



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 19, 2026 – 08:25 PM UTC

PDB ID : 4UOZ / pdb_00004uoz
Title : beta-(1,6)-galactosidase from Bifidobacterium animalis subsp. lactis Bl-04 nucleophile mutant E324A in complex with galactose
Authors : Viborg, A.H.; Fredslund, F.; Katayama, T.; Nielsen, S.K.; Svensson, B.; Kitaoka, M.; Lo Leggio, L.; Abou Hachem, M.
Deposited on : 2014-06-11
Resolution : 2.30 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

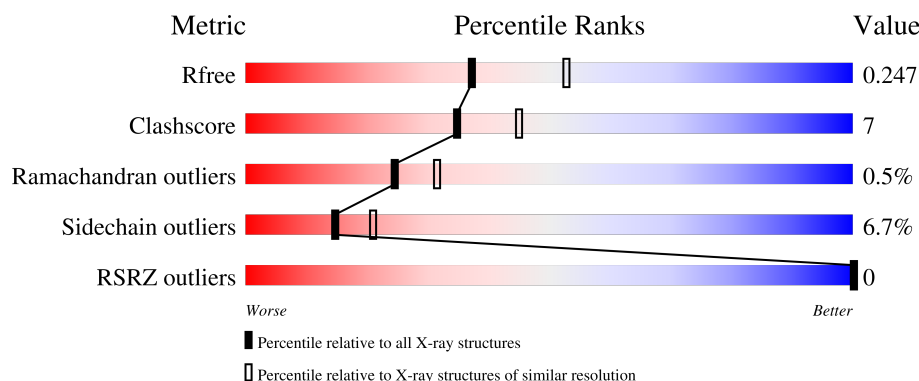
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (2.30-2.30)

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	695	
1	B	695	
1	C	695	

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 17041 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

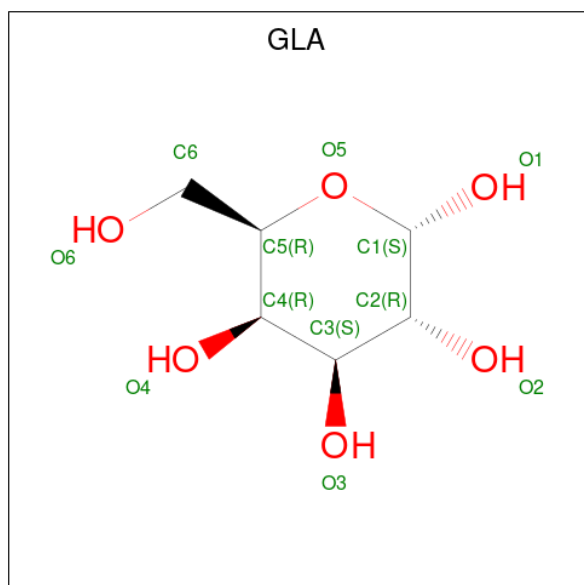
- Molecule 1 is a protein called BETA-GALACTOSIDASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	688	Total	C	N	O	S	0	1	0
			5474	3460	954	1037	23			
1	B	688	Total	C	N	O	S	0	1	0
			5474	3460	955	1036	23			
1	C	688	Total	C	N	O	S	0	0	0
			5469	3457	954	1035	23			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	324	ALA	GLU	engineered mutation	UNP C6A6W5
B	324	ALA	GLU	engineered mutation	UNP C6A6W5
C	324	ALA	GLU	engineered mutation	UNP C6A6W5

- Molecule 2 is alpha-D-galactopyranose (CCD ID: GLA) (formula: C₆H₁₂O₆).

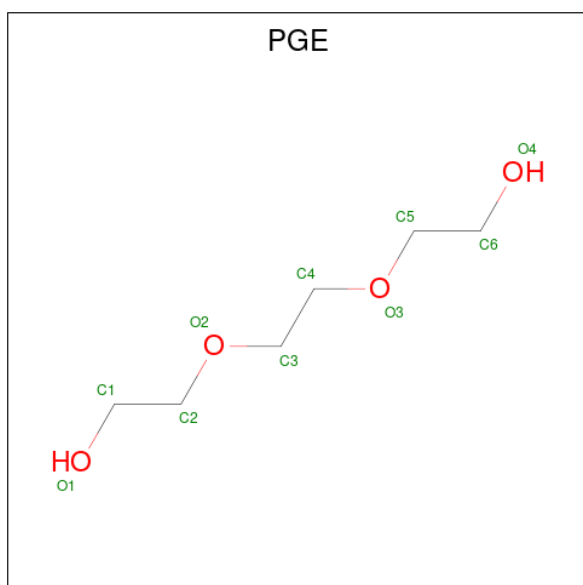


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			12	6	6		
2	B	1	Total	C	O	0	0
			12	6	6		
2	C	1	Total	C	O	0	0
			12	6	6		

- Molecule 3 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Zn	0	0
			1	1		

- Molecule 4 is TRIETHYLENE GLYCOL (CCD ID: PGE) (formula: C₆H₁₄O₄).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			10	6	4		
4	A	1	Total	C	O	0	0
			10	6	4		
4	B	1	Total	C	O	0	0
			10	6	4		
4	B	1	Total	C	O	0	0
			10	6	4		
4	C	1	Total	C	O	0	0
			10	6	4		
4	C	1	Total	C	O	0	0
			10	6	4		

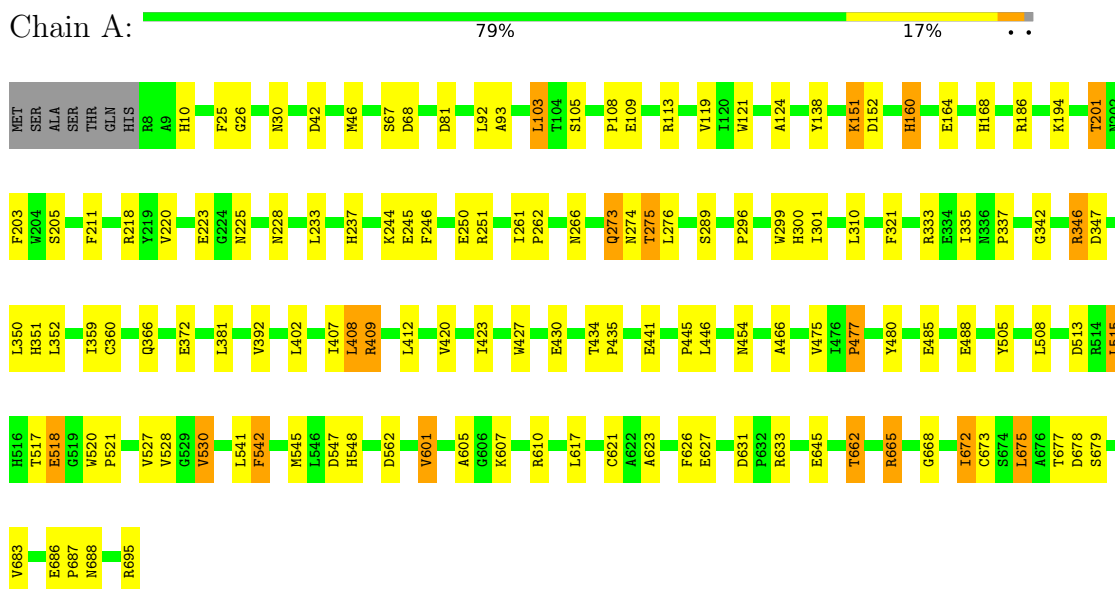
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	185	Total 185	O 185	0	0
5	B	200	Total 200	O 200	0	0
5	C	142	Total 142	O 142	0	0

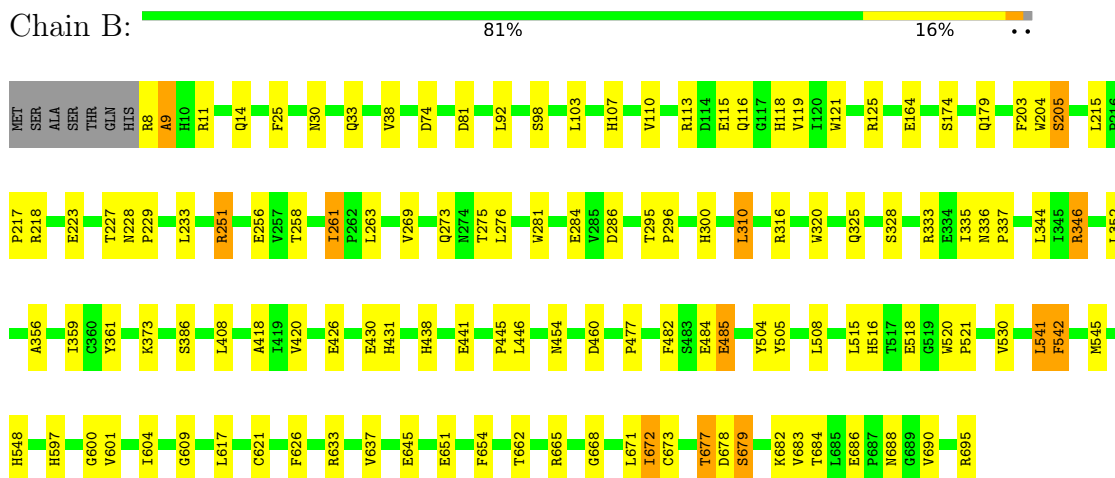
3 Residue-property plots

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.

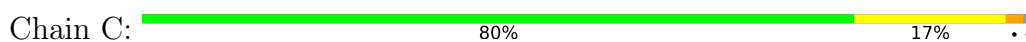
• Molecule 1: BETA-GALACTOSIDASE



• Molecule 1: BETA-GALACTOSIDASE



• Molecule 1: BETA-GALACTOSIDASE





4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	134.20Å 167.97Å 108.58Å 90.00° 115.64° 90.00°	Depositor
Resolution (Å)	28.68 – 2.30 28.68 – 2.30	Depositor EDS
% Data completeness (in resolution range)	99.9 (28.68-2.30) 99.9 (28.68-2.30)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.02 (at 2.31Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.186 , 0.248 0.186 , 0.247	Depositor DCC
R_{free} test set	4795 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	22.3	Xtriage
Anisotropy	0.063	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 27.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.085 for -1/2*h+1/2*k-l,1/2*h-1/2*k-l,-1/2 *h-1/2*k 0.045 for -1/2*h-1/2*k-l,-1/2*h-1/2*k+l,-1/ 2*h+1/2*k	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	17041	wwPDB-VP
Average B, all atoms (Å ²)	23.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.98% 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: ZN, PGE, GLA

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	1.17	9/5631 (0.2%)	1.16	20/7677 (0.3%)
1	B	1.20	11/5631 (0.2%)	1.15	17/7678 (0.2%)
1	C	1.16	7/5623 (0.1%)	1.14	16/7666 (0.2%)
All	All	1.18	27/16885 (0.2%)	1.15	53/23021 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1

All (27) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	124	ALA	CA-C	11.17	1.57	1.52
1	C	275	THR	CA-C	8.10	1.56	1.52
1	B	609	GLY	N-CA	7.21	1.54	1.45
1	A	275	THR	CA-C	6.56	1.55	1.52
1	A	601	VAL	N-CA	6.26	1.54	1.46
1	B	275	THR	CA-C	6.16	1.55	1.52
1	A	201	THR	CA-C	5.59	1.60	1.52
1	B	654	PHE	C-O	5.54	1.30	1.24
1	B	431	HIS	CG-CD2	5.52	1.42	1.35
1	A	10	HIS	CG-CD2	5.37	1.41	1.35
1	C	300	HIS	CG-CD2	5.32	1.41	1.35
1	B	300	HIS	CG-CD2	5.30	1.41	1.35
1	C	168	HIS	CG-CD2	5.29	1.41	1.35
1	C	599	GLY	N-CA	5.23	1.49	1.44
1	C	160	HIS	CG-CD2	5.21	1.41	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	438	HIS	CG-CD2	5.17	1.41	1.35
1	B	438	HIS	CG-CD2	5.15	1.41	1.35
1	B	300	HIS	ND1-CE1	5.11	1.37	1.32
1	B	548	HIS	ND1-CE1	5.11	1.37	1.32
1	A	351	HIS	CE1-NE2	5.09	1.37	1.32
1	B	516	HIS	CG-CD2	5.09	1.41	1.35
1	B	597	HIS	CG-CD2	5.05	1.41	1.35
1	A	168	HIS	CG-CD2	5.05	1.41	1.35
1	A	160	HIS	CG-CD2	5.04	1.41	1.35
1	A	548	HIS	ND1-CE1	5.02	1.37	1.32
1	C	10	HIS	CG-CD2	5.01	1.41	1.35
1	B	548	HIS	CG-CD2	5.01	1.41	1.35

All (53) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	98	SER	CA-C-N	10.90	127.51	119.66
1	C	98	SER	C-N-CA	10.90	127.51	119.66
1	A	601	VAL	N-CA-C	9.41	121.49	107.75
1	C	601	VAL	N-CA-C	9.10	121.24	107.77
1	B	346	ARG	NE-CZ-NH2	-8.85	111.23	119.20
1	B	346	ARG	CG-CD-NE	-7.92	94.57	112.00
1	B	601	VAL	N-CA-C	7.91	120.53	107.24
1	A	631	ASP	CA-C-N	-7.75	111.85	120.45
1	A	631	ASP	C-N-CA	-7.75	111.85	120.45
1	A	686	GLU	CA-C-N	-7.15	112.39	119.76
1	A	686	GLU	C-N-CA	-7.15	112.39	119.76
1	C	346	ARG	CG-CD-NE	-6.87	96.89	112.00
1	A	151	LYS	N-CA-C	-6.77	101.56	110.43
1	B	542	PHE	CA-C-N	-6.69	112.87	119.76
1	B	542	PHE	C-N-CA	-6.69	112.87	119.76
1	B	261	ILE	CA-C-N	6.49	126.47	119.78
1	B	261	ILE	C-N-CA	6.49	126.47	119.78
1	A	346	ARG	NE-CZ-NH2	-6.45	113.40	119.20
1	B	420	VAL	N-CA-C	6.35	117.93	108.54
1	C	665	ARG	CA-C-N	6.23	126.14	119.85
1	C	665	ARG	C-N-CA	6.23	126.14	119.85
1	A	228	ASN	CA-C-N	6.22	125.44	118.97
1	A	228	ASN	C-N-CA	6.22	125.44	118.97
1	C	244	LYS	N-CA-C	-6.13	104.68	111.36
1	B	215	LEU	CA-C-N	-5.95	114.25	120.38
1	B	215	LEU	C-N-CA	-5.95	114.25	120.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	662	THR	N-CA-C	-5.82	99.53	109.24
1	C	70	ASN	N-CA-C	5.78	117.72	108.41
1	C	686	GLU	CA-C-N	-5.75	114.03	119.90
1	C	686	GLU	C-N-CA	-5.75	114.03	119.90
1	B	125	ARG	N-CA-C	5.74	117.25	108.42
1	A	542	PHE	CA-C-N	-5.69	113.90	119.76
1	A	542	PHE	C-N-CA	-5.69	113.90	119.76
1	C	96	THR	N-CA-C	5.68	119.84	113.02
1	B	228	ASN	CA-C-N	5.64	125.10	119.24
1	B	228	ASN	C-N-CA	5.64	125.10	119.24
1	B	686	GLU	CA-C-N	-5.58	114.01	119.76
1	B	686	GLU	C-N-CA	-5.58	114.01	119.76
1	C	379	LEU	CA-C-N	5.56	125.87	119.92
1	C	379	LEU	C-N-CA	5.56	125.87	119.92
1	A	412	LEU	N-CA-C	-5.54	101.71	109.96
1	A	488	GLU	N-CA-C	-5.49	105.22	111.14
1	A	346	ARG	CG-CD-NE	-5.40	100.12	112.00
1	C	71	PHE	N-CA-C	5.27	118.00	107.62
1	A	244	LYS	N-CA-C	-5.24	105.48	111.14
1	A	665	ARG	CA-C-N	-5.22	115.19	120.31
1	A	665	ARG	C-N-CA	-5.22	115.19	120.31
1	B	98	SER	CA-C-N	5.20	125.74	120.38
1	B	98	SER	C-N-CA	5.20	125.74	120.38
1	C	434	THR	CA-C-N	-5.18	114.28	119.56
1	C	434	THR	C-N-CA	-5.18	114.28	119.56
1	A	420	VAL	N-CA-C	5.11	116.10	108.54
1	A	466	ALA	N-CA-C	-5.01	103.43	110.35

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	361	TYR	Peptide

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	5474	0	5179	80	0
1	B	5474	0	5181	86	0
1	C	5469	0	5175	88	0
2	A	12	0	12	1	0
2	B	12	0	12	1	0
2	C	12	0	12	0	0
3	A	1	0	0	0	0
4	A	20	0	28	1	0
4	B	20	0	28	1	0
4	C	20	0	28	1	0
5	A	185	0	0	17	0
5	B	200	0	0	20	0
5	C	142	0	0	16	0
All	All	17041	0	15655	241	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 (241) 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:9:ALA:HB1	5:B:2001:HOH:O	1.20	1.32
1:C:615:GLN:HB2	5:C:2136:HOH:O	1.21	1.31
1:B:118:HIS:HD2	5:B:2052:HOH:O	1.13	1.30
1:C:251:ARG:HD3	5:C:2053:HOH:O	1.27	1.27
1:C:352:LEU:HG	5:C:2085:HOH:O	1.09	1.25
1:B:673:CYS:HB2	5:B:2197:HOH:O	1.41	1.21
1:A:673:CYS:HB2	5:A:2182:HOH:O	1.41	1.19
1:C:251:ARG:HB2	5:C:2053:HOH:O	1.41	1.19
1:C:545:MET:SD	5:C:2120:HOH:O	2.10	1.09
1:B:118:HIS:CD2	5:B:2052:HOH:O	1.93	1.08
1:A:30:ASN:HB2	5:A:2017:HOH:O	1.54	1.04
1:B:673:CYS:CB	5:B:2197:HOH:O	2.02	0.98
1:C:542:PHE:H	1:C:545:MET:CE	1.76	0.96
1:B:673:CYS:SG	5:B:2197:HOH:O	2.22	0.95
1:B:113:ARG:HH21	1:B:119:VAL:HG22	1.35	0.88
1:B:8:ARG:O	1:B:9:ALA:HB3	1.73	0.87
1:B:30[B]:ASN:HD22	1:B:33:GLN:NE2	1.73	0.86
1:B:333:ARG:HD2	5:B:2114:HOH:O	1.74	0.86
1:C:542:PHE:HB2	1:C:545:MET:CE	2.09	0.83
1:A:623:ALA:HA	4:A:1698:PGE:H5	1.62	0.82
1:C:542:PHE:N	1:C:545:MET:HE1	1.93	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:56:LEU:HB3	5:C:2012:HOH:O	1.80	0.81
1:C:251:ARG:CD	5:C:2053:HOH:O	2.02	0.80
1:C:660:THR:O	5:C:2141:HOH:O	1.92	0.80
1:B:542:PHE:H	1:B:545:MET:HE3	1.48	0.79
1:C:56:LEU:CB	5:C:2012:HOH:O	2.31	0.79
1:C:542:PHE:H	1:C:545:MET:HE1	1.43	0.79
1:C:542:PHE:H	1:C:545:MET:HE3	1.46	0.78
1:A:346:ARG:NH2	1:A:688:ASN:OD1	2.17	0.78
1:C:542:PHE:N	1:C:545:MET:CE	2.47	0.77
1:C:694:ARG:HH11	1:C:694:ARG:HG2	1.49	0.77
1:A:542:PHE:HB2	1:A:545:MET:CE	2.15	0.77
1:C:56:LEU:HD12	1:C:92:LEU:HD23	1.66	0.75
1:B:30[B]:ASN:HD22	1:B:33:GLN:CD	1.94	0.75
1:B:203:PHE:HB3	5:B:2071:HOH:O	1.85	0.74
1:C:542:PHE:HB2	1:C:545:MET:HE2	1.68	0.74
1:A:665:ARG:NH2	1:A:668:GLY:O	2.22	0.73
1:B:8:ARG:O	1:B:9:ALA:CB	2.36	0.73
1:A:542:PHE:HD2	1:A:545:MET:HE1	1.54	0.72
1:C:333:ARG:HD3	5:C:2077:HOH:O	1.89	0.72
1:B:333:ARG:CD	5:B:2114:HOH:O	2.35	0.72
5:A:2116:HOH:O	1:B:229:PRO:HG2	1.88	0.71
1:A:409:ARG:HG2	5:A:2001:HOH:O	1.88	0.71
1:C:42:ASP:HB3	1:C:46:MET:HE3	1.75	0.69
1:C:276:LEU:HD12	1:C:276:LEU:H	1.57	0.68
1:C:248:CYS:O	1:C:251:ARG:HG3	1.94	0.68
1:B:665:ARG:NH2	1:B:668:GLY:O	2.27	0.67
1:B:454:ASN:CG	5:B:2165:HOH:O	2.36	0.67
1:B:346:ARG:NH2	1:B:688:ASN:OD1	2.27	0.66
1:B:333:ARG:CG	5:B:2114:HOH:O	2.44	0.66
1:C:205:SER:HA	5:C:2042:HOH:O	1.94	0.66
1:B:30[B]:ASN:ND2	1:B:33:GLN:CD	2.54	0.65
1:B:205:SER:HA	5:B:2072:HOH:O	1.96	0.65
1:B:542:PHE:H	1:B:545:MET:CE	2.10	0.64
1:C:299:TRP:CD1	4:C:1696:PGE:H42	2.34	0.63
1:C:56:LEU:CD1	1:C:92:LEU:HD23	2.28	0.63
1:B:454:ASN:HB3	5:B:2165:HOH:O	1.98	0.62
1:B:671:LEU:O	1:B:672:ILE:HD12	1.99	0.62
1:C:694:ARG:HG2	1:C:694:ARG:NH1	2.14	0.61
1:B:665:ARG:NH1	1:B:678:ASP:OD2	2.33	0.61
1:A:296:PRO:HB2	1:B:545:MET:HE2	1.82	0.61
1:B:333:ARG:HG3	5:B:2114:HOH:O	2.01	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:545:MET:HE2	1:C:296:PRO:HB2	1.83	0.60
1:C:296:PRO:HB3	1:C:337:PRO:HG2	1.81	0.60
1:A:610:ARG:HD2	5:A:2147:HOH:O	2.02	0.60
1:B:8:ARG:O	1:B:8:ARG:CG	2.50	0.60
1:A:372:GLU:OE1	1:B:203:PHE:HZ	1.85	0.59
1:B:276:LEU:HD23	1:B:281:TRP:CZ2	2.38	0.59
1:C:179:GLN:HE21	1:C:179:GLN:HA	1.68	0.59
1:C:255:SER:HB2	5:C:2001:HOH:O	2.02	0.59
1:C:346:ARG:NH2	1:C:688:ASN:OD1	2.35	0.58
1:A:542:PHE:CD2	1:A:545:MET:HE1	2.38	0.58
1:B:542:PHE:HD2	1:B:545:MET:HE1	1.68	0.58
1:A:542:PHE:H	1:A:545:MET:HE3	1.69	0.57
1:A:151:LYS:O	1:A:152:ASP:HB2	2.04	0.57
1:A:333:ARG:NH1	5:A:2085:HOH:O	2.36	0.57
1:B:121:TRP:CD1	1:C:218:ARG:HB3	2.39	0.57
1:A:673:CYS:CB	5:A:2182:HOH:O	2.19	0.56
1:C:55:SER:HA	1:C:91:ASP:O	2.05	0.56
1:C:542:PHE:CB	1:C:545:MET:CE	2.83	0.56
1:A:346:ARG:NH1	1:A:347:ASP:OD1	2.33	0.56
1:A:409:ARG:NH1	5:A:2007:HOH:O	2.39	0.55
1:B:8:ARG:O	1:B:8:ARG:HG2	2.06	0.55
1:C:679:SER:HB3	1:C:682:LYS:O	2.07	0.55
1:B:520:TRP:HA	1:B:521:PRO:C	2.31	0.55
1:A:695:ARG:HG2	1:A:695:ARG:HH11	1.70	0.55
1:B:269:VAL:HG13	1:B:310:LEU:HD13	1.89	0.55
1:B:542:PHE:N	1:B:545:MET:HE3	2.20	0.55
1:A:520:TRP:HA	1:A:521:PRO:C	2.32	0.55
1:B:107:HIS:O	1:B:110:VAL:HG22	2.07	0.55
1:A:109:GLU:O	5:A:2033:HOH:O	2.18	0.54
1:C:352:LEU:HD13	1:C:642:ARG:NH1	2.22	0.54
1:A:513:ASP:OD2	1:C:373:LYS:NZ	2.38	0.54
1:A:203:PHE:HB3	5:A:2057:HOH:O	2.07	0.54
1:A:515:LEU:HB3	1:C:381:LEU:HD13	1.90	0.54
1:B:542:PHE:HB2	1:B:545:MET:CE	2.38	0.54
1:B:333:ARG:HD3	5:B:2113:HOH:O	2.08	0.54
1:C:352:LEU:CD1	1:C:642:ARG:NH1	2.70	0.54
1:C:251:ARG:CB	5:C:2053:HOH:O	2.20	0.54
1:A:93:ALA:HA	1:A:160:HIS:O	2.09	0.53
1:C:570:ASP:OD1	1:C:570:ASP:N	2.39	0.53
1:C:103:LEU:HD11	1:C:138:TYR:CG	2.43	0.53
1:B:296:PRO:HB2	1:C:545:MET:HE2	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:203:PHE:HZ	1:C:372:GLU:OE1	1.92	0.52
1:B:542:PHE:HD2	1:B:545:MET:CE	2.23	0.52
1:A:607:LYS:HE2	5:A:2142:HOH:O	2.09	0.52
1:C:167:CYS:HA	1:C:268:MET:HE1	1.92	0.52
1:C:542:PHE:N	1:C:545:MET:HE3	2.21	0.52
1:B:386:SER:HA	1:C:533:GLU:OE2	2.10	0.51
1:C:201:THR:OG1	1:C:207:ARG:HA	2.09	0.51
1:C:39:GLN:O	1:C:43:ILE:HG12	2.11	0.51
1:C:604:ILE:N	1:C:604:ILE:HD12	2.25	0.51
1:B:269:VAL:CG1	1:B:310:LEU:HD13	2.40	0.51
1:A:113:ARG:HH21	1:A:119:VAL:CG2	2.23	0.51
1:B:276:LEU:HD12	1:B:276:LEU:H	1.76	0.50
1:B:373:LYS:HG3	1:C:515:LEU:HD22	1.92	0.50
1:A:621:CYS:HB3	1:A:626:PHE:O	2.12	0.50
1:A:542:PHE:HB2	1:A:545:MET:HE3	1.90	0.50
1:B:103:LEU:O	1:B:103:LEU:HD23	2.11	0.50
1:B:113:ARG:HG3	1:B:174:SER:HB3	1.94	0.50
1:B:651:GLU:OE1	1:B:695:ARG:NH1	2.45	0.50
1:A:121:TRP:CD1	1:B:218:ARG:HB3	2.47	0.49
1:B:11:ARG:HB2	1:B:286:ASP:HB3	1.95	0.49
1:B:344:LEU:C	1:B:344:LEU:HD23	2.36	0.49
1:B:542:PHE:HB2	1:B:545:MET:HE3	1.94	0.49
1:C:43:ILE:HD13	1:C:83:LEU:HD23	1.95	0.49
1:B:316:ARG:HA	5:B:2102:HOH:O	2.12	0.49
1:B:541:LEU:HB3	1:B:545:MET:HE1	1.94	0.49
1:C:189:TYR:CD2	1:C:195:VAL:HG22	2.48	0.49
1:A:335:ILE:O	1:A:337:PRO:HD3	2.13	0.49
1:B:335:ILE:O	1:B:337:PRO:HD3	2.13	0.49
1:B:346:ARG:HD2	1:B:346:ARG:C	2.38	0.48
1:B:251:ARG:HB2	1:B:263:LEU:HD22	1.96	0.48
1:A:275:THR:O	1:A:427:TRP:HZ2	1.97	0.48
1:C:56:LEU:CD2	5:C:2012:HOH:O	2.60	0.48
1:C:109:GLU:O	5:C:2025:HOH:O	2.19	0.48
1:A:186:ARG:HA	1:A:211:PHE:CE2	2.49	0.48
1:B:679:SER:HB2	1:B:682:LYS:O	2.13	0.48
1:B:118:HIS:HA	5:B:2052:HOH:O	2.14	0.48
1:C:527:VAL:HG12	1:C:601:VAL:HG21	1.96	0.48
1:A:517:THR:C	1:A:518:GLU:HG2	2.39	0.48
1:A:164:GLU:OE2	2:A:701:GLA:H1	2.14	0.47
1:C:151:LYS:HB2	1:C:151:LYS:NZ	2.28	0.47
1:A:25:PHE:HA	1:A:359:ILE:O	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:547:ASP:OD1	1:A:547:ASP:C	2.58	0.47
1:C:43:ILE:CD1	1:C:83:LEU:HD23	2.45	0.47
1:A:299:TRP:CH2	1:A:610:ARG:HD3	2.50	0.47
1:A:67:SER:O	1:A:68:ASP:C	2.58	0.46
1:A:300:HIS:HE1	1:A:347:ASP:OD2	1.97	0.46
1:B:542:PHE:N	1:B:545:MET:CE	2.75	0.46
1:C:276:LEU:HD12	1:C:276:LEU:N	2.29	0.46
1:A:273:GLN:HE22	1:A:423:ILE:HD13	1.81	0.46
1:B:296:PRO:HB3	1:B:337:PRO:HG2	1.97	0.46
1:A:113:ARG:HH21	1:A:119:VAL:HG22	1.80	0.46
1:B:164:GLU:OE2	2:B:701:GLA:H1	2.15	0.46
1:B:203:PHE:CE2	1:B:204:TRP:CE2	3.04	0.46
1:A:26:GLY:O	1:A:360:CYS:HA	2.16	0.46
1:C:346:ARG:HD2	1:C:346:ARG:C	2.41	0.46
1:A:276:LEU:HD12	1:A:276:LEU:H	1.81	0.46
1:B:485:GLU:CD	1:B:485:GLU:H	2.23	0.46
1:C:93:ALA:HA	1:C:160:HIS:HB3	1.98	0.46
1:A:108:PRO:HD2	1:A:109:GLU:OE1	2.16	0.45
1:A:673:CYS:SG	5:A:2182:HOH:O	2.61	0.45
1:A:237:HIS:HE1	5:A:2076:HOH:O	1.99	0.45
1:C:26:GLY:HA3	1:C:53:ILE:O	2.17	0.45
1:A:218:ARG:HB3	1:C:121:TRP:CD1	2.52	0.45
1:A:562:ASP:HB2	1:A:605:ALA:HB1	1.99	0.45
1:A:237:HIS:HD2	5:A:2074:HOH:O	2.00	0.45
1:B:621:CYS:HB3	1:B:626:PHE:O	2.17	0.45
1:C:24:TRP:HB2	1:C:358:ALA:CB	2.46	0.45
1:A:246:PHE:HE1	1:A:250:GLU:OE2	1.98	0.45
1:A:342:GLY:HA3	1:A:675:LEU:HD22	1.98	0.45
1:B:542:PHE:CD2	1:B:545:MET:HE1	2.50	0.45
1:C:464:ILE:HD11	1:C:486:MET:SD	2.56	0.45
1:B:454:ASN:CB	5:B:2165:HOH:O	2.55	0.45
1:C:545:MET:HE3	1:C:545:MET:HB2	1.64	0.45
1:C:103:LEU:HD23	1:C:103:LEU:O	2.17	0.44
1:C:671:LEU:HA	1:C:671:LEU:HD23	1.67	0.44
1:A:205:SER:HA	5:A:2058:HOH:O	2.18	0.44
1:C:68:ASP:HA	1:C:102:TRP:CH2	2.53	0.44
1:A:42:ASP:HB3	1:A:46:MET:HE3	2.00	0.44
1:A:273:GLN:NE2	1:A:423:ILE:HD13	2.33	0.44
1:C:276:LEU:HD23	1:C:281:TRP:CZ2	2.53	0.44
1:C:501:PHE:CD1	1:C:501:PHE:N	2.86	0.44
1:B:251:ARG:NH2	1:B:284:GLU:OE1	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:289:SER:HB3	1:A:321:PHE:HB3	1.99	0.43
1:A:296:PRO:HB3	1:A:337:PRO:HG2	2.00	0.43
1:A:301:ILE:HD11	1:A:346:ARG:NH2	2.34	0.43
1:C:317:LYS:O	1:C:411:LYS:HG2	2.18	0.43
1:A:434:THR:HB	1:A:435:PRO:HD2	2.01	0.43
1:A:475:VAL:O	1:A:477:PRO:HD3	2.19	0.43
1:C:92:LEU:HD13	1:C:159:TRP:CZ3	2.53	0.43
1:A:266:ASN:OD1	1:A:266:ASN:N	2.43	0.43
1:A:527:VAL:HG12	1:A:601:VAL:HG21	2.01	0.43
1:A:103:LEU:HD21	1:A:138:TYR:CD2	2.53	0.43
1:B:74:ASP:HB2	5:B:2040:HOH:O	2.19	0.43
1:B:441:GLU:O	1:B:445:PRO:HD2	2.18	0.43
1:B:604:ILE:N	1:B:604:ILE:HD12	2.33	0.43
1:C:649:ILE:O	1:C:694:ARG:HA	2.19	0.43
1:C:255:SER:HB3	1:C:263:LEU:HD11	2.00	0.43
1:C:520:TRP:HA	1:C:521:PRO:C	2.43	0.43
1:A:151:LYS:O	1:A:152:ASP:CB	2.61	0.42
1:A:441:GLU:O	1:A:445:PRO:HD2	2.20	0.42
1:A:480:TYR:CD1	1:A:480:TYR:C	2.97	0.42
1:A:542:PHE:H	1:A:545:MET:CE	2.33	0.42
1:B:677:THR:HB	1:B:684:THR:HB	2.00	0.42
1:C:129:ARG:NH1	1:C:176:ASP:OD2	2.45	0.42
1:B:320:TRP:O	1:B:356:ALA:HA	2.20	0.42
1:A:408:LEU:O	1:A:409:ARG:HB2	2.18	0.42
1:B:113:ARG:NH2	1:B:119:VAL:HG22	2.18	0.42
1:B:203:PHE:CZ	1:B:204:TRP:NE1	2.87	0.42
1:C:65:GLU:HA	1:C:70:ASN:O	2.20	0.42
1:A:261:ILE:HA	1:A:262:PRO:HD3	1.93	0.42
1:A:408:LEU:HB2	5:A:2124:HOH:O	2.20	0.42
1:C:510:ASP:OD1	1:C:510:ASP:C	2.63	0.42
1:B:14:GLN:HB2	5:B:2011:HOH:O	2.19	0.42
1:A:687:PRO:O	1:A:688:ASN:HB2	2.19	0.42
1:B:295:THR:HG21	4:B:1696:PGE:H2	2.01	0.41
1:A:402:LEU:O	1:A:407:ILE:HG22	2.20	0.41
1:A:665:ARG:NH1	1:A:678:ASP:OD1	2.53	0.41
1:B:258:THR:HB	1:B:261:ILE:HD12	2.02	0.41
1:C:665:ARG:HD2	1:C:679:SER:O	2.20	0.41
1:B:426:GLU:OE2	1:B:430:GLU:OE2	2.38	0.41
1:C:61:TRP:CG	1:C:100:PRO:HD3	2.55	0.41
1:C:251:ARG:HD2	1:C:252:ASP:OD1	2.21	0.41
1:C:56:LEU:HB2	5:C:2012:HOH:O	2.10	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:441:GLU:O	1:C:445:PRO:HD2	2.21	0.41
1:A:274:ASN:HB2	1:A:430:GLU:OE2	2.21	0.41
1:A:672:ILE:HD12	1:A:672:ILE:HA	1.81	0.41
1:B:25:PHE:HA	1:B:359:ILE:O	2.21	0.41
1:B:116:GLN:HB2	1:B:118:HIS:CE1	2.55	0.41
1:C:301:ILE:HD11	1:C:346:ARG:NH2	2.35	0.41
1:C:645:GLU:C	1:C:647:GLY:H	2.28	0.41
1:B:418:ALA:HA	1:B:460:ASP:O	2.21	0.41
5:A:2175:HOH:O	1:C:341:PRO:HG3	2.20	0.40
1:B:346:ARG:C	1:B:346:ARG:CD	2.94	0.40
1:B:336:ASN:O	1:C:537:PRO:HG2	2.22	0.40
1:A:289:SER:HA	1:A:321:PHE:O	2.21	0.40
1:A:366:GLN:HB3	1:A:381:LEU:HG	2.02	0.40
1:A:528:VAL:HG12	1:A:530:VAL:HB	2.03	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	687/695 (99%)	659 (96%)	26 (4%)	2 (0%)	36	46
1	B	687/695 (99%)	654 (95%)	27 (4%)	6 (1%)	14	17
1	C	686/695 (99%)	657 (96%)	26 (4%)	3 (0%)	30	38
All	All	2060/2085 (99%)	1970 (96%)	79 (4%)	11 (0%)	24	31

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	9	ALA
1	B	217	PRO
1	B	477	PRO

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Mol	Chain	Res	Type
1	B	504	TYR
1	C	504	TYR
1	A	201	THR
1	B	600	GLY
1	B	328	SER
1	C	477	PRO
1	C	69	GLY
1	A	477	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	575/580 (99%)	538 (94%)	37 (6%)	16	23
1	B	575/580 (99%)	539 (94%)	36 (6%)	16	23
1	C	574/580 (99%)	531 (92%)	43 (8%)	12	17
All	All	1724/1740 (99%)	1608 (93%)	116 (7%)	15	21

All (116) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	81	ASP
1	A	92	LEU
1	A	103	LEU
1	A	105	SER
1	A	194	LYS
1	A	220	VAL
1	A	223	GLU
1	A	225	ASN
1	A	233	LEU
1	A	245	GLU
1	A	251	ARG
1	A	273	GLN
1	A	310	LEU
1	A	350	LEU

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Mol	Chain	Res	Type
1	A	352	LEU
1	A	392	VAL
1	A	408	LEU
1	A	409	ARG
1	A	446	LEU
1	A	454	ASN
1	A	485	GLU
1	A	505	TYR
1	A	508	LEU
1	A	515	LEU
1	A	518	GLU
1	A	530	VAL
1	A	541	LEU
1	A	617	LEU
1	A	627	GLU
1	A	633	ARG
1	A	645	GLU
1	A	662	THR
1	A	672	ILE
1	A	675	LEU
1	A	677	THR
1	A	679	SER
1	A	683	VAL
1	B	38	VAL
1	B	81	ASP
1	B	92	LEU
1	B	115	GLU
1	B	179	GLN
1	B	205	SER
1	B	223	GLU
1	B	227	THR
1	B	233	LEU
1	B	251	ARG
1	B	256	GLU
1	B	273	GLN
1	B	310	LEU
1	B	325	GLN
1	B	352	LEU
1	B	408	LEU
1	B	446	LEU
1	B	482	PHE
1	B	484	GLU

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Mol	Chain	Res	Type
1	B	485	GLU
1	B	505	TYR
1	B	508	LEU
1	B	515	LEU
1	B	518	GLU
1	B	530	VAL
1	B	541	LEU
1	B	617	LEU
1	B	633	ARG
1	B	637	VAL
1	B	645	GLU
1	B	662	THR
1	B	672	ILE
1	B	677	THR
1	B	679	SER
1	B	683	VAL
1	B	690	VAL
1	C	16	LEU
1	C	38	VAL
1	C	56	LEU
1	C	92	LEU
1	C	105	SER
1	C	113	ARG
1	C	115	GLU
1	C	151	LYS
1	C	179	GLN
1	C	187	ASP
1	C	205	SER
1	C	223	GLU
1	C	233	LEU
1	C	251	ARG
1	C	310	LEU
1	C	346	ARG
1	C	350	LEU
1	C	352	LEU
1	C	373	LYS
1	C	408	LEU
1	C	446	LEU
1	C	454	ASN
1	C	482	PHE
1	C	484	GLU
1	C	485	GLU

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Mol	Chain	Res	Type
1	C	488	GLU
1	C	501	PHE
1	C	505	TYR
1	C	508	LEU
1	C	515	LEU
1	C	530	VAL
1	C	541	LEU
1	C	610	ARG
1	C	617	LEU
1	C	627	GLU
1	C	637	VAL
1	C	662	THR
1	C	665	ARG
1	C	670	MET
1	C	672	ILE
1	C	677	THR
1	C	683	VAL
1	C	694	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	202	ASN
1	A	237	HIS
1	A	273	GLN
1	A	454	ASN
1	A	516	HIS
1	B	33	GLN
1	B	39	GLN
1	B	48	GLN
1	B	273	GLN
1	B	283	HIS
1	B	385	HIS
1	C	10	HIS
1	C	30	ASN
1	C	33	GLN
1	C	48	GLN
1	C	179	GLN
1	C	202	ASN
1	C	237	HIS
1	C	273	GLN
1	C	512	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 10 ligands modelled in this entry, 1 is monoatomic - leaving 9 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
4	PGE	C	1696	-	9,9,9	0.53	0	8,8,8	0.72	0
4	PGE	C	1697	-	9,9,9	0.94	0	8,8,8	0.88	0
4	PGE	A	1697	-	9,9,9	0.51	0	8,8,8	0.49	0
4	PGE	A	1698	-	9,9,9	0.87	0	8,8,8	1.00	0
2	GLA	C	701	-	12,12,12	1.06	1 (8%)	17,17,17	1.75	5 (29%)
2	GLA	B	701	-	12,12,12	0.80	0	17,17,17	1.64	4 (23%)
2	GLA	A	701	-	12,12,12	0.85	0	17,17,17	1.33	3 (17%)
4	PGE	B	1697	-	9,9,9	0.83	0	8,8,8	0.87	1 (12%)
4	PGE	B	1696	-	9,9,9	0.54	0	8,8,8	0.73	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
4	PGE	C	1696	-	-	5/7/7/7	-
4	PGE	C	1697	-	-	3/7/7/7	-
4	PGE	A	1697	-	-	5/7/7/7	-
4	PGE	A	1698	-	-	1/7/7/7	-
2	GLA	C	701	-	-	0/2/22/22	0/1/1/1
2	GLA	B	701	-	-	0/2/22/22	0/1/1/1
2	GLA	A	701	-	-	0/2/22/22	0/1/1/1
4	PGE	B	1697	-	-	4/7/7/7	-
4	PGE	B	1696	-	-	7/7/7/7	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	701	GLA	C4-C5	2.79	1.59	1.53

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	701	GLA	O3-C3-C4	3.67	119.03	110.38
2	B	701	GLA	C1-O5-C5	3.35	120.12	113.65
2	C	701	GLA	C1-O5-C5	3.11	119.66	113.65
2	A	701	GLA	C1-C2-C3	-2.93	104.37	110.36
2	B	701	GLA	O3-C3-C2	-2.83	103.72	110.38
2	B	701	GLA	O3-C3-C4	2.56	116.41	110.38
2	A	701	GLA	O3-C3-C4	2.20	115.57	110.38
2	A	701	GLA	C1-O5-C5	2.17	117.85	113.65
2	C	701	GLA	C6-C5-C4	2.06	118.07	113.02
2	C	701	GLA	O5-C1-C2	2.06	113.92	110.30
2	B	701	GLA	O6-C6-C5	2.05	118.32	111.33
4	B	1697	PGE	O2-C3-C4	2.04	119.67	110.35
2	C	701	GLA	O5-C5-C4	2.02	113.34	109.70

There are no chirality outliers.

All (25) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	1696	PGE	C1-C2-O2-C3
4	C	1696	PGE	C3-C4-O3-C5
4	A	1697	PGE	O3-C5-C6-O4
4	C	1696	PGE	O1-C1-C2-O2
4	C	1696	PGE	O2-C3-C4-O3

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Mol	Chain	Res	Type	Atoms
4	B	1696	PGE	O3-C5-C6-O4
4	A	1697	PGE	O1-C1-C2-O2
4	B	1696	PGE	O1-C1-C2-O2
4	C	1696	PGE	O3-C5-C6-O4
4	B	1697	PGE	O1-C1-C2-O2
4	C	1697	PGE	O2-C3-C4-O3
4	A	1697	PGE	O2-C3-C4-O3
4	B	1696	PGE	O2-C3-C4-O3
4	B	1696	PGE	C4-C3-O2-C2
4	A	1697	PGE	C3-C4-O3-C5
4	B	1697	PGE	O3-C5-C6-O4
4	C	1697	PGE	O1-C1-C2-O2
4	B	1696	PGE	C6-C5-O3-C4
4	B	1697	PGE	O2-C3-C4-O3
4	B	1696	PGE	C3-C4-O3-C5
4	A	1697	PGE	C1-C2-O2-C3
4	C	1697	PGE	C3-C4-O3-C5
4	A	1698	PGE	O2-C3-C4-O3
4	B	1697	PGE	C4-C3-O2-C2
4	C	1696	PGE	C1-C2-O2-C3

There are no ring outliers.

5 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	1696	PGE	1	0
4	A	1698	PGE	1	0
2	B	701	GLA	1	0
2	A	701	GLA	1	0
4	B	1696	PGE	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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	688/695 (98%)	-0.36	0 100 100	11, 22, 38, 52	1 (0%)
1	B	688/695 (98%)	-0.44	0 100 100	8, 18, 36, 51	1 (0%)
1	C	688/695 (98%)	-0.31	0 100 100	10, 23, 41, 62	0
All	All	2064/2085 (98%)	-0.37	0 100 100	8, 21, 39, 62	2 (0%)

There are no RSRZ outliers to report.

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	PGE	B	1697	10/10	0.77	0.15	36,40,44,49	0
4	PGE	A	1698	10/10	0.79	0.14	28,30,39,39	0
4	PGE	C	1697	10/10	0.79	0.14	28,37,44,45	0
4	PGE	B	1696	10/10	0.88	0.13	31,33,44,45	0
2	GLA	A	701	12/12	0.89	0.10	28,33,35,37	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	PGE	C	1696	10/10	0.90	0.11	28,31,47,51	0
4	PGE	A	1697	10/10	0.91	0.11	32,36,51,52	0
2	GLA	C	701	12/12	0.93	0.09	27,30,33,33	0
2	GLA	B	701	12/12	0.94	0.09	23,26,28,28	0
3	ZN	A	1696	1/1	0.99	0.05	43,43,43,43	0

6.5 Other polymers [i](#)

There are no such residues in this entry.