



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 06:39 PM UTC

PDB ID : 4LSF / pdb_00004lsf
Title : Ion selectivity of OmpF soaked in 0.1M KBr
Authors : Balasundaresan, D.; Blachowicz, L.; Roux, B.
Deposited on : 2013-07-22
Resolution : 1.90 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)
Xtrriage (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

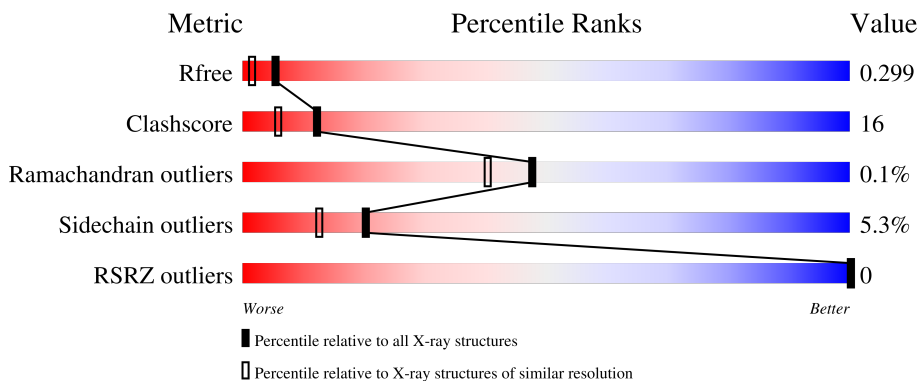
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION



The reported resolution of this entry is 1.90 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	7789 (1.90-1.90)
Clashscore	190562	8410 (1.90-1.90)
Ramachandran outliers	187476	8333 (1.90-1.90)
Sidechain outliers	187428	8333 (1.90-1.90)
RSRZ outliers	180081	7790 (1.90-1.90)

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	341	 76% 22% ..
1	B	341	 73% 24% ..

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	BR	A	402	-	-	X	-
2	BR	A	403	-	-	X	-
2	BR	B	404	-	-	X	-
2	BR	B	405	-	-	X	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 5483 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 Outer membrane protein F.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	339	2634	1659	437	535	3	0	3	0
1	B	339	2629	1656	436	534	3	0	2	0

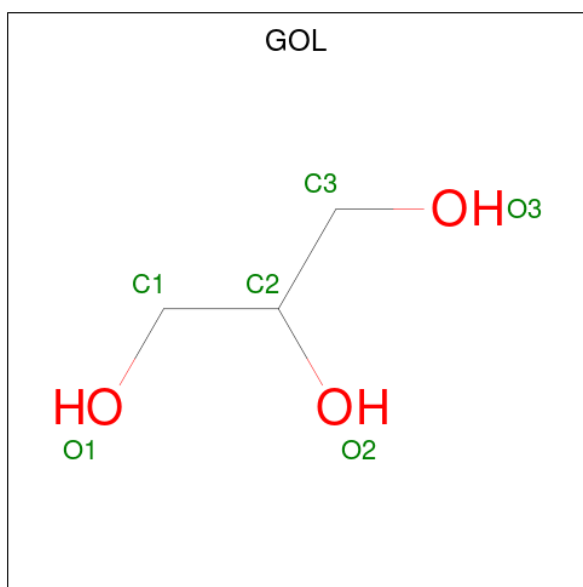
There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	GLY	-	expression tag	UNP P02931
B	0	GLY	-	expression tag	UNP P02931

- Molecule 2 is BROMIDE ION (CCD ID: BR) (formula: Br).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	3	Total	Br	0	0
			3	3		
2	B	4	Total	Br	0	0
			4	4		

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



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

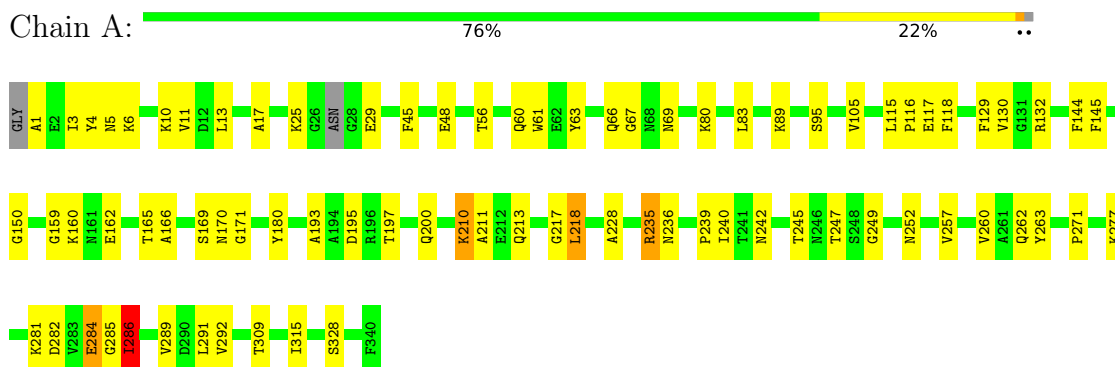
- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	100	Total O 100 100	0	0
4	B	101	Total O 101 101	0	0

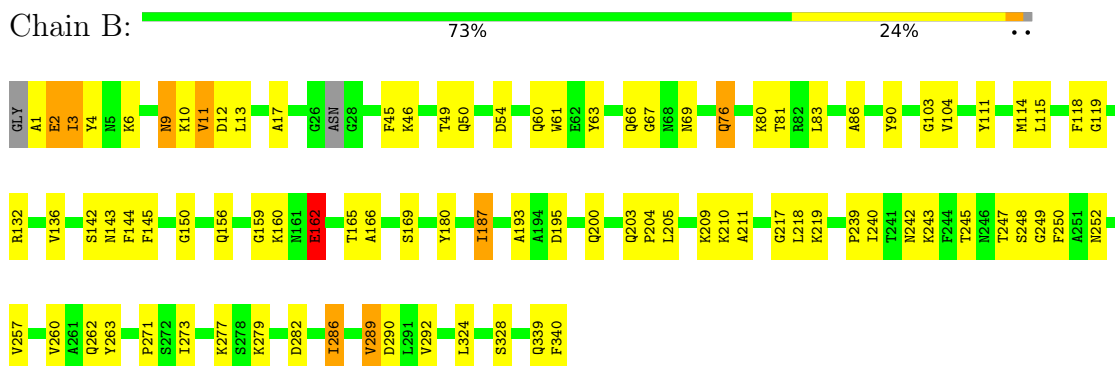
3 Residue-property plots [i](#)

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: Outer membrane protein F



- Molecule 1: Outer membrane protein F



4 Data and refinement statistics i

Property	Value	Source
Space group	P 3	Depositor
Cell constants a, b, c, α , β , γ	116.63Å 116.63Å 51.25Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	29.16 – 1.90 29.16 – 1.90	Depositor EDS
% Data completeness (in resolution range)	99.3 (29.16-1.90) 99.2 (29.16-1.90)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.53 (at 1.89Å)	Xtrriage
Refinement program	PHENIX (phenix.refine: 1.7.2_869)	Depositor
R, R_{free}	0.267 , 0.298 0.266 , 0.299	Depositor DCC
R_{free} test set	3069 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	24.6	Xtrriage
Anisotropy	0.657	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 35.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.42$, $\langle L^2 \rangle = 0.25$	Xtrriage
Estimated twinning fraction	0.367 for -h,-k,l 0.469 for h,-h-k,-l 0.367 for -k,-h,-l	Xtrriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	5483	wwPDB-VP
Average B, all atoms (Å ²)	33.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.05% 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, BR

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	0.82	2/2698 (0.1%)	0.93	2/3647 (0.1%)
1	B	0.86	3/2690 (0.1%)	0.97	3/3636 (0.1%)
All	All	0.84	5/5388 (0.1%)	0.95	5/7283 (0.1%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	9	ASN	C-N	7.42	1.43	1.33
1	B	2	GLU	CA-C	-6.03	1.44	1.52
1	A	286	ILE	C-O	-5.92	1.17	1.24
1	B	86	ALA	CA-CB	-5.82	1.43	1.54
1	A	228	ALA	CA-CB	5.51	1.62	1.53

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	17	ALA	N-CA-C	-6.73	97.93	108.90
1	B	162	GLU	CB-CA-C	-6.06	101.41	111.41
1	B	17	ALA	N-CA-C	-5.51	99.92	108.90
1	A	291	LEU	N-CA-C	-5.26	107.41	113.88
1	B	119	GLY	N-CA-C	-5.25	104.82	112.17

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	2634	0	2451	70	0
1	B	2629	0	2445	86	0
2	A	3	0	0	7	0
2	B	4	0	0	9	0
3	A	6	0	8	2	0
3	B	6	0	8	2	0
4	A	100	0	0	17	0
4	B	101	0	0	15	0
All	All	5483	0	4912	158	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 16.

All (158) 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:180:TYR:HB3	1:B:187:ILE:HD11	1.47	0.94
1:A:105:VAL:HG12	1:A:129:PHE:O	1.70	0.91
1:B:3:ILE:HD13	1:B:13:LEU:HB3	1.53	0.90
1:B:160:LYS:HE2	1:B:162:GLU:OE2	1.73	0.88
1:A:60:GLN:HG2	4:A:556:HOH:O	1.74	0.87
1:B:2:GLU:OE1	1:B:10:LYS:HD2	1.77	0.85
1:B:60:GLN:HG2	4:B:551:HOH:O	1.78	0.84
1:B:245:THR:CG2	1:B:247:THR:HG22	2.08	0.83
1:A:145:PHE:CD2	4:A:565:HOH:O	2.33	0.81
1:B:144:PHE:CD1	4:B:553:HOH:O	2.34	0.80
1:A:144:PHE:CD1	4:A:565:HOH:O	2.35	0.80
1:A:67:GLY:O	2:A:403:BR:BR	2.57	0.77
1:B:160:LYS:NZ	1:B:162:GLU:CD	2.44	0.76
1:B:145:PHE:CD2	4:B:553:HOH:O	2.40	0.74
1:A:277:LYS:HA	1:A:292:VAL:O	1.86	0.74
1:A:105:VAL:HG12	1:A:129:PHE:C	2.13	0.74
1:A:260:VAL:HG11	4:A:549:HOH:O	1.87	0.73
1:A:160:LYS:HD2	1:A:170:ASN:O	1.89	0.71
1:A:67:GLY:C	2:A:402:BR:BR	2.89	0.71
1:A:105:VAL:HG13	1:A:130:VAL:HA	1.74	0.70
1:B:260:VAL:HG11	4:B:564:HOH:O	1.91	0.70
1:A:160:LYS:HD3	1:A:171:GLY:HA2	1.72	0.70
1:A:249:GLY:HA2	4:A:547:HOH:O	1.92	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:46:LYS:HD2	1:B:60:GLN:HB2	1.74	0.69
1:B:160:LYS:CE	1:B:162:GLU:OE2	2.40	0.69
1:A:89:LYS:HD3	1:A:95:SER:HB3	1.76	0.68
1:B:160:LYS:HE2	1:B:162:GLU:CD	2.19	0.67
2:B:404:BR:BR	4:B:526:HOH:O	2.67	0.67
1:A:1:ALA:O	1:A:3:ILE:HG23	1.95	0.67
1:A:83:LEU:HB2	4:A:556:HOH:O	1.94	0.66
1:A:159:GLY:N	4:A:557:HOH:O	2.28	0.66
1:B:180:TYR:HB3	1:B:187:ILE:CD1	2.25	0.65
1:A:262:GLN:NE2	4:A:549:HOH:O	2.30	0.65
1:B:145:PHE:CE2	4:B:553:HOH:O	2.49	0.65
1:B:4:TYR:HB3	1:B:11:VAL:HG12	1.79	0.64
1:B:160:LYS:CE	1:B:162:GLU:CD	2.71	0.63
1:B:115:LEU:HB2	1:B:118:PHE:O	1.98	0.63
1:B:2:GLU:OE1	1:B:10:LYS:CD	2.47	0.63
1:A:105:VAL:CG1	1:A:129:PHE:O	2.45	0.63
1:B:132:ARG:HH12	3:B:401:GOL:H2	1.64	0.63
1:A:116:PRO:HG3	4:A:510:HOH:O	1.98	0.63
1:B:1:ALA:C	1:B:12:ASP:OD1	2.42	0.63
1:B:67:GLY:C	2:B:405:BR:BR	2.98	0.62
1:B:3:ILE:CD1	1:B:13:LEU:HB3	2.26	0.62
1:B:160:LYS:CE	1:B:162:GLU:OE1	2.47	0.62
1:B:45:PHE:HB2	4:B:548:HOH:O	1.99	0.62
1:B:67:GLY:HA2	2:B:405:BR:BR	2.54	0.61
1:A:66:GLN:O	2:A:402:BR:BR	2.73	0.61
1:B:160:LYS:HZ3	1:B:162:GLU:CD	2.08	0.61
1:B:205:LEU:HD21	1:B:240:ILE:HD11	1.81	0.61
1:B:11:VAL:CG2	4:B:548:HOH:O	2.49	0.61
1:B:81:THR:O	2:B:403:BR:BR	2.74	0.60
1:A:67:GLY:HA2	2:A:402:BR:BR	2.57	0.60
1:A:145:PHE:CE2	4:A:565:HOH:O	2.49	0.60
1:A:217:GLY:C	1:A:218:LEU:HD12	2.27	0.59
1:A:218:LEU:HD12	1:A:218:LEU:N	2.18	0.59
1:B:203:GLN:NE2	4:B:593:HOH:O	2.36	0.58
1:B:1:ALA:N	1:B:12:ASP:OD1	2.30	0.58
1:B:1:ALA:O	1:B:12:ASP:OD1	2.21	0.58
1:A:61:TRP:CZ2	1:A:63:TYR:HB2	2.38	0.58
1:A:11:VAL:HG13	4:A:546:HOH:O	2.03	0.58
1:B:245:THR:HG23	1:B:247:THR:HG22	1.85	0.58
1:B:67:GLY:CA	2:B:405:BR:BR	3.07	0.58
1:A:67:GLY:CA	2:A:402:BR:BR	3.07	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:160:LYS:HE2	1:A:162:GLU:OE1	2.04	0.57
1:A:132:ARG:HH12	3:A:404:GOL:H2	1.69	0.57
1:B:160:LYS:NZ	1:B:162:GLU:OE1	2.38	0.56
1:B:205:LEU:HD23	1:B:250:PHE:O	2.05	0.56
1:A:159:GLY:CA	4:A:557:HOH:O	2.54	0.56
1:A:160:LYS:HE2	1:A:197:THR:HG22	1.86	0.56
1:B:61:TRP:CZ2	1:B:63:TYR:HB2	2.41	0.55
1:B:263:TYR:O	1:B:271:PRO:HD2	2.06	0.55
1:B:242:ASN:OD1	1:B:242:ASN:C	2.49	0.55
1:A:160:LYS:NZ	1:A:162:GLU:OE1	2.40	0.55
1:A:242:ASN:HB3	1:A:247:THR:HB	1.88	0.55
1:B:114:MET:HB2	4:B:564:HOH:O	2.06	0.54
1:B:50:GLN:NE2	4:B:586:HOH:O	2.40	0.54
2:A:401:BR:BR	4:A:532:HOH:O	2.74	0.54
1:B:76:GLN:OE1	1:B:76:GLN:N	2.35	0.54
1:A:105:VAL:CG1	1:A:129:PHE:C	2.81	0.53
1:A:252[A]:ASN:ND2	1:A:284:GLU:OE2	2.42	0.53
1:B:262:GLN:NE2	4:B:564:HOH:O	2.41	0.53
1:A:263:TYR:O	1:A:271:PRO:HD2	2.09	0.53
1:A:105:VAL:CG1	1:A:130:VAL:HA	2.38	0.53
1:B:160:LYS:HG2	1:B:162:GLU:OE1	2.09	0.53
1:B:195:ASP:OD1	1:B:209:LYS:HD2	2.10	0.52
1:A:5:ASN:O	1:A:6:LYS:HG3	2.10	0.52
1:B:286:ILE:CG2	1:B:289:VAL:HG22	2.39	0.52
1:A:3:ILE:HD13	1:A:13:LEU:HB3	1.92	0.52
1:A:171:GLY:HA3	1:A:195:ASP:O	2.09	0.51
1:A:5:ASN:HD22	1:A:6:LYS:N	2.10	0.50
1:A:242:ASN:OD1	1:A:242:ASN:C	2.54	0.50
1:B:150:GLY:O	1:B:180:TYR:HA	2.12	0.50
1:B:66:GLN:O	2:B:405:BR:BR	2.85	0.50
1:A:45:PHE:HB2	4:A:546:HOH:O	2.11	0.49
1:B:12:ASP:N	1:B:46:LYS:O	2.41	0.49
1:B:205:LEU:HD21	1:B:240:ILE:CG1	2.42	0.49
1:A:4:TYR:O	1:A:10:LYS:HA	2.12	0.49
1:A:245:THR:HG22	1:A:245:THR:O	2.12	0.49
1:B:132:ARG:NH1	3:B:401:GOL:H2	2.27	0.49
1:A:165:THR:O	1:A:169:SER:OG	2.28	0.49
1:A:170:ASN:HB3	4:A:586:HOH:O	2.12	0.48
1:A:115:LEU:HD23	4:A:549:HOH:O	2.12	0.48
1:A:160:LYS:CE	1:A:162:GLU:OE1	2.60	0.48
1:B:160:LYS:HE2	1:B:162:GLU:OE1	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:205:LEU:HB3	1:B:249:GLY:HA3	1.96	0.47
1:B:1:ALA:N	1:B:340:PHE:OXT	2.47	0.47
1:B:46:LYS:HD3	1:B:60:GLN:CD	2.39	0.47
1:B:111:TYR:CD2	1:B:219:LYS:HB3	2.50	0.47
1:B:83:LEU:HB2	4:B:551:HOH:O	2.14	0.47
1:B:205:LEU:HD21	1:B:240:ILE:CD1	2.45	0.47
1:A:132:ARG:NH1	3:A:404:GOL:H2	2.30	0.46
1:A:48:GLU:HG3	1:A:56:THR:HG21	1.98	0.46
1:A:252[B]:ASN:OD1	1:A:282:ASP:O	2.34	0.46
1:B:160:LYS:CG	1:B:162:GLU:OE1	2.63	0.46
1:B:205:LEU:HD22	1:B:250:PHE:N	2.31	0.46
1:B:286:ILE:CG2	1:B:289:VAL:CG2	2.94	0.46
1:A:5:ASN:ND2	1:A:5:ASN:C	2.74	0.46
1:A:150:GLY:O	1:A:180:TYR:HA	2.16	0.45
1:A:236:ASN:ND2	1:A:252[A]:ASN:HA	2.30	0.45
1:B:61:TRP:C	4:B:551:HOH:O	2.59	0.45
1:A:130:VAL:HG13	1:A:213:GLN:CD	2.40	0.45
1:A:236:ASN:ND2	1:A:252[B]:ASN:HA	2.31	0.45
1:B:217:GLY:C	1:B:218:LEU:HG	2.42	0.45
1:A:239:PRO:C	1:A:240:ILE:HG23	2.41	0.45
1:B:69:ASN:N	2:B:405:BR:BR	2.95	0.45
1:B:252:ASN:ND2	1:B:282:ASP:O	2.38	0.44
1:A:193:ALA:HA	1:A:211:ALA:O	2.17	0.44
1:B:69:ASN:O	2:B:405:BR:BR	2.90	0.44
1:B:339:GLN:HG2	2:B:404:BR:BR	2.73	0.44
1:B:12:ASP:O	1:B:45:PHE:HA	2.18	0.43
1:B:166:ALA:HB1	1:B:200:GLN:HA	2.01	0.43
1:B:286:ILE:HG21	1:B:289:VAL:HG21	2.00	0.43
1:B:286:ILE:HG21	1:B:289:VAL:CG2	2.48	0.43
1:A:105:VAL:HG11	1:A:130:VAL:HG12	2.00	0.43
1:B:160:LYS:NZ	1:B:162:GLU:OE2	2.49	0.43
1:B:193:ALA:HA	1:B:211:ALA:O	2.17	0.43
1:B:9:ASN:OD1	1:B:49:THR:HB	2.17	0.43
1:A:29:GLU:CD	4:A:564:HOH:O	2.62	0.43
1:A:166:ALA:HB1	1:A:200:GLN:HA	2.01	0.43
1:B:142:SER:O	1:B:143:ASN:HB2	2.19	0.43
1:B:279:LYS:HB3	1:B:290:ASP:OD1	2.19	0.43
1:A:285:GLY:C	1:A:286:ILE:HD12	2.44	0.42
1:B:54:ASP:O	1:B:90:TYR:HD1	2.02	0.42
1:A:69:ASN:O	2:A:403:BR:BR	2.92	0.42
1:B:204:PRO:HG2	1:B:247:THR:OG1	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:103:GLY:HA2	1:B:156:GLN:OE1	2.20	0.41
1:B:277:LYS:HA	1:B:292:VAL:O	2.19	0.41
1:B:2:GLU:OE1	1:B:10:LYS:HG3	2.20	0.41
1:B:243:LYS:HD3	1:B:324:LEU:O	2.20	0.41
1:A:117:GLU:HA	1:A:117:GLU:OE1	2.20	0.41
1:B:239:PRO:C	1:B:240:ILE:HG23	2.45	0.41
1:B:159:GLY:N	4:B:554:HOH:O	2.54	0.41
1:B:165:THR:O	1:B:169:SER:OG	2.36	0.41
1:A:210:LYS:HB3	1:A:210:LYS:HE3	1.84	0.41
1:A:115:LEU:HB2	1:A:118:PHE:O	2.21	0.40
1:A:5:ASN:O	1:A:6:LYS:CG	2.69	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	338/341 (99%)	316 (94%)	21 (6%)	1 (0%)	36	29
1	B	337/341 (99%)	317 (94%)	20 (6%)	0	100	100
All	All	675/682 (99%)	633 (94%)	41 (6%)	1 (0%)	48	40

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	284	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	265/263 (101%)	253 (96%)	12 (4%)	24	17
1	B	264/263 (100%)	248 (94%)	16 (6%)	17	9
All	All	529/526 (101%)	501 (95%)	28 (5%)	20	12

All (28) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	25	LYS
1	A	80	LYS
1	A	210	LYS
1	A	218	LEU
1	A	235	ARG
1	A	257	VAL
1	A	281	LYS
1	A	286	ILE
1	A	289	VAL
1	A	309	THR
1	A	315	ILE
1	A	328	SER
1	B	3	ILE
1	B	6	LYS
1	B	11	VAL
1	B	76	GLN
1	B	80	LYS
1	B	104	VAL
1	B	136	VAL
1	B	162	GLU
1	B	187	ILE
1	B	210	LYS
1	B	248	SER
1	B	257	VAL
1	B	273	ILE
1	B	286	ILE
1	B	289	VAL
1	B	328	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	5	ASN
1	A	230	ASN
1	A	236	ASN
1	B	161	ASN
1	B	203	GLN
1	B	224	ASN
1	B	230	ASN
1	B	339	GLN

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 9 ligands modelled in this entry, 7 are monoatomic - leaving 2 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	B	401	-	5,5,5	0.63	0	5,5,5	1.44	2 (40%)
3	GOL	A	404	-	5,5,5	0.66	0	5,5,5	1.06	1 (20%)

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	B	401	-	-	1/4/4/4	-
3	GOL	A	404	-	-	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($^{\circ}$)	Ideal($^{\circ}$)
3	B	401	GOL	O1-C1-C2	-2.24	100.31	110.38
3	B	401	GOL	O3-C3-C2	-2.13	100.77	110.38
3	A	404	GOL	O1-C1-C2	-2.09	100.97	110.38

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	401	GOL	O1-C1-C2-O2
3	A	404	GOL	O1-C1-C2-O2

There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	401	GOL	2	0
3	A	404	GOL	2	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	339/341 (99%)	-0.76	0 100 100	20, 29, 55, 65	3 (0%)
1	B	339/341 (99%)	-0.72	0 100 100	19, 29, 56, 65	2 (0%)
All	All	678/682 (99%)	-0.74	0 100 100	19, 29, 56, 65	5 (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
3	GOL	B	401	6/6	0.92	0.09	25,25,32,33	0
3	GOL	A	404	6/6	0.96	0.08	25,25,35,36	0
2	BR	B	403	1/1	0.98	0.11	27,27,27,27	1
2	BR	B	402	1/1	0.99	0.03	30,30,30,30	1
2	BR	A	401	1/1	0.99	0.04	30,30,30,30	1
2	BR	B	404	1/1	1.00	0.03	28,28,28,28	1
2	BR	B	405	1/1	1.00	0.02	26,26,26,26	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	BR	A	402	1/1	1.00	0.01	24,24,24,24	1
2	BR	A	403	1/1	1.00	0.04	25,25,25,25	1

6.5 Other polymers [i](#)

There are no such residues in this entry.