



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 05:35 PM UTC

PDB ID : 4FZW / pdb_00004fzw
Title : Crystal Structure of the PaaF-PaaG Hydratase-Isomerase Complex from E.coli
Authors : Grishin, A.M.; Cygler, M.; Montreal-Kingston Bacterial Structural Genomics Initiative (BSGI)
Deposited on : 2012-07-08
Resolution : 2.55 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

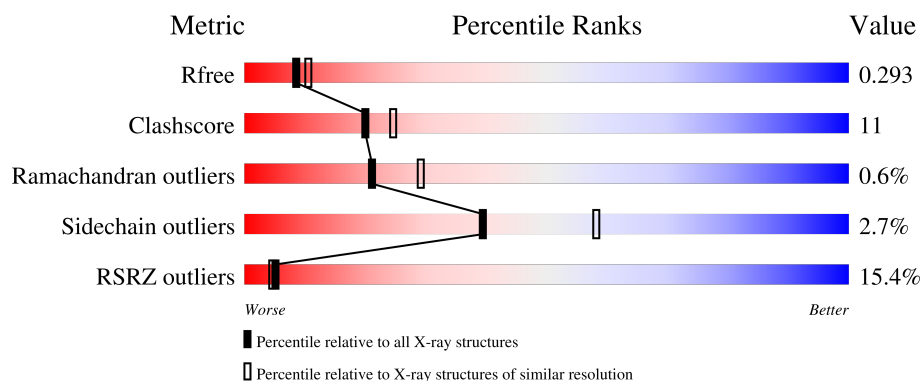
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.55 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	1091 (2.54-2.54)
Clashscore	190562	1120 (2.54-2.54)
Ramachandran outliers	187476	1106 (2.54-2.54)
Sidechain outliers	187428	1106 (2.54-2.54)
RSRZ outliers	180081	1091 (2.54-2.54)

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	258	18% 72% 24% ..
1	B	258	14% 76% 22% ..
2	C	274	15% 71% 18% 9%
2	D	274	12% 73% 16% 9%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 7617 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 2,3-dehydroadipyl-CoA hydratase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	254	Total	C	N	O	S	0	0	0
			1885	1180	339	358	8			
1	B	256	Total	C	N	O	S	0	0	0
			1878	1177	336	356	9			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	MET	-	initiating methionine	UNP P76082
A	-1	ARG	-	expression tag	UNP P76082
A	0	SER	-	expression tag	UNP P76082
B	-2	MET	-	expression tag	UNP P76082
B	-1	ARG	-	expression tag	UNP P76082
B	0	SER	-	expression tag	UNP P76082

- Molecule 2 is a protein called 1,2-epoxyphenylacetyl-CoA isomerase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	249	Total	C	N	O	S	0	0	0
			1846	1159	329	347	11			
2	D	250	Total	C	N	O	S	0	1	0
			1869	1174	333	351	11			

There are 24 discrepancies between the modelled and reference sequences:

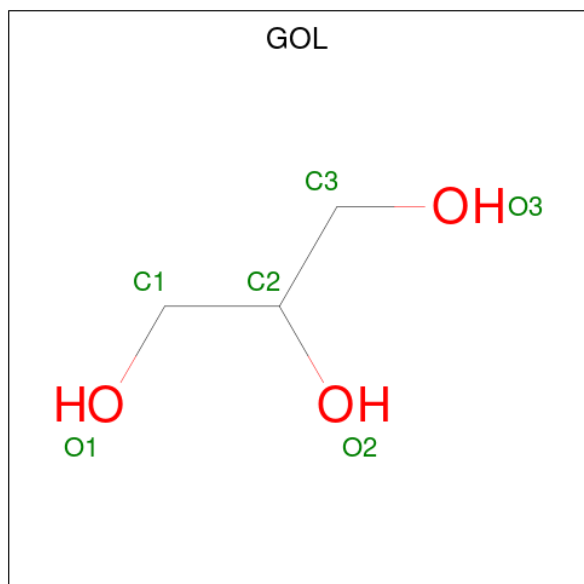
Chain	Residue	Modelled	Actual	Comment	Reference
C	-11	MET	-	initiating methionine	UNP P77467
C	-10	GLY	-	expression tag	UNP P77467
C	-9	SER	-	expression tag	UNP P77467
C	-8	SER	-	expression tag	UNP P77467
C	-7	HIS	-	expression tag	UNP P77467
C	-6	HIS	-	expression tag	UNP P77467

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-5	HIS	-	expression tag	UNP P77467
C	-4	HIS	-	expression tag	UNP P77467
C	-3	HIS	-	expression tag	UNP P77467
C	-2	HIS	-	expression tag	UNP P77467
C	-1	GLY	-	expression tag	UNP P77467
C	0	SER	-	expression tag	UNP P77467
D	-11	MET	-	initiating methionine	UNP P77467
D	-10	GLY	-	expression tag	UNP P77467
D	-9	SER	-	expression tag	UNP P77467
D	-8	SER	-	expression tag	UNP P77467
D	-7	HIS	-	expression tag	UNP P77467
D	-6	HIS	-	expression tag	UNP P77467
D	-5	HIS	-	expression tag	UNP P77467
D	-4	HIS	-	expression tag	UNP P77467
D	-3	HIS	-	expression tag	UNP P77467
D	-2	HIS	-	expression tag	UNP P77467
D	-1	GLY	-	expression tag	UNP P77467
D	0	SER	-	expression tag	UNP P77467

- Molecule 3 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



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

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

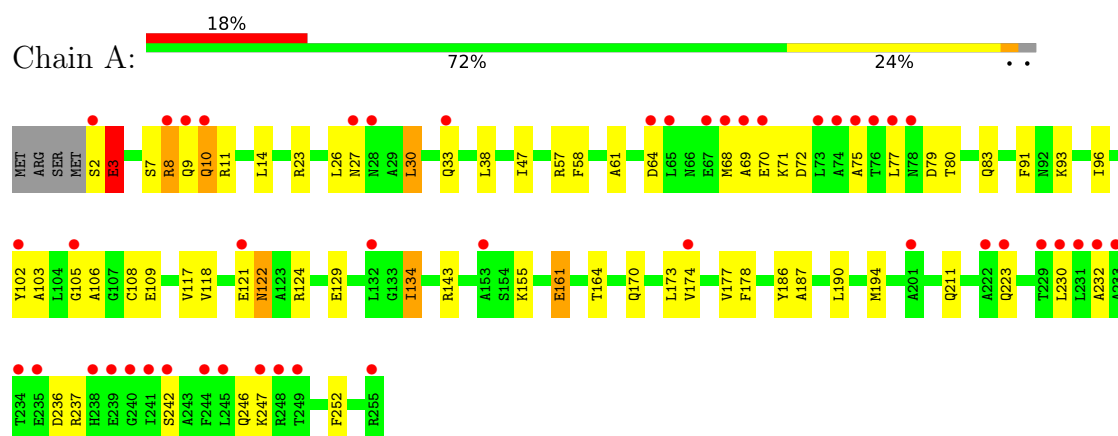
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	29	Total	O	0	0
			29	29		
4	B	36	Total	O	0	0
			36	36		
4	C	25	Total	O	0	0
			25	25		
4	D	31	Total	O	0	0
			31	31		

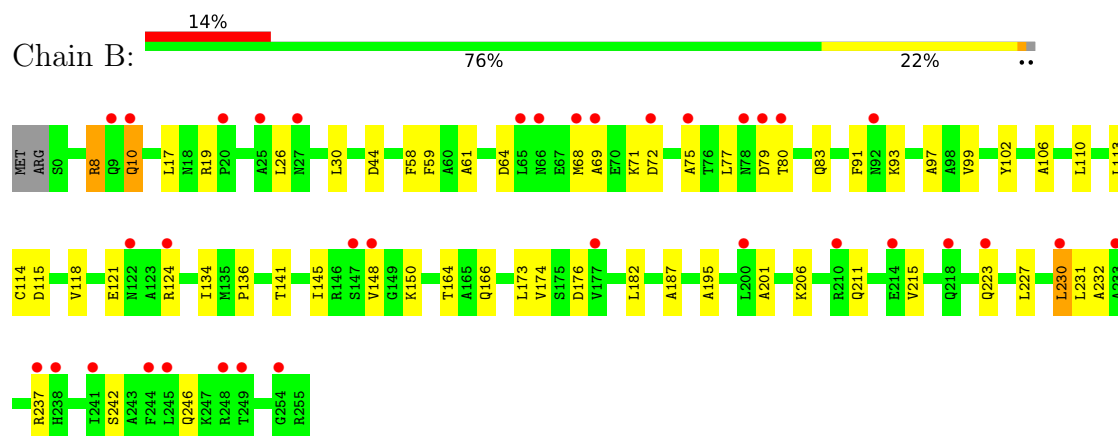
3 Residue-property plots [i](#)

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.

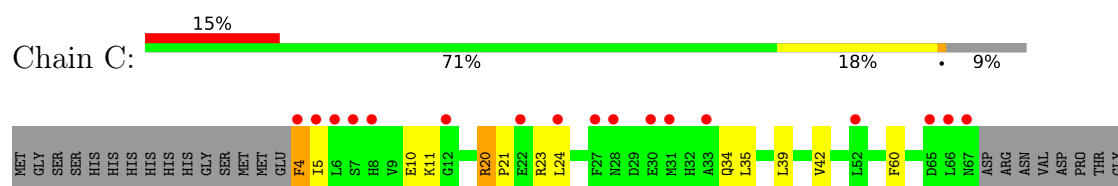
- Molecule 1: 2,3-dehydroadipyl-CoA hydratase

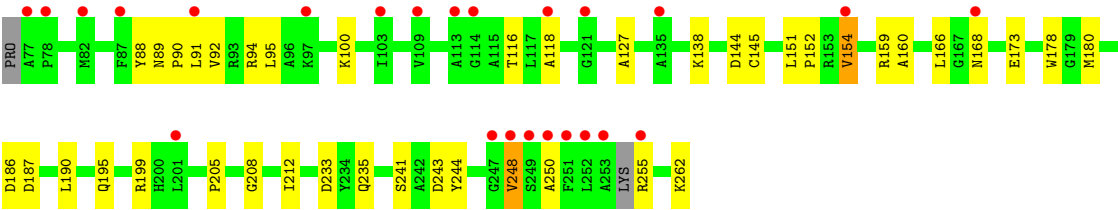


- Molecule 1: 2,3-dehydroadipyl-CoA hydratase

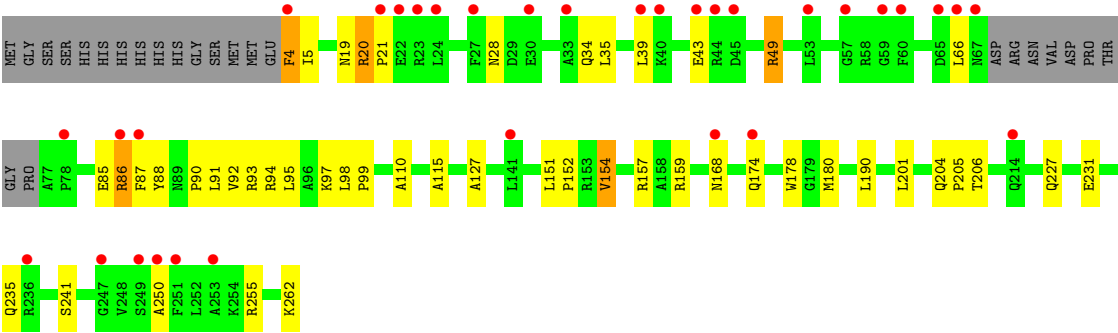


- Molecule 2: 1,2-epoxyphenylacetyl-CoA isomerase





● Molecule 2: 1,2-epoxyphenylacetyl-CoA isomerase



4 Data and refinement statistics

Property	Value	Source
Space group	P 3 2 1	Depositor
Cell constants a, b, c, α , β , γ	131.98Å 131.98Å 153.87Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	46.79 – 2.55 46.79 – 2.55	Depositor EDS
% Data completeness (in resolution range)	96.4 (46.79-2.55) 99.7 (46.79-2.55)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.01 (at 2.54Å)	Xtriage
Refinement program	PHENIX 1.6.4_486	Depositor
R, R_{free}	0.280 , 0.321 0.285 , 0.293	Depositor DCC
R_{free} test set	2589 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å ²)	40.9	Xtriage
Anisotropy	0.719	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 37.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	0.044 for -h,-k,l	Xtriage
F_o, F_c correlation	0.87	EDS
Total number of atoms	7617	wwPDB-VP
Average B, all atoms (Å ²)	49.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 24.12 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 4.0751e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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: 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	0.59	0/1906	0.90	3/2583 (0.1%)
1	B	0.60	0/1899	0.90	3/2574 (0.1%)
2	C	0.59	0/1873	0.95	6/2536 (0.2%)
2	D	0.58	0/1901	0.91	3/2576 (0.1%)
All	All	0.59	0/7579	0.92	15/10269 (0.1%)

There are no bond length outliers.

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	20	ARG	CA-C-N	7.30	128.97	119.84
2	C	20	ARG	C-N-CA	7.30	128.97	119.84
2	D	20	ARG	CA-C-N	6.49	127.96	119.84
2	D	20	ARG	C-N-CA	6.49	127.96	119.84
1	A	102	TYR	N-CA-C	6.39	118.99	109.59
1	A	10	GLN	CB-CA-C	-5.89	109.76	116.54
2	C	248	VAL	CB-CA-C	-5.81	102.84	112.26
2	D	157	ARG	N-CA-C	5.58	117.17	111.14
1	B	10	GLN	CB-CA-C	-5.43	109.85	117.23
2	C	89	ASN	CA-C-N	-5.38	113.08	119.05
2	C	89	ASN	C-N-CA	-5.38	113.08	119.05
1	B	19	ARG	CA-C-N	5.21	124.66	119.24
1	B	19	ARG	C-N-CA	5.21	124.66	119.24
2	C	160	ALA	N-CA-C	-5.15	105.58	111.14
1	A	247	LYS	N-CA-C	5.12	117.43	111.02

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	1885	0	1925	55	0
1	B	1878	0	1911	45	0
2	C	1846	0	1821	40	0
2	D	1869	0	1853	38	0
3	A	6	0	8	0	0
3	B	12	0	15	1	0
4	A	29	0	0	1	0
4	B	36	0	0	0	0
4	C	25	0	0	2	0
4	D	31	0	0	0	0
All	All	7617	0	7533	171	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 11.

All (171) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:77:LEU:HD21	1:B:230:LEU:HD11	1.39	1.04
2:D:154:VAL:HG13	2:D:180:MET:HA	1.43	0.99
2:C:4:PHE:HD1	2:C:34:GLN:HE22	1.15	0.92
2:D:4:PHE:HD1	2:D:34:GLN:HE22	1.17	0.89
2:C:39:LEU:HB2	2:C:94:ARG:HH11	1.41	0.86
2:D:93:ARG:O	2:D:97:LYS:HG2	1.78	0.83
1:B:118:VAL:HG21	1:B:187:ALA:HB2	1.62	0.81
1:A:9:GLN:O	1:A:10:GLN:HG2	1.81	0.80
1:A:230:LEU:HD21	1:B:77:LEU:HD21	1.65	0.78
1:A:80:THR:O	1:A:83:GLN:HG2	1.84	0.77
1:B:211:GLN:HE21	1:B:223:GLN:HE22	1.33	0.77
1:B:80:THR:O	1:B:83:GLN:HG2	1.84	0.76
1:A:232:ALA:HA	1:A:237:ARG:CD	2.17	0.74
2:C:244:TYR:O	2:C:248:VAL:HG23	1.87	0.74
1:B:242:SER:O	1:B:246:GLN:HG2	1.89	0.73
2:D:39:LEU:HB2	2:D:94:ARG:HH11	1.53	0.73
1:A:242:SER:O	1:A:246:GLN:HG2	1.90	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:182:LEU:CD1	2:C:233:ASP:HB3	2.20	0.71
1:B:232:ALA:HA	1:B:237:ARG:NE	2.05	0.71
2:C:154:VAL:HG13	2:C:180:MET:HA	1.73	0.70
1:A:118:VAL:HG21	1:A:187:ALA:HB2	1.72	0.70
1:A:2:SER:O	1:A:3:GLU:HB2	1.93	0.69
2:C:39:LEU:HB2	2:C:94:ARG:NH1	2.08	0.69
2:D:159:ARG:NH1	2:D:178:TRP:NE1	2.41	0.69
2:D:90:PRO:O	2:D:94:ARG:HG2	1.96	0.66
2:D:159:ARG:HH11	2:D:178:TRP:NE1	1.92	0.66
2:C:4:PHE:N	2:C:4:PHE:HD2	1.93	0.65
1:A:9:GLN:O	1:A:10:GLN:CG	2.45	0.65
2:C:4:PHE:HD1	2:C:34:GLN:NE2	1.90	0.65
2:D:19:ASN:C	2:D:21:PRO:HD3	2.21	0.65
2:D:159:ARG:NH1	2:D:178:TRP:CD1	2.66	0.64
1:A:68:MET:HE1	1:A:134:ILE:HD13	1.78	0.64
1:A:77:LEU:CD2	1:B:230:LEU:HD11	2.24	0.63
1:A:121:GLU:OE2	1:A:177:VAL:HG12	1.97	0.63
1:A:230:LEU:HD21	1:B:77:LEU:CD2	2.28	0.63
1:B:72:ASP:H	1:B:75:ALA:HB3	1.64	0.63
1:A:211:GLN:HE21	1:A:223:GLN:HE22	1.47	0.63
2:D:39:LEU:HB2	2:D:94:ARG:NH1	2.13	0.62
2:D:4:PHE:HD2	2:D:4:PHE:N	1.97	0.62
1:A:211:GLN:HB3	1:A:223:GLN:HE21	1.63	0.62
2:D:4:PHE:N	2:D:4:PHE:CD2	2.64	0.61
2:D:66:LEU:O	2:D:66:LEU:HD12	2.00	0.61
2:C:159:ARG:NH1	2:C:178:TRP:CD1	2.69	0.61
2:C:241:SER:HB2	2:C:262:LYS:OXT	2.00	0.60
2:D:86:ARG:HG2	2:D:87:PHE:CE2	2.36	0.60
1:B:211:GLN:HG3	1:B:223:GLN:NE2	2.17	0.59
2:C:5:ILE:CD1	2:C:35:LEU:HB2	2.33	0.59
2:C:4:PHE:N	2:C:4:PHE:CD2	2.65	0.57
1:A:173:LEU:HD23	1:A:173:LEU:O	2.03	0.57
1:A:211:GLN:CB	1:A:223:GLN:HE21	2.17	0.57
1:B:121:GLU:HG3	1:B:166:GLN:NE2	2.19	0.57
1:A:10:GLN:HG3	1:A:11:ARG:N	2.20	0.57
1:B:211:GLN:HB3	1:B:223:GLN:HE21	1.70	0.57
1:B:211:GLN:CB	1:B:223:GLN:HE21	2.18	0.57
1:B:227:LEU:O	1:B:230:LEU:HB3	2.04	0.56
1:A:57:ARG:HE	1:A:58:PHE:HE2	1.53	0.56
2:C:116:THR:OG1	2:C:145:CYS:HB2	2.04	0.56
1:A:3:GLU:HB3	1:A:33:GLN:HE22	1.70	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:8:ARG:HD2	1:A:10:GLN:O	2.06	0.56
1:B:26:LEU:HD12	1:B:106:ALA:HB1	1.88	0.55
1:A:91:PHE:CZ	1:A:93:LYS:HB2	2.41	0.55
2:C:235:GLN:HA	2:C:235:GLN:OE1	2.07	0.54
2:C:173:GLU:HG3	4:C:317:HOH:O	2.07	0.54
1:B:211:GLN:HE21	1:B:223:GLN:NE2	2.03	0.54
2:C:159:ARG:HH11	2:C:178:TRP:NE1	2.06	0.54
1:A:122:ASN:OD1	1:A:122:ASN:N	2.41	0.54
2:C:90:PRO:O	2:C:94:ARG:HG2	2.08	0.53
1:A:121:GLU:CD	1:A:177:VAL:HG12	2.34	0.53
2:D:85:GLU:O	2:D:85:GLU:HG3	2.07	0.53
1:A:27:ASN:HB3	1:A:30:LEU:H	1.72	0.53
1:A:8:ARG:HH12	1:A:47:ILE:HG13	1.74	0.52
2:C:35:LEU:O	2:C:39:LEU:HG	2.10	0.52
1:B:91:PHE:CZ	1:B:93:LYS:HB2	2.44	0.52
1:A:103:ALA:O	1:A:108:CYS:HB2	2.10	0.52
1:B:182:LEU:HD13	2:C:233:ASP:HB3	1.92	0.52
2:D:154:VAL:HG13	2:D:180:MET:CA	2.30	0.52
2:D:86:ARG:HG2	2:D:87:PHE:CZ	2.44	0.52
2:C:250:ALA:HA	2:C:255:ARG:NE	2.24	0.52
2:C:159:ARG:NH1	2:C:178:TRP:NE1	2.58	0.52
2:D:88:TYR:O	2:D:92:VAL:HG23	2.10	0.51
2:C:208:GLY:O	2:C:212:ILE:HG13	2.11	0.51
1:A:69:ALA:C	1:A:71:LYS:H	2.19	0.51
1:A:232:ALA:HA	1:A:237:ARG:HD2	1.91	0.51
2:D:86:ARG:HG2	2:D:87:PHE:CD2	2.46	0.51
1:A:105:GLY:O	1:A:109:GLU:HG3	2.11	0.50
1:A:9:GLN:C	1:A:10:GLN:HG2	2.37	0.50
2:C:23:ARG:O	2:C:24:LEU:HB2	2.12	0.50
1:A:10:GLN:HG3	1:A:11:ARG:H	1.76	0.49
2:D:35:LEU:O	2:D:39:LEU:HG	2.11	0.49
2:D:151:LEU:N	2:D:152:PRO:CD	2.76	0.49
1:B:145:ILE:HD11	1:B:150:LYS:HG3	1.95	0.49
1:A:124:ARG:NH1	1:A:164:THR:HG22	2.28	0.49
1:B:97:ALA:HB2	1:B:114:CYS:SG	2.53	0.48
1:B:79:ASP:OD1	1:B:80:THR:N	2.47	0.48
2:D:20:ARG:N	2:D:21:PRO:HD3	2.28	0.48
1:A:236:ASP:HB3	1:A:252:PHE:CD1	2.49	0.48
1:B:58:PHE:CD1	1:B:61:ALA:HB2	2.49	0.48
1:A:118:VAL:O	1:A:118:VAL:HG23	2.14	0.48
1:B:201:ALA:HA	1:B:231:LEU:HD21	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:69:ALA:C	1:B:71:LYS:H	2.20	0.47
1:A:230:LEU:HD11	1:B:77:LEU:HD21	1.97	0.47
2:C:127:ALA:HB2	2:C:190:LEU:HD22	1.95	0.47
1:A:155:LYS:HE2	1:A:161:GLU:CD	2.39	0.47
1:B:211:GLN:CG	1:B:223:GLN:NE2	2.78	0.47
1:A:58:PHE:CD1	1:A:61:ALA:HB2	2.50	0.47
1:B:118:VAL:HG23	1:B:118:VAL:O	2.13	0.47
1:A:96:ILE:HD11	1:A:194:MET:HE2	1.97	0.47
1:A:7:SER:OG	1:A:14:LEU:HB3	2.15	0.47
2:D:241:SER:HB2	2:D:262:LYS:OXT	2.15	0.46
1:B:58:PHE:CD1	1:B:102:TYR:HB2	2.50	0.46
1:A:68:MET:HE1	1:A:134:ILE:CD1	2.43	0.46
2:D:91:LEU:O	2:D:95:LEU:HD13	2.15	0.46
2:D:174:GLN:HE21	2:D:178:TRP:NE1	2.14	0.46
2:C:250:ALA:HA	2:C:255:ARG:HG2	1.98	0.46
2:D:227:GLN:O	2:D:231:GLU:HG3	2.15	0.46
2:C:88:TYR:O	2:C:92:VAL:HG23	2.16	0.46
2:D:127:ALA:HB2	2:D:190:LEU:HD22	1.97	0.46
2:D:43:GLU:HG2	2:D:98:LEU:HD13	1.98	0.45
1:A:23:ARG:HD3	1:A:58:PHE:CZ	2.51	0.45
1:A:211:GLN:HG3	1:A:223:GLN:NE2	2.32	0.45
1:A:68:MET:HE1	1:A:134:ILE:HG21	1.99	0.45
2:D:250:ALA:HA	2:D:255:ARG:HG2	1.99	0.45
2:C:195:GLN:O	2:C:199:ARG:HG2	2.16	0.45
1:B:173:LEU:HD23	1:B:173:LEU:O	2.17	0.44
1:A:178:PHE:CD1	1:A:186:TYR:HD2	2.35	0.44
1:B:211:GLN:CG	1:B:223:GLN:HE21	2.30	0.44
2:D:154:VAL:CG1	2:D:180:MET:HA	2.31	0.44
1:B:118:VAL:HG21	1:B:187:ALA:CB	2.40	0.44
2:C:151:LEU:HB2	2:C:152:PRO:HD3	1.98	0.44
2:C:168:ASN:HB2	4:C:307:HOH:O	2.17	0.44
2:C:138:LYS:HE3	2:C:166:LEU:O	2.18	0.44
1:A:26:LEU:HD12	1:A:106:ALA:HB1	2.00	0.43
2:C:60:PHE:CE2	2:C:118:ALA:HB2	2.52	0.43
2:D:98:LEU:HD12	2:D:99:PRO:HD2	2.00	0.43
1:B:59:PHE:HB2	1:B:99:VAL:HG13	1.99	0.43
1:B:115:ASP:OD1	1:B:206:LYS:HE3	2.19	0.43
2:C:144:ASP:O	2:C:145:CYS:HB2	2.17	0.43
2:C:20:ARG:N	2:C:21:PRO:HD3	2.34	0.43
2:D:49:ARG:HB3	2:D:206:THR:OG1	2.18	0.43
2:D:235:GLN:HA	2:D:235:GLN:OE1	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:105:GLY:HA2	1:A:129:GLU:OE2	2.19	0.42
2:C:39:LEU:HD12	2:C:94:ARG:HD2	2.00	0.42
1:A:117:VAL:O	1:A:174:VAL:HG13	2.19	0.42
1:B:8:ARG:HD2	1:B:10:GLN:O	2.19	0.42
2:C:91:LEU:O	2:C:95:LEU:HD13	2.19	0.42
1:B:232:ALA:HA	1:B:237:ARG:HE	1.84	0.42
2:D:168[B]:ASN:HD22	2:D:168[B]:ASN:HA	1.73	0.42
1:A:79:ASP:OD1	1:A:80:THR:N	2.53	0.42
1:B:44:ASP:OD1	1:B:44:ASP:C	2.61	0.42
1:B:58:PHE:HZ	3:B:301:GOL:H32	1.85	0.42
1:A:8:ARG:NH1	1:A:47:ILE:HG13	2.35	0.42
2:D:28:ASN:OD1	2:D:28:ASN:C	2.63	0.42
1:B:174:VAL:HG12	1:B:176:ASP:H	1.84	0.42
2:C:42:VAL:O	2:C:100:LYS:NZ	2.41	0.42
1:B:69:ALA:C	1:B:71:LYS:N	2.77	0.41
2:C:186:ASP:O	2:C:187:ASP:C	2.60	0.41
1:A:143:ARG:NH2	4:A:418:HOH:O	2.52	0.41
1:B:17:LEU:HD23	1:B:30:LEU:HD21	2.02	0.41
2:D:201:LEU:HD23	2:D:201:LEU:HA	1.76	0.41
2:C:205:PRO:HA	2:C:243:ASP:OD2	2.21	0.41
2:D:110:ALA:O	2:D:115:ALA:HB2	2.20	0.41
1:A:236:ASP:HB3	1:A:252:PHE:HD1	1.85	0.41
1:B:136:PRO:HB2	1:B:141:THR:HG23	2.01	0.41
2:C:10:GLU:O	2:C:11:LYS:C	2.64	0.41
1:B:124:ARG:NH1	1:B:164:THR:HG22	2.35	0.41
1:B:110:LEU:O	1:B:113:LEU:HB3	2.20	0.41
1:A:72:ASP:H	1:A:75:ALA:HB3	1.86	0.41
1:A:96:ILE:HD13	1:A:190:LEU:HD23	2.03	0.40
1:A:38:LEU:HD23	1:A:38:LEU:HA	1.90	0.40
2:D:204:GLN:O	2:D:206:THR:N	2.54	0.40
2:C:248:VAL:O	2:C:248:VAL:HG12	2.20	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	252/258 (98%)	236 (94%)	13 (5%)	3 (1%)	10	13
1	B	254/258 (98%)	243 (96%)	9 (4%)	2 (1%)	16	22
2	C	243/274 (89%)	224 (92%)	19 (8%)	0	100	100
2	D	247/274 (90%)	235 (95%)	11 (4%)	1 (0%)	30	39
All	All	996/1064 (94%)	938 (94%)	52 (5%)	6 (1%)	21	29

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	3	GLU
1	A	70	GLU
1	B	195	ALA
1	A	134	ILE
2	D	205	PRO
1	B	134	ILE

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	192/200 (96%)	185 (96%)	7 (4%)	31	46
1	B	189/200 (94%)	183 (97%)	6 (3%)	34	51
2	C	184/216 (85%)	182 (99%)	2 (1%)	65	79
2	D	188/216 (87%)	183 (97%)	5 (3%)	39	58
All	All	753/832 (90%)	733 (97%)	20 (3%)	39	58

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	GLU
1	A	8	ARG

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Mol	Chain	Res	Type
1	A	30	LEU
1	A	64	ASP
1	A	122	ASN
1	A	161	GLU
1	A	170	GLN
1	B	8	ARG
1	B	64	ASP
1	B	68	MET
1	B	148	VAL
1	B	215	VAL
1	B	230	LEU
2	C	4	PHE
2	C	154	VAL
2	D	4	PHE
2	D	5	ILE
2	D	49	ARG
2	D	86	ARG
2	D	154	VAL

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	28	ASN
1	A	33	GLN
1	A	89	GLN
1	A	142	GLN
1	A	169	GLN
1	A	223	GLN
1	A	246	GLN
1	B	142	GLN
1	B	211	GLN
1	B	223	GLN
1	B	246	GLN
2	C	195	GLN
2	D	174	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

3 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	GOL	B	302	-	5,5,5	0.60	0	5,5,5	1.71	2 (40%)
3	GOL	B	301	-	5,5,5	0.40	0	5,5,5	2.05	2 (40%)
3	GOL	A	301	-	5,5,5	0.46	0	5,5,5	1.15	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	B	302	-	-	2/4/4/4	-
3	GOL	B	301	-	-	2/4/4/4	-
3	GOL	A	301	-	-	4/4/4/4	-

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	301	GOL	C3-C2-C1	3.35	124.07	111.80
3	B	302	GOL	C3-C2-C1	2.48	120.89	111.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	301	GOL	O2-C2-C1	2.47	119.41	109.18
3	B	302	GOL	O2-C2-C3	2.18	118.19	109.18

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	301	GOL	O1-C1-C2-C3
3	A	301	GOL	O2-C2-C3-O3
3	B	302	GOL	O1-C1-C2-C3
3	A	301	GOL	C1-C2-C3-O3
3	A	301	GOL	O1-C1-C2-O2
3	B	301	GOL	O1-C1-C2-O2
3	B	302	GOL	O1-C1-C2-O2
3	B	301	GOL	O2-C2-C3-O3

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	301	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	254/258 (98%)	1.02	46 (18%) 3 3	31, 42, 86, 95	0
1	B	256/258 (99%)	0.88	35 (13%) 6 5	33, 41, 82, 94	0
2	C	249/274 (90%)	1.04	41 (16%) 4 3	33, 45, 76, 113	0
2	D	250/274 (91%)	1.01	33 (13%) 7 6	34, 48, 76, 115	1 (0%)
All	All	1009/1064 (94%)	0.99	155 (15%) 5 4	31, 44, 80, 115	1 (0%)

All (155) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	78	ASN	8.2
1	A	233	ALA	6.4
2	C	33	ALA	6.1
1	A	242	SER	5.8
1	A	241	ILE	5.6
1	A	10	GLN	5.4
1	A	68	MET	4.7
2	C	4	PHE	4.6
2	C	78	PRO	4.5
2	C	251	PHE	4.4
1	B	230	LEU	4.4
2	C	67	ASN	4.4
2	D	67	ASN	4.3
1	A	240	GLY	4.3
2	D	78	PRO	4.1
2	C	87	PHE	4.1
1	A	67	GLU	4.1
1	B	241	ILE	4.1
1	B	9	GLN	3.9
1	A	9	GLN	3.9
2	D	168[A]	ASN	3.9

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Mol	Chain	Res	Type	RSRZ
1	A	69	ALA	3.7
1	B	245	LEU	3.7
1	B	10	GLN	3.6
1	A	33	GLN	3.5
2	C	114	GLY	3.5
2	D	4	PHE	3.5
2	C	135	ALA	3.4
2	D	40	LYS	3.4
1	A	245	LEU	3.4
2	D	44	ARG	3.4
1	A	2	SER	3.4
2	D	66	LEU	3.4
1	B	75	ALA	3.4
2	C	250	ALA	3.3
2	C	248	VAL	3.3
1	B	124	ARG	3.3
2	C	77	ALA	3.3
1	A	76	THR	3.2
1	A	234	THR	3.2
1	B	68	MET	3.2
2	C	97	LYS	3.1
2	D	60	PHE	3.1
1	A	27	ASN	3.1
2	D	253	ALA	3.1
2	D	250	ALA	3.0
2	D	57	GLY	3.0
1	B	122	ASN	3.0
1	A	229	THR	2.9
2	C	253	ALA	2.9
1	B	78	ASN	2.9
2	C	24	LEU	2.9
1	B	244	PHE	2.9
2	C	168	ASN	2.9
1	A	73	LEU	2.9
2	C	103	ILE	2.8
1	B	80	THR	2.8
2	C	65	ASP	2.8
1	A	121	GLU	2.8
2	D	21	PRO	2.8
1	A	74	ALA	2.8
1	B	72	ASP	2.8
2	C	249	SER	2.8

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Mol	Chain	Res	Type	RSRZ
1	B	69	ALA	2.7
1	A	70	GLU	2.7
2	C	30	GLU	2.7
2	D	22	GLU	2.7
1	A	235	GLU	2.7
2	D	27	PHE	2.7
1	A	174	VAL	2.7
1	A	249	THR	2.7
1	A	230	LEU	2.6
1	A	75	ALA	2.6
2	C	8	HIS	2.6
1	B	20	PRO	2.6
1	A	239	GLU	2.6
1	B	147	SER	2.6
1	B	233	ALA	2.6
2	D	247	GLY	2.6
1	A	231	LEU	2.6
2	D	86	ARG	2.6
1	A	77	LEU	2.6
2	D	30	GLU	2.5
2	D	87	PHE	2.5
2	D	174	GLN	2.5
2	D	236	ARG	2.5
2	C	52	LEU	2.5
2	D	249	SER	2.5
2	C	121	GLY	2.5
1	B	65	LEU	2.5
1	B	27	ASN	2.5
2	C	28	ASN	2.5
1	B	249	THR	2.5
1	B	237	ARG	2.5
1	A	232	ALA	2.5
2	C	113	ALA	2.5
2	C	66	LEU	2.4
1	A	238	HIS	2.4
1	A	8	ARG	2.4
1	A	244	PHE	2.4
1	B	214	GLU	2.4
1	B	79	ASP	2.4
1	B	92	ASN	2.4
2	D	59	GLY	2.4
2	D	65	ASP	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	177	VAL	2.4
1	A	201	ALA	2.4
2	C	12	GLY	2.3
2	C	82	MET	2.3
1	A	222	ALA	2.3
2	C	118	ALA	2.3
2	C	154	VAL	2.3
1	A	153	ALA	2.3
1	B	254	GLY	2.3
2	D	214	GLN	2.3
1	A	65	LEU	2.3
1	B	200	LEU	2.3
2	C	201	LEU	2.3
1	A	64	ASP	2.3
1	A	102	TYR	2.3
1	B	66	ASN	2.3
1	A	255	ARG	2.3
2	D	23	ARG	2.3
1	A	132	LEU	2.3
2	C	91	LEU	2.3
2	C	109	VAL	2.3
1	B	218	GLN	2.2
2	C	252	LEU	2.2
2	D	33	ALA	2.2
1	A	28	ASN	2.2
1	B	223	GLN	2.2
1	A	248	ARG	2.2
2	C	27	PHE	2.2
2	D	39	LEU	2.1
2	C	255	ARG	2.1
1	A	247	LYS	2.1
2	D	251	PHE	2.1
1	B	238	HIS	2.1
1	B	210	ARG	2.1
1	B	248	ARG	2.1
1	B	25	ALA	2.1
2	C	247	GLY	2.1
2	C	7	SER	2.1
1	A	223	GLN	2.1
1	B	148	VAL	2.1
2	D	24	LEU	2.1
2	D	141	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
2	C	22	GLU	2.1
1	A	105	GLY	2.0
2	D	43	GLU	2.0
2	D	45	ASP	2.0
2	C	6	LEU	2.0
2	D	53	LEU	2.0
2	C	5	ILE	2.0
2	C	31	MET	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($\text{\AA}^2$)	Q<0.9
3	GOL	B	301	6/6	0.63	0.23	61,77,84,89	0
3	GOL	A	301	6/6	0.65	0.26	49,63,67,70	0
3	GOL	B	302	6/6	0.76	0.19	44,54,58,63	0

6.5 Other polymers [i](#)

There are no such residues in this entry.