



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 08:38 PM UTC

PDB ID : 9LHI / pdb_00009lhi
Title : Crystal structure of BglB
Authors : Chen, A.; Liu, K.; Ji, C.
Deposited on : 2025-01-12
Resolution : 1.74 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

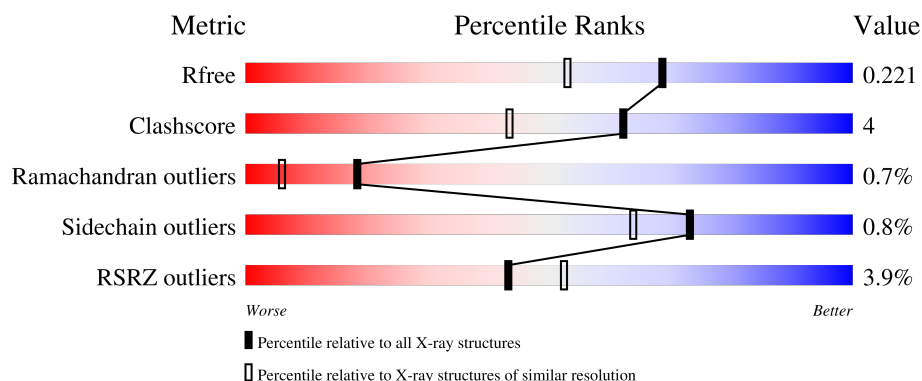
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.74 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	1187 (1.74-1.74)
Clashscore	190562	1207 (1.74-1.74)
Ramachandran outliers	187476	1200 (1.74-1.74)
Sidechain outliers	187428	1200 (1.74-1.74)
RSRZ outliers	180081	1188 (1.74-1.74)

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	494	3% 89% 10% .
1	B	494	2% 88% 10% .
1	C	494	4% 91% 7% .
1	D	494	5% 89% 9% ..

2 Entry composition [i](#)

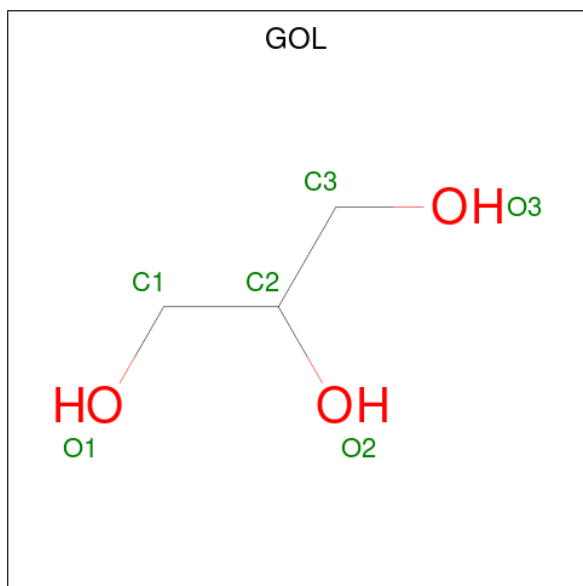
There are 5 unique types of molecules in this entry. The entry contains 16926 atoms, of which 0 are hydrogens and 0 are deuteriums.

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	486	Total	C	N	O	S	0	0	0
			3921	2534	672	707	8			
1	B	486	Total	C	N	O	S	0	0	0
			3921	2535	673	705	8			
1	C	488	Total	C	N	O	S	0	0	0
			3918	2532	671	707	8			
1	D	488	Total	C	N	O	S	0	0	0
			3918	2533	673	704	8			

- Molecule 2 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



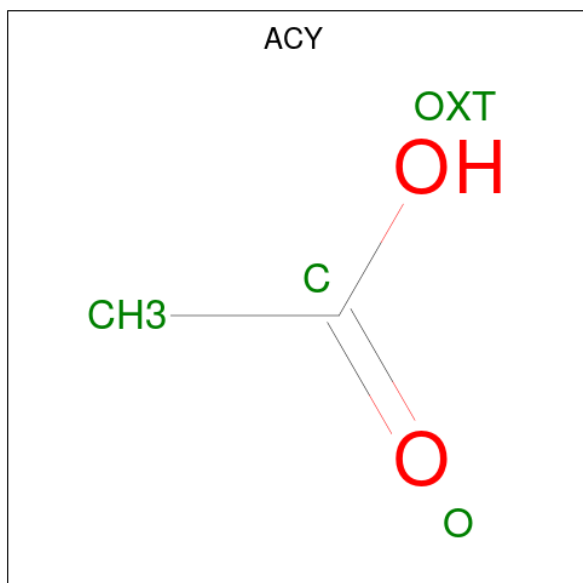
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			6	3	3		
2	A	1	Total	C	O	0	0
			6	3	3		

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

- Molecule 3 is ACETIC ACID (CCD ID: ACY) (formula: C₂H₄O₂).



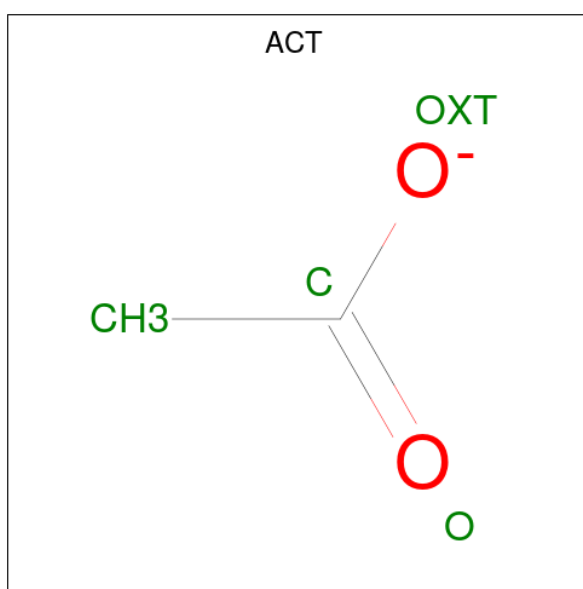
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			4	2	2		

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

- Molecule 4 is ACETATE ION (CCD ID: ACT) (formula: $C_2H_3O_2$).



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

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	331	Total	O	0	0
			331	331		
5	B	339	Total	O	0	0
			339	339		
5	C	243	Total	O	0	0
			243	243		

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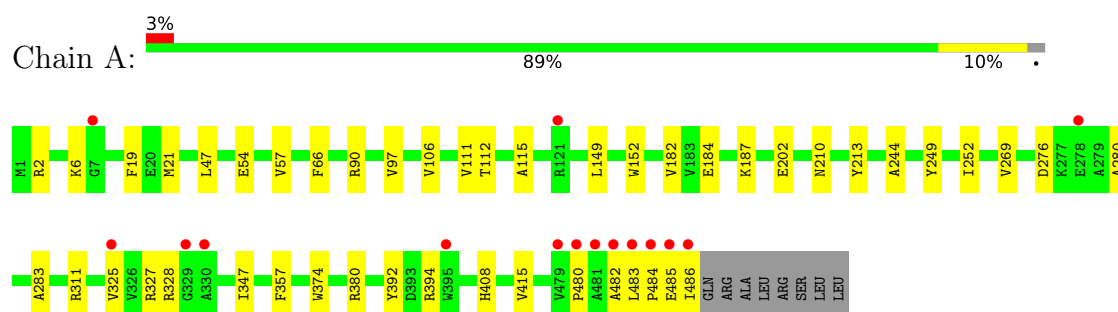
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	D	235	Total 235	O 235	0	0

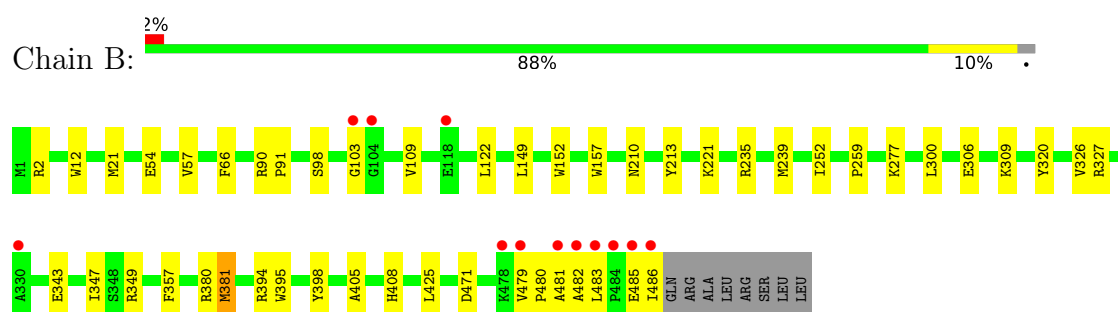
3 Residue-property plots [i](#)

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.

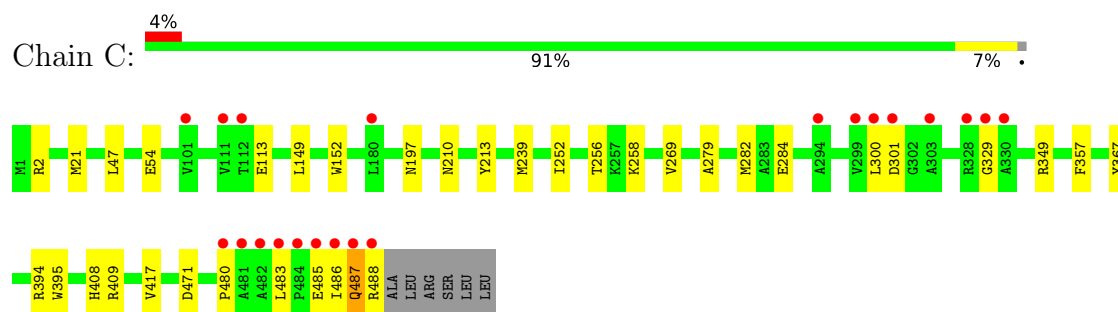
• Molecule 1: Beta-galactosidase



• Molecule 1: Beta-galactosidase

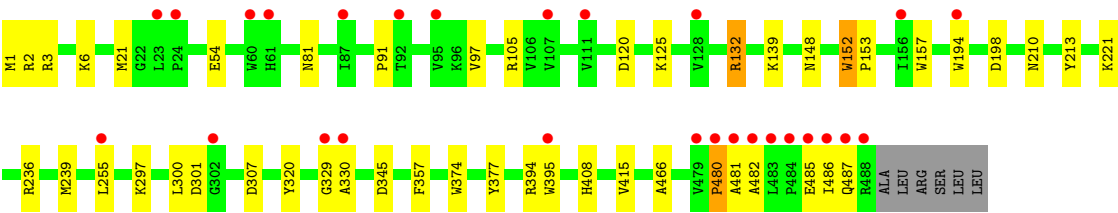


• Molecule 1: Beta-galactosidase



• 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	100.03Å 91.05Å 116.36Å 90.00° 90.85° 90.00°	Depositor
Resolution (Å)	31.93 – 1.74 31.93 – 1.74	Depositor EDS
% Data completeness (in resolution range)	99.8 (31.93-1.74) 99.8 (31.93-1.74)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.30 (at 1.74Å)	Xtriage
Refinement program	PHENIX (1.10_2155: ???)	Depositor
R, R_{free}	0.190 , 0.221 0.191 , 0.221	Depositor DCC
R_{free} test set	10598 reflections (4.93%)	wwPDB-VP
Wilson B-factor (Å ²)	24.4	Xtriage
Anisotropy	0.739	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 32.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.017 for h,-k,-l	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	16926	wwPDB-VP
Average B, all atoms (Å ²)	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.51% 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: ACT, ACY, GOL

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.40	0/4046	0.63	1/5512 (0.0%)
1	B	0.42	1/4046 (0.0%)	0.61	0/5511
1	C	0.34	0/4043	0.56	0/5513
1	D	0.35	0/4043	0.56	0/5512
All	All	0.38	1/16178 (0.0%)	0.59	1/22048 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	381	MET	SD-CE	-5.03	1.67	1.79

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	19	PHE	CB-CA-C	-6.15	99.53	109.13

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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	3921	0	3744	31	0
1	B	3921	0	3751	38	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	3918	0	3720	30	0
1	D	3918	0	3729	36	0
2	A	18	0	24	0	0
2	B	18	0	24	1	0
2	C	18	0	24	0	0
2	D	18	0	24	1	0
3	A	4	0	3	1	0
3	B	4	0	3	0	0
3	C	8	0	6	0	0
3	D	4	0	3	0	0
4	A	4	0	3	0	0
4	B	4	0	3	0	0
5	A	331	0	0	5	0
5	B	339	0	0	5	0
5	C	243	0	0	4	0
5	D	235	0	0	5	0
All	All	16926	0	15061	125	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 (125) 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:306:GLU:OE1	1:B:309:LYS:NZ	1.66	1.29
1:B:380:ARG:NH1	5:B:601:HOH:O	1.78	1.16
1:C:239:MET:HE1	1:C:300:LEU:HD11	1.53	0.91
1:A:328:ARG:NH1	5:A:601:HOH:O	2.08	0.84
1:D:6:LYS:O	5:D:601:HOH:O	1.95	0.83
1:C:394:ARG:HH11	1:C:395:TRP:HE1	1.27	0.82
1:B:57:VAL:HG12	1:B:66:PHE:HZ	1.49	0.78
1:C:485:GLU:OE2	5:C:601:HOH:O	2.05	0.74
1:B:259:PRO:HB3	5:B:601:HOH:O	1.88	0.73
1:C:395:TRP:HZ2	1:C:485:GLU:OE1	1.70	0.73
1:D:105:ARG:NH1	1:D:307:ASP:OD2	2.21	0.73
1:A:57:VAL:HG12	1:A:66:PHE:HZ	1.54	0.71
1:A:482:ALA:N	1:A:485:GLU:OE2	2.23	0.71
1:C:113:GLU:H	1:C:113:GLU:CD	1.97	0.71
1:A:276:ASP:OD1	1:A:327:ARG:HG2	1.92	0.70
1:D:487:GLN:NE2	5:D:603:HOH:O	2.24	0.70
1:A:6:LYS:O	5:A:602:HOH:O	2.09	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:482:ALA:N	1:B:485:GLU:OE2	2.22	0.69
1:B:306:GLU:CD	1:B:309:LYS:HZ1	1.89	0.69
1:B:394:ARG:HD3	1:B:395:TRP:NE1	2.10	0.67
1:A:483:LEU:HD23	1:A:484:PRO:HD3	1.77	0.66
1:B:306:GLU:HA	1:B:309:LYS:HE2	1.77	0.66
1:C:349:ARG:NH2	5:C:604:HOH:O	2.27	0.65
1:D:132:ARG:NH1	1:D:198:ASP:OD1	2.30	0.65
1:D:236:ARG:NH1	5:D:604:HOH:O	2.31	0.64
1:B:103:GLY:O	5:B:602:HOH:O	2.15	0.64
1:B:149:LEU:HD11	1:B:252:ILE:HD11	1.80	0.62
1:D:1:MET:HE1	1:D:466:ALA:HB1	1.80	0.61
1:D:132:ARG:HH12	1:D:198:ASP:CG	2.10	0.59
1:A:483:LEU:HD21	1:D:345:ASP:OD2	2.03	0.59
1:B:90:ARG:NH1	1:B:122:LEU:O	2.36	0.59
1:B:306:GLU:CD	1:B:309:LYS:NZ	2.53	0.58
1:A:112:THR:HG23	1:A:115:ALA:H	1.69	0.57
1:B:482:ALA:O	1:B:485:GLU:HG2	2.04	0.57
1:B:394:ARG:CZ	1:C:394:ARG:HH21	2.18	0.56
1:D:120:ASP:OD1	1:D:125:LYS:HE2	2.05	0.56
3:A:504:ACY:H1	1:B:343:GLU:OE2	2.05	0.56
1:C:394:ARG:HH11	1:C:395:TRP:NE1	2.00	0.56
1:A:392:TYR:HE2	1:D:480:PRO:HB2	1.71	0.56
1:B:239:MET:HE1	1:B:300:LEU:HD21	1.87	0.56
1:A:202:GLU:OE2	1:A:380:ARG:NH1	2.39	0.54
1:A:249:TYR:CD1	1:A:311:ARG:HG2	2.43	0.53
1:A:269:VAL:HG11	1:A:283:ALA:HB3	1.89	0.53
1:B:471:ASP:OD1	5:B:603:HOH:O	2.19	0.53
1:C:488:ARG:O	5:C:602:HOH:O	2.19	0.53
1:C:394:ARG:NH1	1:C:485:GLU:CD	2.67	0.52
1:B:398:TYR:HB3	1:B:479:VAL:HG12	1.92	0.52
1:D:482:ALA:O	1:D:486:ILE:HG13	2.09	0.52
1:B:349:ARG:NH2	5:B:610:HOH:O	2.42	0.52
1:D:1:MET:HG2	1:D:3:ARG:HG3	1.91	0.52
1:B:235:ARG:O	1:B:239:MET:HG2	2.10	0.52
1:B:347:ILE:HG12	1:B:486:ILE:CB	2.40	0.52
1:A:210:ASN:HA	1:A:213:TYR:CE2	2.45	0.52
1:C:197:ASN:O	1:C:258:LYS:NZ	2.36	0.51
1:A:484:PRO:HB2	5:A:660:HOH:O	2.10	0.50
1:D:139:LYS:O	5:D:602:HOH:O	2.19	0.50
1:C:471:ASP:OD2	5:C:603:HOH:O	2.19	0.50
5:A:680:HOH:O	1:C:487:GLN:HB3	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:483:LEU:HG	1:C:487:GLN:HE22	1.76	0.49
1:D:297:LYS:HE2	1:D:377:TYR:CD1	2.47	0.49
1:D:239:MET:HE1	1:D:300:LEU:HD13	1.95	0.49
1:B:483:LEU:O	1:D:487:GLN:O	2.31	0.48
1:A:90:ARG:NH2	5:A:606:HOH:O	2.39	0.48
1:A:21:MET:HB3	1:A:54:GLU:HA	1.96	0.48
1:A:482:ALA:O	1:A:485:GLU:HG2	2.14	0.47
1:C:113:GLU:CD	1:C:113:GLU:N	2.71	0.47
1:A:486:ILE:HA	1:C:487:GLN:HA	1.96	0.47
1:B:306:GLU:OE1	1:B:309:LYS:CE	2.57	0.47
1:D:194:TRP:HB2	1:D:255:LEU:HD13	1.95	0.47
1:B:380:ARG:C	1:B:381:MET:HG3	2.39	0.47
1:D:2:ARG:HB3	1:D:408:HIS:CE1	2.50	0.47
1:B:326:VAL:HG22	1:B:327:ARG:O	2.13	0.47
1:A:112:THR:CG2	1:A:115:ALA:H	2.27	0.47
1:B:239:MET:CE	1:B:300:LEU:HD21	2.44	0.46
1:A:57:VAL:CG1	1:A:66:PHE:HZ	2.25	0.46
1:D:482:ALA:H	1:D:485:GLU:CD	2.23	0.46
1:B:210:ASN:HA	1:B:213:TYR:CE2	2.51	0.46
1:D:482:ALA:HB3	1:D:485:GLU:OE1	2.15	0.46
1:C:210:ASN:HA	1:C:213:TYR:CE2	2.50	0.46
1:A:327:ARG:HG2	1:A:327:ARG:H	1.48	0.45
1:B:394:ARG:HG3	1:C:394:ARG:HG3	1.98	0.45
1:C:394:ARG:HH12	1:C:485:GLU:CD	2.23	0.45
1:C:485:GLU:H	1:C:485:GLU:HG2	1.59	0.45
1:D:210:ASN:HA	1:D:213:TYR:CE2	2.51	0.45
1:D:329:GLY:HA2	1:D:330:ALA:HA	1.60	0.45
1:A:182:VAL:HG13	1:A:244:ALA:HA	1.98	0.45
1:C:149:LEU:HD11	1:C:252:ILE:HD11	1.99	0.45
1:C:300:LEU:O	1:C:301:ASP:HB2	2.16	0.45
1:D:395:TRP:HZ2	1:D:485:GLU:OE2	2.00	0.45
1:A:2:ARG:HB3	1:A:408:HIS:CE1	2.52	0.45
1:C:367:TYR:CE1	1:C:409:ARG:HG2	2.52	0.44
1:A:149:LEU:HD11	1:A:252:ILE:HD11	2.00	0.44
1:D:91:PRO:HA	1:D:157:TRP:CE2	2.53	0.44
1:C:269:VAL:HB	1:C:284:GLU:CG	2.48	0.43
1:C:279:ALA:HA	1:C:282:MET:HE3	1.98	0.43
1:D:374:TRP:HB2	1:D:415:VAL:HG13	2.00	0.43
1:B:91:PRO:HA	1:B:157:TRP:CE2	2.53	0.43
1:D:482:ALA:HB1	5:D:624:HOH:O	2.18	0.43
1:B:277:LYS:HE2	1:B:277:LYS:HB3	1.85	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:47:LEU:HD23	1:D:221:LYS:HD2	2.00	0.43
1:D:105:ARG:HH12	1:D:307:ASP:CG	2.25	0.43
1:B:21:MET:HB3	1:B:54:GLU:HA	2.00	0.43
1:A:184:GLU:HA	1:A:187:LYS:HD3	2.00	0.43
1:C:486:ILE:O	1:C:488:ARG:N	2.50	0.42
1:A:280:ALA:HA	1:A:325:VAL:HG11	2.01	0.42
1:A:374:TRP:HB2	1:A:415:VAL:HG13	2.01	0.42
1:D:81:ASN:HA	1:D:148:ASN:O	2.19	0.42
1:A:394:ARG:HG3	1:D:394:ARG:HG3	2.02	0.42
1:C:269:VAL:HB	1:C:284:GLU:HG3	2.02	0.42
1:B:320:TYR:CD1	2:B:502:GOL:H11	2.54	0.41
1:D:1:MET:HE2	1:D:3:ARG:HG2	2.01	0.41
1:D:139:LYS:HA	1:D:139:LYS:HD3	1.79	0.41
1:B:394:ARG:HD3	1:B:395:TRP:CD1	2.55	0.41
1:A:347:ILE:HG23	1:A:485:GLU:HG3	2.02	0.41
1:A:47:LEU:HD23	1:B:221:LYS:HD2	2.02	0.41
1:D:320:TYR:CD2	2:D:503:GOL:H11	2.56	0.41
1:B:2:ARG:HH21	1:B:408:HIS:HB3	1.86	0.40
1:B:2:ARG:NH2	1:B:405:ALA:O	2.54	0.40
1:B:12:TRP:CD2	1:B:425:LEU:HB2	2.56	0.40
1:D:152:TRP:HB2	1:D:153:PRO:HD3	2.03	0.40
1:A:392:TYR:HE2	1:D:480:PRO:CB	2.34	0.40
1:C:21:MET:HB3	1:C:54:GLU:HA	2.02	0.40
1:D:21:MET:HB3	1:D:54:GLU:HA	2.02	0.40
1:B:2:ARG:HB3	1:B:408:HIS:CE1	2.57	0.40
1:C:2:ARG:HB3	1:C:408:HIS:CE1	2.56	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	484/494 (98%)	472 (98%)	10 (2%)	2 (0%)	30	16
1	B	484/494 (98%)	470 (97%)	11 (2%)	3 (1%)	21	8
1	C	486/494 (98%)	471 (97%)	11 (2%)	4 (1%)	16	4
1	D	486/494 (98%)	467 (96%)	15 (3%)	4 (1%)	16	4
All	All	1940/1976 (98%)	1880 (97%)	47 (2%)	13 (1%)	18	6

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	152	TRP
1	B	152	TRP
1	B	481	ALA
1	C	152	TRP
1	D	152	TRP
1	D	480	PRO
1	D	481	ALA
1	B	480	PRO
1	D	301	ASP
1	A	480	PRO
1	C	329	GLY
1	C	487	GLN
1	C	480	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	396/408 (97%)	392 (99%)	4 (1%)	68	54
1	B	396/408 (97%)	393 (99%)	3 (1%)	73	64
1	C	393/408 (96%)	390 (99%)	3 (1%)	73	64
1	D	393/408 (96%)	390 (99%)	3 (1%)	73	64
All	All	1578/1632 (97%)	1565 (99%)	13 (1%)	73	64

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	97	VAL
1	A	106	VAL
1	A	111	VAL
1	A	357	PHE
1	B	98	SER
1	B	109	VAL
1	B	357	PHE
1	C	256	THR
1	C	357	PHE
1	C	417	VAL
1	D	97	VAL
1	D	132	ARG
1	D	357	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	124	ASN
1	A	207	ASN
1	A	378	ASN
1	A	386	ASN
1	B	386	ASN
1	B	475	HIS
1	C	65	GLN
1	C	207	ASN
1	C	219	ASN
1	C	475	HIS
1	C	487	GLN
1	D	65	GLN
1	D	305	GLN

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](#)

19 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	GOL	D	502	-	5,5,5	0.32	0	5,5,5	1.30	0
3	ACY	C	505	-	3,3,3	0.82	0	3,3,3	0.93	0
3	ACY	B	504	-	3,3,3	0.68	0	3,3,3	1.17	0
4	ACT	B	505	-	3,3,3	0.83	0	3,3,3	1.40	0
2	GOL	C	502	-	5,5,5	0.24	0	5,5,5	1.63	1 (20%)
4	ACT	A	505	-	3,3,3	0.82	0	3,3,3	1.41	0
2	GOL	B	501	-	5,5,5	0.31	0	5,5,5	0.25	0
2	GOL	D	503	-	5,5,5	0.33	0	5,5,5	0.60	0
2	GOL	D	501	-	5,5,5	0.29	0	5,5,5	0.22	0
2	GOL	C	501	-	5,5,5	0.49	0	5,5,5	0.89	0
3	ACY	A	504	-	3,3,3	0.71	0	3,3,3	0.81	0
2	GOL	A	503	-	5,5,5	0.21	0	5,5,5	0.78	0
2	GOL	A	502	-	5,5,5	0.37	0	5,5,5	0.87	0
2	GOL	C	503	-	5,5,5	0.39	0	5,5,5	1.09	1 (20%)
2	GOL	B	503	-	5,5,5	0.31	0	5,5,5	0.53	0
3	ACY	D	504	-	3,3,3	0.79	0	3,3,3	0.80	0
2	GOL	A	501	-	5,5,5	0.27	0	5,5,5	1.57	1 (20%)
3	ACY	C	504	-	3,3,3	0.77	0	3,3,3	0.91	0
2	GOL	B	502	-	5,5,5	0.25	0	5,5,5	0.65	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GOL	C	503	-	-	4/4/4/4	-
2	GOL	D	501	-	-	0/4/4/4	-
2	GOL	B	503	-	-	0/4/4/4	-
2	GOL	D	502	-	-	2/4/4/4	-
2	GOL	B	501	-	-	0/4/4/4	-
2	GOL	C	501	-	-	2/4/4/4	-
2	GOL	A	501	-	-	2/4/4/4	-
2	GOL	B	502	-	-	2/4/4/4	-
2	GOL	C	502	-	-	2/4/4/4	-
2	GOL	A	503	-	-	1/4/4/4	-
2	GOL	A	502	-	-	2/4/4/4	-
2	GOL	D	503	-	-	1/4/4/4	-

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	502	GOL	C3-C2-C1	-3.15	100.25	111.80
2	A	501	GOL	C3-C2-C1	-3.01	100.74	111.80
2	C	503	GOL	C3-C2-C1	-2.13	103.99	111.80

There are no chirality outliers.

All (18) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	501	GOL	O1-C1-C2-C3
2	C	502	GOL	O1-C1-C2-C3
2	C	503	GOL	O1-C1-C2-C3
2	C	503	GOL	C1-C2-C3-O3
2	A	502	GOL	C1-C2-C3-O3
2	A	503	GOL	C1-C2-C3-O3
2	B	502	GOL	O1-C1-C2-C3
2	C	501	GOL	O1-C1-C2-C3
2	D	502	GOL	O1-C1-C2-C3
2	A	501	GOL	O1-C1-C2-O2
2	C	502	GOL	O1-C1-C2-O2
2	C	503	GOL	O1-C1-C2-O2
2	D	502	GOL	O1-C1-C2-O2
2	C	503	GOL	O2-C2-C3-O3
2	B	502	GOL	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
2	C	501	GOL	O2-C2-C3-O3
2	A	502	GOL	O2-C2-C3-O3
2	D	503	GOL	O1-C1-C2-C3

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	503	GOL	1	0
3	A	504	ACY	1	0
2	B	502	GOL	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ > 2			OWAB(Å ²)	Q < 0.9
1	A	486/494 (98%)	0.22	15 (3%)	51	60	20, 27, 42, 61	0
1	B	486/494 (98%)	0.17	12 (2%)	58	66	20, 27, 42, 52	0
1	C	488/494 (98%)	0.39	21 (4%)	40	49	22, 32, 48, 65	0
1	D	488/494 (98%)	0.68	27 (5%)	30	37	24, 34, 50, 64	0
All	All	1948/1976 (98%)	0.37	75 (3%)	43	52	20, 30, 47, 65	0

All (75) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	486	ILE	6.1
1	A	486	ILE	6.0
1	D	483	LEU	5.9
1	B	483	LEU	5.5
1	D	481	ALA	5.4
1	C	486	ILE	5.3
1	D	486	ILE	5.2
1	A	483	LEU	5.2
1	C	483	LEU	5.1
1	D	482	ALA	5.0
1	C	481	ALA	4.5
1	A	482	ALA	4.4
1	C	484	PRO	4.4
1	B	482	ALA	4.2
1	D	329	GLY	4.1
1	B	481	ALA	4.0
1	A	480	PRO	3.9
1	B	479	VAL	3.9
1	D	484	PRO	3.8
1	B	103	GLY	3.8
1	A	329	GLY	3.6

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Mol	Chain	Res	Type	RSRZ
1	A	484	PRO	3.6
1	D	479	VAL	3.6
1	A	485	GLU	3.5
1	C	329	GLY	3.5
1	C	480	PRO	3.4
1	D	302	GLY	3.3
1	C	303	ALA	3.3
1	B	484	PRO	3.3
1	A	481	ALA	3.3
1	D	485	GLU	3.2
1	C	485	GLU	3.1
1	D	330	ALA	3.0
1	A	479	VAL	2.9
1	D	488	ARG	2.8
1	D	61	HIS	2.8
1	C	101	VAL	2.8
1	C	482	ALA	2.8
1	D	23	LEU	2.7
1	D	194	TRP	2.7
1	D	480	PRO	2.6
1	A	121	ARG	2.6
1	C	300	LEU	2.6
1	A	330	ALA	2.5
1	C	112	THR	2.5
1	D	60	TRP	2.5
1	D	87	ILE	2.5
1	B	478	LYS	2.4
1	D	255	LEU	2.4
1	C	111	VAL	2.4
1	D	111	VAL	2.4
1	D	156	ILE	2.3
1	D	487	GLN	2.3
1	D	95	VAL	2.3
1	C	301	ASP	2.3
1	D	24	PRO	2.3
1	C	294	ALA	2.2
1	C	180	LEU	2.2
1	A	7	GLY	2.2
1	B	104	GLY	2.2
1	B	118	GLU	2.2
1	D	107	VAL	2.1
1	C	330	ALA	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	278	GLU	2.1
1	A	395	TRP	2.1
1	D	395	TRP	2.1
1	B	330	ALA	2.1
1	C	299	VAL	2.1
1	C	487	GLN	2.1
1	C	328	ARG	2.1
1	D	92	THR	2.1
1	B	485	GLU	2.0
1	A	325	VAL	2.0
1	C	488	ARG	2.0
1	D	128	VAL	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(Å ²)	Q<0.9
4	ACT	B	505	4/4	0.75	0.16	42,49,49,49	0
2	GOL	A	502	6/6	0.81	0.14	24,25,28,35	0
4	ACT	A	505	4/4	0.82	0.14	46,46,48,50	0
3	ACY	D	504	4/4	0.84	0.13	42,47,50,51	0
2	GOL	A	501	6/6	0.85	0.12	26,28,36,37	0
2	GOL	C	503	6/6	0.87	0.12	33,34,37,40	0
3	ACY	B	504	4/4	0.88	0.10	28,32,33,40	0
2	GOL	C	501	6/6	0.88	0.11	24,29,35,38	0
3	ACY	C	505	4/4	0.89	0.10	24,32,38,39	0
2	GOL	C	502	6/6	0.89	0.11	26,32,38,39	0
2	GOL	B	502	6/6	0.90	0.10	30,30,33,37	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	ACY	A	504	4/4	0.91	0.09	24,26,34,36	0
2	GOL	D	502	6/6	0.91	0.12	28,34,39,41	0
2	GOL	A	503	6/6	0.92	0.09	29,30,35,35	0
2	GOL	B	503	6/6	0.93	0.08	24,28,32,34	0
3	ACY	C	504	4/4	0.93	0.09	27,29,31,35	0
2	GOL	D	501	6/6	0.93	0.08	29,29,31,36	0
2	GOL	B	501	6/6	0.94	0.07	22,23,23,29	0
2	GOL	D	503	6/6	0.95	0.07	30,34,35,37	0

6.5 Other polymers [i](#)

There are no such residues in this entry.