



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 18, 2026 – 06:12 PM UTC

PDB ID : 4UOQ / pdb_00004uoq
Title : Nucleophile mutant (E324A) of beta-(1,6)-galactosidase from Bifidobacterium animalis subsp. lactis Bl-04
Authors : Viborg, A.H.; Fredslund, F.; Katayama, T.; Nielsen, S.K.; Svensson, B.; Kitaoka, M.; Lo Leggio, L.; Abou Hachem, M.
Deposited on : 2014-06-09
Resolution : 2.70 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

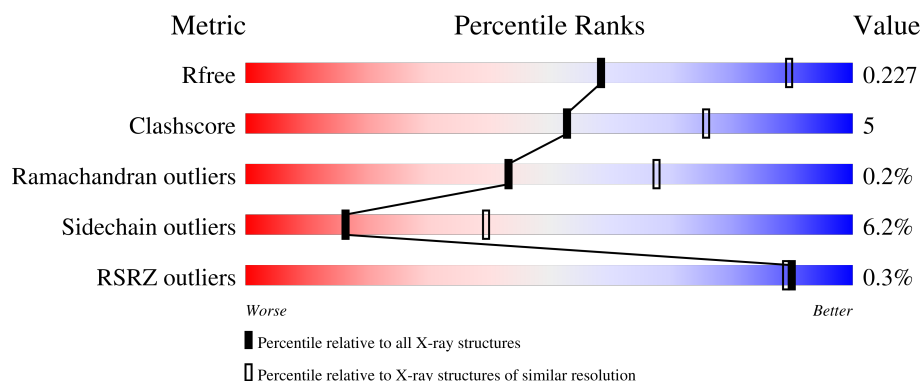
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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	3538 (2.70-2.70)
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (2.70-2.70)

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 6 unique types of molecules in this entry. The entry contains 16764 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.

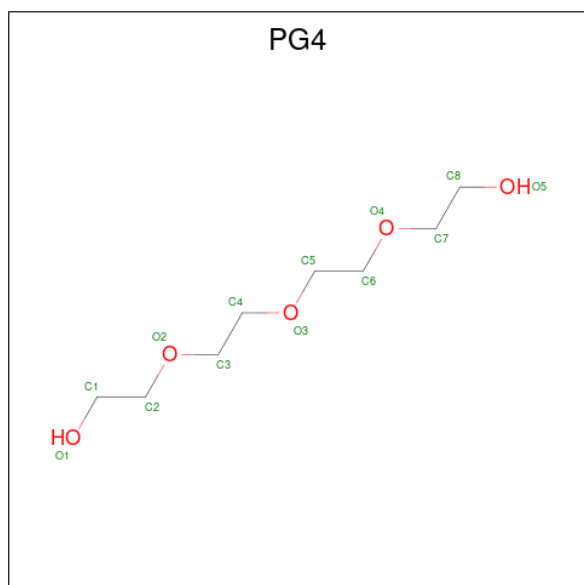
- Molecule 1 is a protein called BETA-GALACTOSIDASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	683	Total	C	N	O	S	0	0	0
			5443	3443	950	1027	23			
1	B	684	Total	C	N	O	S	0	0	0
			5452	3448	952	1029	23			
1	C	682	Total	C	N	O	S	0	0	0
			5433	3437	947	1026	23			

There are 3 discrepancies between the modelled and reference sequences:

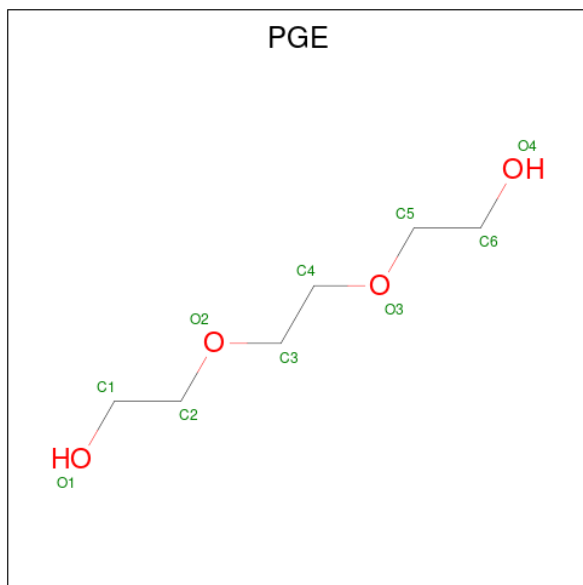
Chain	Residue	Modelled	Actual	Comment	Reference
A	324	ALA	GLU	engineered mutation	UNP C6A6W5
B	324	ALA	GLU	engineered mutation	UNP C6A6W5
C	324	ALA	GLU	engineered mutation	UNP C6A6W5

- Molecule 2 is TETRAETHYLENE GLYCOL (CCD ID: PG4) (formula: C₈H₁₈O₅).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			13	8	5		
2	C	1	Total	C	O	0	0
			13	8	5		

- Molecule 3 is TRIETHYLENE GLYCOL (CCD ID: PGE) (formula: $C_6H_{14}O_4$).



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

- Molecule 4 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: $C_4H_{10}O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			7	4	3		
4	A	1	Total	C	O	0	0
			7	4	3		
4	A	1	Total	C	O	0	0
			7	4	3		
4	A	1	Total	C	O	0	0
			7	4	3		
4	B	1	Total	C	O	0	0
			7	4	3		
4	B	1	Total	C	O	0	0
			7	4	3		
4	B	1	Total	C	O	0	0
			7	4	3		
4	B	1	Total	C	O	0	0
			7	4	3		
4	C	1	Total	C	O	0	0
			7	4	3		
4	C	1	Total	C	O	0	0
			7	4	3		

- Molecule 5 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

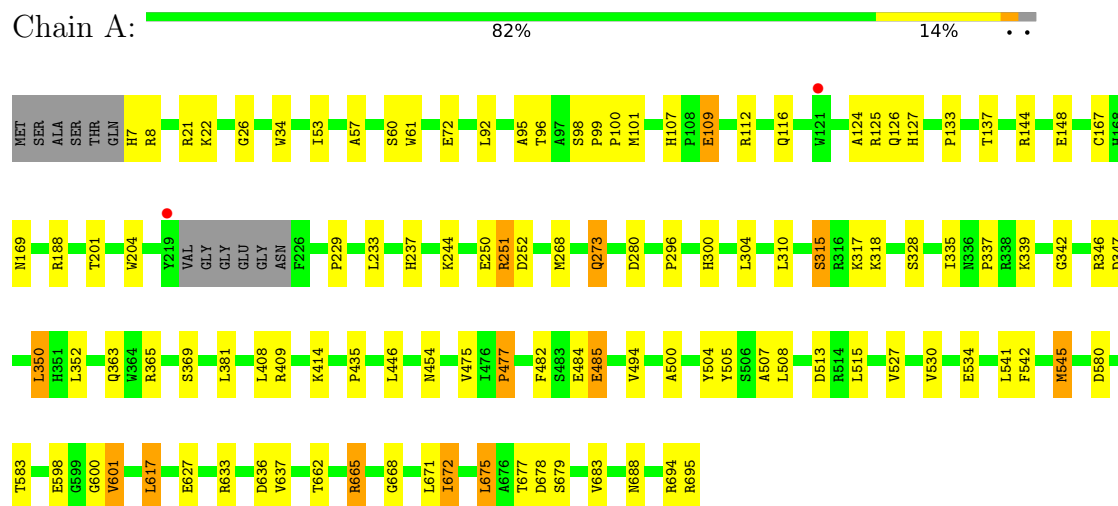
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	114	Total 114	O 114	0	0
6	B	101	Total 101	O 101	0	0
6	C	84	Total 84	O 84	0	0

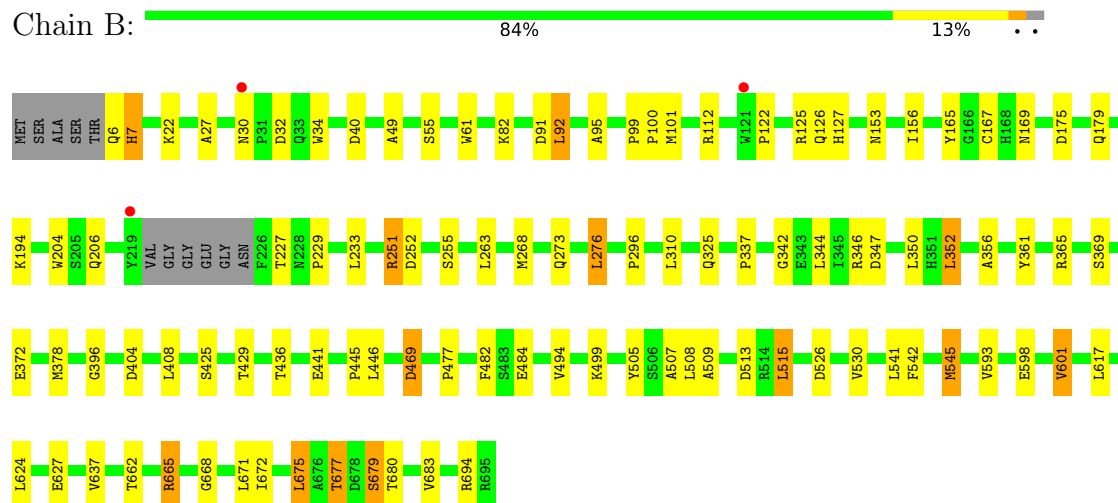
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

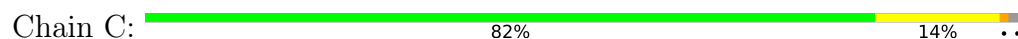
• Molecule 1: BETA-GALACTOSIDASE

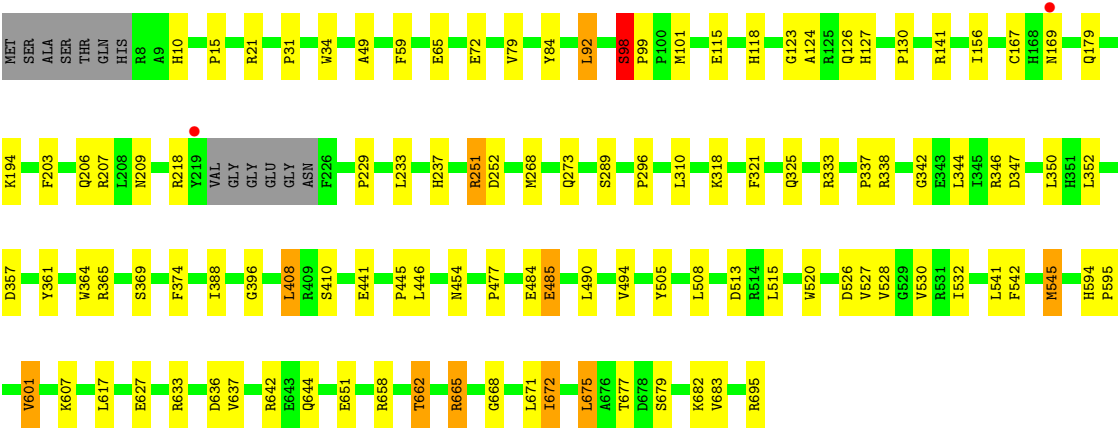


• Molecule 1: BETA-GALACTOSIDASE



• Molecule 1: BETA-GALACTOSIDASE





4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α , β , γ	150.56Å 150.56Å 237.25Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	19.93 – 2.70 19.93 – 2.70	Depositor EDS
% Data completeness (in resolution range)	99.8 (19.93-2.70) 99.5 (19.93-2.70)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.50 (at 2.71Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.181 , 0.227 0.184 , 0.227	Depositor DCC
R_{free} test set	2000 reflections (2.34%)	wwPDB-VP
Wilson B-factor (Å ²)	46.7	Xtriage
Anisotropy	0.397	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 29.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.011 for -h,-k,l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	16764	wwPDB-VP
Average B, all atoms (Å ²)	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.41% 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, PG4, PEG

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.55	0/5597	0.88	6/7630 (0.1%)
1	B	0.52	0/5606	0.83	1/7642 (0.0%)
1	C	0.52	0/5586	0.84	4/7615 (0.1%)
All	All	0.53	0/16789	0.85	11/22887 (0.0%)

There are no bond length outliers.

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	98	SER	CA-C-N	9.81	126.83	119.66
1	A	98	SER	C-N-CA	9.81	126.83	119.66
1	B	601	VAL	N-CA-C	8.98	121.06	107.77
1	A	8	ARG	N-CA-C	8.26	120.98	110.24
1	C	98	SER	CA-C-N	7.82	125.37	119.66
1	C	98	SER	C-N-CA	7.82	125.37	119.66
1	C	601	VAL	N-CA-C	6.46	117.33	107.77
1	A	601	VAL	N-CA-C	6.28	117.07	107.77
1	A	7	HIS	CA-C-N	5.16	128.41	120.82
1	A	7	HIS	C-N-CA	5.16	128.41	120.82
1	C	123	GLY	N-CA-C	-5.12	107.60	114.25

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	5443	0	5151	64	0
1	B	5452	0	5159	49	0
1	C	5433	0	5144	56	0
2	A	13	0	18	0	0
2	C	13	0	18	0	0
3	A	10	0	14	3	0
3	B	10	0	14	1	0
3	C	20	0	28	1	0
4	A	28	0	40	2	0
4	B	28	0	40	0	0
4	C	14	0	20	0	0
5	A	1	0	0	0	0
6	A	114	0	0	3	0
6	B	101	0	0	2	0
6	C	84	0	0	5	0
All	All	16764	0	15646	161	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 5.

All (161) 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:A:251:ARG:HH11	1:A:251:ARG:HG2	1.40	0.86
1:C:251:ARG:HG2	1:C:251:ARG:HH11	1.40	0.85
1:B:251:ARG:HH11	1:B:251:ARG:HG2	1.43	0.83
1:A:346:ARG:NH1	1:A:347:ASP:OD1	2.13	0.82
1:C:346:ARG:NH1	1:C:347:ASP:OD1	2.13	0.81
1:B:542:PHE:HD1	1:B:545:MET:HE3	1.50	0.77
1:A:201:THR:O	6:A:2021:HOH:O	2.06	0.74
1:A:665:ARG:NH2	1:A:668:GLY:O	2.23	0.72
1:C:115:GLU:O	1:C:218:ARG:NH1	2.25	0.69
1:C:542:PHE:HD1	1:C:545:MET:HE3	1.58	0.68
1:C:665:ARG:NH2	1:C:668:GLY:O	2.28	0.67
1:B:665:ARG:NH2	1:B:668:GLY:O	2.28	0.66
1:B:40:ASP:OD1	1:B:82:LYS:NZ	2.29	0.66
1:A:633:ARG:NH1	1:A:636:ASP:OD1	2.29	0.66
1:B:671:LEU:HD11	1:B:694:ARG:HB2	1.78	0.65
1:B:346:ARG:NH1	1:B:347:ASP:OD1	2.31	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:333:ARG:NH1	6:C:2035:HOH:O	2.30	0.63
1:A:527:VAL:HG12	1:A:601:VAL:HG21	1.81	0.63
1:A:414:LYS:HE3	3:A:1697:PGE:H4	1.81	0.63
1:C:251:ARG:HG2	1:C:251:ARG:NH1	2.13	0.62
1:B:6:GLN:N	6:B:2001:HOH:O	2.33	0.60
1:B:296:PRO:HB3	1:B:337:PRO:HG2	1.83	0.60
1:B:251:ARG:HG2	1:B:251:ARG:NH1	2.10	0.60
1:A:125:ARG:HB3	1:B:204:TRP:CD1	2.37	0.59
1:A:485:GLU:N	1:A:485:GLU:OE1	2.34	0.59
1:C:207:ARG:NH1	1:C:209:ASN:OD1	2.36	0.58
1:C:485:GLU:OE1	1:C:485:GLU:N	2.35	0.58
1:C:126:GLN:O	1:C:169:ASN:HB3	2.05	0.57
1:A:342:GLY:HA3	1:A:675:LEU:HD22	1.87	0.56
1:C:296:PRO:HB3	1:C:337:PRO:HG2	1.88	0.56
1:A:144:ARG:O	1:A:148:GLU:HG2	2.05	0.56
1:A:542:PHE:HD2	1:A:545:MET:HE3	1.71	0.55
1:B:92:LEU:HB2	1:B:156:ILE:HG23	1.89	0.55
1:A:251:ARG:NH1	1:A:252:ASP:OD1	2.40	0.55
1:C:527:VAL:HG12	1:C:601:VAL:HG21	1.89	0.54
1:C:441:GLU:O	1:C:445:PRO:HD2	2.08	0.54
1:C:124:ALA:O	1:C:127:HIS:ND1	2.38	0.54
1:B:229:PRO:HB2	1:B:513:ASP:OD2	2.08	0.53
1:C:237:HIS:HE1	6:C:2027:HOH:O	1.91	0.53
1:A:296:PRO:HB3	1:A:337:PRO:HG2	1.91	0.53
1:A:335:ILE:O	1:A:337:PRO:HD3	2.08	0.53
1:C:229:PRO:HB2	1:C:513:ASP:OD2	2.09	0.52
1:C:662:THR:HG23	1:C:682:LYS:HD2	1.91	0.52
1:B:251:ARG:NH1	1:B:252:ASP:OD1	2.43	0.52
1:B:126:GLN:O	1:B:169:ASN:HB3	2.10	0.52
1:A:96:THR:OG1	1:A:250:GLU:OE2	2.24	0.52
1:A:112:ARG:HD3	1:A:169:ASN:HB2	1.90	0.52
1:C:251:ARG:NH1	1:C:252:ASP:OD1	2.44	0.51
1:A:485:GLU:H	1:A:485:GLU:CD	2.18	0.51
1:A:126:GLN:O	1:A:169:ASN:HB3	2.10	0.51
1:A:229:PRO:HB2	1:A:513:ASP:OD2	2.10	0.51
1:A:116:GLN:OE1	1:C:118:HIS:ND1	2.44	0.51
1:A:409:ARG:HH21	4:A:1700:PEG:H31	1.75	0.51
1:C:633:ARG:NH1	1:C:636:ASP:OD1	2.44	0.50
1:A:251:ARG:HG2	1:A:251:ARG:NH1	2.15	0.50
1:A:317:LYS:HD2	3:A:1697:PGE:H22	1.93	0.50
1:B:255:SER:HB3	1:B:263:LEU:HD11	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:342:GLY:HA3	1:B:675:LEU:HD22	1.94	0.50
1:A:315:SER:OG	1:A:318:LYS:O	2.30	0.50
1:A:296:PRO:HG2	1:B:542:PHE:CD1	2.47	0.50
1:A:542:PHE:O	1:A:545:MET:HB2	2.13	0.49
1:A:409:ARG:HE	4:A:1700:PEG:H31	1.78	0.49
1:C:520:TRP:O	1:C:532:ILE:N	2.43	0.49
1:B:101:MET:HB3	1:B:101:MET:HE2	1.74	0.49
1:B:6:GLN:O	1:B:7:HIS:HB2	2.12	0.48
1:C:15:PRO:HG3	1:C:21:ARG:HA	1.94	0.48
1:B:165:TYR:O	1:B:276:LEU:HD21	2.14	0.48
1:B:352:LEU:HD22	1:B:356:ALA:O	2.14	0.48
1:B:441:GLU:O	1:B:445:PRO:HD2	2.14	0.48
1:C:494:VAL:HG11	1:C:601:VAL:HG23	1.97	0.47
1:A:109:GLU:H	1:A:109:GLU:HG3	1.37	0.47
1:C:130:PRO:HG2	6:C:2008:HOH:O	2.13	0.47
1:C:357:ASP:OD1	1:C:642:ARG:NH2	2.30	0.47
1:B:509:ALA:HB2	1:B:515:LEU:HD12	1.96	0.47
1:C:101:MET:HB3	1:C:101:MET:HE2	1.84	0.47
1:A:244:LYS:NZ	1:A:280:ASP:OD2	2.39	0.47
1:A:204:TRP:HA	1:C:59:PHE:CG	2.50	0.47
1:B:32:ASP:OD1	1:B:32:ASP:N	2.47	0.47
1:A:671:LEU:HD11	1:A:694:ARG:HB2	1.97	0.46
1:A:304:LEU:HD22	1:A:350:LEU:HB3	1.98	0.46
1:C:84:TYR:CD2	3:C:1700:PGE:H1	2.50	0.46
1:C:651:GLU:OE1	1:C:695:ARG:NH1	2.27	0.46
1:A:26:GLY:HA3	1:A:53:ILE:O	2.16	0.46
1:A:665:ARG:NH1	1:A:678:ASP:OD2	2.49	0.46
1:B:677:THR:HG22	6:B:2101:HOH:O	2.14	0.46
1:C:485:GLU:H	1:C:485:GLU:CD	2.22	0.46
1:A:124:ALA:O	1:A:127:HIS:ND1	2.48	0.46
1:A:475:VAL:O	1:A:477:PRO:HD3	2.16	0.46
1:C:410:SER:HB3	1:C:644:GLN:HG2	1.97	0.46
1:B:153:ASN:ND2	3:B:1697:PGE:O2	2.49	0.45
1:A:617:LEU:HD12	1:A:617:LEU:HA	1.82	0.45
1:A:188:ARG:HB2	6:A:2017:HOH:O	2.17	0.45
1:A:328:SER:HA	1:A:339:LYS:HG3	1.99	0.45
1:C:31:PRO:HG3	1:C:79:VAL:HG21	1.98	0.45
1:A:346:ARG:NH2	1:A:688:ASN:OD1	2.49	0.45
1:B:49:ALA:O	1:B:396:GLY:HA3	2.17	0.45
1:B:167:CYS:HA	1:B:268:MET:HE1	1.98	0.45
1:B:499:LYS:HE2	1:B:624:LEU:O	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:21:ARG:O	1:A:22:LYS:HD2	2.17	0.45
1:A:671:LEU:O	1:A:672:ILE:HD12	2.17	0.45
1:C:49:ALA:O	1:C:396:GLY:HA3	2.17	0.44
1:A:414:LYS:CE	3:A:1697:PGE:H4	2.48	0.44
1:C:594:HIS:HA	1:C:595:PRO:HD2	1.89	0.44
1:A:237:HIS:HD2	6:A:2026:HOH:O	1.99	0.44
1:B:296:PRO:CB	1:B:337:PRO:HG2	2.46	0.44
1:A:167:CYS:HA	1:A:268:MET:HE1	2.00	0.44
1:C:671:LEU:O	1:C:672:ILE:HD12	2.18	0.44
1:A:57:ALA:HA	1:A:60:SER:OG	2.18	0.44
1:B:325:GLN:HG3	1:B:361:TYR:CD1	2.52	0.44
1:C:289:SER:HA	1:C:321:PHE:O	2.18	0.44
1:B:22:LYS:NZ	1:B:404:ASP:OD1	2.51	0.43
1:B:679:SER:OG	1:B:680:THR:N	2.50	0.43
1:C:10:HIS:HB2	1:C:318:LYS:HD3	2.00	0.43
1:B:344:LEU:C	1:B:344:LEU:HD23	2.44	0.43
1:B:372:GLU:HB3	1:C:203:PHE:HD2	1.83	0.43
1:C:65:GLU:OE2	1:C:141:ARG:NH2	2.49	0.43
1:C:92:LEU:HB2	1:C:156:ILE:HG23	2.00	0.43
1:A:534:GLU:OE2	1:C:338:ARG:HD2	2.18	0.43
1:B:494:VAL:HG11	1:B:601:VAL:HG23	2.01	0.42
1:C:607:LYS:HE3	6:C:2063:HOH:O	2.18	0.42
1:B:27:ALA:HB2	1:B:378:MET:SD	2.60	0.42
1:C:325:GLN:HG3	1:C:361:TYR:CD1	2.55	0.42
1:A:34:TRP:CZ2	1:A:365:ARG:HD3	2.54	0.42
1:B:526:ASP:OD1	1:B:526:ASP:N	2.52	0.42
1:A:500:ALA:N	1:A:600:GLY:O	2.40	0.42
1:C:388:ILE:HA	6:C:2054:HOH:O	2.19	0.42
1:A:482:PHE:HB2	1:A:507:ALA:HA	2.02	0.42
1:B:425:SER:O	1:B:429:THR:HG23	2.20	0.42
1:C:490:LEU:O	1:C:494:VAL:HG23	2.20	0.42
1:A:107:HIS:ND1	1:A:109:GLU:OE2	2.52	0.42
1:A:381:LEU:HD13	1:B:515:LEU:HB3	2.02	0.42
1:B:99:PRO:HA	1:B:100:PRO:HD3	1.85	0.42
1:B:482:PHE:HB2	1:B:507:ALA:HA	2.02	0.42
1:A:61:TRP:CE3	1:A:96:THR:HA	2.55	0.41
1:C:98:SER:HA	1:C:99:PRO:HD2	1.77	0.41
1:C:528:VAL:HA	1:C:601:VAL:HG11	2.02	0.41
1:C:167:CYS:HA	1:C:268:MET:HE1	2.02	0.41
1:B:542:PHE:O	1:B:545:MET:HB2	2.20	0.41
1:C:342:GLY:HA3	1:C:675:LEU:HD22	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:363:GLN:H	1:A:363:GLN:HG2	1.79	0.41
1:A:435:PRO:HD3	1:C:374:PHE:CG	2.56	0.41
1:A:494:VAL:HG11	1:A:601:VAL:HG23	2.02	0.41
1:A:580:ASP:HB3	1:A:583:THR:HG23	2.01	0.41
1:A:300:HIS:HE1	1:A:347:ASP:OD2	2.03	0.41
1:B:175:ASP:O	1:B:179:GLN:HG3	2.20	0.41
1:A:133:PRO:O	1:A:137:THR:HG23	2.21	0.41
1:A:273:GLN:HE21	1:A:273:GLN:HB2	1.59	0.41
1:B:55:SER:HA	1:B:91:ASP:O	2.21	0.41
1:B:469:ASP:OD1	1:B:469:ASP:N	2.42	0.41
1:C:34:TRP:CZ2	1:C:365:ARG:HD3	2.56	0.41
1:B:122:PRO:HA	1:B:127:HIS:ND1	2.36	0.41
1:C:364:TRP:CD1	1:C:365:ARG:HB2	2.56	0.41
1:C:658:ARG:HA	1:C:658:ARG:HD2	1.93	0.41
1:C:344:LEU:C	1:C:344:LEU:HD23	2.46	0.40
1:C:526:ASP:OD1	1:C:526:ASP:N	2.53	0.40
1:A:99:PRO:HA	1:A:100:PRO:HD3	1.87	0.40
1:B:34:TRP:CZ2	1:B:365:ARG:HD3	2.56	0.40
1:A:101:MET:HE2	1:A:101:MET:HB3	1.96	0.40
1:B:61:TRP:HB2	1:B:95:ALA:O	2.22	0.40
1:C:408:LEU:O	1:C:644:GLN:NE2	2.55	0.40
1:A:61:TRP:HB2	1:A:95:ALA:O	2.20	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	679/695 (98%)	660 (97%)	17 (2%)	2 (0%)	36 60
1	B	680/695 (98%)	663 (98%)	15 (2%)	2 (0%)	36 60
1	C	678/695 (98%)	660 (97%)	17 (2%)	1 (0%)	48 73

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	2037/2085 (98%)	1983 (97%)	49 (2%)	5 (0%)	43 68

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	7	HIS
1	A	477	PRO
1	B	477	PRO
1	C	477	PRO
1	A	504	TYR

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	572/580 (99%)	538 (94%)	34 (6%)	18 42
1	B	573/580 (99%)	535 (93%)	38 (7%)	15 36
1	C	571/580 (98%)	537 (94%)	34 (6%)	17 41
All	All	1716/1740 (99%)	1610 (94%)	106 (6%)	16 39

All (106) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	72	GLU
1	A	92	LEU
1	A	109	GLU
1	A	233	LEU
1	A	251	ARG
1	A	273	GLN
1	A	310	LEU
1	A	315	SER
1	A	350	LEU
1	A	352	LEU
1	A	369	SER

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Mol	Chain	Res	Type
1	A	408	LEU
1	A	446	LEU
1	A	454	ASN
1	A	484	GLU
1	A	485	GLU
1	A	505	TYR
1	A	508	LEU
1	A	515	LEU
1	A	530	VAL
1	A	541	LEU
1	A	545	MET
1	A	598	GLU
1	A	617	LEU
1	A	627	GLU
1	A	637	VAL
1	A	662	THR
1	A	665	ARG
1	A	672	ILE
1	A	675	LEU
1	A	677	THR
1	A	679	SER
1	A	683	VAL
1	A	695	ARG
1	B	30	ASN
1	B	92	LEU
1	B	112	ARG
1	B	125	ARG
1	B	194	LYS
1	B	206	GLN
1	B	227	THR
1	B	233	LEU
1	B	251	ARG
1	B	273	GLN
1	B	276	LEU
1	B	310	LEU
1	B	350	LEU
1	B	352	LEU
1	B	369	SER
1	B	408	LEU
1	B	436	THR
1	B	446	LEU
1	B	469	ASP

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Mol	Chain	Res	Type
1	B	484	GLU
1	B	505	TYR
1	B	508	LEU
1	B	515	LEU
1	B	530	VAL
1	B	541	LEU
1	B	545	MET
1	B	593	VAL
1	B	598	GLU
1	B	617	LEU
1	B	627	GLU
1	B	637	VAL
1	B	662	THR
1	B	665	ARG
1	B	672	ILE
1	B	675	LEU
1	B	677	THR
1	B	679	SER
1	B	683	VAL
1	C	72	GLU
1	C	92	LEU
1	C	98	SER
1	C	179	GLN
1	C	194	LYS
1	C	206	GLN
1	C	233	LEU
1	C	251	ARG
1	C	273	GLN
1	C	310	LEU
1	C	350	LEU
1	C	352	LEU
1	C	369	SER
1	C	408	LEU
1	C	446	LEU
1	C	454	ASN
1	C	484	GLU
1	C	485	GLU
1	C	505	TYR
1	C	508	LEU
1	C	515	LEU
1	C	530	VAL
1	C	541	LEU

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Mol	Chain	Res	Type
1	C	545	MET
1	C	617	LEU
1	C	627	GLU
1	C	637	VAL
1	C	662	THR
1	C	665	ARG
1	C	672	ILE
1	C	675	LEU
1	C	677	THR
1	C	679	SER
1	C	683	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	7	HIS
1	A	30	ASN
1	A	48	GLN
1	A	70	ASN
1	A	273	GLN
1	A	300	HIS
1	A	363	GLN
1	A	467	GLN
1	B	7	HIS
1	B	30	ASN
1	B	70	ASN
1	B	116	GLN
1	B	283	HIS
1	B	597	HIS
1	C	10	HIS
1	C	48	GLN
1	C	70	ASN
1	C	237	HIS
1	C	273	GLN

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](#)

Of 17 ligands modelled in this entry, 1 is monoatomic - leaving 16 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	PEG	A	1700	-	6,6,6	0.49	0	5,5,5	0.43	0
4	PEG	A	1701	-	6,6,6	0.53	0	5,5,5	0.20	0
2	PG4	A	1696	-	12,12,12	0.73	0	11,11,11	0.57	0
4	PEG	B	1696	-	6,6,6	0.65	0	5,5,5	0.57	0
3	PGE	C	1700	-	9,9,9	0.61	0	8,8,8	0.22	0
4	PEG	A	1699	-	6,6,6	0.50	0	5,5,5	0.31	0
4	PEG	C	1697	-	6,6,6	0.57	0	5,5,5	0.10	0
4	PEG	B	1700	-	6,6,6	0.61	0	5,5,5	0.25	0
3	PGE	C	1698	-	9,9,9	0.68	0	8,8,8	1.14	0
2	PG4	C	1696	-	12,12,12	0.64	0	11,11,11	0.46	0
4	PEG	A	1698	-	6,6,6	0.71	0	5,5,5	0.73	0
4	PEG	B	1699	-	6,6,6	0.60	0	5,5,5	0.18	0
4	PEG	B	1698	-	6,6,6	0.57	0	5,5,5	0.24	0
3	PGE	B	1697	-	9,9,9	0.68	0	8,8,8	0.44	0
4	PEG	C	1699	-	6,6,6	0.54	0	5,5,5	0.35	0
3	PGE	A	1697	-	9,9,9	0.65	0	8,8,8	0.47	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	PEG	A	1700	-	-	3/4/4/4	-
4	PEG	A	1701	-	-	2/4/4/4	-
2	PG4	A	1696	-	-	2/10/10/10	-
4	PEG	B	1696	-	-	0/4/4/4	-
3	PGE	C	1700	-	-	2/7/7/7	-
4	PEG	A	1699	-	-	2/4/4/4	-
4	PEG	C	1697	-	-	0/4/4/4	-
4	PEG	B	1700	-	-	1/4/4/4	-
3	PGE	C	1698	-	-	3/7/7/7	-
2	PG4	C	1696	-	-	1/10/10/10	-
4	PEG	A	1698	-	-	0/4/4/4	-
4	PEG	B	1699	-	-	0/4/4/4	-
4	PEG	B	1698	-	-	1/4/4/4	-
3	PGE	B	1697	-	-	0/7/7/7	-
4	PEG	C	1699	-	-	1/4/4/4	-
3	PGE	A	1697	-	-	3/7/7/7	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (21) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	1698	PEG	O1-C1-C2-O2
3	A	1697	PGE	O3-C5-C6-O4
3	C	1700	PGE	O3-C5-C6-O4
4	B	1700	PEG	O2-C3-C4-O4
4	A	1700	PEG	O2-C3-C4-O4
4	A	1701	PEG	O1-C1-C2-O2
2	A	1696	PG4	O3-C5-C6-O4
3	C	1698	PGE	O2-C3-C4-O3
4	A	1699	PEG	O1-C1-C2-O2
4	A	1699	PEG	C1-C2-O2-C3
3	A	1697	PGE	C4-C3-O2-C2
3	C	1700	PGE	O2-C3-C4-O3
4	A	1700	PEG	O1-C1-C2-O2
2	A	1696	PG4	O2-C3-C4-O3
3	A	1697	PGE	C1-C2-O2-C3
4	C	1699	PEG	O2-C3-C4-O4
3	C	1698	PGE	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
2	C	1696	PG4	O4-C7-C8-O5
3	C	1698	PGE	O3-C5-C6-O4
4	A	1700	PEG	C4-C3-O2-C2
4	A	1701	PEG	C4-C3-O2-C2

There are no ring outliers.

4 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1700	PEG	2	0
3	C	1700	PGE	1	0
3	B	1697	PGE	1	0
3	A	1697	PGE	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 [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	683/695 (98%)	-0.63	2 (0%) 90 89	22, 35, 56, 95	0
1	B	684/695 (98%)	-0.64	3 (0%) 88 87	20, 36, 58, 86	0
1	C	682/695 (98%)	-0.57	2 (0%) 90 89	24, 38, 57, 93	0
All	All	2049/2085 (98%)	-0.61	7 (0%) 90 89	20, 36, 57, 95	0

All (7) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	219	TYR	3.3
1	B	121	TRP	3.1
1	C	169	ASN	2.8
1	B	30	ASN	2.8
1	B	219	TYR	2.7
1	A	219	TYR	2.6
1	A	121	TRP	2.2

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
3	PGE	C	1698	10/10	0.67	0.16	35,40,53,57	0
4	PEG	A	1701	7/7	0.70	0.14	58,61,63,63	0
4	PEG	C	1697	7/7	0.80	0.14	37,45,55,55	0
4	PEG	C	1699	7/7	0.83	0.11	54,58,66,70	0
3	PGE	C	1700	10/10	0.85	0.12	50,56,62,62	0
4	PEG	B	1700	7/7	0.85	0.14	32,46,52,54	0
3	PGE	A	1697	10/10	0.86	0.12	31,41,48,48	0
4	PEG	A	1700	7/7	0.86	0.11	39,50,60,61	0
3	PGE	B	1697	10/10	0.87	0.11	48,57,61,64	0
4	PEG	A	1698	7/7	0.88	0.09	30,33,39,40	0
2	PG4	A	1696	13/13	0.89	0.10	25,37,48,49	0
4	PEG	B	1699	7/7	0.90	0.10	46,48,52,54	0
4	PEG	B	1698	7/7	0.90	0.10	28,33,44,45	0
4	PEG	A	1699	7/7	0.91	0.10	33,40,44,46	0
2	PG4	C	1696	13/13	0.93	0.10	26,42,49,50	0
4	PEG	B	1696	7/7	0.94	0.08	27,29,37,39	0
5	ZN	A	1702	1/1	0.98	0.06	77,77,77,77	0

6.5 Other polymers [i](#)

There are no such residues in this entry.