



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 7, 2026 – 02:25 AM UTC

PDB ID : 5ZXL / pdb_00005zxl
Title : Structure of GldA from E.coli
Authors : Zhang, J.; Lin, L.
Deposited on : 2018-05-21
Resolution : 2.79 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

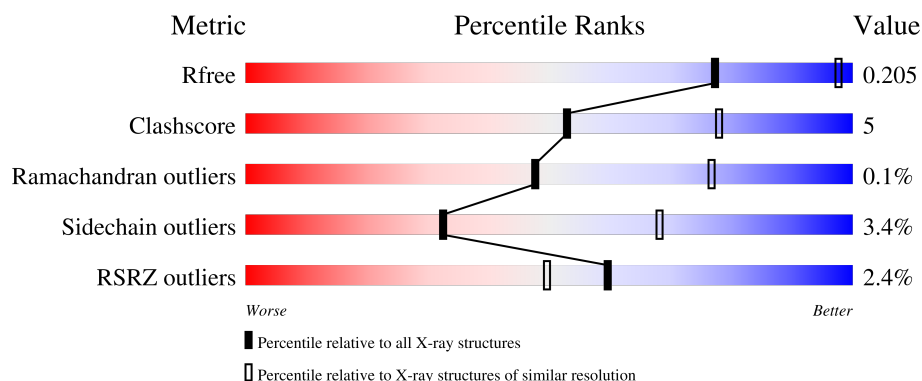
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.79 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	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

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	367	2% 89% 10%
1	B	367	% 87% 11%
1	C	367	4% 87% 12%
1	D	367	2% 89% 11%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 11102 atoms, of which 96 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 Glycerol dehydrogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	367	Total	C	N	O	S	0	0	0
			2697	1704	455	524	14			
1	B	367	Total	C	N	O	S	0	1	0
			2693	1703	455	521	14			
1	C	367	Total	C	N	O	S	0	0	0
			2658	1680	451	513	14			
1	D	367	Total	C	N	O	S	0	1	0
			2717	1720	460	523	14			

- Molecule 2 is ZINC ION (CCD ID: ZN) (formula: Zn).

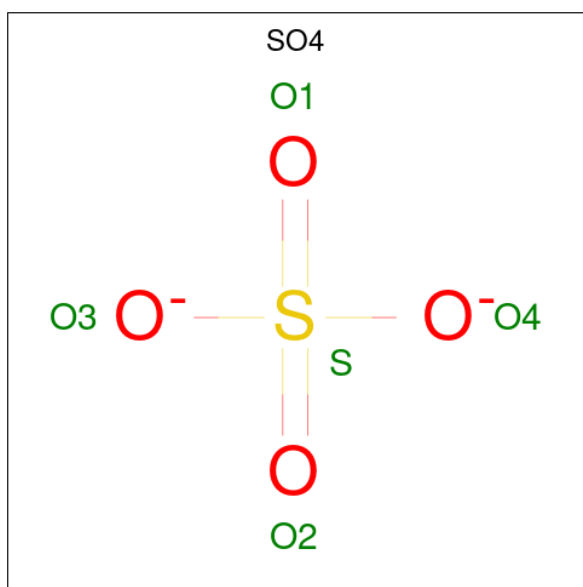
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Zn	0	0
			1	1		
2	B	1	Total	Zn	0	0
			1	1		
2	C	1	Total	Zn	0	0
			1	1		
2	D	2	Total	Zn	0	0
			2	2		

- Molecule 3 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	H	O	0	0
			14	3	8	3		
3	A	1	Total	C	H	O	0	0
			14	3	8	3		
3	B	1	Total	C	H	O	0	0
			14	3	8	3		
3	B	1	Total	C	H	O	0	0
			14	3	8	3		
3	B	1	Total	C	H	O	0	0
			14	3	8	3		
3	C	1	Total	C	H	O	0	0
			14	3	8	3		
3	C	1	Total	C	H	O	0	0
			14	3	8	3		
3	C	1	Total	C	H	O	0	0
			14	3	8	3		
3	D	1	Total	C	H	O	0	0
			14	3	8	3		
3	D	1	Total	C	H	O	0	0
			14	3	8	3		
3	D	1	Total	C	H	O	0	0
			14	3	8	3		

- Molecule 4 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	O	S	0	0
			5	4	1		
4	C	1	Total	O	S	0	0
			5	4	1		
4	C	1	Total	O	S	0	0
			5	4	1		
4	D	1	Total	O	S	0	0
			5	4	1		
4	D	1	Total	O	S	0	0
			5	4	1		

- Molecule 5 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	D	1	Total	Cl	0	0
			1	1		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	36	Total	O	0	0
			36	36		
6	B	44	Total	O	0	0
			44	44		
6	C	17	Total	O	0	0
			17	17		

Continued on next page...

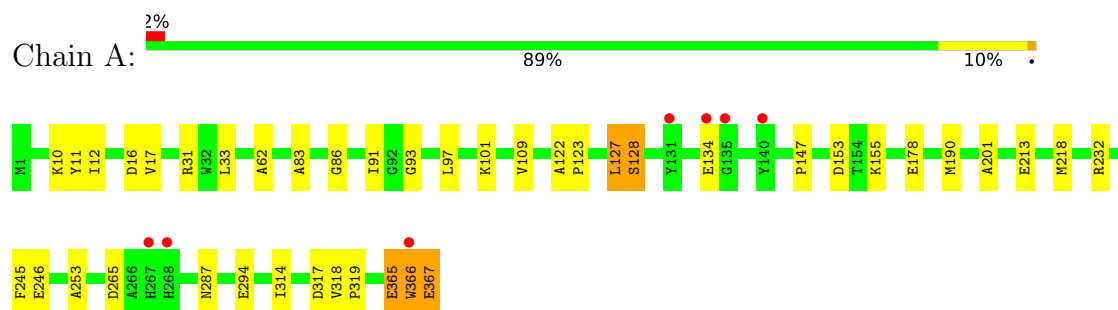
Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	D	41	Total	O	0	0
			41	41		

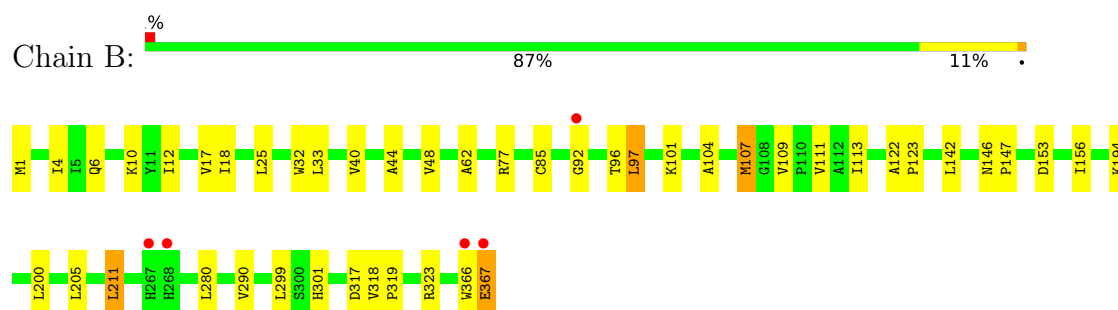
3 Residue-property plots

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.

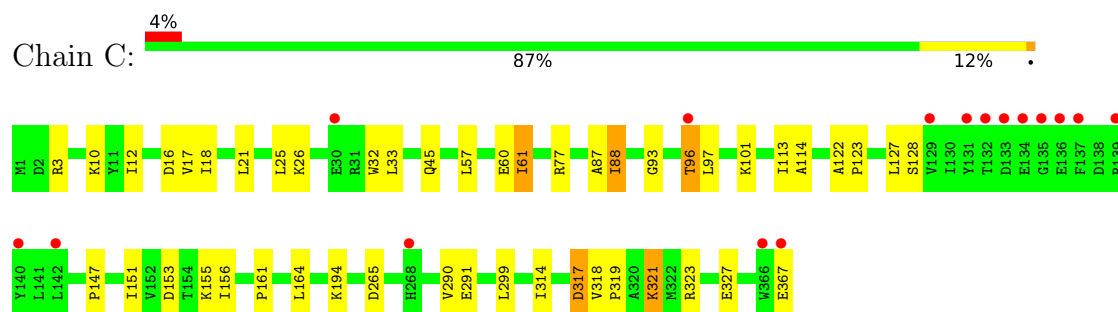
- Molecule 1: Glycerol dehydrogenase



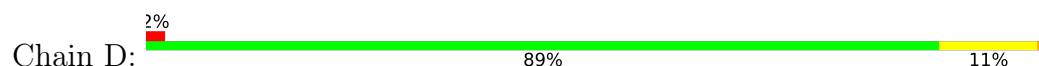
- Molecule 1: Glycerol dehydrogenase

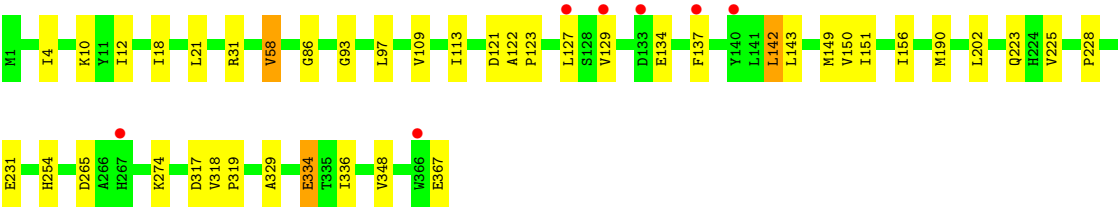


- Molecule 1: Glycerol dehydrogenase



- Molecule 1: Glycerol dehydrogenase





4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α , β , γ	162.45Å 162.45Å 293.13Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.61 – 2.79 40.61 – 2.79	Depositor EDS
% Data completeness (in resolution range)	99.5 (40.61-2.79) 95.4 (40.61-2.79)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.69 (at 2.81Å)	Xtriage
Refinement program	PHENIX 1.11.1_2575	Depositor
R, R_{free}	0.173 , 0.204 0.177 , 0.205	Depositor DCC
R_{free} test set	2000 reflections (2.06%)	wwPDB-VP
Wilson B-factor (Å ²)	59.7	Xtriage
Anisotropy	0.096	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 34.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	11102	wwPDB-VP
Average B, all atoms (Å ²)	62.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.56% 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: GOL, ZN, SO4, CL

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	0.38	0/2744	0.57	0/3737
1	B	0.37	0/2740	0.57	0/3733
1	C	0.34	0/2704	0.55	0/3687
1	D	0.39	1/2766 (0.0%)	0.57	0/3764
All	All	0.37	1/10954 (0.0%)	0.57	0/14921

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	254	HIS	C-O	-5.18	1.17	1.24

There are no bond angle outliers.

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	2697	0	2673	28	0
1	B	2693	0	2661	32	0
1	C	2658	0	2624	30	0
1	D	2717	0	2704	23	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	1	0	0	0	0
2	D	2	0	0	0	0
3	A	12	16	16	1	0
3	B	18	24	23	0	0
3	C	24	32	32	0	0
3	D	18	24	22	2	0
4	B	5	0	0	0	0
4	C	10	0	0	0	0
4	D	10	0	0	0	0
5	D	1	0	0	0	0
6	A	36	0	0	1	0
6	B	44	0	0	0	0
6	C	17	0	0	0	0
6	D	41	0	0	1	0
All	All	11006	96	10755	107	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 (107) 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:77:ARG:HG3	1:B:107:MET:HE1	1.43	1.01
1:D:31:ARG:NH2	1:D:58:VAL:HG11	2.04	0.73
1:B:323[B]:ARG:O	1:B:323[B]:ARG:HD3	1.88	0.72
1:A:365:GLU:O	1:A:367:GLU:HG3	1.91	0.71
1:C:101:LYS:HD3	1:C:147:PRO:HG3	1.71	0.71
1:B:97:LEU:HG	1:B:113:ILE:HG23	1.72	0.71
1:B:18:ILE:HG13	1:B:156:ILE:HD11	1.77	0.67
1:B:301:HIS:NE2	1:B:367:GLU:HG2	2.10	0.67
1:D:121:ASP:OD1	3:D:405:GOL:O3	2.13	0.66
1:B:33:LEU:HD11	1:B:62:ALA:HB2	1.79	0.64
1:A:101:LYS:HD3	1:A:147:PRO:HG3	1.81	0.62
1:D:231:GLU:HG2	6:D:501:HOH:O	1.99	0.62
1:B:10:LYS:HD3	1:B:12:ILE:HD11	1.82	0.61
1:C:25:LEU:HB3	1:C:32:TRP:CZ2	2.37	0.60
1:D:127:LEU:HD13	1:D:142:LEU:HD12	1.83	0.59
1:B:101:LYS:HD3	1:B:147:PRO:HG3	1.84	0.58
1:C:3:ARG:HD3	1:C:194:LYS:HB2	1.86	0.57
1:B:92:GLY:H	1:B:96:THR:HG21	1.69	0.57
1:A:218:MET:HE2	1:A:218:MET:CA	2.32	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:33:LEU:HB2	1:B:85:CYS:SG	2.45	0.56
1:B:17:VAL:HG12	1:B:153:ASP:HA	1.88	0.56
1:B:107:MET:HE3	1:B:107:MET:HA	1.87	0.56
1:A:365:GLU:HG2	1:A:366:TRP:N	2.21	0.54
1:C:317:ASP:H	1:C:321:LYS:NZ	2.06	0.54
1:C:88:ILE:N	1:C:88:ILE:HD12	2.24	0.53
1:B:107:MET:HB3	1:B:109:VAL:HG22	1.90	0.53
1:A:12:ILE:HG12	1:B:4:ILE:HG12	1.91	0.52
1:A:17:VAL:HG12	1:A:153:ASP:HA	1.92	0.51
1:B:366:TRP:O	1:B:367:GLU:HB3	2.09	0.51
1:C:161:PRO:HD2	1:C:164:LEU:HD12	1.92	0.51
1:D:318:VAL:HB	1:D:319:PRO:HD3	1.93	0.51
1:D:329:ALA:O	1:D:334:GLU:HG3	2.11	0.50
1:A:31:ARG:NH2	1:A:83:ALA:O	2.44	0.50
1:C:33:LEU:HD12	1:C:60:GLU:O	2.12	0.50
1:C:10:LYS:HD3	1:C:12:ILE:HD11	1.93	0.49
1:C:265:ASP:OD2	1:C:321:LYS:HE2	2.12	0.49
1:B:122:ALA:N	1:B:123:PRO:CD	2.76	0.49
1:A:10:LYS:HD3	1:A:12:ILE:HD11	1.94	0.48
1:C:318:VAL:HB	1:C:319:PRO:HD3	1.95	0.48
1:A:287:ASN:HB2	1:D:228:PRO:HB2	1.96	0.48
1:D:336:ILE:HD13	1:D:348:VAL:HG21	1.96	0.48
1:A:246:GLU:HB3	6:A:501:HOH:O	2.14	0.48
1:C:127:LEU:C	1:C:127:LEU:HD13	2.40	0.47
1:A:91:ILE:O	1:A:91:ILE:HG23	2.14	0.47
1:B:44:ALA:O	1:B:48:VAL:HG23	2.13	0.47
1:C:18:ILE:HD13	1:C:156:ILE:HD11	1.97	0.47
1:A:232:ARG:HH12	3:A:403:GOL:C1	2.27	0.47
1:C:291:GLU:H	1:C:291:GLU:CD	2.23	0.47
1:A:33:LEU:HD11	1:A:62:ALA:HB2	1.98	0.46
1:D:18:ILE:HD12	1:D:156:ILE:HD11	1.98	0.46
1:C:93:GLY:O	1:C:96:THR:HG23	2.15	0.46
1:A:265:ASP:HB2	1:A:314:ILE:HG12	1.98	0.46
1:A:318:VAL:HB	1:A:319:PRO:HD3	1.98	0.46
1:C:265:ASP:HB2	1:C:314:ILE:HG12	1.99	0.45
1:B:101:LYS:CD	1:B:147:PRO:HG3	2.45	0.45
1:C:45:GLN:OE1	1:C:61:ILE:HD13	2.16	0.45
1:A:178:GLU:CD	1:A:253:ALA:HB3	2.42	0.45
1:B:6:GLN:HB3	1:B:146:ASN:OD1	2.17	0.45
1:D:129:VAL:HG13	1:D:137[A]:PHE:HE2	1.82	0.45
1:B:1:MET:SD	1:B:194:LYS:HE3	2.57	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:122:ALA:N	1:D:123:PRO:CD	2.80	0.44
1:B:122:ALA:O	1:B:123:PRO:C	2.60	0.44
1:D:93:GLY:O	1:D:97:LEU:HG	2.18	0.44
1:B:25:LEU:HB3	1:B:32:TRP:CZ2	2.53	0.44
1:C:16:ASP:OD1	1:C:155:LYS:HD3	2.18	0.44
1:C:17:VAL:HG12	1:C:153:ASP:HA	1.99	0.43
1:C:93:GLY:O	1:C:97:LEU:HG	2.18	0.43
1:A:16:ASP:OD1	1:A:155:LYS:HD3	2.19	0.43
1:B:77:ARG:CG	1:B:107:MET:HE1	2.30	0.43
1:D:86:GLY:O	1:D:109:VAL:HB	2.18	0.43
1:B:40:VAL:HG21	1:B:92:GLY:HA2	2.00	0.43
1:D:265:ASP:N	1:D:265:ASP:OD1	2.49	0.43
1:C:18:ILE:HA	1:C:21:LEU:HG	1.99	0.43
1:B:18:ILE:HG13	1:B:156:ILE:CD1	2.47	0.43
1:C:12:ILE:HG12	1:D:4:ILE:HG12	2.01	0.43
1:D:149:MET:CE	1:D:151:ILE:HD11	2.49	0.43
1:C:21:LEU:O	1:C:25:LEU:HD13	2.18	0.43
1:D:10:LYS:HD3	1:D:12:ILE:HD11	1.99	0.43
1:A:93:GLY:O	1:A:97:LEU:HG	2.19	0.43
1:C:122:ALA:N	1:C:123:PRO:CD	2.82	0.43
1:C:323:ARG:O	1:C:327:GLU:HG2	2.19	0.43
1:D:122:ALA:O	1:D:123:PRO:C	2.61	0.43
1:C:25:LEU:HD12	1:C:25:LEU:N	2.34	0.42
1:D:58:VAL:HG21	3:D:404:GOL:H12	2.02	0.42
1:A:190:MET:HB3	1:A:190:MET:HE2	1.77	0.42
1:B:104:ALA:CB	1:B:111:VAL:HB	2.49	0.42
1:C:113:ILE:HD13	1:C:113:ILE:HA	1.81	0.42
1:D:223:GLN:O	1:D:225:VAL:HG13	2.19	0.42
1:B:211:LEU:HD12	1:B:211:LEU:HA	1.92	0.42
1:A:365:GLU:O	1:A:367:GLU:N	2.47	0.42
1:B:318:VAL:HB	1:B:319:PRO:HD3	2.02	0.42
1:A:127:LEU:HD23	1:A:128:SER:N	2.36	0.41
1:A:201:ALA:HB2	1:B:205:LEU:HD22	2.02	0.41
1:C:114:ALA:HA	1:C:151:ILE:O	2.21	0.41
1:D:113:ILE:O	1:D:150:VAL:HA	2.20	0.41
1:B:113:ILE:HD13	1:B:113:ILE:HA	1.82	0.41
1:C:87:ALA:C	1:C:88:ILE:HD12	2.45	0.41
1:A:11:TYR:O	1:B:4:ILE:HA	2.21	0.41
1:D:149:MET:HE2	1:D:151:ILE:HD11	2.01	0.41
1:A:122:ALA:N	1:A:123:PRO:CD	2.82	0.41
1:A:86:GLY:O	1:A:109:VAL:HB	2.21	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:367:GLU:HG3	1:A:367:GLU:H	1.47	0.40
1:D:129:VAL:HG13	1:D:137[A]:PHE:CE2	2.56	0.40
1:A:10:LYS:HE2	1:B:6:GLN:OE1	2.22	0.40
1:A:245:PHE:CD1	1:A:245:PHE:C	3.00	0.40
1:C:26:LYS:HG3	1:C:57:LEU:HD21	2.04	0.40
1:C:77:ARG:HH11	1:C:77:ARG:HD3	1.78	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	365/367 (100%)	356 (98%)	7 (2%)	2 (0%)	24	55
1	B	366/367 (100%)	358 (98%)	8 (2%)	0	100	100
1	C	365/367 (100%)	356 (98%)	9 (2%)	0	100	100
1	D	366/367 (100%)	359 (98%)	7 (2%)	0	100	100
All	All	1462/1468 (100%)	1429 (98%)	31 (2%)	2 (0%)	48	77

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	366	TRP
1	A	365	GLU

5.3.2 Protein sidechains [i](#)

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	271/275 (98%)	264 (97%)	7 (3%)	40	75
1	B	268/275 (98%)	258 (96%)	10 (4%)	30	65
1	C	263/275 (96%)	254 (97%)	9 (3%)	32	68
1	D	274/275 (100%)	263 (96%)	11 (4%)	28	63
All	All	1076/1100 (98%)	1039 (97%)	37 (3%)	32	68

All (37) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	127	LEU
1	A	128	SER
1	A	134	GLU
1	A	213	GLU
1	A	294	GLU
1	A	317	ASP
1	A	367	GLU
1	B	97	LEU
1	B	107	MET
1	B	142	LEU
1	B	200	LEU
1	B	211	LEU
1	B	280	LEU
1	B	290	VAL
1	B	299	LEU
1	B	317	ASP
1	B	367	GLU
1	C	61	ILE
1	C	88	ILE
1	C	96	THR
1	C	128	SER
1	C	290	VAL
1	C	299	LEU
1	C	317	ASP
1	C	321	LYS
1	C	367	GLU
1	D	21	LEU
1	D	58	VAL
1	D	134	GLU
1	D	142	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	143	LEU
1	D	190	MET
1	D	202	LEU
1	D	274	LYS
1	D	317	ASP
1	D	334	GLU
1	D	367	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	13	GLN
1	A	360	GLN
1	B	45	GLN
1	B	337	HIS
1	D	208	ASN
1	D	223	GLN
1	D	301	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 23 ligands modelled in this entry, 6 are monoatomic - leaving 17 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	$\# Z > 2$
3	GOL	D	403	-	5,5,5	0.44	0	5,5,5	0.70	0
3	GOL	A	402	2	5,5,5	0.21	0	5,5,5	0.44	0
3	GOL	B	404	-	5,5,5	0.30	0	5,5,5	0.66	0
3	GOL	C	405	-	5,5,5	0.36	0	5,5,5	0.45	0
3	GOL	D	404	-	5,5,5	0.29	0	5,5,5	0.44	0
4	SO4	C	406	-	4,4,4	0.32	0	6,6,6	0.21	0
4	SO4	D	407	-	4,4,4	0.31	0	6,6,6	0.30	0
3	GOL	A	403	-	5,5,5	0.42	0	5,5,5	0.26	0
4	SO4	D	408	-	4,4,4	0.28	0	6,6,6	0.11	0
4	SO4	C	407	-	4,4,4	0.32	0	6,6,6	0.12	0
3	GOL	C	402	2	5,5,5	0.37	0	5,5,5	0.15	0
3	GOL	B	403	-	5,5,5	0.34	0	5,5,5	0.47	0
3	GOL	B	402	2	5,5,5	0.45	0	5,5,5	0.20	0
4	SO4	B	405	-	4,4,4	0.26	0	6,6,6	0.39	0
3	GOL	C	404	-	5,5,5	0.34	0	5,5,5	0.37	0
3	GOL	C	403	-	5,5,5	0.44	0	5,5,5	0.51	0
3	GOL	D	405	2	5,5,5	0.21	0	5,5,5	0.70	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	GOL	D	403	-	-	2/4/4/4	-
3	GOL	A	402	2	-	2/4/4/4	-
3	GOL	B	404	-	-	0/4/4/4	-
3	GOL	C	405	-	-	0/4/4/4	-
3	GOL	D	404	-	-	0/4/4/4	-
3	GOL	A	403	-	-	2/4/4/4	-
3	GOL	C	402	2	-	2/4/4/4	-
3	GOL	B	403	-	-	0/4/4/4	-
3	GOL	B	402	2	-	0/4/4/4	-
3	GOL	C	404	-	-	0/4/4/4	-
3	GOL	C	403	-	-	2/4/4/4	-
3	GOL	D	405	2	-	0/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	402	GOL	O1-C1-C2-C3
3	A	403	GOL	O1-C1-C2-C3
3	C	402	GOL	O1-C1-C2-C3
3	C	403	GOL	O1-C1-C2-C3
3	D	403	GOL	O1-C1-C2-C3
3	A	402	GOL	O1-C1-C2-O2
3	C	402	GOL	O1-C1-C2-O2
3	C	403	GOL	O1-C1-C2-O2
3	D	403	GOL	O1-C1-C2-O2
3	A	403	GOL	O1-C1-C2-O2

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	404	GOL	1	0
3	A	403	GOL	1	0
3	D	405	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	367/367 (100%)	-0.47	7 (1%) 66 57	39, 54, 85, 121	0
1	B	367/367 (100%)	-0.43	5 (1%) 73 64	30, 56, 74, 120	1 (0%)
1	C	367/367 (100%)	-0.11	16 (4%) 39 31	45, 64, 105, 135	0
1	D	367/367 (100%)	-0.47	7 (1%) 66 57	41, 54, 83, 111	1 (0%)
All	All	1468/1468 (100%)	-0.37	35 (2%) 59 49	30, 56, 92, 135	2 (0%)

All (35) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	137[A]	PHE	7.3
1	C	133	ASP	5.5
1	C	137	PHE	4.9
1	C	136	GLU	4.7
1	C	129	VAL	4.7
1	B	366	TRP	4.5
1	D	366	TRP	4.3
1	D	140	TYR	4.3
1	C	139	ARG	3.8
1	C	131	TYR	3.8
1	C	142	LEU	3.5
1	C	134	GLU	3.5
1	A	366	TRP	3.2
1	C	366	TRP	3.2
1	B	268	HIS	3.2
1	C	135	GLY	3.2
1	A	268	HIS	2.8
1	A	135	GLY	2.7
1	B	367	GLU	2.7
1	C	367	GLU	2.6
1	B	92	GLY	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	267	HIS	2.5
1	D	133	ASP	2.5
1	A	131	TYR	2.5
1	B	267	HIS	2.5
1	A	140	TYR	2.4
1	C	140	TYR	2.3
1	C	132	THR	2.3
1	C	30	GLU	2.2
1	C	268	HIS	2.2
1	D	129	VAL	2.2
1	A	134	GLU	2.1
1	D	267	HIS	2.1
1	D	127	LEU	2.1
1	C	96	THR	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
3	GOL	C	405	6/6	0.56	0.18	93,112,127,127	0
3	GOL	B	403	6/6	0.63	0.23	88,109,137,137	0
4	SO4	B	405	5/5	0.64	0.12	116,117,134,161	0
3	GOL	C	403	6/6	0.70	0.26	93,112,130,130	0
4	SO4	C	407	5/5	0.73	0.11	125,125,153,175	0
3	GOL	A	403	6/6	0.76	0.14	89,110,118,132	0
3	GOL	D	403	6/6	0.77	0.16	86,106,132,132	0
3	GOL	B	404	6/6	0.78	0.24	81,109,131,137	0
4	SO4	D	407	5/5	0.78	0.24	84,89,130,145	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	SO4	C	406	5/5	0.80	0.10	106,106,128,151	0
3	GOL	D	404	6/6	0.80	0.16	88,111,129,134	0
3	GOL	C	404	6/6	0.80	0.21	90,110,121,132	0
5	CL	D	406	1/1	0.80	0.26	100,100,100,100	0
4	SO4	D	408	5/5	0.83	0.12	116,116,124,158	0
3	GOL	D	405	6/6	0.85	0.24	75,94,121,145	0
3	GOL	A	402	6/6	0.88	0.27	83,101,126,127	0
3	GOL	C	402	6/6	0.90	0.22	82,105,123,132	0
3	GOL	B	402	6/6	0.91	0.18	92,112,134,135	0
2	ZN	D	401	1/1	0.96	0.10	103,103,103,103	0
2	ZN	D	402	1/1	0.97	0.06	104,104,104,104	0
2	ZN	B	401	1/1	0.98	0.06	109,109,109,109	0
2	ZN	A	401	1/1	1.00	0.06	93,93,93,93	0
2	ZN	C	401	1/1	1.00	0.04	93,93,93,93	0

6.5 Other polymers [i](#)

There are no such residues in this entry.