



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 10:15 AM UTC

PDB ID : 8H25 / pdb_00008h25
Title : Lacticaseibacillus casei GH35 beta-galactosidase LBCZ_0230
Authors : Saburi, W.; Ota, T.; Kato, K.; Tagami, T.; Yamashita, K.; Yao, M.; Mori, H.
Deposited on : 2022-10-04
Resolution : 2.29 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

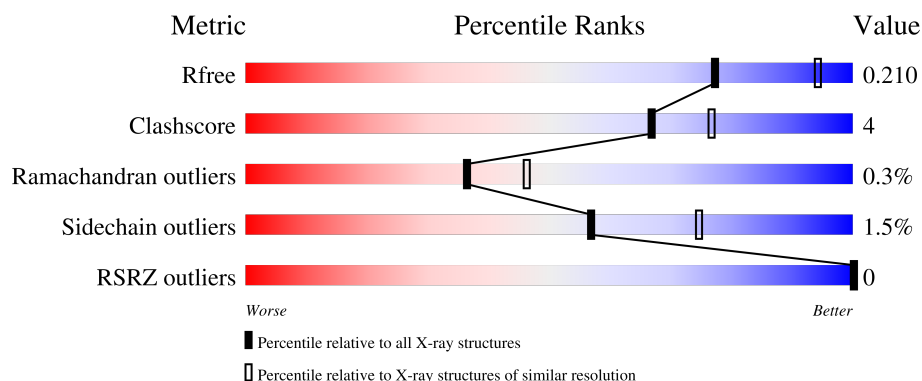
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

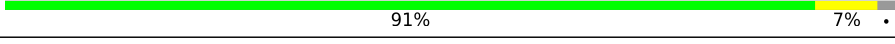
The reported resolution of this entry is 2.29 Å.

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	604	 91% 7% .
1	B	604	 87% 11% .
1	C	604	 91% 7% .
1	D	604	 88% 9% ..

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 19500 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	592	Total	C	N	O	S	0	0	0
			4754	3060	792	883	19			
1	B	592	Total	C	N	O	S	0	0	0
			4754	3060	792	883	19			
1	C	592	Total	C	N	O	S	0	1	0
			4762	3064	794	885	19			
1	D	592	Total	C	N	O	S	0	0	0
			4754	3060	792	883	19			

There are 24 discrepancies between the modelled and reference sequences:

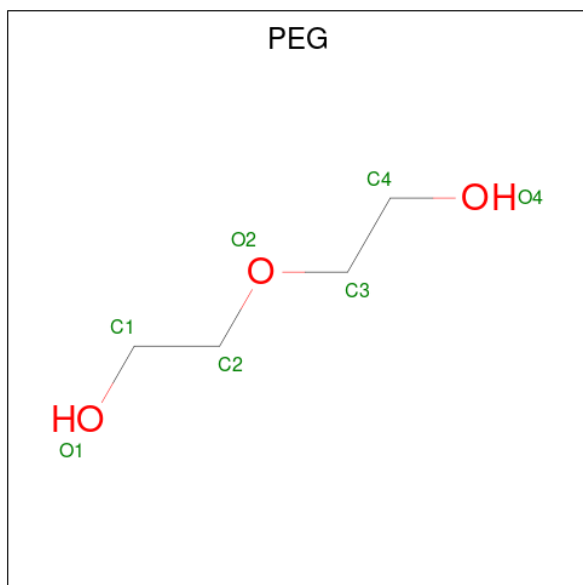
Chain	Residue	Modelled	Actual	Comment	Reference
A	599	HIS	-	expression tag	UNP A0A5R8LFD3
A	600	HIS	-	expression tag	UNP A0A5R8LFD3
A	601	HIS	-	expression tag	UNP A0A5R8LFD3
A	602	HIS	-	expression tag	UNP A0A5R8LFD3
A	603	HIS	-	expression tag	UNP A0A5R8LFD3
A	604	HIS	-	expression tag	UNP A0A5R8LFD3
B	599	HIS	-	expression tag	UNP A0A5R8LFD3
B	600	HIS	-	expression tag	UNP A0A5R8LFD3
B	601	HIS	-	expression tag	UNP A0A5R8LFD3
B	602	HIS	-	expression tag	UNP A0A5R8LFD3
B	603	HIS	-	expression tag	UNP A0A5R8LFD3
B	604	HIS	-	expression tag	UNP A0A5R8LFD3
C	599	HIS	-	expression tag	UNP A0A5R8LFD3
C	600	HIS	-	expression tag	UNP A0A5R8LFD3
C	601	HIS	-	expression tag	UNP A0A5R8LFD3
C	602	HIS	-	expression tag	UNP A0A5R8LFD3
C	603	HIS	-	expression tag	UNP A0A5R8LFD3
C	604	HIS	-	expression tag	UNP A0A5R8LFD3
D	599	HIS	-	expression tag	UNP A0A5R8LFD3
D	600	HIS	-	expression tag	UNP A0A5R8LFD3
D	601	HIS	-	expression tag	UNP A0A5R8LFD3

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Chain	Residue	Modelled	Actual	Comment	Reference
D	602	HIS	-	expression tag	UNP A0A5R8LFD3
D	603	HIS	-	expression tag	UNP A0A5R8LFD3
D	604	HIS	-	expression tag	UNP A0A5R8LFD3

- Molecule 2 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: $C_4H_{10}O_3$).



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

- Molecule 3 is 4-(2-HYDROXYETHYL)-1-PIPERAZINE ETHANESULFONIC ACID (CCD ID: EPE) (formula: $C_8H_{18}N_2O_4S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	B	1	Total	C	N	O	S	0	0
			15	8	2	4	1		
3	C	1	Total	C	N	O	S	0	0
			15	8	2	4	1		
3	C	1	Total	C	N	O	S	0	0
			15	8	2	4	1		
3	D	1	Total	C	N	O	S	0	0
			15	8	2	4	1		

- Molecule 4 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



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

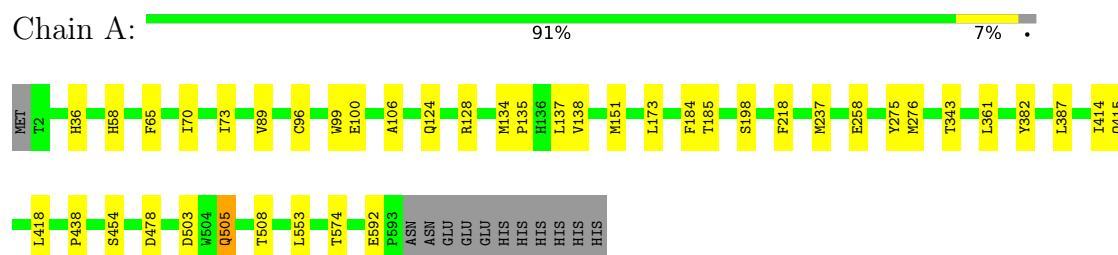
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	79	Total	O	0	0
			79	79		
5	B	97	Total	O	0	0
			97	97		
5	C	99	Total	O	0	0
			99	99		
5	D	93	Total	O	0	0
			93	93		

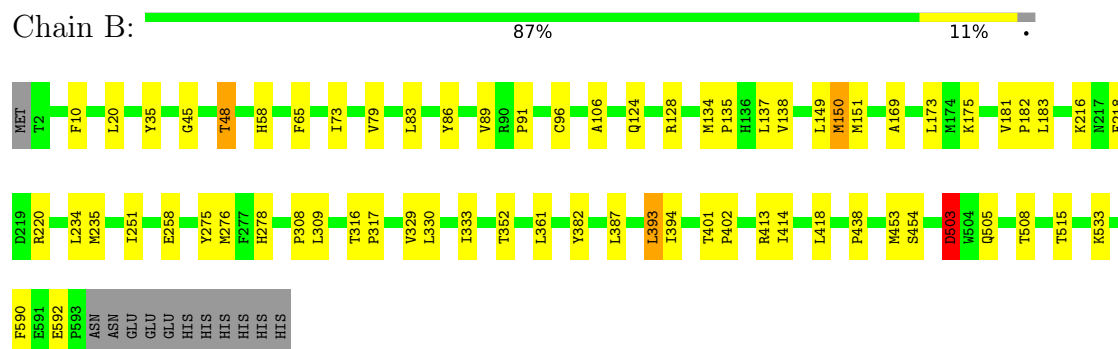
3 Residue-property plots

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.

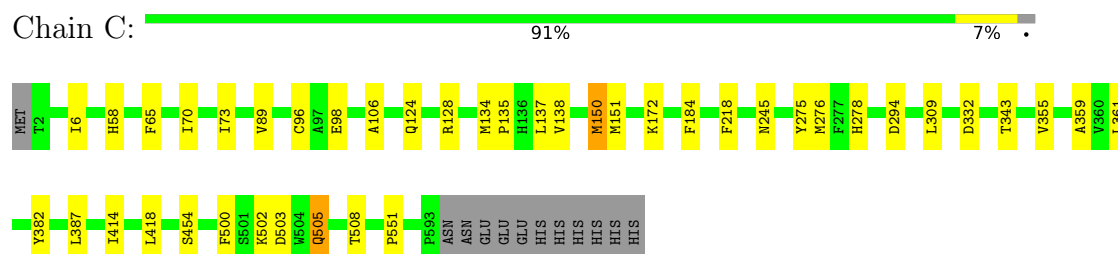
• Molecule 1: Beta-galactosidase



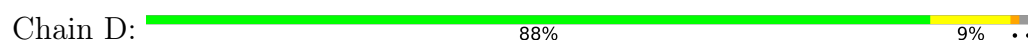
• Molecule 1: Beta-galactosidase

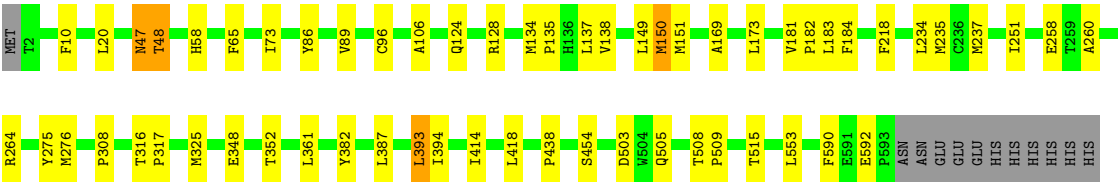


• Molecule 1: Beta-galactosidase



• Molecule 1: Beta-galactosidase





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	92.38Å 111.00Å 120.34Å 90.00° 90.02° 90.00°	Depositor
Resolution (Å)	45.90 – 2.29 45.90 – 2.29	Depositor EDS
% Data completeness (in resolution range)	99.6 (45.90-2.29) 99.6 (45.90-2.29)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.11 (at 2.29Å)	Xtriage
Refinement program	REFMAC 5.8.0352	Depositor
R, R_{free}	0.195 , 0.232 0.179 , 0.210	Depositor DCC
R_{free} test set	5399 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å ²)	40.8	Xtriage
Anisotropy	0.577	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 16.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	0.467 for h,-k,-l	Xtriage
Reported twinning fraction	0.512 for H, K, L 0.488 for -h,-k,l	Depositor
Outliers	0 of 108220 reflections	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	19500	wwPDB-VP
Average B, all atoms (Å ²)	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.47% 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: PEG, GOL, EPE

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	0.46	0/4900	0.77	2/6674 (0.0%)
1	B	0.46	0/4900	0.77	1/6674 (0.0%)
1	C	0.45	0/4908	0.76	0/6685
1	D	0.46	0/4900	0.77	0/6674
All	All	0.46	0/19608	0.77	3/26707 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	36	HIS	CB-CG-CD2	-7.19	121.86	131.20
1	B	503	ASP	CA-CB-CG	7.05	119.65	112.60
1	A	36	HIS	CB-CG-ND1	6.21	132.02	122.70

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	4754	0	4531	20	0
1	B	4754	0	4531	57	0
1	C	4762	0	4536	24	0
1	D	4754	0	4531	39	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	28	0	40	1	0
2	C	14	0	20	0	0
3	B	15	0	18	0	0
3	C	30	0	34	2	0
3	D	15	0	17	0	0
4	B	6	0	8	2	0
5	A	79	0	0	1	0
5	B	97	0	0	0	0
5	C	99	0	0	1	0
5	D	93	0	0	1	0
All	All	19500	0	18266	140	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 4.

All (140) 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:413:ARG:CD	1:B:453:MET:HE1	1.98	0.92
1:D:308:PRO:O	1:D:316:THR:HG22	1.71	0.91
1:B:308:PRO:O	1:B:316:THR:HG22	1.72	0.90
1:B:181:VAL:HG22	1:B:182:PRO:HD2	1.57	0.84
1:B:413:ARG:HD2	1:B:453:MET:HE1	1.60	0.83
1:D:181:VAL:HG22	1:D:182:PRO:HD2	1.59	0.81
1:B:413:ARG:HD3	1:B:453:MET:HE1	1.64	0.78
1:D:150:MET:HE1	1:D:235:MET:HE1	1.68	0.75
1:B:453:MET:HE2	1:B:533:LYS:NZ	2.02	0.73
1:B:10:PHE:HZ	1:B:235:MET:HE2	1.55	0.71
1:D:150:MET:CE	1:D:235:MET:HE1	2.22	0.69
1:D:10:PHE:HZ	1:D:235:MET:HE2	1.55	0.69
1:D:47:ASN:HD22	1:D:48:THR:HG23	1.58	0.68
1:D:149:LEU:O	1:D:181:VAL:HG22	1.93	0.68
1:A:70:ILE:HG21	2:A:701:PEG:H12	1.76	0.67
1:D:149:LEU:O	1:D:181:VAL:CG2	2.43	0.67
1:B:48:THR:HG22	1:B:86:TYR:HB2	1.76	0.66
1:B:91:PRO:HG3	1:B:151:MET:HE2	1.76	0.66
1:A:185:THR:HG21	1:A:198:SER:HA	1.77	0.66
1:B:149:LEU:O	1:B:181:VAL:HG22	1.95	0.66
1:D:10:PHE:CZ	1:D:235:MET:HE2	2.30	0.66
1:B:10:PHE:CZ	1:B:235:MET:HE2	2.31	0.65
1:D:150:MET:HE1	1:D:235:MET:CE	2.25	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:316:THR:OG1	1:B:317:PRO:HD2	1.96	0.65
1:B:137:LEU:HD13	1:B:151:MET:HE1	1.79	0.64
1:D:48:THR:HG22	1:D:86:TYR:HB2	1.79	0.64
1:B:149:LEU:O	1:B:181:VAL:CG2	2.46	0.63
1:A:478:ASP:HA	5:A:833:HOH:O	1.98	0.63
1:B:251:ILE:HD11	1:B:590:PHE:CD1	2.34	0.62
1:B:137:LEU:HD13	1:B:151:MET:CE	2.30	0.62
1:D:316:THR:OG1	1:D:317:PRO:HD2	2.00	0.61
1:D:169:ALA:O	1:D:173:LEU:HD13	2.00	0.61
1:B:150:MET:CE	1:B:235:MET:HE1	2.30	0.61
1:B:169:ALA:O	1:B:173:LEU:HD13	2.01	0.60
1:D:251:ILE:HD11	1:D:590:PHE:CD1	2.38	0.59
1:B:216:LYS:HG2	1:B:220:ARG:HH12	1.68	0.58
1:B:352:THR:OG1	1:B:515:THR:HG22	2.04	0.58
1:B:150:MET:HE1	1:B:235:MET:CE	2.34	0.57
1:A:184:PHE:CE2	1:A:237:MET:HE3	2.40	0.57
1:B:150:MET:HE1	1:B:235:MET:HE1	1.87	0.57
1:A:503:ASP:OD2	1:A:505:GLN:NE2	2.34	0.57
1:D:352:THR:OG1	1:D:515:THR:HG22	2.04	0.56
1:C:503:ASP:OD2	1:C:505:GLN:NE2	2.34	0.56
1:D:503:ASP:OD2	1:D:505:GLN:NE2	2.39	0.56
1:B:175:LYS:NZ	4:B:702:GOL:O1	2.37	0.55
1:B:329:VAL:HG23	1:B:330:LEU:HD23	1.88	0.55
1:D:184:PHE:CE2	1:D:237:MET:HE3	2.41	0.55
1:B:181:VAL:CG2	1:B:182:PRO:HD2	2.34	0.54
1:B:329:VAL:O	1:B:330:LEU:HD22	2.07	0.54
1:D:181:VAL:HG22	1:D:182:PRO:CD	2.35	0.54
1:B:181:VAL:HG22	1:B:182:PRO:CD	2.35	0.54
1:B:503:ASP:OD2	1:B:505:GLN:NE2	2.41	0.54
1:D:264:ARG:HG2	1:D:325:MET:CG	2.38	0.53
1:C:359:ALA:HB1	1:C:502:LYS:HG3	1.91	0.52
1:A:415:GLN:HE22	1:A:574:THR:HB	1.75	0.51
1:B:48:THR:CG2	1:B:86:TYR:HB2	2.40	0.51
1:D:181:VAL:CG2	1:D:182:PRO:HD2	2.38	0.51
1:B:592:GLU:H	1:B:592:GLU:CD	2.18	0.51
1:D:48:THR:CG2	1:D:86:TYR:HB2	2.40	0.51
1:B:35:TYR:CE1	1:B:83:LEU:HD11	2.46	0.51
1:B:106:ALA:HB3	1:B:382:TYR:HB3	1.93	0.51
1:C:359:ALA:HB1	1:C:502:LYS:CG	2.41	0.50
1:B:329:VAL:C	1:B:330:LEU:HD22	2.36	0.50
1:A:418:LEU:HD22	1:A:438:PRO:HD2	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:592:GLU:H	1:D:592:GLU:CD	2.19	0.50
1:C:6:ILE:HD11	1:C:150:MET:CE	2.41	0.49
1:B:79:VAL:O	1:B:83:LEU:HD13	2.13	0.49
1:B:453:MET:HE2	1:B:533:LYS:HZ2	1.77	0.48
1:D:234:LEU:HD22	1:D:234:LEU:N	2.29	0.47
1:D:106:ALA:HB3	1:D:382:TYR:HB3	1.97	0.47
1:B:418:LEU:HD22	1:B:438:PRO:HD2	1.95	0.47
1:D:418:LEU:HD22	1:D:438:PRO:HD2	1.97	0.46
1:B:234:LEU:N	1:B:234:LEU:HD22	2.30	0.46
1:B:20:LEU:HD22	1:B:20:LEU:N	2.29	0.46
1:D:20:LEU:HD22	1:D:20:LEU:N	2.31	0.46
1:C:106:ALA:HB3	1:C:382:TYR:HB3	1.98	0.46
1:A:361:LEU:HD21	1:A:387:LEU:HD23	1.97	0.46
1:C:355:VAL:HG12	1:C:500:PHE:CD1	2.51	0.46
1:C:361:LEU:HD21	1:C:387:LEU:HD23	1.97	0.45
1:D:58:HIS:O	1:D:65:PHE:HA	2.16	0.45
1:B:73:ILE:HD13	1:B:137:LEU:HD21	1.97	0.45
1:B:150:MET:HE2	1:B:235:MET:HE1	1.97	0.45
1:B:134:MET:O	1:B:138:VAL:HG23	2.17	0.45
1:B:413:ARG:HD3	1:B:453:MET:CE	2.42	0.45
1:C:6:ILE:HD11	1:C:150:MET:HE1	1.98	0.45
1:A:275:TYR:HA	1:A:276:MET:HA	1.80	0.44
1:B:58:HIS:O	1:B:65:PHE:HA	2.17	0.44
1:B:275:TYR:HA	1:B:276:MET:HA	1.80	0.44
1:A:106:ALA:HB3	1:A:382:TYR:HB3	1.99	0.44
1:C:58:HIS:O	1:C:65:PHE:HA	2.16	0.44
1:C:275:TYR:HA	1:C:276:MET:HA	1.80	0.44
1:D:134:MET:N	1:D:135:PRO:CD	2.80	0.44
1:A:414:ILE:C	1:A:414:ILE:HD12	2.43	0.44
1:C:245[B]:ASN:HD21	1:C:551:PRO:CG	2.31	0.44
1:A:58:HIS:O	1:A:65:PHE:HA	2.17	0.44
1:C:70:ILE:HG21	3:C:702:EPE:H72	1.98	0.44
1:B:453:MET:HE2	1:B:533:LYS:CE	2.47	0.44
1:D:183:LEU:HD12	1:D:183:LEU:N	2.33	0.44
1:A:73:ILE:HD13	1:A:137:LEU:HD21	1.99	0.43
1:B:183:LEU:HD12	1:B:183:LEU:N	2.33	0.43
1:B:134:MET:N	1:B:135:PRO:CD	2.80	0.43
1:B:453:MET:HE2	1:B:533:LYS:HZ1	1.81	0.43
1:C:414:ILE:HD12	1:C:414:ILE:C	2.43	0.43
1:A:361:LEU:HD11	1:A:387:LEU:CD2	2.49	0.43
1:B:414:ILE:C	1:B:414:ILE:HD12	2.43	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:134:MET:N	1:C:135:PRO:CD	2.81	0.43
1:D:414:ILE:HD12	1:D:414:ILE:C	2.43	0.43
1:C:98:GLU:OE2	3:C:703:EPE:H32	2.18	0.43
1:D:89:VAL:O	1:D:151:MET:HA	2.19	0.43
1:A:134:MET:N	1:A:135:PRO:CD	2.81	0.43
1:B:89:VAL:O	1:B:151:MET:HA	2.19	0.43
1:D:260:ALA:O	1:D:264:ARG:HG3	2.19	0.43
1:C:361:LEU:HD11	1:C:387:LEU:CD2	2.50	0.42
1:B:175:LYS:CE	4:B:702:GOL:O1	2.67	0.42
1:D:134:MET:O	1:D:138:VAL:HG23	2.20	0.42
1:D:73:ILE:HD13	1:D:137:LEU:HD21	2.00	0.42
1:D:393:LEU:HD22	1:D:394:ILE:N	2.34	0.42
1:B:361:LEU:HD11	1:B:387:LEU:CD2	2.50	0.42
1:C:73:ILE:HD13	1:C:137:LEU:HD21	2.00	0.42
1:B:393:LEU:HD22	1:B:394:ILE:N	2.34	0.42
1:A:134:MET:O	1:A:138:VAL:HG23	2.20	0.41
1:D:124:GLN:O	1:D:128:ARG:HG3	2.21	0.41
1:C:332:ASP:HB2	5:C:867:HOH:O	2.20	0.41
1:D:509:PRO:HD3	5:D:810:HOH:O	2.19	0.41
1:B:124:GLN:O	1:B:128:ARG:HG3	2.20	0.41
1:C:134:MET:O	1:C:138:VAL:HG23	2.21	0.41
1:D:275:TYR:HA	1:D:276:MET:HA	1.79	0.41
1:C:89:VAL:O	1:C:151:MET:HA	2.19	0.41
1:B:45:GLY:HA3	1:B:333:ILE:HD13	2.02	0.41
1:C:124:GLN:O	1:C:128:ARG:HG3	2.21	0.41
1:C:418:LEU:HD13	1:C:418:LEU:C	2.46	0.41
1:A:89:VAL:O	1:A:151:MET:HA	2.20	0.41
1:D:361:LEU:HD11	1:D:387:LEU:CD2	2.51	0.41
1:B:278:HIS:HB2	1:B:309:LEU:HD12	2.02	0.40
1:A:99:TRP:O	1:A:100:GLU:C	2.64	0.40
1:A:124:GLN:O	1:A:128:ARG:HG3	2.21	0.40
1:B:401:THR:HB	1:B:402:PRO:HD2	2.03	0.40
1:C:150:MET:HE2	1:C:184:PHE:HD2	1.86	0.40
1:A:173:LEU:HD23	1:A:173:LEU:HA	1.94	0.40
1:C:278:HIS:HB2	1:C:309:LEU:HD12	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	590/604 (98%)	568 (96%)	20 (3%)	2 (0%)	36	46
1	B	590/604 (98%)	568 (96%)	20 (3%)	2 (0%)	36	46
1	C	591/604 (98%)	567 (96%)	22 (4%)	2 (0%)	36	46
1	D	590/604 (98%)	567 (96%)	21 (4%)	2 (0%)	36	46
All	All	2361/2416 (98%)	2270 (96%)	83 (4%)	8 (0%)	36	46

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	454	SER
1	B	454	SER
1	C	454	SER
1	D	454	SER
1	A	96	CYS
1	C	96	CYS
1	D	96	CYS
1	B	96	CYS

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	498/510 (98%)	491 (99%)	7 (1%)	59	76
1	B	498/510 (98%)	491 (99%)	7 (1%)	59	76

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	499/510 (98%)	492 (99%)	7 (1%)	59	76
1	D	498/510 (98%)	489 (98%)	9 (2%)	51	70
All	All	1993/2040 (98%)	1963 (98%)	30 (2%)	57	75

All (30) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	218	PHE
1	A	258	GLU
1	A	343	THR
1	A	505	GLN
1	A	508	THR
1	A	553	LEU
1	A	592	GLU
1	B	48	THR
1	B	150	MET
1	B	218	PHE
1	B	258	GLU
1	B	393	LEU
1	B	503	ASP
1	B	508	THR
1	C	150	MET
1	C	172	LYS
1	C	218	PHE
1	C	294	ASP
1	C	343	THR
1	C	505	GLN
1	C	508	THR
1	D	47	ASN
1	D	48	THR
1	D	150	MET
1	D	218	PHE
1	D	258	GLU
1	D	348	GLU
1	D	393	LEU
1	D	508	THR
1	D	553	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (31) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	139	ASN
1	A	195	ASN
1	A	226	GLN
1	A	299	GLN
1	A	415	GLN
1	A	420	GLN
1	A	445	GLN
1	A	493	ASN
1	A	522	HIS
1	B	8	HIS
1	B	139	ASN
1	B	195	ASN
1	B	323	GLN
1	B	420	GLN
1	B	445	GLN
1	B	522	HIS
1	B	566	GLN
1	C	139	ASN
1	C	195	ASN
1	C	299	GLN
1	C	420	GLN
1	C	493	ASN
1	C	522	HIS
1	D	47	ASN
1	D	139	ASN
1	D	230	GLN
1	D	312	GLN
1	D	323	GLN
1	D	420	GLN
1	D	445	GLN
1	D	522	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

11 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
3	EPE	D	701	-	15,15,15	0.99	1 (6%)	19,20,20	1.14	2 (10%)
2	PEG	A	703	-	6,6,6	0.14	0	5,5,5	0.07	0
2	PEG	C	701	-	6,6,6	0.17	0	5,5,5	0.08	0
3	EPE	B	701	-	15,15,15	0.65	1 (6%)	19,20,20	0.64	0
3	EPE	C	702	-	15,15,15	1.01	1 (6%)	19,20,20	0.90	1 (5%)
3	EPE	C	703	-	15,15,15	0.97	1 (6%)	19,20,20	1.76	2 (10%)
4	GOL	B	702	-	5,5,5	0.10	0	5,5,5	0.26	0
2	PEG	A	702	-	6,6,6	0.19	0	5,5,5	0.13	0
2	PEG	C	704	-	6,6,6	0.17	0	5,5,5	0.09	0
2	PEG	A	701	-	6,6,6	0.20	0	5,5,5	0.12	0
2	PEG	A	704	-	6,6,6	0.20	0	5,5,5	0.06	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
3	EPE	D	701	-	-	3/9/19/19	0/1/1/1
2	PEG	A	703	-	-	1/4/4/4	-
2	PEG	C	701	-	-	2/4/4/4	-
3	EPE	B	701	-	-	1/9/19/19	0/1/1/1
3	EPE	C	702	-	-	3/9/19/19	0/1/1/1
3	EPE	C	703	-	-	1/9/19/19	0/1/1/1
4	GOL	B	702	-	-	4/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	PEG	A	702	-	-	1/4/4/4	-
2	PEG	C	704	-	-	2/4/4/4	-
2	PEG	A	701	-	-	1/4/4/4	-
2	PEG	A	704	-	-	1/4/4/4	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	702	EPE	O1S-S	3.71	1.55	1.45
3	D	701	EPE	O2S-S	3.66	1.55	1.45
3	C	703	EPE	O2S-S	3.55	1.55	1.45
3	B	701	EPE	O3S-S	2.26	1.55	1.47

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	703	EPE	O2S-S-C10	-6.41	97.04	106.73
3	D	701	EPE	O2S-S-C10	-3.40	101.59	106.73
3	C	703	EPE	O3S-S-O1S	2.98	118.86	111.40
3	C	702	EPE	O3S-S-O2S	2.88	118.61	111.40
3	D	701	EPE	O3S-S-O1S	2.48	117.61	111.40

There are no chirality outliers.

All (20) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	702	EPE	S-C10-C9-N1
3	C	703	EPE	S-C10-C9-N1
3	D	701	EPE	C9-C10-S-O1S
3	D	701	EPE	C9-C10-S-O3S
4	B	702	GOL	C1-C2-C3-O3
4	B	702	GOL	O2-C2-C3-O3
2	C	701	PEG	O1-C1-C2-O2
2	C	704	PEG	O1-C1-C2-O2
2	C	704	PEG	O2-C3-C4-O4
4	B	702	GOL	O1-C1-C2-C3
2	A	704	PEG	O2-C3-C4-O4
2	C	701	PEG	O2-C3-C4-O4
4	B	702	GOL	O1-C1-C2-O2
3	C	702	EPE	C8-C7-N4-C3
3	D	701	EPE	C9-C10-S-O2S

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Mol	Chain	Res	Type	Atoms
3	C	702	EPE	C8-C7-N4-C5
2	A	701	PEG	O1-C1-C2-O2
2	A	702	PEG	C1-C2-O2-C3
2	A	703	PEG	O2-C3-C4-O4
3	B	701	EPE	C9-C10-S-O2S

There are no ring outliers.

4 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	702	EPE	1	0
3	C	703	EPE	1	0
4	B	702	GOL	2	0
2	A	701	PEG	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	592/604 (98%)	-1.05	0 100 100	30, 46, 63, 82	0
1	B	592/604 (98%)	-1.11	0 100 100	25, 42, 62, 84	0
1	C	592/604 (98%)	-1.09	0 100 100	24, 47, 68, 97	1 (0%)
1	D	592/604 (98%)	-1.12	0 100 100	28, 42, 59, 94	0
All	All	2368/2416 (98%)	-1.09	0 100 100	24, 44, 63, 97	1 (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
2	PEG	A	704	7/7	0.97	0.10	49,51,53,53	0
2	PEG	A	703	7/7	0.98	0.05	59,60,63,65	0
2	PEG	A	702	7/7	0.98	0.04	53,54,57,59	0
2	PEG	C	701	7/7	0.98	0.05	58,62,66,68	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	PEG	C	704	7/7	0.98	0.05	52,55,57,57	0
3	EPE	B	701	15/15	0.98	0.05	47,52,54,55	0
3	EPE	C	702	15/15	0.98	0.05	52,61,67,68	0
3	EPE	C	703	15/15	0.98	0.06	41,57,68,71	0
3	EPE	D	701	15/15	0.98	0.06	49,55,58,58	0
4	GOL	B	702	6/6	0.98	0.05	51,54,57,59	0
2	PEG	A	701	7/7	0.99	0.04	59,63,67,68	0

6.5 Other polymers [i](#)

There are no such residues in this entry.