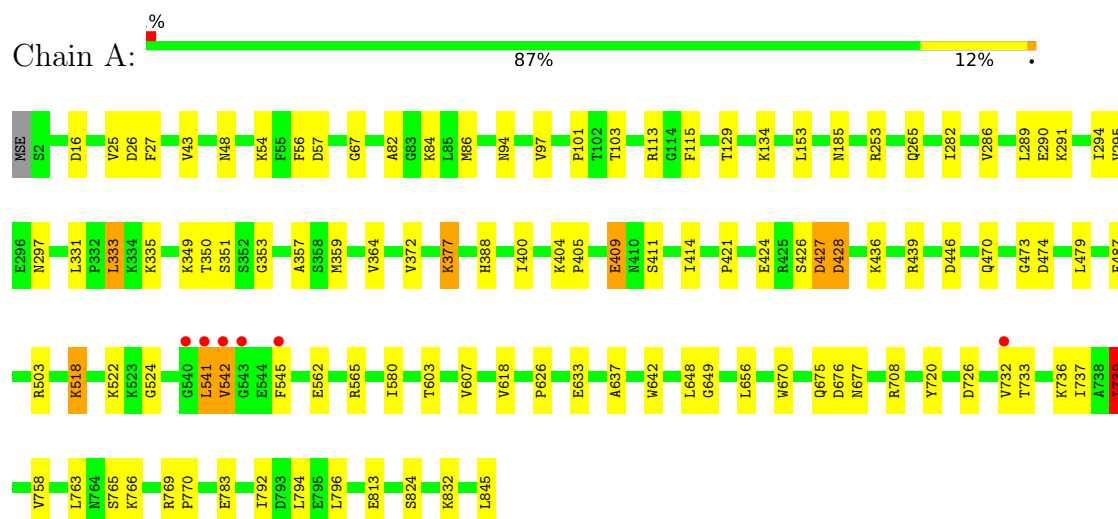
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	875	Total	O	0	0
			875	875		
3	B	828	Total	O	0	0
			828	828		
3	C	701	Total	O	0	0
			701	701		
3	D	674	Total	O	0	0
			674	674		

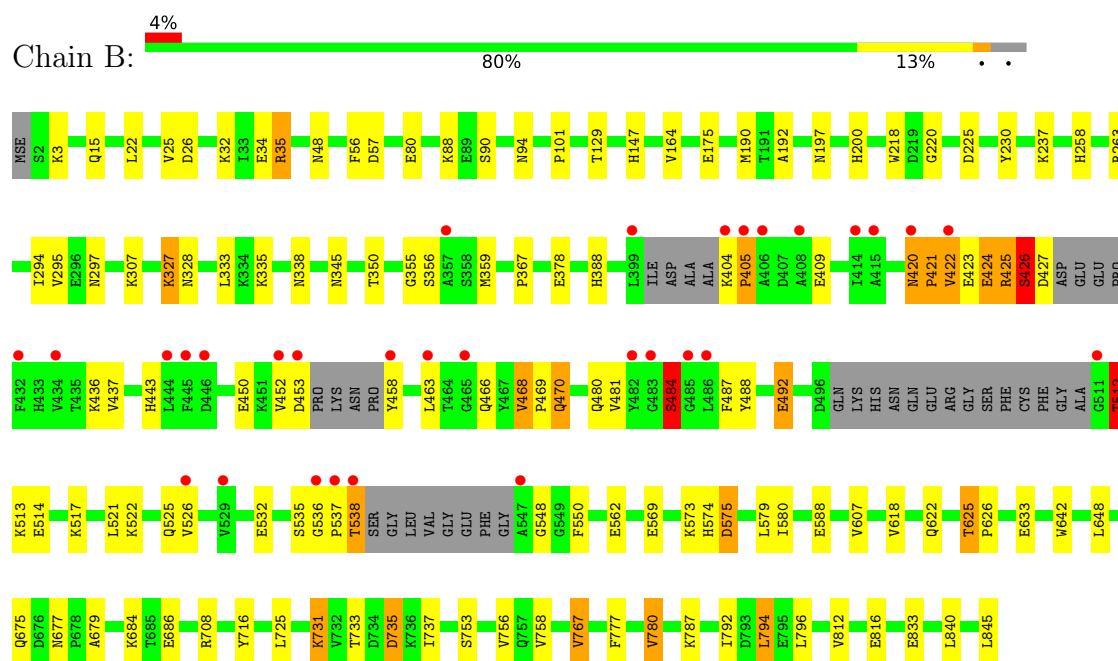
3 Residue-property plots

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.

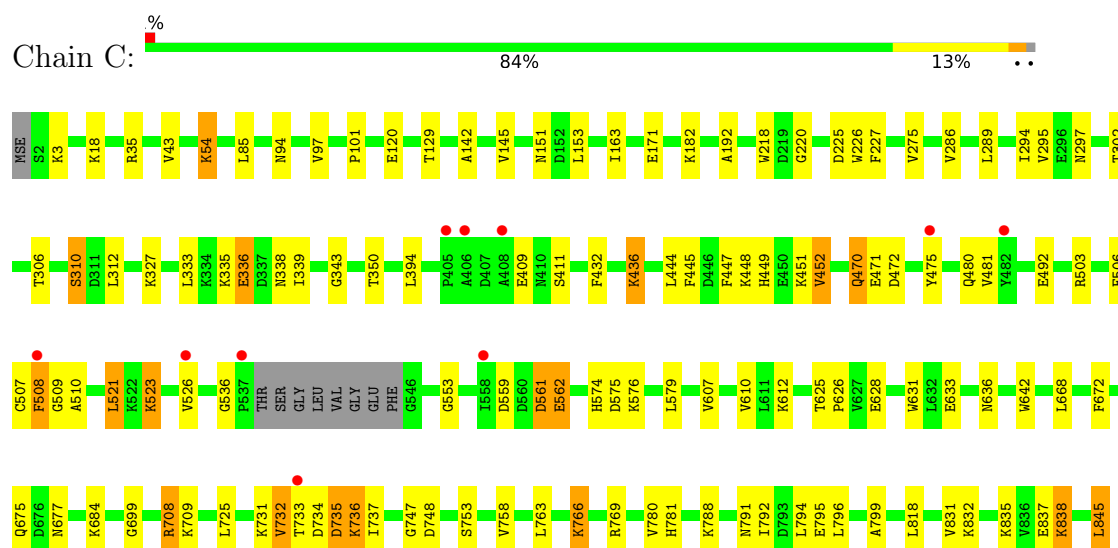
• Molecule 1: Beta-glucosidase I



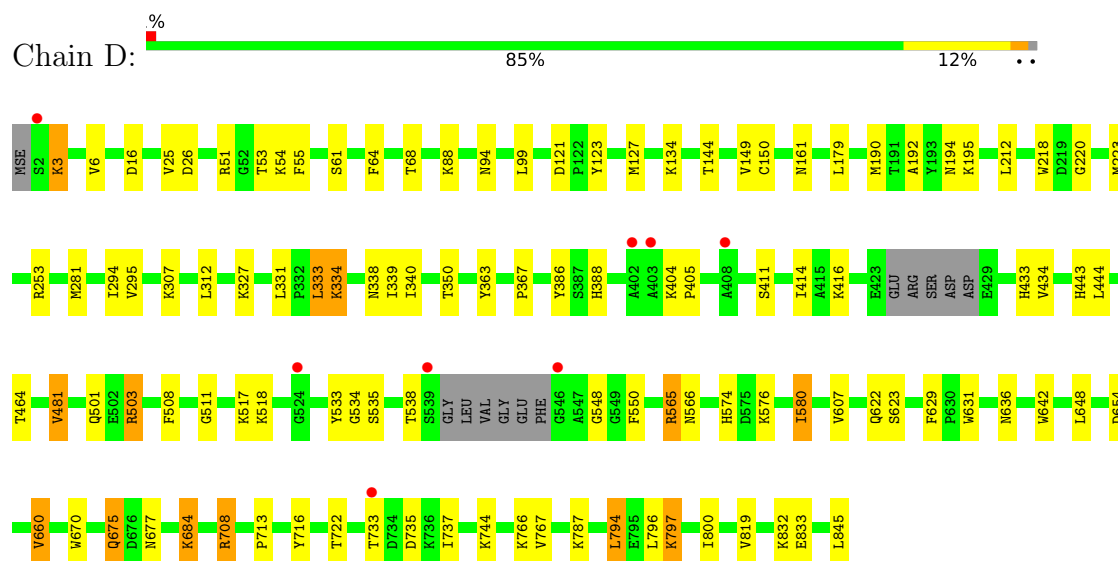
• Molecule 1: Beta-glucosidase I



• Molecule 1: Beta-glucosidase I



• Molecule 1: Beta-glucosidase I



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	245.68Å 148.64Å 119.78Å 90.00° 112.95° 90.00°	Depositor
Resolution (Å)	50.00 – 2.15 50.00 – 2.15	Depositor EDS
% Data completeness (in resolution range)	99.8 (50.00-2.15) 99.8 (50.00-2.15)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.03 (at 2.16Å)	Xtriage
Refinement program	REFMAC 5.5.0072	Depositor
R, R_{free}	0.160 , 0.218 0.156 , 0.213	Depositor DCC
R_{free} test set	10724 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	28.4	Xtriage
Anisotropy	0.039	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 48.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	29154	wwPDB-VP
Average B, all atoms (Å ²)	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.30% 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:
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	1.27	11/6733 (0.2%)	1.12	11/9088 (0.1%)
1	B	1.30	11/6466 (0.2%)	1.14	20/8720 (0.2%)
1	C	1.21	7/6675 (0.1%)	1.10	11/9008 (0.1%)
1	D	1.17	4/6645 (0.1%)	1.09	15/8967 (0.2%)
All	All	1.24	33/26519 (0.1%)	1.11	57/35783 (0.2%)

All (33) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	642	TRP	C-O	-7.53	1.16	1.24
1	A	185	ASN	CA-CB	7.17	1.57	1.52
1	B	26	ASP	C-O	-6.60	1.17	1.24
1	A	542	VAL	CA-CB	6.06	1.61	1.54
1	A	25	VAL	C-O	-5.96	1.17	1.24
1	B	716	TYR	C-O	5.89	1.31	1.23
1	A	265	GLN	C-O	-5.82	1.16	1.24
1	B	22	LEU	N-CA	5.75	1.53	1.46
1	A	27	PHE	C-O	-5.70	1.16	1.24
1	B	80	GLU	C-O	-5.66	1.17	1.24
1	B	679	ALA	CA-CB	5.60	1.61	1.53
1	A	282	ILE	CA-C	5.55	1.59	1.52
1	B	588	GLU	CA-C	-5.47	1.46	1.52
1	C	536	GLY	C-O	-5.44	1.18	1.24
1	C	642	TRP	C-O	-5.43	1.18	1.24
1	A	26	ASP	C-O	-5.42	1.19	1.24
1	C	625	THR	CA-CB	5.41	1.60	1.53
1	B	642	TRP	C-O	-5.36	1.18	1.24
1	B	625	THR	N-CA	5.28	1.50	1.46
1	D	26	ASP	C-O	-5.28	1.19	1.24
1	C	163	ILE	CA-CB	5.23	1.60	1.53
1	B	25	VAL	C-O	-5.22	1.18	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	90	SER	CA-C	5.13	1.59	1.52
1	C	171	GLU	N-CA	5.13	1.52	1.46
1	B	356	SER	CA-C	5.09	1.59	1.52
1	D	25	VAL	C-O	-5.09	1.18	1.24
1	D	797	LYS	C-O	-5.09	1.17	1.24
1	D	660	VAL	CA-CB	5.07	1.60	1.54
1	C	145	VAL	CA-C	5.07	1.58	1.52
1	C	452	VAL	CA-CB	5.06	1.60	1.53
1	A	294	ILE	CG1-CD1	-5.03	1.32	1.51
1	A	103	THR	CA-CB	5.02	1.58	1.53
1	A	626	PRO	C-O	5.01	1.29	1.23

All (57) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	548	GLY	N-CA-C	10.33	124.61	110.56
1	A	291	LYS	N-CA-C	8.18	119.83	111.07
1	B	424	GLU	N-CA-C	6.27	118.84	108.49
1	B	225	ASP	N-CA-C	-6.26	102.70	110.41
1	A	720	TYR	N-CA-C	-6.23	105.68	113.28
1	B	355	GLY	N-CA-C	6.21	120.49	111.24
1	A	783	GLU	CA-C-N	-6.17	113.32	119.93
1	A	783	GLU	C-N-CA	-6.17	113.32	119.93
1	D	121	ASP	CA-C-N	-6.10	113.40	119.56
1	D	121	ASP	C-N-CA	-6.10	113.40	119.56
1	C	339	ILE	N-CA-C	6.10	117.54	108.46
1	C	574	HIS	CA-C-N	5.90	128.10	120.44
1	C	574	HIS	C-N-CA	5.90	128.10	120.44
1	A	473	GLY	N-CA-C	5.83	118.30	110.43
1	A	739	ILE	CB-CA-C	5.81	118.81	110.33
1	B	25	VAL	N-CA-C	5.80	116.57	110.72
1	D	51	ARG	N-CA-C	5.74	118.48	111.82
1	B	175	GLU	CA-C-N	-5.71	113.14	119.19
1	B	175	GLU	C-N-CA	-5.71	113.14	119.19
1	D	68	THR	CA-C-N	5.70	126.15	119.94
1	D	68	THR	C-N-CA	5.70	126.15	119.94
1	B	575	ASP	CB-CA-C	-5.67	101.98	110.88
1	D	6	VAL	N-CA-C	5.65	116.10	110.23
1	D	464	THR	N-CA-C	5.60	117.90	109.23
1	A	113	ARG	NE-CZ-NH1	-5.55	115.95	121.50
1	B	468	VAL	N-CA-C	5.50	113.60	108.15
1	B	15	GLN	N-CA-C	5.49	117.27	111.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	512	THR	N-CA-C	5.47	117.75	110.53
1	B	484	SER	N-CA-C	5.47	118.32	108.48
1	D	670	TRP	CA-C-N	-5.40	115.02	120.31
1	D	670	TRP	C-N-CA	-5.40	115.02	120.31
1	D	53	THR	N-CA-C	5.39	119.72	113.20
1	C	747	GLY	N-CA-C	-5.36	103.31	112.64
1	C	171	GLU	CA-C-N	-5.36	117.67	123.08
1	C	171	GLU	C-N-CA	-5.36	117.67	123.08
1	D	481	VAL	N-CA-C	5.33	117.75	108.90
1	A	25	VAL	N-CA-C	5.33	116.11	110.72
1	B	767	VAL	N-CA-CB	-5.29	102.76	111.44
1	B	421	PRO	CA-C-N	5.29	127.70	120.46
1	B	421	PRO	C-N-CA	5.29	127.70	120.46
1	B	569	GLU	N-CA-C	-5.27	105.43	111.07
1	B	426	SER	N-CA-C	5.22	116.97	111.28
1	A	67	GLY	N-CA-C	5.21	119.19	112.83
1	D	3	LYS	N-CA-C	-5.21	106.93	113.28
1	A	763	LEU	CA-C-N	-5.21	114.14	122.62
1	A	763	LEU	C-N-CA	-5.21	114.14	122.62
1	B	422	VAL	N-CA-C	-5.18	105.34	110.62
1	C	732	VAL	N-CA-C	5.14	114.15	106.85
1	D	629	PHE	CA-C-N	-5.11	114.40	119.56
1	D	629	PHE	C-N-CA	-5.11	114.40	119.56
1	B	359	MSE	N-CA-C	5.06	115.01	107.88
1	B	263	ARG	NE-CZ-NH2	5.05	123.75	119.20
1	C	225	ASP	N-CA-C	-5.05	104.20	110.41
1	D	363	TYR	N-CA-C	-5.02	100.69	108.42
1	C	302	THR	N-CA-C	-5.02	106.90	112.57
1	C	343	GLY	CA-C-N	5.01	124.79	119.28
1	C	343	GLY	C-N-CA	5.01	124.79	119.28

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	6606	0	6514	71	0
1	B	6351	0	6279	90	0
1	C	6550	0	6460	80	0
1	D	6521	0	6439	65	0
2	A	24	0	32	10	0
2	B	12	0	16	5	0
2	C	6	0	8	0	0
2	D	6	0	8	0	0
3	A	875	0	0	14	0
3	B	828	0	0	18	0
3	C	701	0	0	15	0
3	D	674	0	0	10	0
All	All	29154	0	25756	304	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 6.

All (304) 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)
2:A:5001:GOL:H32	3:A:1983:HOH:O	1.54	1.05
1:C:734:ASP:O	1:C:735:ASP:HB3	1.57	1.04
1:A:737:ILE:HD11	1:A:796:LEU:HD23	1.41	1.01
1:C:338:ASN:HB3	1:C:575:ASP:HB2	1.53	0.91
1:D:134:LYS:HE2	3:D:2595:HOH:O	1.70	0.91
1:D:565:ARG:HG2	1:D:565:ARG:HH11	1.35	0.90
1:A:708:ARG:NH2	1:B:708:ARG:NH2	2.27	0.82
1:C:472:ASP:OD2	1:C:523:LYS:HB2	1.80	0.82
1:C:449:HIS:HD2	1:C:451:LYS:H	1.27	0.81
1:D:127:MSE:CE	1:D:179:LEU:HD22	2.12	0.80
1:B:48:ASN:HB3	3:B:2353:HOH:O	1.83	0.79
1:B:517:LYS:HD2	3:B:2238:HOH:O	1.82	0.79
1:B:484:SER:HB3	1:B:538:THR:OG1	1.83	0.78
1:A:84:LYS:HB3	1:A:84:LYS:HZ2	1.47	0.78
1:B:481:VAL:H	1:B:512:THR:HG22	1.48	0.78
1:A:404:LYS:HB3	1:A:405:PRO:HD2	1.66	0.77
1:C:736:LYS:HD2	1:C:737:ILE:N	1.99	0.77
1:A:297:ASN:HB2	3:A:2042:HOH:O	1.86	0.76
3:A:2133:HOH:O	1:B:675:GLN:HG2	1.86	0.75
1:B:350:THR:HG22	3:B:2411:HOH:O	1.88	0.74
1:C:411:SER:O	1:C:436:LYS:HE2	1.87	0.73
1:B:297:ASN:HB3	3:B:2349:HOH:O	1.88	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:758:VAL:HG21	1:A:792:ILE:HD13	1.71	0.72
1:A:439:ARG:H	2:A:5002:GOL:H11	1.54	0.72
1:A:57:ASP:H	2:A:5002:GOL:C3	2.02	0.72
1:B:562:GLU:HG2	3:B:2413:HOH:O	1.90	0.72
1:A:439:ARG:HB2	2:A:5002:GOL:H12	1.70	0.72
1:B:437:VAL:HG13	2:B:5006:GOL:H32	1.70	0.72
1:C:837:GLU:HB3	3:C:863:HOH:O	1.90	0.71
1:C:94:ASN:ND2	1:C:295:VAL:H	1.89	0.71
1:C:471:GLU:HA	1:C:523:LYS:HG2	1.73	0.71
1:B:737:ILE:HD11	1:B:796:LEU:HD23	1.72	0.70
1:D:350:THR:HG22	3:D:2389:HOH:O	1.92	0.70
1:B:164:VAL:H	1:B:197:ASN:HD21	1.39	0.69
1:A:84:LYS:HB3	1:A:84:LYS:NZ	2.06	0.69
1:B:307:LYS:HE2	3:B:2259:HOH:O	1.93	0.69
1:C:794:LEU:HD12	1:C:799:ALA:HB2	1.73	0.69
1:B:426:SER:O	1:B:427:ASP:CB	2.41	0.69
1:D:127:MSE:HE1	1:D:179:LEU:HD22	1.74	0.68
1:D:565:ARG:HH11	1:D:565:ARG:CG	2.06	0.68
1:C:737:ILE:HD11	1:C:796:LEU:HD23	1.76	0.68
1:B:404:LYS:HB2	1:B:405:PRO:HD3	1.75	0.67
1:B:56:PHE:HB2	3:B:2942:HOH:O	1.95	0.67
1:D:327:LYS:HE3	1:D:636:ASN:HD22	1.61	0.66
1:C:733:THR:HB	1:C:736:LYS:HB3	1.75	0.66
1:C:794:LEU:CD1	1:C:799:ALA:HB2	2.26	0.66
1:D:123:TYR:CE1	1:D:127:MSE:HE3	2.30	0.66
1:B:420:ASN:O	1:B:425:ARG:NH1	2.29	0.66
1:C:409:GLU:HB2	3:C:2536:HOH:O	1.96	0.66
1:C:763:LEU:HD21	1:C:818:LEU:HD22	1.76	0.66
1:B:481:VAL:H	1:B:512:THR:CG2	2.08	0.66
1:C:838:LYS:HE2	3:C:1742:HOH:O	1.96	0.66
1:B:94:ASN:ND2	1:B:295:VAL:H	1.95	0.65
1:B:218:TRP:CZ2	1:B:220:GLY:HA3	2.32	0.65
1:B:458:TYR:CZ	1:B:537:PRO:HB2	2.32	0.64
1:B:422:VAL:HG21	1:B:532:GLU:OE1	1.97	0.64
1:B:452:VAL:O	1:B:453:ASP:C	2.41	0.64
1:A:562:GLU:OE1	1:A:565:ARG:NH1	2.30	0.64
1:C:734:ASP:O	1:C:735:ASP:CB	2.38	0.64
1:B:32:LYS:HE3	1:B:34:GLU:HG2	1.79	0.64
1:D:737:ILE:HB	1:D:794:LEU:HD12	1.80	0.63
1:C:628:GLU:HG3	1:C:672:PHE:O	1.99	0.62
1:D:684:LYS:HD2	3:D:1811:HOH:O	1.97	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:684:LYS:HD3	1:B:686:GLU:HG2	1.82	0.62
1:D:331:LEU:HD23	1:D:333:LEU:HD13	1.82	0.61
1:D:733:THR:C	1:D:735:ASP:H	2.07	0.61
1:D:535:SER:O	1:D:538:THR:HB	2.00	0.61
1:D:503:ARG:HG2	1:D:511:GLY:O	2.01	0.61
1:A:388:HIS:CD2	3:A:2944:HOH:O	2.53	0.60
1:A:541:LEU:O	1:A:545:PHE:HE1	1.84	0.60
1:B:468:VAL:CG2	1:B:526:VAL:HG22	2.31	0.60
1:B:816:GLU:HB3	1:B:833:GLU:OE2	2.02	0.59
1:C:791:ASN:HB3	3:C:2502:HOH:O	2.01	0.59
1:D:127:MSE:HE2	1:D:179:LEU:HD22	1.85	0.59
1:B:466:GLN:NE2	3:B:1879:HOH:O	2.35	0.58
1:D:675:GLN:H	1:D:675:GLN:NE2	2.00	0.58
1:A:439:ARG:NH2	2:A:5002:GOL:O3	2.23	0.58
1:A:54:LYS:HE2	3:A:2291:HOH:O	2.04	0.58
1:A:84:LYS:HD2	3:A:2372:HOH:O	2.04	0.58
1:D:94:ASN:ND2	1:D:295:VAL:H	2.02	0.57
1:C:472:ASP:OD2	1:C:472:ASP:N	2.36	0.57
1:B:522:LYS:HE2	1:B:525:GLN:NE2	2.20	0.57
1:C:735:ASP:CG	1:C:735:ASP:O	2.48	0.57
1:C:508:PHE:N	1:C:508:PHE:HD2	2.02	0.56
1:B:426:SER:O	1:B:427:ASP:HB2	2.04	0.56
1:A:708:ARG:HH22	1:B:708:ARG:NH2	2.04	0.56
1:A:331:LEU:HD21	1:A:618:VAL:HG21	1.88	0.56
1:B:725:LEU:HD12	1:B:725:LEU:C	2.31	0.56
1:C:43:VAL:HG12	1:C:97:VAL:HB	1.88	0.56
1:A:737:ILE:HD11	1:A:796:LEU:CD2	2.24	0.56
1:B:388:HIS:CD2	3:B:2561:HOH:O	2.59	0.56
1:C:753:SER:HA	1:C:780:VAL:O	2.06	0.56
1:A:56:PHE:CD1	2:A:5002:GOL:H32	2.41	0.56
1:B:816:GLU:OE1	1:B:833:GLU:OE2	2.22	0.56
1:C:85:LEU:HD22	1:C:312:LEU:HD23	1.88	0.55
1:A:794:LEU:O	1:A:794:LEU:HD12	2.06	0.55
1:A:479:LEU:HD22	1:A:487:PHE:HB2	1.89	0.55
1:B:388:HIS:HD2	3:B:2561:HOH:O	1.87	0.55
1:D:161:ASN:HA	1:D:195:LYS:HB2	1.89	0.55
1:B:469:PRO:HG3	1:B:521:LEU:HD23	1.89	0.55
1:C:781:HIS:O	1:C:788:LYS:HE3	2.07	0.55
1:C:336:GLU:H	1:C:336:GLU:CD	2.14	0.55
1:A:350:THR:HG22	3:A:853:HOH:O	2.07	0.54
1:B:522:LYS:HE2	1:B:525:GLN:HE21	1.72	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:258:HIS:HD2	3:B:2515:HOH:O	1.91	0.54
1:C:576:LYS:HA	3:C:2855:HOH:O	2.08	0.54
1:A:57:ASP:N	2:A:5002:GOL:O3	2.38	0.53
1:A:94:ASN:ND2	1:A:295:VAL:H	2.06	0.53
1:D:565:ARG:HG2	1:D:565:ARG:NH1	2.15	0.53
1:A:101:PRO:HG2	1:A:129:THR:HG23	1.89	0.53
1:A:16:ASP:CG	1:A:253:ARG:HD2	2.33	0.53
1:A:474:ASP:HB3	1:A:518:LYS:HD2	1.91	0.53
1:C:732:VAL:HG12	3:C:2193:HOH:O	2.08	0.53
1:A:57:ASP:H	2:A:5002:GOL:H32	1.72	0.53
1:C:508:PHE:N	1:C:508:PHE:CD2	2.74	0.53
1:A:758:VAL:CG2	1:A:792:ILE:HD13	2.39	0.52
1:A:388:HIS:HD2	3:A:2944:HOH:O	1.92	0.52
1:A:794:LEU:HD12	1:A:794:LEU:C	2.34	0.52
1:B:512:THR:HG23	1:B:513:LYS:O	2.10	0.52
1:C:475:TYR:HB2	1:C:521:LEU:HD22	1.90	0.52
1:A:670:TRP:CD1	3:A:2131:HOH:O	2.61	0.52
1:D:443:HIS:CE1	1:D:508:PHE:HE2	2.28	0.52
1:A:409:GLU:HB3	3:A:1423:HOH:O	2.09	0.52
1:A:470:GLN:HA	1:A:470:GLN:NE2	2.25	0.52
1:D:404:LYS:HB3	1:D:405:PRO:HD2	1.92	0.52
1:B:422:VAL:HG21	1:B:532:GLU:CD	2.34	0.51
1:B:675:GLN:H	1:B:675:GLN:NE2	2.08	0.51
1:B:443:HIS:C	3:B:2942:HOH:O	2.53	0.51
1:D:339:ILE:HG22	1:D:576:LYS:HB2	1.91	0.51
1:B:422:VAL:CG2	1:B:532:GLU:OE1	2.58	0.51
1:D:416:LYS:HG2	1:D:434:VAL:HG22	1.93	0.51
1:B:758:VAL:HG21	1:B:792:ILE:HD13	1.93	0.51
1:D:675:GLN:H	1:D:675:GLN:HE21	1.59	0.51
1:B:453:ASP:OD1	1:B:453:ASP:O	2.30	0.50
1:A:349:LYS:HE2	1:A:364:VAL:O	2.11	0.50
1:D:566:ASN:ND2	3:D:2876:HOH:O	2.43	0.50
1:A:708:ARG:HH22	1:B:708:ARG:HH22	1.58	0.50
1:B:404:LYS:O	1:B:405:PRO:O	2.30	0.50
1:B:536:GLY:N	1:B:537:PRO:CD	2.75	0.50
1:D:443:HIS:HE1	1:D:508:PHE:HE2	1.57	0.50
1:B:57:ASP:H	2:B:5006:GOL:C1	2.24	0.49
1:B:404:LYS:O	1:B:405:PRO:C	2.54	0.49
1:A:134:LYS:HE2	3:A:3057:HOH:O	2.11	0.49
1:A:765:SER:HB3	1:A:813:GLU:OE1	2.13	0.49
1:B:458:TYR:N	3:B:2207:HOH:O	2.46	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:153:LEU:C	1:A:153:LEU:HD12	2.38	0.49
1:B:470:GLN:CA	1:B:470:GLN:HE21	2.25	0.49
1:C:97:VAL:HG22	1:C:142:ALA:HB3	1.94	0.49
1:C:182:LYS:HB2	1:C:845:LEU:HG	1.94	0.49
1:D:501:GLN:HG3	3:D:2137:HOH:O	2.13	0.49
1:A:48:ASN:HD21	1:A:357:ALA:HB1	1.78	0.49
1:B:378:GLU:HG2	3:B:2471:HOH:O	2.13	0.49
1:C:503:ARG:HH21	1:C:510:ALA:HA	1.76	0.49
1:C:736:LYS:HD2	1:C:736:LYS:C	2.37	0.49
1:D:733:THR:C	1:D:735:ASP:N	2.69	0.49
1:C:449:HIS:CD2	1:C:451:LYS:H	2.18	0.49
1:D:367:PRO:HG2	1:D:580:ILE:HG21	1.95	0.49
1:A:84:LYS:NZ	1:A:84:LYS:CB	2.73	0.48
1:A:333:LEU:HD22	1:A:656:LEU:HB3	1.95	0.48
1:C:675:GLN:H	1:C:675:GLN:NE2	2.11	0.48
1:D:737:ILE:HB	1:D:794:LEU:CD1	2.43	0.48
1:D:796:LEU:HD22	1:D:800:ILE:HD11	1.94	0.48
1:A:421:PRO:HG2	1:A:424:GLU:HB2	1.95	0.48
1:B:335:LYS:HE2	3:B:2440:HOH:O	2.14	0.48
1:D:54:LYS:HE2	3:D:2324:HOH:O	2.14	0.48
1:D:622:GLN:NE2	1:D:648:LEU:HD13	2.28	0.48
1:C:151:ASN:HB2	1:C:192:ALA:HB1	1.95	0.48
1:C:736:LYS:HD2	1:C:737:ILE:H	1.75	0.48
1:D:127:MSE:HE2	1:D:179:LEU:HD13	1.95	0.48
1:B:338:ASN:ND2	1:B:574:HIS:HA	2.28	0.48
1:D:607:VAL:HG11	1:D:631:TRP:CE2	2.49	0.48
1:B:409:GLU:HA	1:B:436:LYS:NZ	2.29	0.48
1:D:733:THR:O	1:D:735:ASP:N	2.47	0.48
1:B:458:TYR:CE1	1:B:537:PRO:HB2	2.49	0.47
1:D:338:ASN:ND2	1:D:574:HIS:HA	2.30	0.47
1:D:433:HIS:ND1	3:D:2743:HOH:O	2.35	0.47
1:B:404:LYS:C	1:B:405:PRO:O	2.53	0.47
1:B:735:ASP:OD1	1:B:735:ASP:N	2.47	0.47
1:C:470:GLN:HE21	1:C:470:GLN:HA	1.79	0.47
1:B:463:LEU:HD22	1:B:550:PHE:CE1	2.49	0.47
1:B:480:GLN:HG2	1:B:514:GLU:HA	1.96	0.47
1:C:503:ARG:HB3	1:C:503:ARG:CZ	2.44	0.47
1:C:559:ASP:CG	1:C:562:GLU:HB3	2.40	0.47
1:A:439:ARG:H	2:A:5002:GOL:C1	2.27	0.47
1:D:334:LYS:HE2	3:D:2244:HOH:O	2.15	0.47
1:A:769:ARG:HB3	1:A:770:PRO:HD2	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:676:ASP:HB3	1:A:708:ARG:HD3	1.96	0.46
1:C:472:ASP:OD2	1:C:523:LYS:CB	2.57	0.46
1:A:427:ASP:O	3:A:1704:HOH:O	2.20	0.46
1:D:713:PRO:HG2	1:D:716:TYR:HB2	1.98	0.46
1:A:400:ILE:HD12	1:A:414:ILE:HG12	1.98	0.46
1:C:338:ASN:O	1:C:575:ASP:HB3	2.16	0.46
1:D:281:MSE:SE	1:D:281:MSE:C	3.09	0.46
1:A:648:LEU:HD12	1:A:649:GLY:N	2.31	0.46
1:D:192:ALA:HB1	1:D:194:ASN:OD1	2.16	0.46
1:D:607:VAL:HG11	1:D:631:TRP:CD2	2.51	0.46
1:B:345:ASN:HB3	1:B:622:GLN:OE1	2.16	0.46
1:C:218:TRP:CZ2	1:C:220:GLY:HA3	2.52	0.45
1:C:327:LYS:HE2	1:C:636:ASN:HD22	1.81	0.45
1:C:432:PHE:O	1:C:449:HIS:CE1	2.69	0.45
1:B:725:LEU:HD12	1:B:725:LEU:O	2.16	0.45
1:C:54:LYS:HE3	3:C:1010:HOH:O	2.16	0.45
1:C:766:LYS:HB3	3:C:2866:HOH:O	2.16	0.45
1:C:286:VAL:HA	1:C:289:LEU:HG	1.99	0.45
1:C:769:ARG:HH11	1:C:769:ARG:HD3	1.51	0.45
1:A:769:ARG:HB3	1:A:770:PRO:CD	2.47	0.45
1:A:43:VAL:HG12	1:A:97:VAL:HB	1.99	0.45
1:B:327:LYS:O	1:B:328:ASN:HB2	2.17	0.45
1:D:88:LYS:HB3	1:D:88:LYS:HE3	1.74	0.45
1:C:561:ASP:HB2	3:C:2617:HOH:O	2.17	0.45
1:A:82:ALA:O	1:A:86:MSE:HG3	2.16	0.44
1:B:338:ASN:HD22	1:B:575:ASP:H	1.65	0.44
1:B:487:PHE:HD2	1:B:488:TYR:N	2.15	0.44
1:C:607:VAL:HG11	1:C:631:TRP:CE2	2.51	0.44
1:C:626:PRO:HD3	1:C:668:LEU:HD13	1.98	0.44
1:B:57:ASP:H	2:B:5006:GOL:H11	1.82	0.44
1:C:763:LEU:HD11	1:C:818:LEU:HD13	1.99	0.44
1:B:338:ASN:HD21	1:B:574:HIS:HA	1.83	0.44
1:C:471:GLU:CA	1:C:523:LYS:HG2	2.46	0.44
1:D:534:GLY:HA3	1:D:538:THR:HG21	1.98	0.44
1:C:153:LEU:C	1:C:153:LEU:HD12	2.43	0.44
1:C:838:LYS:HB2	1:C:838:LYS:HE3	1.84	0.44
1:C:708:ARG:HD3	3:C:2241:HOH:O	2.17	0.44
1:D:212:LEU:HD23	1:D:212:LEU:HA	1.92	0.44
1:C:503:ARG:NH2	1:C:509:GLY:O	2.51	0.43
1:A:331:LEU:HD23	1:A:333:LEU:HD13	2.01	0.43
1:A:404:LYS:HB3	1:A:405:PRO:CD	2.41	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:123:TYR:HE1	1:D:127:MSE:HE3	1.79	0.43
1:D:833:GLU:HB3	3:D:2378:HOH:O	2.17	0.43
1:A:675:GLN:H	1:A:675:GLN:NE2	2.15	0.43
1:B:625:THR:HB	1:B:626:PRO:CD	2.49	0.43
1:B:731:LYS:HE3	1:B:733:THR:HG23	2.00	0.43
1:D:744:LYS:HB2	1:D:787:LYS:HG3	2.01	0.43
1:A:541:LEU:O	1:A:545:PHE:CE1	2.68	0.43
1:C:758:VAL:HG21	1:C:792:ILE:HD13	2.00	0.43
1:C:725:LEU:C	1:C:725:LEU:HD12	2.43	0.43
1:D:339:ILE:HA	1:D:576:LYS:O	2.18	0.43
1:B:420:ASN:HB3	1:B:421:PRO:HD2	2.00	0.43
1:D:190:MSE:HG3	1:D:223:MSE:HG3	2.00	0.43
1:C:579:LEU:HD22	1:C:610:VAL:HG11	2.00	0.42
1:D:149:VAL:O	1:D:150:CYS:HB2	2.19	0.42
1:B:480:GLN:HG3	3:B:949:HOH:O	2.18	0.42
1:D:99:LEU:HA	1:D:144:THR:HB	2.01	0.42
1:D:444:LEU:HB2	1:D:548:GLY:O	2.19	0.42
1:D:533:TYR:CZ	1:D:535:SER:HA	2.53	0.42
1:D:218:TRP:CZ2	1:D:220:GLY:HA3	2.54	0.42
1:A:411:SER:O	1:A:436:LYS:HD3	2.18	0.42
1:B:237:LYS:HE3	3:B:2183:HOH:O	2.18	0.42
1:A:115:PHE:CE1	1:A:353:GLY:HA3	2.55	0.42
1:A:737:ILE:HG22	1:A:739:ILE:HG22	2.01	0.42
1:B:56:PHE:CD1	2:B:5006:GOL:H11	2.55	0.42
1:B:812:VAL:HB	1:B:840:LEU:HB3	2.01	0.42
1:C:101:PRO:HG2	1:C:129:THR:HG23	2.00	0.42
1:C:708:ARG:NE	3:C:2241:HOH:O	2.52	0.42
1:A:372:VAL:HG13	1:A:377:LYS:O	2.20	0.42
1:A:351:SER:HA	1:A:648:LEU:HD23	2.02	0.42
1:B:101:PRO:HG2	1:B:129:THR:HG23	2.00	0.42
1:D:708:ARG:HD3	3:D:2947:HOH:O	2.19	0.42
1:A:618:VAL:HA	1:A:637:ALA:HB3	2.01	0.42
1:A:824:SER:HB3	2:A:5003:GOL:H32	2.02	0.42
1:C:394:LEU:HB2	1:C:553:GLY:HA2	2.02	0.42
1:D:481:VAL:HG12	1:D:550:PHE:CB	2.50	0.42
1:B:684:LYS:HD3	1:B:686:GLU:CG	2.49	0.42
1:B:753:SER:HA	1:B:780:VAL:O	2.19	0.42
1:D:623:SER:O	1:D:642:TRP:HA	2.19	0.42
1:A:54:LYS:HA	1:A:446:ASP:OD2	2.20	0.42
1:A:286:VAL:HA	1:A:289:LEU:HG	2.01	0.42
1:B:756:VAL:O	1:B:777:PHE:HA	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:708:ARG:NE	3:B:2054:HOH:O	2.51	0.41
1:B:794:LEU:HD12	1:B:794:LEU:N	2.34	0.41
1:B:88:LYS:HB3	1:B:88:LYS:HE3	1.73	0.41
1:C:350:THR:HG22	3:C:2559:HOH:O	2.20	0.41
1:B:34:GLU:O	1:B:35:ARG:C	2.63	0.41
1:C:448:LYS:HE2	3:C:1705:HOH:O	2.19	0.41
1:C:684:LYS:HD3	3:C:1417:HOH:O	2.20	0.41
1:A:428:ASP:HA	3:A:1704:HOH:O	2.20	0.41
1:B:147:HIS:HB3	1:B:192:ALA:HA	2.02	0.41
1:B:190:MSE:SE	2:B:5005:GOL:H31	2.70	0.41
1:C:18:LYS:HB3	1:C:275:VAL:HG21	2.03	0.41
1:B:492:GLU:O	1:B:492:GLU:HG3	2.20	0.41
1:B:579:LEU:HD21	1:B:607:VAL:HA	2.01	0.41
1:C:226:TRP:O	1:C:227:PHE:HB2	2.21	0.41
1:C:306:THR:O	1:C:310:SER:HB2	2.20	0.41
1:D:796:LEU:HD22	1:D:800:ILE:CD1	2.50	0.41
1:D:55:PHE:CG	1:D:443:HIS:HD2	2.38	0.41
1:D:64:PHE:N	1:D:64:PHE:CD2	2.89	0.41
1:A:297:ASN:CB	3:A:2042:HOH:O	2.55	0.41
1:D:16:ASP:OD1	1:D:253:ARG:HD2	2.20	0.41
1:B:200:HIS:CD2	1:B:230:TYR:CE2	3.09	0.41
1:B:731:LYS:HE3	1:B:733:THR:CG2	2.50	0.41
1:C:120:GLU:CD	1:C:699:GLY:HA3	2.46	0.41
1:C:447:PHE:HE2	1:C:452:VAL:HG21	1.85	0.41
1:C:733:THR:HG22	1:C:734:ASP:O	2.21	0.41
1:D:654:ASP:HB3	1:D:660:VAL:HG23	2.03	0.41
1:A:16:ASP:OD1	1:A:253:ARG:HD2	2.20	0.41
1:A:359:MSE:HE2	1:A:359:MSE:HB3	2.02	0.41
1:C:795:GLU:O	1:C:796:LEU:C	2.64	0.40
1:D:386:TYR:HB3	1:D:388:HIS:CD2	2.56	0.40
1:C:411:SER:C	1:C:436:LYS:HE2	2.45	0.40
1:C:444:LEU:O	1:C:445:PHE:C	2.64	0.40
1:C:709:LYS:HD2	3:C:895:HOH:O	2.21	0.40
1:B:367:PRO:HD3	1:B:648:LEU:HD11	2.03	0.40
1:A:603:THR:O	1:A:607:VAL:HG23	2.21	0.40
1:C:480:GLN:NE2	1:C:506:PHE:HB2	2.36	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	842/845 (100%)	808 (96%)	33 (4%)	1 (0%)	48	50
1	B	798/845 (94%)	764 (96%)	33 (4%)	1 (0%)	48	50
1	C	832/845 (98%)	796 (96%)	36 (4%)	0	100	100
1	D	827/845 (98%)	789 (95%)	38 (5%)	0	100	100
All	All	3299/3380 (98%)	3157 (96%)	140 (4%)	2 (0%)	48	50

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	524	GLY
1	B	405	PRO

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	716/706 (101%)	692 (97%)	24 (3%)	32	33
1	B	690/706 (98%)	661 (96%)	29 (4%)	26	25
1	C	710/706 (101%)	676 (95%)	34 (5%)	23	20
1	D	707/706 (100%)	680 (96%)	27 (4%)	29	29
All	All	2823/2824 (100%)	2709 (96%)	114 (4%)	28	27

All (114) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	290	GLU
1	A	333	LEU
1	A	335	LYS
1	A	377	LYS
1	A	409	GLU
1	A	426	SER
1	A	427	ASP
1	A	428	ASP
1	A	503	ARG
1	A	518	LYS
1	A	522	LYS
1	A	541	LEU
1	A	542	VAL
1	A	580	ILE
1	A	633	GLU
1	A	677	ASN
1	A	726	ASP
1	A	732	VAL
1	A	733	THR
1	A	736	LYS
1	A	739	ILE
1	A	766	LYS
1	A	832	LYS
1	A	845	LEU
1	B	3	LYS
1	B	35	ARG
1	B	294	ILE
1	B	327	LYS
1	B	333	LEU
1	B	420	ASN
1	B	423	GLU
1	B	424	GLU
1	B	425	ARG
1	B	426	SER
1	B	450	GLU
1	B	470	GLN
1	B	484	SER
1	B	492	GLU
1	B	512	THR
1	B	535	SER
1	B	538	THR
1	B	573	LYS
1	B	580	ILE

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Mol	Chain	Res	Type
1	B	618	VAL
1	B	633	GLU
1	B	677	ASN
1	B	731	LYS
1	B	735	ASP
1	B	767	VAL
1	B	780	VAL
1	B	787	LYS
1	B	794	LEU
1	B	845	LEU
1	C	3	LYS
1	C	35	ARG
1	C	54	LYS
1	C	294	ILE
1	C	297	ASN
1	C	310	SER
1	C	333	LEU
1	C	335	LYS
1	C	336	GLU
1	C	436	LYS
1	C	470	GLN
1	C	481	VAL
1	C	492	GLU
1	C	507	CYS
1	C	508	PHE
1	C	521	LEU
1	C	523	LYS
1	C	526	VAL
1	C	561	ASP
1	C	562	GLU
1	C	612	LYS
1	C	633	GLU
1	C	677	ASN
1	C	708	ARG
1	C	731	LYS
1	C	735	ASP
1	C	736	LYS
1	C	748	ASP
1	C	766	LYS
1	C	831	VAL
1	C	832	LYS
1	C	835	LYS

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Mol	Chain	Res	Type
1	C	838	LYS
1	C	845	LEU
1	D	3	LYS
1	D	61	SER
1	D	294	ILE
1	D	307	LYS
1	D	312	LEU
1	D	333	LEU
1	D	334	LYS
1	D	340	ILE
1	D	411	SER
1	D	414	ILE
1	D	503	ARG
1	D	517	LYS
1	D	518	LYS
1	D	565	ARG
1	D	580	ILE
1	D	675	GLN
1	D	677	ASN
1	D	684	LYS
1	D	708	ARG
1	D	722	THR
1	D	766	LYS
1	D	767	VAL
1	D	794	LEU
1	D	797	LYS
1	D	819	VAL
1	D	832	LYS
1	D	845	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (50) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	15	GLN
1	A	48	ASN
1	A	94	ASN
1	A	288	ASN
1	A	388	HIS
1	A	420	ASN
1	A	438	ASN
1	A	470	GLN
1	A	480	GLN

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Mol	Chain	Res	Type
1	A	525	GLN
1	A	551	GLN
1	A	636	ASN
1	A	675	GLN
1	A	781	HIS
1	B	48	ASN
1	B	94	ASN
1	B	197	ASN
1	B	258	HIS
1	B	265	GLN
1	B	288	ASN
1	B	338	ASN
1	B	388	HIS
1	B	470	GLN
1	B	480	GLN
1	B	525	GLN
1	B	551	GLN
1	B	636	ASN
1	B	675	GLN
1	B	781	HIS
1	C	94	ASN
1	C	265	GLN
1	C	345	ASN
1	C	388	HIS
1	C	420	ASN
1	C	438	ASN
1	C	449	HIS
1	C	470	GLN
1	C	480	GLN
1	C	499	HIS
1	C	525	GLN
1	C	551	GLN
1	C	636	ASN
1	C	675	GLN
1	D	48	ASN
1	D	94	ASN
1	D	338	ASN
1	D	388	HIS
1	D	443	HIS
1	D	525	GLN
1	D	636	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

8 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	5003	-	5,5,5	0.35	0	5,5,5	0.65	0
2	GOL	B	5005	-	5,5,5	0.56	0	5,5,5	1.07	0
2	GOL	A	5004	-	5,5,5	0.44	0	5,5,5	0.86	0
2	GOL	B	5006	-	5,5,5	0.31	0	5,5,5	0.39	0
2	GOL	C	5007	-	5,5,5	0.59	0	5,5,5	0.77	0
2	GOL	A	5002	-	5,5,5	0.82	0	5,5,5	1.78	1 (20%)
2	GOL	A	5001	-	5,5,5	0.47	0	5,5,5	0.75	0
2	GOL	D	5008	-	5,5,5	0.51	0	5,5,5	1.02	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	5003	-	-	0/4/4/4	-
2	GOL	B	5005	-	-	2/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GOL	A	5004	-	-	4/4/4/4	-
2	GOL	B	5006	-	-	4/4/4/4	-
2	GOL	C	5007	-	-	2/4/4/4	-
2	GOL	A	5002	-	-	2/4/4/4	-
2	GOL	A	5001	-	-	2/4/4/4	-
2	GOL	D	5008	-	-	2/4/4/4	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	5002	GOL	C3-C2-C1	-3.24	99.91	111.80

There are no chirality outliers.

All (18) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	5001	GOL	O2-C2-C3-O3
2	A	5002	GOL	C1-C2-C3-O3
2	A	5004	GOL	O1-C1-C2-C3
2	B	5006	GOL	O1-C1-C2-C3
2	B	5006	GOL	C1-C2-C3-O3
2	A	5002	GOL	O2-C2-C3-O3
2	A	5001	GOL	C1-C2-C3-O3
2	A	5004	GOL	C1-C2-C3-O3
2	B	5005	GOL	O1-C1-C2-C3
2	C	5007	GOL	O1-C1-C2-C3
2	D	5008	GOL	C1-C2-C3-O3
2	A	5004	GOL	O1-C1-C2-O2
2	A	5004	GOL	O2-C2-C3-O3
2	B	5006	GOL	O2-C2-C3-O3
2	B	5005	GOL	O1-C1-C2-O2
2	B	5006	GOL	O1-C1-C2-O2
2	C	5007	GOL	O1-C1-C2-O2
2	D	5008	GOL	O2-C2-C3-O3

There are no ring outliers.

5 monomers are involved in 15 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	5003	GOL	1	0
2	B	5005	GOL	1	0
2	B	5006	GOL	4	0
2	A	5002	GOL	8	0
2	A	5001	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	834/845 (98%)	-0.57	6 (0%) 84 85	12, 25, 51, 69	0
1	B	800/845 (94%)	-0.40	31 (3%) 43 48	12, 22, 67, 98	0
1	C	826/845 (97%)	-0.16	10 (1%) 76 79	14, 32, 65, 94	0
1	D	823/845 (97%)	-0.14	8 (0%) 79 82	14, 34, 58, 73	0
All	All	3283/3380 (97%)	-0.31	55 (1%) 69 73	12, 28, 61, 98	0

All (55) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	445	PHE	5.1
1	B	408	ALA	4.5
1	B	538	THR	4.2
1	B	406	ALA	4.0
1	B	357	ALA	3.9
1	B	422	VAL	3.8
1	B	404	LYS	3.7
1	C	405	PRO	3.6
1	B	432	PHE	3.5
1	C	733	THR	3.4
1	B	547	ALA	3.4
1	C	408	ALA	3.2
1	C	526	VAL	3.2
1	B	452	VAL	3.1
1	B	434	VAL	3.1
1	B	526	VAL	3.1
1	A	541	LEU	3.1
1	B	405	PRO	3.0
1	B	453	ASP	3.0
1	A	543	GLY	2.9
1	A	545	PHE	2.9

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Mol	Chain	Res	Type	RSRZ
1	C	537	PRO	2.8
1	C	406	ALA	2.8
1	D	408	ALA	2.7
1	B	482	TYR	2.7
1	B	465	GLY	2.7
1	B	536	GLY	2.7
1	B	458	TYR	2.7
1	D	539	SER	2.7
1	B	399	LEU	2.6
1	D	733	THR	2.6
1	A	542	VAL	2.6
1	B	483	GLY	2.6
1	B	446	ASP	2.6
1	B	414	ILE	2.5
1	B	529	VAL	2.5
1	B	415	ALA	2.4
1	D	403	ALA	2.4
1	B	511	GLY	2.4
1	B	463	LEU	2.3
1	B	486	LEU	2.3
1	B	444	LEU	2.3
1	C	558	ILE	2.2
1	D	524	GLY	2.2
1	D	546	GLY	2.2
1	D	2	SER	2.2
1	C	508	PHE	2.1
1	A	540	GLY	2.1
1	C	475	TYR	2.1
1	D	402	ALA	2.1
1	B	420	ASN	2.1
1	C	482	TYR	2.0
1	A	732	VAL	2.0
1	B	537	PRO	2.0
1	B	485	GLY	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
2	GOL	C	5007	6/6	0.84	0.12	33,38,40,46	0
2	GOL	D	5008	6/6	0.87	0.11	35,37,38,39	0
2	GOL	B	5006	6/6	0.88	0.09	50,51,54,58	0
2	GOL	A	5002	6/6	0.89	0.14	27,31,39,41	0
2	GOL	A	5001	6/6	0.91	0.11	29,37,38,41	0
2	GOL	A	5004	6/6	0.92	0.08	37,39,40,44	0
2	GOL	A	5003	6/6	0.93	0.10	30,37,44,48	0
2	GOL	B	5005	6/6	0.94	0.08	34,40,41,45	0

6.5 Other polymers [i](#)

There are no such residues in this entry.