



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 07:09 AM UTC

PDB ID : 3AC0 / pdb_00003ac0
Title : Crystal structure of Beta-glucosidase from Kluyveromyces marxianus in complex with glucose
Authors : Yoshida, E.; Hidaka, M.; Fushinobu, S.; Katayama, T.; Kumagai, H.
Deposited on : 2009-12-25
Resolution : 2.54 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

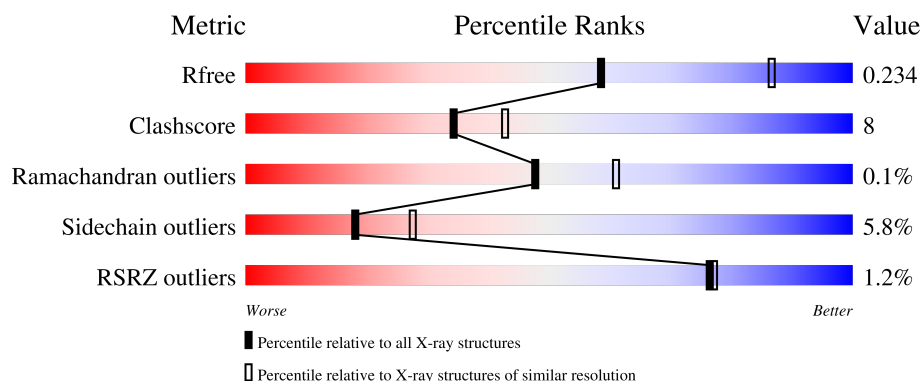
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

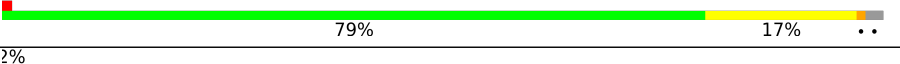
The reported resolution of this entry is 2.54 Å.

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	1091 (2.54-2.54)
Clashscore	190562	1120 (2.54-2.54)
Ramachandran outliers	187476	1106 (2.54-2.54)
Sidechain outliers	187428	1106 (2.54-2.54)
RSRZ outliers	180081	1091 (2.54-2.54)

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	
1	B	845	
1	C	845	
1	D	845	

2 Entry composition [i](#)

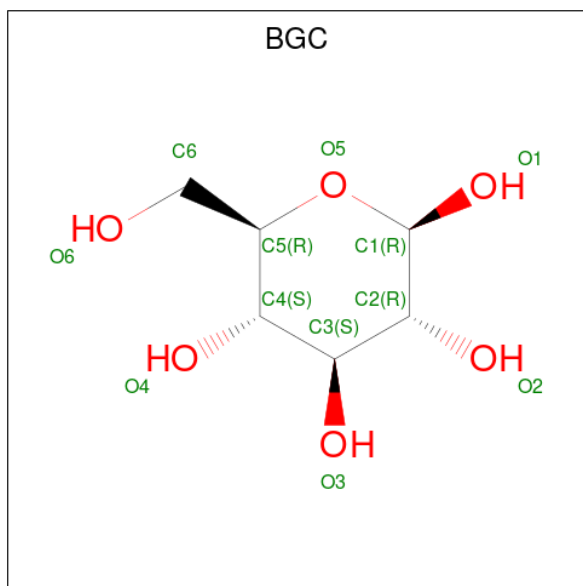
There are 3 unique types of molecules in this entry. The entry contains 27663 atoms, of which 0 are hydrogens and 0 are deuteriums.

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	841	Total	C	N	O	S	0	0	0
			6587	4184	1107	1281	15			
1	B	825	Total	C	N	O	S	0	0	0
			6462	4104	1091	1253	14			
1	C	831	Total	C	N	O	S	0	0	0
			6514	4143	1093	1263	15			
1	D	829	Total	C	N	O	S	0	0	0
			6488	4128	1092	1253	15			

- Molecule 2 is beta-D-glucopyranose (CCD ID: BGC) (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		

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

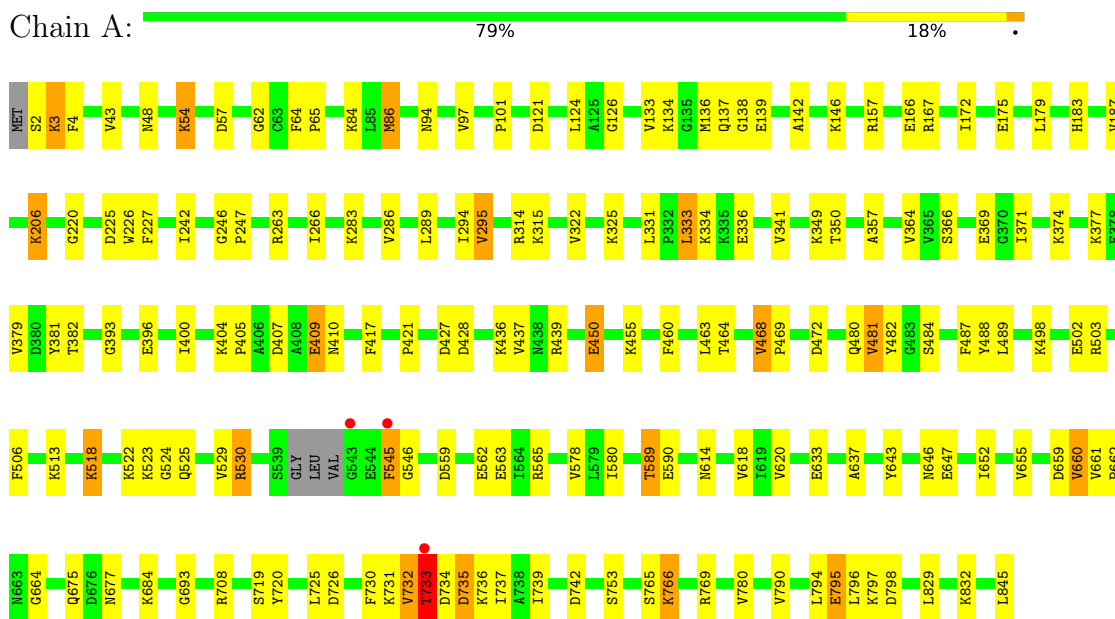
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	448	Total	O	0	0
			448	448		
3	B	446	Total	O	0	0
			446	446		
3	C	345	Total	O	0	0
			345	345		
3	D	325	Total	O	0	0
			325	325		

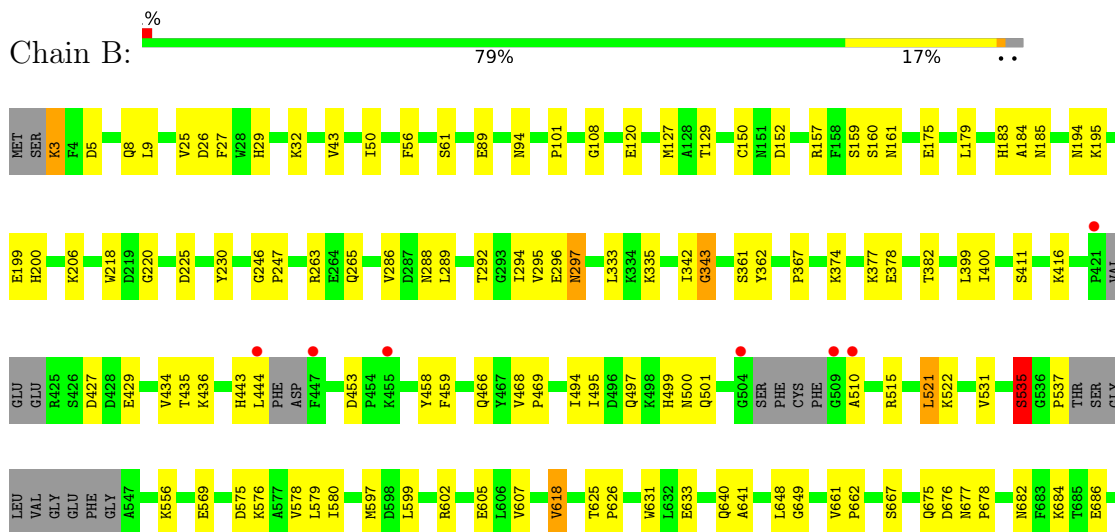
3 Residue-property plots

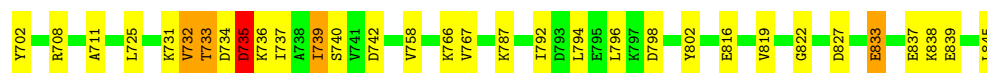
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

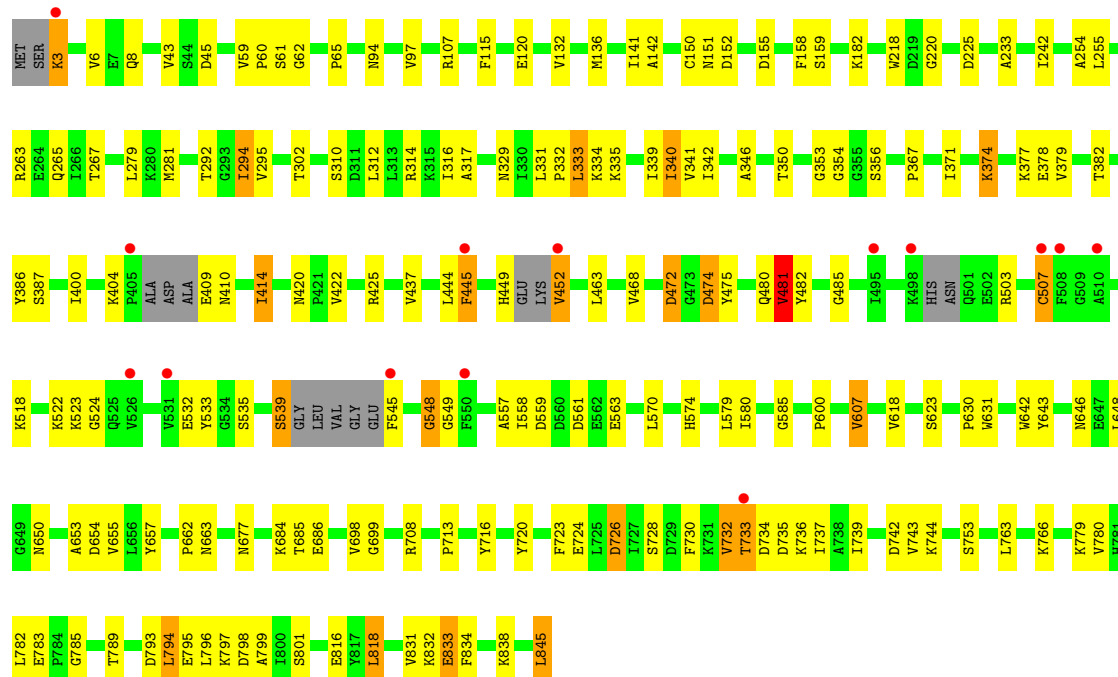
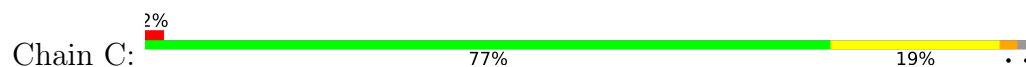


• Molecule 1: Beta-glucosidase I

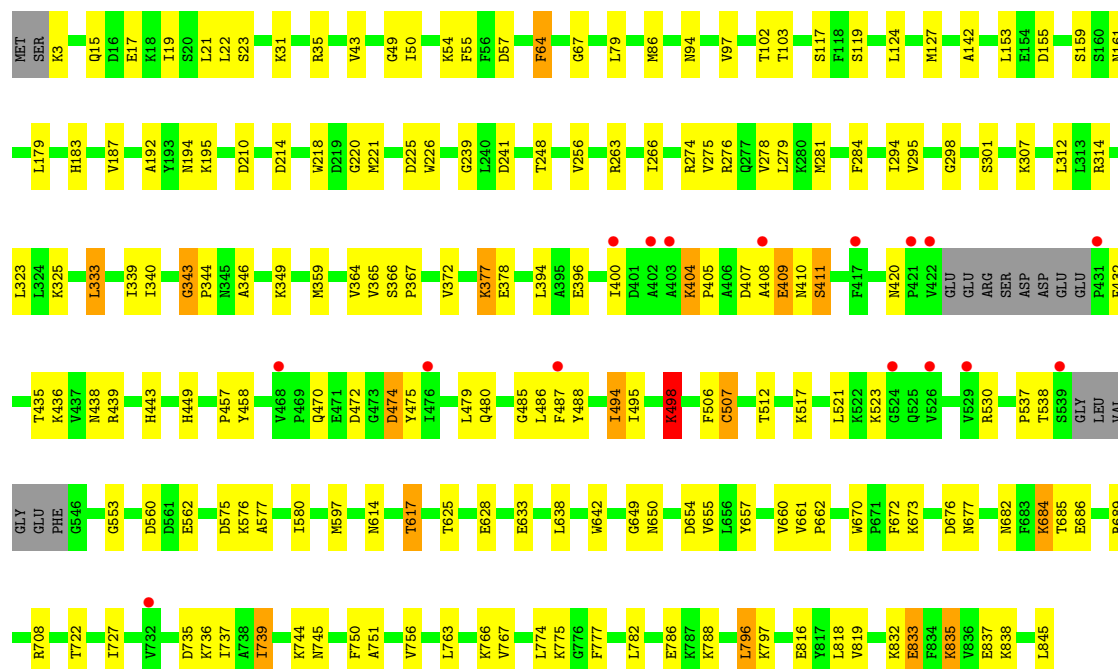
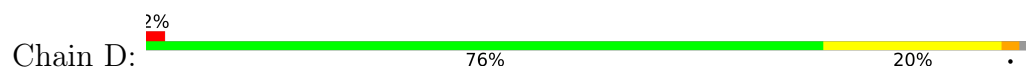




• Molecule 1: Beta-glucosidase I



• 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	245.85Å 148.41Å 119.64Å 90.00° 112.84° 90.00°	Depositor
Resolution (Å)	50.00 – 2.54 50.00 – 2.54	Depositor EDS
% Data completeness (in resolution range)	99.5 (50.00-2.54) 99.6 (50.00-2.54)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.11 (at 2.54Å)	Xtriage
Refinement program	REFMAC 5.5.0072	Depositor
R, R_{free}	0.169 , 0.242 0.165 , 0.234	Depositor DCC
R_{free} test set	6526 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	36.7	Xtriage
Anisotropy	0.011	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 41.9	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	27663	wwPDB-VP
Average B, all atoms (Å ²)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.24% 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: BGC

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	1.04	3/6723 (0.0%)	1.11	28/9089 (0.3%)
1	B	1.12	6/6591 (0.1%)	1.14	30/8907 (0.3%)
1	C	0.99	5/6646 (0.1%)	1.09	13/8981 (0.1%)
1	D	0.98	2/6622 (0.0%)	1.10	20/8952 (0.2%)
All	All	1.03	16/26582 (0.1%)	1.11	91/35929 (0.3%)

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	26	ASP	C-O	-8.05	1.16	1.24
1	A	242	ILE	CA-CB	6.56	1.63	1.54
1	B	822	GLY	C-O	-6.30	1.17	1.23
1	B	175	GLU	C-O	-6.18	1.18	1.24
1	A	220	GLY	C-O	6.18	1.29	1.23
1	C	263	ARG	C-O	-6.00	1.16	1.23
1	B	265	GLN	C-O	-5.45	1.17	1.24
1	C	267	THR	C-O	-5.35	1.16	1.23
1	C	254	ALA	CA-C	5.31	1.59	1.52
1	B	535	SER	C-N	-5.24	1.30	1.34
1	D	642	TRP	C-O	-5.16	1.19	1.24
1	D	266	ILE	C-O	-5.10	1.18	1.24
1	C	607	VAL	CA-CB	5.09	1.60	1.54
1	B	819	VAL	CA-CB	5.05	1.60	1.54
1	A	295	VAL	CA-CB	5.04	1.60	1.54
1	C	141	ILE	CA-CB	-5.01	1.48	1.54

All (91) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	499	HIS	N-CA-C	12.47	124.42	111.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	735	ASP	N-CA-C	9.29	124.62	113.28
1	B	641	ALA	N-CA-C	8.85	121.01	111.36
1	A	175	GLU	CA-C-N	-8.39	110.29	119.19
1	A	175	GLU	C-N-CA	-8.39	110.29	119.19
1	C	548	GLY	N-CA-C	8.38	119.38	111.67
1	D	343	GLY	CA-C-N	7.64	127.69	119.28
1	D	343	GLY	C-N-CA	7.64	127.69	119.28
1	A	121	ASP	CA-C-N	-7.52	111.22	119.19
1	A	121	ASP	C-N-CA	-7.52	111.22	119.19
1	B	499	HIS	CA-C-N	-7.48	111.22	122.74
1	B	499	HIS	C-N-CA	-7.48	111.22	122.74
1	D	298	GLY	CA-C-N	-7.47	113.13	120.52
1	D	298	GLY	C-N-CA	-7.47	113.13	120.52
1	A	693	GLY	N-CA-C	7.12	121.28	112.73
1	D	64	PHE	CA-C-N	-7.06	113.04	120.03
1	D	64	PHE	C-N-CA	-7.06	113.04	120.03
1	B	343	GLY	CA-C-N	7.05	127.03	119.28
1	B	343	GLY	C-N-CA	7.05	127.03	119.28
1	A	769	ARG	CA-C-N	-6.92	113.18	120.03
1	A	769	ARG	C-N-CA	-6.92	113.18	120.03
1	C	507	CYS	N-CA-C	6.58	120.17	111.28
1	B	453	ASP	CA-C-N	6.54	128.02	119.84
1	B	453	ASP	C-N-CA	6.54	128.02	119.84
1	C	242	ILE	N-CA-C	6.51	117.19	108.27
1	A	468	VAL	CA-C-N	6.42	126.37	119.76
1	A	468	VAL	C-N-CA	6.42	126.37	119.76
1	B	599	LEU	CA-C-N	-6.40	113.36	120.14
1	B	599	LEU	C-N-CA	-6.40	113.36	120.14
1	D	507	CYS	N-CA-C	6.27	119.74	111.28
1	C	733	THR	CB-CA-C	-6.26	99.19	113.33
1	B	711	ALA	N-CA-C	-6.20	104.44	111.14
1	A	589	THR	N-CA-C	6.07	118.52	108.99
1	B	25	VAL	N-CA-C	6.06	116.84	110.72
1	C	783	GLU	N-CA-C	-6.04	102.27	110.36
1	A	733	THR	N-CA-C	-5.98	100.82	109.31
1	A	498	LYS	N-CA-C	-5.95	105.01	112.93
1	B	27	PHE	N-CA-C	5.94	118.54	111.71
1	B	510	ALA	N-CA-C	5.93	117.74	111.28
1	C	437	VAL	N-CA-C	5.92	115.88	106.88
1	B	640	GLN	CA-C-N	5.89	128.65	120.29
1	B	640	GLN	C-N-CA	5.89	128.65	120.29
1	C	481	VAL	N-CA-C	5.79	117.41	108.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	481	VAL	N-CA-C	5.72	116.60	108.42
1	A	157	ARG	N-CA-C	5.69	119.03	111.75
1	A	124	LEU	N-CA-C	-5.67	105.18	111.36
1	C	302	THR	N-CA-C	-5.66	104.78	112.26
1	C	8	GLN	N-CA-C	-5.64	104.77	111.03
1	C	339	ILE	N-CA-C	5.63	118.04	108.86
1	D	625	THR	CA-C-N	-5.62	114.17	119.85
1	D	625	THR	C-N-CA	-5.62	114.17	119.85
1	D	670	TRP	CA-C-N	-5.60	114.48	120.03
1	D	670	TRP	C-N-CA	-5.60	114.48	120.03
1	A	545	PHE	N-CA-C	5.59	118.83	109.95
1	B	802	TYR	N-CA-C	-5.59	100.80	109.24
1	B	50	ILE	N-CA-C	5.58	115.63	107.37
1	A	54	LYS	N-CA-C	5.51	117.47	108.76
1	B	575	ASP	CB-CA-C	-5.45	102.32	110.88
1	B	468	VAL	N-CA-C	5.43	113.52	108.15
1	A	614	ASN	CA-C-N	5.42	125.09	119.56
1	A	614	ASN	C-N-CA	5.42	125.09	119.56
1	D	485	GLY	N-CA-C	5.39	120.01	110.80
1	A	86	MET	N-CA-C	-5.37	105.50	111.36
1	A	138	GLY	N-CA-C	-5.31	106.36	112.73
1	B	157	ARG	N-CA-C	5.30	117.81	111.71
1	B	579	LEU	CA-CB-CG	5.30	134.86	116.30
1	D	684	LYS	N-CA-C	-5.28	100.69	108.99
1	A	765	SER	N-CA-C	-5.27	103.57	110.53
1	B	120	GLU	N-CA-C	-5.27	106.11	112.54
1	A	437	VAL	N-CA-C	5.23	115.39	107.80
1	D	67	GLY	N-CA-C	5.22	119.20	112.83
1	A	660	VAL	CA-C-N	5.21	126.34	122.59
1	A	660	VAL	C-N-CA	5.21	126.34	122.59
1	C	281	MET	N-CA-C	-5.19	105.53	111.14
1	C	374	LYS	N-CA-C	-5.19	107.49	113.88
1	A	266	ILE	N-CA-C	5.18	117.08	108.99
1	B	667	SER	N-CA-C	-5.17	106.75	113.16
1	B	29	HIS	N-CA-C	5.15	117.79	109.40
1	D	103	THR	N-CA-C	5.14	116.61	110.44
1	D	498	LYS	N-CA-C	-5.12	106.16	112.72
1	D	642	TRP	CB-CA-C	-5.12	109.13	115.89
1	B	175	GLU	CA-C-N	-5.12	113.76	119.19
1	B	175	GLU	C-N-CA	-5.12	113.76	119.19
1	A	172	ILE	CB-CA-C	-5.12	106.58	111.44
1	C	730	PHE	N-CA-C	5.12	115.78	107.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	266	ILE	N-CA-C	5.10	116.64	108.89
1	D	179	LEU	N-CA-C	-5.07	105.84	111.36
1	B	108	GLY	CA-C-N	5.03	124.72	119.64
1	B	108	GLY	C-N-CA	5.03	124.72	119.64
1	D	575	ASP	N-CA-C	-5.01	105.71	111.07
1	A	393	GLY	N-CA-C	5.00	122.50	115.30

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	6587	0	6490	100	0
1	B	6462	0	6387	74	0
1	C	6514	0	6427	108	0
1	D	6488	0	6417	118	0
2	A	12	0	12	2	0
2	B	12	0	12	1	0
2	C	12	0	12	1	0
2	D	12	0	12	3	0
3	A	448	0	0	18	0
3	B	446	0	0	11	0
3	C	345	0	0	12	0
3	D	325	0	0	10	0
All	All	27663	0	25769	394	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 8.

All (394) 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:B:827:ASP:HB3	3:B:1558:HOH:O	1.46	1.12
1:D:562:GLU:HG2	3:D:1448:HOH:O	1.60	1.01

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:633:GLU:HG2	3:B:999:HOH:O	1.63	0.97
1:A:737:ILE:HD11	1:A:796:LEU:HD23	1.45	0.96
1:C:763:LEU:HD11	1:C:818:LEU:HD13	1.47	0.94
1:D:346:ALA:O	1:D:367:PRO:HD2	1.69	0.93
1:C:735:ASP:O	1:C:736:LYS:HG2	1.70	0.92
1:B:225:ASP:OD1	2:B:5002:BGC:H1	1.70	0.92
1:D:49:GLY:HA3	1:D:359:MET:HE1	1.47	0.92
1:D:432:PHE:HB2	1:D:449:HIS:CE1	2.05	0.92
1:C:735:ASP:C	1:C:736:LYS:HG2	1.91	0.91
1:B:798:ASP:HA	3:B:956:HOH:O	1.69	0.91
1:A:334:LYS:HD3	3:A:1186:HOH:O	1.70	0.91
1:B:378:GLU:HB3	3:B:1186:HOH:O	1.70	0.91
1:D:3:LYS:HB3	3:D:1064:HOH:O	1.73	0.89
1:A:86:MET:HE3	3:A:1538:HOH:O	1.73	0.89
1:C:449:HIS:O	1:C:452:VAL:HG12	1.74	0.88
1:B:500:ASN:O	1:B:515:ARG:NH2	2.07	0.86
1:D:404:LYS:HD3	1:D:405:PRO:HD2	1.57	0.86
1:C:225:ASP:OD1	2:C:5003:BGC:H1	1.75	0.85
1:B:733:THR:HG21	3:B:1129:HOH:O	1.80	0.82
1:A:334:LYS:HB3	3:A:1186:HOH:O	1.79	0.81
1:B:297:ASN:HB2	3:B:897:HOH:O	1.81	0.79
1:C:472:ASP:OD1	1:C:523:LYS:HB2	1.82	0.79
1:C:728:SER:HB3	1:C:742:ASP:OD2	1.82	0.79
1:D:432:PHE:HB2	1:D:449:HIS:HE1	1.46	0.79
1:C:482:TYR:HD2	1:C:548:GLY:HA3	1.46	0.79
1:B:816:GLU:OE1	1:B:833:GLU:OE2	2.02	0.77
1:A:263:ARG:HB2	1:C:159:SER:HB2	1.67	0.76
1:B:127:MET:HE1	1:B:183:HIS:CD2	2.21	0.76
1:D:49:GLY:CA	1:D:359:MET:HE1	2.14	0.76
1:B:199:GLU:HG2	3:B:862:HOH:O	1.85	0.76
1:B:459:PHE:H	1:B:535:SER:HB3	1.50	0.76
1:D:472:ASP:OD2	1:D:523:LYS:HB2	1.86	0.76
1:D:407:ASP:CG	1:D:408:ALA:H	1.94	0.74
1:D:737:ILE:HD11	1:D:796:LEU:HD23	1.70	0.74
1:D:409:GLU:CA	1:D:409:GLU:OE2	2.33	0.73
1:A:404:LYS:HB3	1:A:405:PRO:HD2	1.71	0.72
1:C:763:LEU:HD11	1:C:818:LEU:CD1	2.19	0.71
1:C:732:VAL:CG1	1:C:737:ILE:HG12	2.20	0.71
1:A:766:LYS:HG3	3:A:1512:HOH:O	1.90	0.71
1:A:84:LYS:HE3	1:A:139:GLU:OE2	1.91	0.70
1:A:832:LYS:HE2	3:A:1396:HOH:O	1.91	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:459:PHE:H	1:B:535:SER:CB	2.05	0.70
1:D:43:VAL:HG12	1:D:97:VAL:HB	1.74	0.69
1:A:482:TYR:HH	1:A:545:PHE:HD2	1.41	0.69
1:D:577:ALA:HB3	1:D:617:THR:HG23	1.75	0.69
1:C:798:ASP:HB3	3:C:900:HOH:O	1.92	0.68
1:D:54:LYS:HE2	3:D:950:HOH:O	1.93	0.68
1:C:452:VAL:HG12	1:C:452:VAL:O	1.91	0.68
1:A:404:LYS:HB3	1:A:405:PRO:CD	2.25	0.67
1:D:480:GLN:NE2	1:D:506:PHE:HB2	2.09	0.66
1:C:452:VAL:O	1:C:452:VAL:CG1	2.44	0.66
1:A:86:MET:CE	3:A:1538:HOH:O	2.37	0.66
1:D:479:LEU:HB3	1:D:495:ILE:CG2	2.26	0.66
1:D:17:GLU:OE2	1:D:35:ARG:NH2	2.27	0.65
1:D:17:GLU:CD	1:D:35:ARG:HH21	2.03	0.65
1:D:409:GLU:OE2	1:D:409:GLU:N	2.30	0.65
1:A:733:THR:OG1	1:A:734:ASP:N	2.30	0.64
1:B:734:ASP:HB3	1:B:838:LYS:HD3	1.80	0.64
1:C:655:VAL:HG13	1:C:662:PRO:HG3	1.78	0.64
1:D:407:ASP:CG	1:D:408:ALA:N	2.55	0.64
1:D:479:LEU:HB3	1:D:495:ILE:HG21	1.79	0.64
1:D:628:GLU:HG3	1:D:672:PHE:O	1.98	0.64
1:C:733:THR:OG1	1:C:735:ASP:N	2.30	0.64
1:C:444:LEU:HD12	1:C:549:GLY:HA2	1.78	0.63
1:C:474:ASP:HB3	1:C:518:LYS:HE3	1.81	0.63
3:A:1110:HOH:O	1:B:675:GLN:HG2	1.98	0.63
1:B:735:ASP:N	1:B:735:ASP:OD2	2.30	0.63
1:A:502:GLU:CB	1:A:513:LYS:HE3	2.29	0.63
1:B:459:PHE:O	1:B:535:SER:HB3	1.99	0.63
1:D:833:GLU:HG3	3:D:958:HOH:O	1.97	0.63
1:A:633:GLU:HG3	3:A:942:HOH:O	1.98	0.62
1:C:346:ALA:O	1:C:367:PRO:HD2	1.98	0.62
1:D:494:ILE:HD12	1:D:517:LYS:HB3	1.81	0.62
1:D:735:ASP:HB2	1:D:736:LYS:NZ	2.14	0.62
1:D:409:GLU:OE2	1:D:409:GLU:C	2.43	0.62
1:A:736:LYS:HD2	3:A:1138:HOH:O	2.01	0.61
1:A:795:GLU:HG3	1:A:798:ASP:OD2	2.00	0.61
1:D:407:ASP:O	1:D:411:SER:HB2	2.00	0.61
1:B:469:PRO:HG3	1:B:521:LEU:HD23	1.82	0.61
1:D:763:LEU:HD11	1:D:818:LEU:HB2	1.81	0.61
1:B:737:ILE:HD11	1:B:796:LEU:HD23	1.83	0.60
1:A:97:VAL:HG22	1:A:142:ALA:HB3	1.82	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:686:GLU:O	1:D:689:ARG:HG3	2.02	0.60
1:C:43:VAL:HG12	1:C:97:VAL:HB	1.83	0.59
1:C:382:THR:OG1	1:C:563:GLU:OE2	2.20	0.59
1:D:475:TYR:HB2	1:D:521:LEU:HD13	1.84	0.59
1:C:115:PHE:CE1	1:C:353:GLY:HA3	2.37	0.59
1:C:735:ASP:N	1:C:735:ASP:OD2	2.30	0.59
1:A:349:LYS:HE2	1:A:364:VAL:O	2.03	0.59
1:D:727:ILE:HG23	1:D:739:ILE:HD12	1.83	0.59
1:A:225:ASP:OD2	2:A:5001:BGC:H1	2.03	0.59
1:B:416:LYS:HG2	1:B:434:VAL:HG22	1.84	0.59
1:D:479:LEU:CB	1:D:495:ILE:HG21	2.33	0.59
1:D:727:ILE:HG23	1:D:739:ILE:CD1	2.32	0.59
1:C:387:SER:HB2	1:C:600:PRO:HG2	1.85	0.58
1:C:292:THR:HB	1:C:294:ILE:HD12	1.85	0.58
1:C:474:ASP:HB2	1:C:557:ALA:HB3	1.86	0.58
1:C:65:PRO:HA	1:C:643:TYR:O	2.04	0.58
1:A:502:GLU:HB2	1:A:513:LYS:HE3	1.86	0.57
1:C:753:SER:HA	1:C:780:VAL:O	2.05	0.57
1:C:794:LEU:HD13	1:C:799:ALA:HB2	1.85	0.57
1:C:833:GLU:HG3	1:C:834:PHE:N	2.05	0.57
1:C:65:PRO:HG2	1:C:316:ILE:HG22	1.85	0.57
1:A:655:VAL:HG13	1:A:662:PRO:HG3	1.85	0.57
1:D:225:ASP:OD1	2:D:5004:BGC:H1	2.04	0.57
1:A:336:GLU:CD	1:A:336:GLU:H	2.12	0.56
1:D:367:PRO:HG2	1:D:580:ILE:HG21	1.87	0.56
1:A:62:GLY:HA2	1:A:646:ASN:ND2	2.21	0.56
1:B:676:ASP:O	1:B:708:ARG:NH1	2.39	0.56
1:C:292:THR:CB	1:C:294:ILE:HD12	2.35	0.56
1:C:732:VAL:HG12	1:C:737:ILE:HG12	1.88	0.56
1:D:94:ASN:ND2	1:D:295:VAL:H	2.03	0.56
1:A:226:TRP:O	1:A:227:PHE:HB2	2.04	0.56
1:D:487:PHE:HB3	1:D:495:ILE:HB	1.86	0.56
1:C:445:PHE:HB2	3:C:1053:HOH:O	2.05	0.56
1:D:782:LEU:HD21	1:D:788:LYS:HB2	1.88	0.55
1:C:737:ILE:HD11	1:C:796:LEU:HD23	1.86	0.55
1:D:396:GLU:OE2	1:D:439:ARG:HA	2.06	0.55
1:C:482:TYR:HD2	1:C:548:GLY:CA	2.18	0.55
1:A:620:VAL:HG11	1:A:652:ILE:HD13	1.88	0.55
1:D:661:VAL:HG21	1:D:751:ALA:O	2.06	0.55
1:D:127:MET:HE1	1:D:183:HIS:CD2	2.42	0.55
1:D:192:ALA:HB1	1:D:194:ASN:OD1	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:578:VAL:HG22	1:B:618:VAL:CG1	2.37	0.55
1:A:62:GLY:HA2	1:A:646:ASN:HD21	1.70	0.54
1:D:226:TRP:CD2	2:D:5004:BGC:H6C2	2.42	0.54
1:D:774:LEU:O	1:D:775:LYS:HD3	2.08	0.54
1:A:126:GLY:HA3	1:A:179:LEU:HD12	1.89	0.54
1:B:56:PHE:HB2	1:B:443:HIS:O	2.07	0.54
1:B:733:THR:OG1	1:B:735:ASP:N	2.39	0.54
1:D:339:ILE:HA	1:D:576:LYS:O	2.07	0.54
1:B:342:ILE:HA	1:B:382:THR:O	2.07	0.54
1:A:450:GLU:HG3	3:A:1105:HOH:O	2.08	0.54
1:B:497:GLN:O	1:B:501:GLN:NE2	2.41	0.54
1:C:97:VAL:HG22	1:C:142:ALA:HB3	1.89	0.54
1:B:399:LEU:HD23	1:B:411:SER:HA	1.90	0.54
1:B:459:PHE:O	1:B:535:SER:CB	2.56	0.54
1:C:94:ASN:ND2	1:C:295:VAL:H	2.05	0.53
1:D:474:ASP:OD1	1:D:474:ASP:N	2.41	0.53
1:A:331:LEU:HD23	1:A:333:LEU:HD13	1.91	0.53
1:D:654:ASP:HB3	1:D:660:VAL:HG23	1.90	0.53
1:A:65:PRO:HA	1:A:643:TYR:O	2.09	0.53
1:A:482:TYR:OH	1:A:545:PHE:HD2	1.91	0.53
1:B:342:ILE:HG22	1:B:343:GLY:N	2.22	0.53
1:A:487:PHE:HD2	1:A:488:TYR:N	2.07	0.53
1:C:607:VAL:HG11	1:C:631:TRP:CE2	2.43	0.53
1:A:719:SER:OG	1:A:720:TYR:N	2.42	0.52
1:C:686:GLU:HG3	3:C:966:HOH:O	2.09	0.52
1:A:315:LYS:HE3	3:A:1295:HOH:O	2.10	0.52
1:A:341:VAL:O	1:A:381:TYR:HA	2.09	0.52
1:C:182:LYS:HB2	1:C:845:LEU:HG	1.91	0.52
1:C:218:TRP:CZ2	1:C:220:GLY:HA3	2.44	0.52
1:C:684:LYS:HG2	3:C:849:HOH:O	2.08	0.52
1:C:120:GLU:CD	1:C:699:GLY:HA3	2.34	0.52
1:A:732:VAL:HG12	1:A:737:ILE:HG13	1.92	0.51
1:D:816:GLU:HG3	1:D:835:LYS:HD2	1.91	0.51
1:C:420:ASN:O	1:C:425:ARG:NH2	2.42	0.51
1:A:64:PHE:CZ	1:A:86:MET:HG3	2.46	0.51
1:B:200:HIS:CD2	1:B:230:TYR:CE2	2.98	0.51
1:D:325:LYS:HB2	1:D:638:LEU:HB3	1.92	0.51
1:A:382:THR:OG1	1:A:563:GLU:OE2	2.29	0.51
1:B:733:THR:OG1	1:B:734:ASP:N	2.42	0.51
1:D:682:ASN:HB3	3:D:1436:HOH:O	2.11	0.51
1:C:485:GLY:HA2	1:C:532:GLU:O	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:15:GLN:HG3	3:D:941:HOH:O	2.10	0.51
1:A:4:PHE:CD2	1:A:283:LYS:HB2	2.46	0.51
1:C:713:PRO:HG2	1:C:716:TYR:HB2	1.92	0.51
1:A:421:PRO:HB3	1:A:460:PHE:CE1	2.46	0.50
1:B:458:TYR:CZ	1:B:537:PRO:HB2	2.47	0.50
1:B:678:PRO:HB3	1:B:702:TYR:CG	2.46	0.50
1:C:132:VAL:O	1:C:136:MET:HG3	2.12	0.50
1:D:400:ILE:HD12	1:D:409:GLU:O	2.11	0.50
1:D:432:PHE:HD1	1:D:449:HIS:ND1	2.09	0.50
1:A:94:ASN:ND2	1:A:295:VAL:H	2.10	0.50
1:C:414:ILE:O	1:C:463:LEU:HA	2.11	0.50
1:D:333:LEU:HB3	1:D:657:TYR:CE2	2.47	0.50
1:D:432:PHE:HD1	1:D:449:HIS:CE1	2.28	0.50
1:A:133:VAL:O	1:A:137:GLN:HG3	2.11	0.50
1:A:101:PRO:HB3	3:A:1050:HOH:O	2.12	0.49
1:C:292:THR:OG1	1:C:294:ILE:HD12	2.12	0.49
1:D:22:LEU:HD21	1:D:275:VAL:CG2	2.42	0.49
1:A:518:LYS:HE3	3:A:1288:HOH:O	2.11	0.49
1:C:570:LEU:O	1:C:574:HIS:ND1	2.45	0.49
1:D:458:TYR:CE2	1:D:538:THR:HA	2.47	0.49
1:B:494:ILE:O	1:B:495:ILE:HG13	2.12	0.49
1:A:371:ILE:HG22	1:A:379:VAL:HG21	1.94	0.49
1:D:745:ASN:ND2	1:D:750:PHE:O	2.36	0.49
1:B:758:VAL:HG21	1:B:792:ILE:HD12	1.94	0.49
1:D:218:TRP:CZ2	1:D:220:GLY:HA3	2.48	0.49
1:C:726:ASP:CB	3:C:909:HOH:O	2.60	0.49
1:C:6:VAL:HG22	1:C:279:LEU:HB3	1.95	0.49
1:C:150:CYS:HA	1:C:152:ASP:OD2	2.13	0.49
1:A:331:LEU:HD21	1:A:618:VAL:HG21	1.95	0.48
1:A:523:LYS:C	1:A:525:GLN:H	2.21	0.48
1:B:734:ASP:O	1:B:796:LEU:HD12	2.14	0.48
1:D:735:ASP:HB2	1:D:736:LYS:HZ1	1.76	0.48
1:A:366:SER:OG	1:A:369:GLU:HG3	2.14	0.48
1:A:502:GLU:HB3	1:A:513:LYS:HE3	1.94	0.48
1:C:472:ASP:HB2	3:C:921:HOH:O	2.13	0.48
1:D:457:PRO:HD2	1:D:537:PRO:HG2	1.95	0.48
1:B:127:MET:HE1	1:B:183:HIS:HD2	1.74	0.48
1:C:545:PHE:HB2	3:C:934:HOH:O	2.12	0.48
1:C:735:ASP:O	1:C:736:LYS:CG	2.54	0.48
1:D:782:LEU:HD23	1:D:788:LYS:HD2	1.96	0.48
1:B:297:ASN:CB	3:B:897:HOH:O	2.49	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:725:LEU:HA	1:B:742:ASP:O	2.14	0.48
1:C:742:ASP:OD1	1:C:789:THR:OG1	2.27	0.48
1:D:486:LEU:HD11	1:D:498:LYS:HE2	1.95	0.48
1:B:3:LYS:HE3	3:B:1007:HOH:O	2.13	0.48
1:B:94:ASN:ND2	1:B:295:VAL:H	2.12	0.47
1:C:648:LEU:C	1:C:648:LEU:HD12	2.39	0.47
1:C:354:GLY:HA3	1:C:585:GLY:O	2.14	0.47
1:C:797:LYS:O	1:C:801:SER:OG	2.27	0.47
1:D:102:THR:O	1:D:117:SER:HA	2.14	0.47
1:C:107:ARG:HA	1:C:698:VAL:HG13	1.97	0.47
1:D:21:LEU:HD23	1:D:31:LYS:HB3	1.97	0.47
1:D:735:ASP:HB2	1:D:736:LYS:HZ3	1.79	0.47
1:D:49:GLY:C	1:D:359:MET:HE1	2.39	0.47
1:D:673:LYS:O	1:D:676:ASP:HB2	2.15	0.47
1:C:62:GLY:HA2	1:C:646:ASN:HD21	1.80	0.47
1:C:561:ASP:N	1:C:561:ASP:OD1	2.46	0.47
1:D:64:PHE:CZ	1:D:86:MET:HG3	2.50	0.47
1:B:161:ASN:HA	1:B:195:LYS:HB2	1.97	0.47
1:C:733:THR:OG1	1:C:734:ASP:N	2.40	0.47
1:C:3:LYS:HD2	1:C:3:LYS:O	2.15	0.46
1:D:23:SER:OG	1:D:248:THR:HB	2.15	0.46
1:D:432:PHE:CD1	1:D:449:HIS:ND1	2.83	0.46
1:C:422:VAL:HA	1:C:425:ARG:CZ	2.45	0.46
1:C:115:PHE:CZ	1:C:353:GLY:HA3	2.51	0.46
1:A:336:GLU:CD	1:A:336:GLU:N	2.74	0.46
1:B:101:PRO:HG2	1:B:129:THR:HG23	1.98	0.46
1:B:159:SER:HB2	1:D:263:ARG:HB2	1.96	0.46
1:A:84:LYS:HE3	1:A:139:GLU:CD	2.41	0.46
1:A:187:VAL:HG13	3:A:924:HOH:O	2.16	0.46
1:A:86:MET:HE2	1:A:136:MET:CE	2.46	0.46
1:A:407:ASP:HB3	1:A:409:GLU:H	1.81	0.46
1:C:630:PRO:HB2	3:C:1067:HOH:O	2.14	0.46
1:D:94:ASN:HD22	1:D:295:VAL:H	1.64	0.46
1:A:725:LEU:HG	1:A:829:LEU:HD12	1.96	0.46
1:D:142:ALA:HB1	1:D:187:VAL:HB	1.98	0.46
1:D:407:ASP:OD2	1:D:408:ALA:N	2.37	0.46
1:A:84:LYS:HE2	1:A:84:LYS:HB3	1.76	0.46
1:B:678:PRO:HB3	1:B:702:TYR:CD1	2.50	0.46
1:D:210:ASP:O	1:D:214:ASP:HB2	2.16	0.46
1:A:3:LYS:HA	1:A:3:LYS:HD3	1.50	0.46
1:A:708:ARG:NH2	1:B:708:ARG:NH2	2.64	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:333:LEU:HB3	1:C:657:TYR:CE2	2.51	0.46
1:B:578:VAL:HG22	1:B:618:VAL:HG13	1.98	0.45
1:C:724:GLU:HB2	3:C:1122:HOH:O	2.16	0.45
1:A:407:ASP:HB3	1:A:410:ASN:H	1.81	0.45
1:B:246:GLY:HA2	1:B:247:PRO:C	2.41	0.45
1:B:297:ASN:CG	3:B:897:HOH:O	2.59	0.45
1:A:246:GLY:HA2	1:A:247:PRO:C	2.42	0.45
1:A:684:LYS:HG2	3:A:1002:HOH:O	2.16	0.45
1:A:708:ARG:HG3	3:A:880:HOH:O	2.16	0.45
1:A:725:LEU:HA	1:A:742:ASP:O	2.17	0.45
1:B:263:ARG:HB2	1:D:159:SER:HB2	1.99	0.45
1:D:57:ASP:HB2	1:D:435:THR:HG21	1.97	0.45
1:D:432:PHE:CD1	1:D:449:HIS:CE1	3.04	0.45
1:A:733:THR:CG2	1:A:736:LYS:HB2	2.45	0.45
1:B:607:VAL:HG11	1:B:631:TRP:CE2	2.52	0.45
1:C:474:ASP:C	1:C:475:TYR:CD1	2.94	0.45
1:D:377:LYS:O	1:D:378:GLU:C	2.57	0.45
1:C:350:THR:HG22	3:C:1030:HOH:O	2.16	0.45
1:B:739:ILE:HG13	1:B:740:SER:N	2.29	0.45
1:D:55:PHE:CG	1:D:443:HIS:CD2	3.05	0.45
1:B:184:ALA:O	1:B:185:ASN:C	2.60	0.44
1:C:533:TYR:OH	1:C:535:SER:HA	2.17	0.44
1:A:43:VAL:HG12	1:A:97:VAL:HB	1.99	0.44
1:B:206:LYS:HE2	3:B:884:HOH:O	2.18	0.44
1:B:625:THR:HB	1:B:626:PRO:CD	2.48	0.44
1:D:349:LYS:HG2	1:D:364:VAL:HB	2.00	0.44
1:C:155:ASP:O	1:C:685:THR:OG1	2.17	0.44
1:C:449:HIS:O	1:C:452:VAL:CG1	2.54	0.44
1:C:158:PHE:HB2	3:C:896:HOH:O	2.17	0.44
1:A:314:ARG:HB2	1:A:647:GLU:HG3	1.99	0.44
1:C:795:GLU:O	1:C:796:LEU:C	2.59	0.44
1:D:153:LEU:HD13	1:D:155:ASP:HB3	1.99	0.44
1:D:655:VAL:HG13	1:D:662:PRO:HG3	2.00	0.44
1:C:45:ASP:OD2	1:C:356:SER:HB2	2.17	0.44
1:A:396:GLU:OE2	1:A:439:ARG:HA	2.18	0.44
1:B:150:CYS:HA	1:B:152:ASP:OD2	2.17	0.44
1:C:400:ILE:HG12	1:C:410:ASN:O	2.18	0.44
1:B:5:ASP:O	1:B:9:LEU:HD12	2.18	0.43
1:D:276:ARG:NH2	3:D:1130:HOH:O	2.35	0.43
1:D:409:GLU:H	1:D:409:GLU:CD	2.26	0.43
1:A:57:ASP:CG	1:A:57:ASP:O	2.60	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:655:VAL:HA	1:A:660:VAL:O	2.19	0.43
1:C:474:ASP:O	1:C:475:TYR:CD1	2.72	0.43
1:D:400:ILE:HD11	1:D:436:LYS:HG3	2.00	0.43
1:B:286:VAL:HA	1:B:289:LEU:HG	1.99	0.43
1:C:708:ARG:NH2	1:D:708:ARG:NH2	2.66	0.43
1:A:86:MET:HE2	1:A:136:MET:HE3	2.00	0.43
1:A:464:THR:HG22	1:A:530:ARG:HG3	2.01	0.43
1:D:314:ARG:NE	1:D:650:ASN:HB3	2.32	0.43
1:A:263:ARG:HD2	1:C:159:SER:HB2	2.01	0.43
1:A:546:GLY:HA3	3:A:871:HOH:O	2.17	0.43
1:C:331:LEU:HA	1:C:332:PRO:C	2.44	0.43
1:B:160:SER:O	1:B:194:ASN:HB2	2.18	0.43
1:C:3:LYS:HD2	1:C:3:LYS:C	2.44	0.43
1:B:602:ARG:NH1	1:B:605:GLU:OE1	2.52	0.43
1:A:322:VAL:HG22	1:A:664:GLY:C	2.44	0.43
1:D:301:SER:HA	3:D:898:HOH:O	2.19	0.43
1:D:284:PHE:HD1	3:D:1486:HOH:O	2.02	0.43
1:A:734:ASP:C	1:A:735:ASP:CG	2.87	0.42
1:B:367:PRO:HD3	1:B:648:LEU:HD11	2.00	0.42
1:C:151:ASN:ND2	3:C:851:HOH:O	2.52	0.42
1:C:374:LYS:HA	1:C:374:LYS:HD3	1.94	0.42
1:A:489:LEU:HD12	1:A:489:LEU:HA	1.81	0.42
1:B:374:LYS:HA	1:B:374:LYS:HD3	1.79	0.42
1:B:578:VAL:HG12	1:B:580:ILE:HD11	2.02	0.42
1:A:134:LYS:HE3	1:A:183:HIS:O	2.19	0.42
1:A:374:LYS:NZ	1:A:659:ASP:OD2	2.46	0.42
1:B:648:LEU:HD12	1:B:649:GLY:N	2.34	0.42
1:A:166:GLU:OE1	1:A:206:LYS:NZ	2.48	0.42
1:D:21:LEU:HD23	1:D:21:LEU:HA	1.91	0.42
1:A:523:LYS:O	1:A:525:GLN:N	2.51	0.42
1:A:589:THR:O	1:A:590:GLU:C	2.60	0.42
1:C:314:ARG:CZ	1:C:650:ASN:HB3	2.50	0.42
1:C:386:TYR:CE2	1:C:558:ILE:HG12	2.55	0.42
1:C:539:SER:O	1:C:539:SER:OG	2.38	0.42
1:C:563:GLU:OE1	1:C:563:GLU:HA	2.19	0.42
1:C:723:PHE:HA	1:C:744:LYS:O	2.19	0.42
1:D:79:LEU:HD23	1:D:79:LEU:HA	1.76	0.42
1:D:281:MET:SD	1:D:281:MET:C	3.03	0.42
1:B:218:TRP:CZ2	1:B:220:GLY:HA3	2.55	0.42
1:C:371:ILE:HG22	1:C:379:VAL:HG21	2.00	0.42
1:C:744:LYS:HE3	1:C:785:GLY:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:489:LEU:CD1	1:A:529:VAL:HG12	2.49	0.42
1:B:288:ASN:O	1:B:292:THR:HG23	2.19	0.42
1:D:161:ASN:HA	1:D:195:LYS:HB2	2.01	0.42
1:C:233:ALA:HB1	1:C:265:GLN:HB2	2.02	0.42
1:D:49:GLY:C	1:D:50:ILE:HD13	2.45	0.42
1:D:323:LEU:HD22	1:D:662:PRO:HG2	2.02	0.42
1:D:744:LYS:HA	1:D:786:GLU:O	2.20	0.42
1:A:661:VAL:HG13	1:A:720:TYR:HB2	2.02	0.41
1:A:146:LYS:HE3	2:A:5001:BGC:O3	2.20	0.41
1:B:736:LYS:HB2	1:B:736:LYS:HE2	1.58	0.41
1:D:279:LEU:HD23	1:D:279:LEU:HA	1.88	0.41
1:A:286:VAL:HA	1:A:289:LEU:HG	2.02	0.41
1:A:350:THR:O	1:A:350:THR:OG1	2.33	0.41
1:A:417:PHE:HA	1:A:460:PHE:O	2.21	0.41
1:B:494:ILE:C	1:B:495:ILE:HG13	2.45	0.41
1:B:661:VAL:O	1:B:662:PRO:C	2.63	0.41
1:C:331:LEU:HB3	1:C:720:TYR:OH	2.20	0.41
1:D:226:TRP:CE2	2:D:5004:BGC:H6C2	2.55	0.41
1:A:167:ARG:NH2	3:A:887:HOH:O	2.51	0.41
1:A:730:PHE:CD2	1:A:832:LYS:HD2	2.56	0.41
1:A:733:THR:HG23	1:A:736:LYS:H	1.85	0.41
1:D:19:ILE:HG12	1:D:256:VAL:HG11	2.02	0.41
1:D:22:LEU:HD21	1:D:275:VAL:HG22	2.03	0.41
1:A:559:ASP:HB3	1:A:562:GLU:HB3	2.02	0.41
1:D:394:LEU:HB2	1:D:553:GLY:HA2	2.02	0.41
1:D:614:ASN:O	1:D:617:THR:OG1	2.38	0.41
1:A:468:VAL:HA	1:A:469:PRO:HD2	1.88	0.41
1:C:65:PRO:HG3	1:C:317:ALA:HA	2.02	0.41
1:C:340:ILE:HG13	1:C:341:VAL:N	2.34	0.41
1:C:386:TYR:HE2	1:C:558:ILE:HG12	1.86	0.41
1:D:241:ASP:HA	1:D:274:ARG:HD3	2.02	0.41
1:B:361:SER:O	1:B:362:TYR:C	2.63	0.41
1:C:62:GLY:HA2	1:C:646:ASN:ND2	2.36	0.41
1:C:623:SER:O	1:C:642:TRP:HA	2.21	0.41
1:C:684:LYS:HE3	1:C:684:LYS:HB2	2.00	0.41
1:C:743:VAL:HG12	1:C:782:LEU:HD11	2.03	0.41
1:D:119:SER:CB	1:D:124:LEU:HD23	2.50	0.41
1:D:221:MET:SD	1:D:278:VAL:HA	2.60	0.41
1:D:343:GLY:HA2	1:D:344:PRO:HD3	1.84	0.41
1:D:394:LEU:CB	1:D:553:GLY:HA2	2.51	0.41
1:A:48:ASN:HD21	1:A:357:ALA:HB1	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:89:GLU:OE2	1:B:362:TYR:OH	2.28	0.41
1:C:341:VAL:C	1:C:342:ILE:HG13	2.46	0.41
1:C:480:GLN:C	1:C:481:VAL:CG1	2.94	0.41
1:D:349:LYS:HE2	1:D:364:VAL:O	2.21	0.41
1:A:463:LEU:O	1:A:530:ARG:HA	2.21	0.40
1:A:720:TYR:HD1	1:A:720:TYR:HA	1.76	0.40
1:B:296:GLU:O	1:B:297:ASN:C	2.63	0.40
1:D:685:THR:HG22	3:D:927:HOH:O	2.21	0.40
1:B:127:MET:HE3	1:B:179:LEU:HD22	2.03	0.40
1:C:59:VAL:HA	1:C:60:PRO:HD3	1.92	0.40
1:C:653:ALA:O	1:C:654:ASP:C	2.62	0.40
1:C:663:ASN:OD1	1:C:779:LYS:NZ	2.53	0.40
1:A:480:GLN:NE2	1:A:506:PHE:HB2	2.36	0.40
1:A:753:SER:HA	1:A:780:VAL:O	2.21	0.40
1:B:732:VAL:O	1:B:732:VAL:CG2	2.64	0.40
1:D:314:ARG:CZ	1:D:650:ASN:HB3	2.50	0.40
1:D:367:PRO:HA	1:D:649:GLY:HA2	2.02	0.40
1:D:409:GLU:OE2	1:D:410:ASN:N	2.54	0.40
1:D:737:ILE:CD1	1:D:796:LEU:HD23	2.47	0.40
1:A:325:LYS:O	1:A:637:ALA:HA	2.22	0.40
1:A:578:VAL:HG22	1:A:618:VAL:CG1	2.52	0.40
1:D:239:GLY:HA2	1:D:274:ARG:CZ	2.52	0.40
1:D:756:VAL:O	1:D:777:PHE:HA	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	837/845 (99%)	792 (95%)	44 (5%)	1 (0%)	48 61
1	B	815/845 (96%)	776 (95%)	38 (5%)	1 (0%)	48 61

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	821/845 (97%)	773 (94%)	46 (6%)	2 (0%)	43	56
1	D	823/845 (97%)	773 (94%)	50 (6%)	0	100	100
All	All	3296/3380 (98%)	3114 (94%)	178 (5%)	4 (0%)	48	61

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	524	GLY
1	B	297	ASN
1	C	329	ASN
1	C	524	GLY

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	714/717 (100%)	677 (95%)	37 (5%)	21	32
1	B	700/717 (98%)	658 (94%)	42 (6%)	17	26
1	C	707/717 (99%)	664 (94%)	43 (6%)	17	25
1	D	703/717 (98%)	662 (94%)	41 (6%)	18	27
All	All	2824/2868 (98%)	2661 (94%)	163 (6%)	18	27

All (163) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	SER
1	A	3	LYS
1	A	54	LYS
1	A	206	LYS
1	A	294	ILE
1	A	333	LEU
1	A	377	LYS
1	A	400	ILE

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Mol	Chain	Res	Type
1	A	409	GLU
1	A	427	ASP
1	A	428	ASP
1	A	436	LYS
1	A	450	GLU
1	A	455	LYS
1	A	472	ASP
1	A	481	VAL
1	A	484	SER
1	A	503	ARG
1	A	518	LYS
1	A	522	LYS
1	A	530	ARG
1	A	565	ARG
1	A	580	ILE
1	A	675	GLN
1	A	677	ASN
1	A	726	ASP
1	A	731	LYS
1	A	732	VAL
1	A	733	THR
1	A	735	ASP
1	A	739	ILE
1	A	766	LYS
1	A	790	VAL
1	A	794	LEU
1	A	795	GLU
1	A	797	LYS
1	A	845	LEU
1	B	3	LYS
1	B	8	GLN
1	B	32	LYS
1	B	43	VAL
1	B	61	SER
1	B	294	ILE
1	B	333	LEU
1	B	335	LYS
1	B	377	LYS
1	B	400	ILE
1	B	427	ASP
1	B	429	GLU
1	B	435	THR

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Mol	Chain	Res	Type
1	B	436	LYS
1	B	444	LEU
1	B	466	GLN
1	B	521	LEU
1	B	522	LYS
1	B	531	VAL
1	B	535	SER
1	B	556	LYS
1	B	569	GLU
1	B	576	LYS
1	B	597	MET
1	B	618	VAL
1	B	677	ASN
1	B	682	ASN
1	B	684	LYS
1	B	686	GLU
1	B	731	LYS
1	B	732	VAL
1	B	733	THR
1	B	735	ASP
1	B	739	ILE
1	B	766	LYS
1	B	767	VAL
1	B	787	LYS
1	B	794	LEU
1	B	833	GLU
1	B	837	GLU
1	B	839	GLU
1	B	845	LEU
1	C	3	LYS
1	C	61	SER
1	C	255	LEU
1	C	294	ILE
1	C	310	SER
1	C	312	LEU
1	C	333	LEU
1	C	334	LYS
1	C	335	LYS
1	C	340	ILE
1	C	377	LYS
1	C	378	GLU
1	C	404	LYS

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Mol	Chain	Res	Type
1	C	409	GLU
1	C	414	ILE
1	C	445	PHE
1	C	452	VAL
1	C	468	VAL
1	C	472	ASP
1	C	474	ASP
1	C	481	VAL
1	C	503	ARG
1	C	507	CYS
1	C	522	LYS
1	C	539	SER
1	C	559	ASP
1	C	579	LEU
1	C	580	ILE
1	C	618	VAL
1	C	677	ASN
1	C	726	ASP
1	C	732	VAL
1	C	739	ILE
1	C	766	LYS
1	C	793	ASP
1	C	794	LEU
1	C	816	GLU
1	C	818	LEU
1	C	831	VAL
1	C	832	LYS
1	C	833	GLU
1	C	838	LYS
1	C	845	LEU
1	D	294	ILE
1	D	307	LYS
1	D	312	LEU
1	D	333	LEU
1	D	340	ILE
1	D	365	VAL
1	D	366	SER
1	D	372	VAL
1	D	377	LYS
1	D	404	LYS
1	D	409	GLU
1	D	411	SER

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Mol	Chain	Res	Type
1	D	420	ASN
1	D	438	ASN
1	D	470	GLN
1	D	474	ASP
1	D	488	TYR
1	D	494	ILE
1	D	498	LYS
1	D	507	CYS
1	D	512	THR
1	D	530	ARG
1	D	560	ASP
1	D	597	MET
1	D	617	THR
1	D	633	GLU
1	D	677	ASN
1	D	684	LYS
1	D	722	THR
1	D	739	ILE
1	D	766	LYS
1	D	767	VAL
1	D	796	LEU
1	D	797	LYS
1	D	819	VAL
1	D	832	LYS
1	D	833	GLU
1	D	835	LYS
1	D	837	GLU
1	D	838	LYS
1	D	845	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (46) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	15	GLN
1	A	48	ASN
1	A	94	ASN
1	A	373	ASN
1	A	388	HIS
1	A	480	GLN
1	A	525	GLN
1	A	616	ASN
1	A	621	ASN

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Mol	Chain	Res	Type
1	A	636	ASN
1	A	650	ASN
1	A	675	GLN
1	A	781	HIS
1	B	15	GLN
1	B	94	ASN
1	B	151	ASN
1	B	288	ASN
1	B	388	HIS
1	B	525	GLN
1	B	636	ASN
1	B	781	HIS
1	C	94	ASN
1	C	151	ASN
1	C	433	HIS
1	C	438	ASN
1	C	443	HIS
1	C	470	GLN
1	C	497	GLN
1	C	525	GLN
1	C	616	ASN
1	C	636	ASN
1	C	646	ASN
1	C	682	ASN
1	C	764	ASN
1	D	48	ASN
1	D	94	ASN
1	D	151	ASN
1	D	373	ASN
1	D	388	HIS
1	D	443	HIS
1	D	480	GLN
1	D	500	ASN
1	D	551	GLN
1	D	636	ASN
1	D	675	GLN
1	D	764	ASN

5.3.3 RNA ⓘ

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](#)

4 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
2	BGC	A	5001	-	12,12,12	0.68	0	17,17,17	1.58	3 (17%)
2	BGC	B	5002	-	12,12,12	0.79	0	17,17,17	2.15	4 (23%)
2	BGC	C	5003	-	12,12,12	0.58	0	17,17,17	0.74	0
2	BGC	D	5004	-	12,12,12	0.84	0	17,17,17	1.65	3 (17%)

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	BGC	A	5001	-	-	0/2/22/22	0/1/1/1
2	BGC	B	5002	-	-	0/2/22/22	0/1/1/1
2	BGC	C	5003	-	-	0/2/22/22	0/1/1/1
2	BGC	D	5004	-	-	0/2/22/22	0/1/1/1

There are no bond length outliers.

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	5002	BGC	C1-O5-C5	5.43	124.15	113.65

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	5002	BGC	O1-C1-O5	-5.02	95.51	110.41
2	A	5001	BGC	C1-O5-C5	4.39	122.15	113.65
2	D	5004	BGC	O1-C1-O5	-3.29	100.63	110.41
2	D	5004	BGC	C3-C4-C5	-3.12	104.57	110.23
2	B	5002	BGC	O5-C1-C2	2.96	115.50	110.30
2	B	5002	BGC	O4-C4-C5	-2.70	102.67	109.32
2	D	5004	BGC	O2-C2-C1	2.66	115.39	109.25
2	A	5001	BGC	O1-C1-O5	-2.57	102.78	110.41
2	A	5001	BGC	O5-C1-C2	2.44	114.59	110.30

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	5001	BGC	2	0
2	B	5002	BGC	1	0
2	C	5003	BGC	1	0
2	D	5004	BGC	3	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	841/845 (99%)	-0.60	3 (0%) 88 90	15, 31, 60, 77	0
1	B	825/845 (97%)	-0.60	7 (0%) 82 84	15, 26, 76, 97	0
1	C	831/845 (98%)	-0.26	14 (1%) 69 69	18, 38, 87, 105	0
1	D	829/845 (98%)	-0.14	16 (1%) 66 66	19, 43, 80, 99	0
All	All	3326/3380 (98%)	-0.40	40 (1%) 76 77	15, 35, 80, 105	0

All (40) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	543	GLY	5.2
1	B	504	GLY	4.6
1	B	509	GLY	4.6
1	B	444	LEU	4.1
1	D	422	VAL	3.9
1	D	431	PRO	3.8
1	C	405	PRO	3.7
1	B	421	PRO	3.6
1	C	508	PHE	3.1
1	B	447	PHE	2.8
1	A	545	PHE	2.8
1	D	421	PRO	2.7
1	D	524	GLY	2.6
1	D	417	PHE	2.5
1	D	408	ALA	2.5
1	D	526	VAL	2.5
1	D	400	ILE	2.4
1	B	510	ALA	2.4
1	D	402	ALA	2.4
1	C	3	LYS	2.4
1	C	545	PHE	2.4

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Mol	Chain	Res	Type	RSRZ
1	D	529	VAL	2.4
1	C	445	PHE	2.3
1	C	733	THR	2.3
1	B	455	LYS	2.3
1	D	732	VAL	2.3
1	D	476	ILE	2.2
1	D	468	VAL	2.2
1	C	498	LYS	2.2
1	C	452	VAL	2.1
1	C	526	VAL	2.1
1	D	487	PHE	2.1
1	C	510	ALA	2.1
1	A	733	THR	2.1
1	D	403	ALA	2.1
1	C	507	CYS	2.1
1	D	539	SER	2.1
1	C	550	PHE	2.0
1	C	531	VAL	2.0
1	C	495	ILE	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	BGC	A	5001	12/12	0.95	0.07	20,28,32,37	0
2	BGC	B	5002	12/12	0.96	0.07	25,28,30,33	0
2	BGC	D	5004	12/12	0.96	0.06	32,36,38,41	0
2	BGC	C	5003	12/12	0.97	0.05	28,34,38,42	0

6.5 Other polymers ⓘ

There are no such residues in this entry.