



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 14, 2026 – 07:13 PM UTC

PDB ID : 4LRX / pdb_00004lrx
Title : Crystal Structure of the E.coli DhaR(N)-DhaK complex
Authors : Shi, R.; McDonald, L.; Cygler, M.; Ekiel, I.
Deposited on : 2013-07-21
Resolution : 3.25 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:

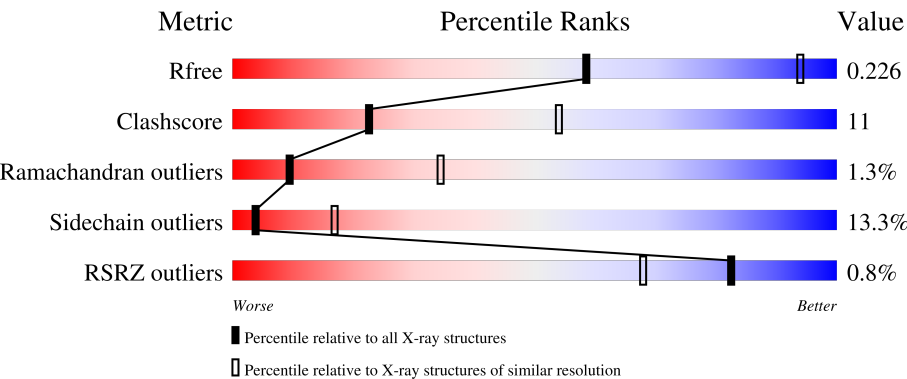
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.25 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	1605 (3.30-3.22)
Clashscore	190562	1660 (3.30-3.22)
Ramachandran outliers	187476	1630 (3.30-3.22)
Sidechain outliers	187428	1629 (3.30-3.22)
RSRZ outliers	180081	1605 (3.30-3.22)

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	356	74%25%.
1	B	356	% 75%23%.
2	C	318	% 57%31%5%7%
2	D	318	% 60%25%7%.7%

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
3	GOL	A	401	-	-	X	-
3	GOL	B	401	-	-	X	-

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 9912 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.

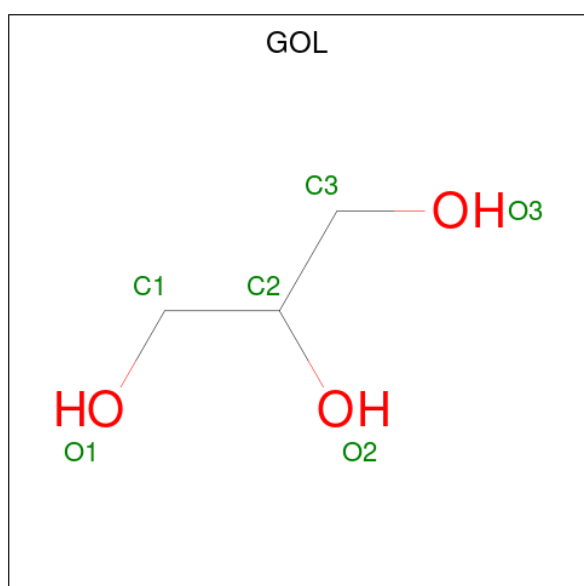
- Molecule 1 is a protein called PTS-dependent dihydroxyacetone kinase, dihydroxyacetone-binding subunit DhaK.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	356	Total	C	N	O	S	0	0	0
			2681	1679	460	529	13			
1	B	356	Total	C	N	O	S	0	0	0
			2681	1679	460	529	13			

- Molecule 2 is a protein called PTS-dependent dihydroxyacetone kinase operon regulatory protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	295	Total	C	N	O	S	0	0	0
			2269	1438	393	426	12			
2	D	295	Total	C	N	O	S	0	0	0
			2269	1438	393	426	12			

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

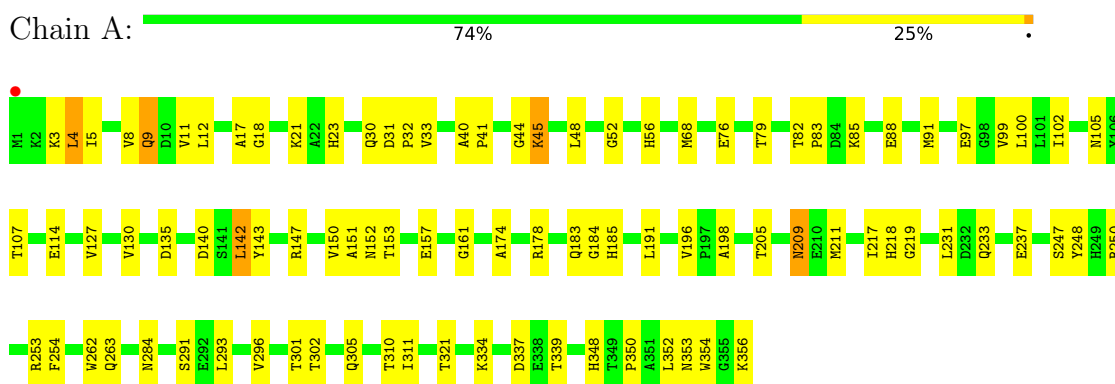


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			6	3	3		
3	B	1	Total	C	O	0	0
			6	3	3		

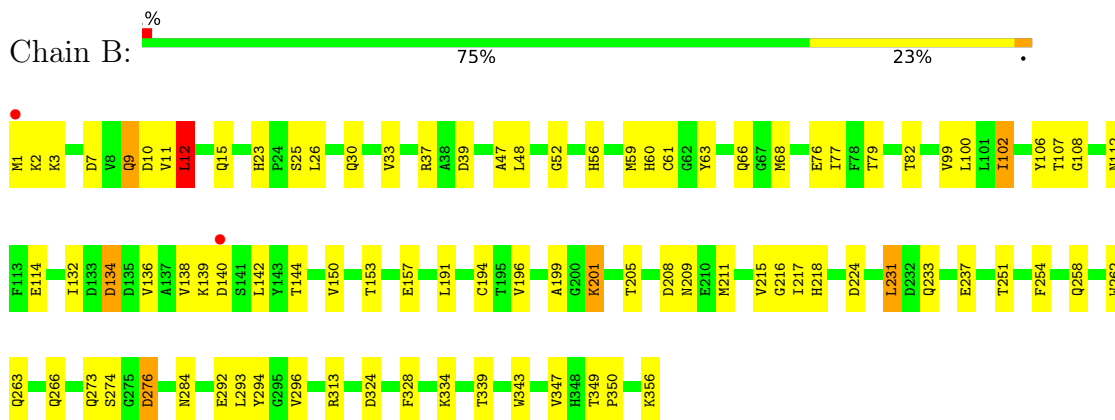
3 Residue-property plots

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.

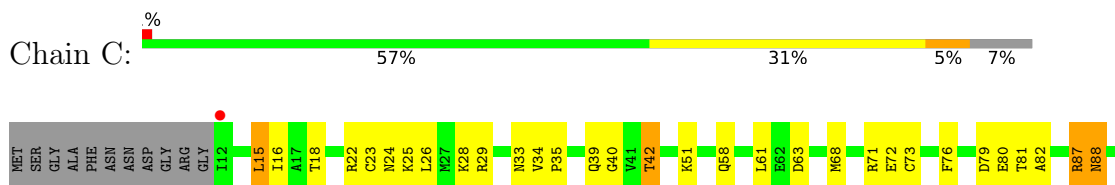
- Molecule 1: PTS-dependent dihydroxyacetone kinase, dihydroxyacetone-binding subunit DhaK

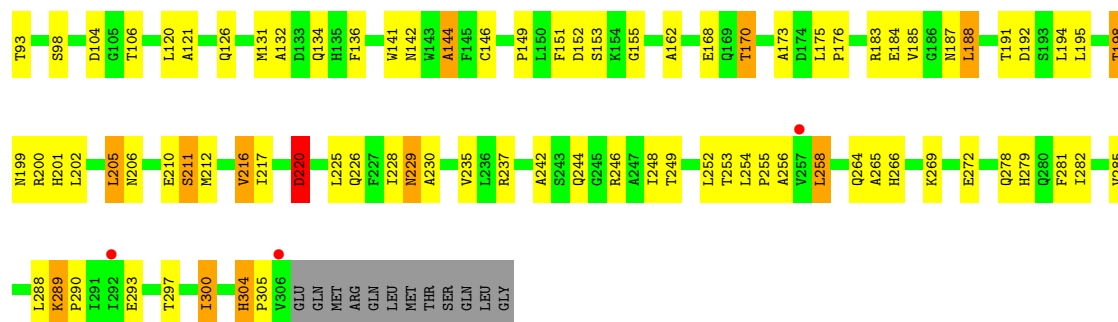


- Molecule 1: PTS-dependent dihydroxyacetone kinase, dihydroxyacetone-binding subunit DhaK

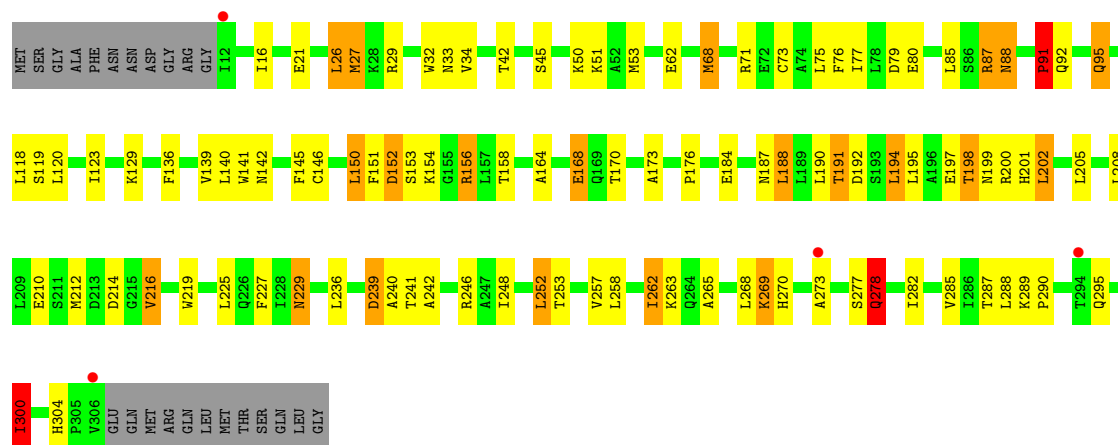


- Molecule 2: PTS-dependent dihydroxyacetone kinase operon regulatory protein





● Molecule 2: PTS-dependent dihydroxyacetone kinase operon regulatory protein



4 Data and refinement statistics

Property	Value	Source
Space group	P 61	Depositor
Cell constants a, b, c, α , β , γ	232.13Å 232.13Å 79.89Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	50.00 – 3.25 50.00 – 3.25	Depositor EDS
% Data completeness (in resolution range)	99.5 (50.00-3.25) 99.7 (50.00-3.25)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.66 (at 3.25Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.191 , 0.228 0.188 , 0.226	Depositor DCC
R_{free} test set	1959 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	58.0	Xtriage
Anisotropy	0.775	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 36.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.034 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	9912	wwPDB-VP
Average B, all atoms (Å ²)	68.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.57% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.83	0/2730	1.04	3/3710 (0.1%)
1	B	0.79	0/2730	1.03	5/3710 (0.1%)
2	C	0.98	5/2311 (0.2%)	1.14	6/3147 (0.2%)
2	D	0.99	3/2311 (0.1%)	1.16	7/3147 (0.2%)
All	All	0.90	8/10082 (0.1%)	1.09	21/13714 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	D	0	1

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	273	ALA	C-O	-8.99	1.12	1.23
2	C	304	HIS	CB-CG	-8.17	1.38	1.50
2	D	273	ALA	C-N	6.50	1.42	1.33
2	C	304	HIS	ND1-CE1	-5.82	1.26	1.32
2	C	144	ALA	CA-CB	-5.58	1.43	1.53
2	C	281	PHE	CA-CB	5.57	1.62	1.53
2	C	304	HIS	CD2-NE2	-5.24	1.32	1.37
2	D	262	ILE	CA-CB	5.24	1.61	1.54

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	300	ILE	CB-CA-C	-7.73	99.64	111.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	152	ASP	N-CA-CB	-6.62	100.26	110.85
2	D	273	ALA	CA-C-O	-6.30	114.28	121.40
1	A	151	ALA	N-CA-C	6.22	118.86	111.71
1	B	61	CYS	N-CA-C	6.04	119.48	111.75
1	A	337	ASP	N-CA-C	5.98	117.88	111.36
2	D	68	MET	N-CA-C	-5.79	106.86	114.04
1	B	12	LEU	N-CA-C	5.73	118.47	111.82
1	B	349	THR	CA-C-N	-5.50	113.23	119.28
1	B	349	THR	C-N-CA	-5.50	113.23	119.28
1	A	45	LYS	N-CA-C	5.46	118.60	110.14
2	D	26	LEU	N-CA-C	5.45	117.85	110.88
2	C	98	SER	N-CA-C	-5.42	105.40	112.23
2	C	185	VAL	N-CA-C	5.34	115.48	110.30
2	C	88	ASN	N-CA-C	5.32	116.36	108.86
2	C	23	CYS	N-CA-C	5.27	117.03	111.28
1	B	276	ASP	N-CA-C	5.17	117.20	110.43
2	D	88	ASN	N-CA-C	5.14	114.93	108.45
2	C	87	ARG	CA-C-N	-5.07	114.37	122.53
2	C	87	ARG	C-N-CA	-5.07	114.37	122.53
2	D	265	ALA	N-CA-C	5.02	118.13	111.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	D	151	PHE	Peptide

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	2681	0	2637	47	0
1	B	2681	0	2637	51	0
2	C	2269	0	2282	65	0
2	D	2269	0	2282	73	0
3	A	6	0	8	6	0
3	B	6	0	8	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	9912	0	9854	208	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 (208) 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:218:HIS:NE2	3:B:401:GOL:H2	1.50	1.25
2:C:212:MET:HE3	2:D:212:MET:HE3	1.26	1.13
1:A:218:HIS:NE2	3:A:401:GOL:H2	1.66	1.10
2:C:211:SER:HB3	2:D:300:ILE:HD11	1.08	1.07
1:B:218:HIS:NE2	3:B:401:GOL:C2	2.20	1.04
1:A:88:GLU:OE2	2:C:42:THR:HG21	1.58	1.04
2:D:216:VAL:H	2:D:229:ASN:ND2	1.55	1.03
1:A:218:HIS:CE1	3:A:401:GOL:H2	1.94	1.00
2:C:211:SER:CB	2:D:300:ILE:HD11	1.92	0.99
1:B:218:HIS:CE1	3:B:401:GOL:H2	2.00	0.96
2:C:217:ILE:HG12	2:C:228:ILE:HG13	1.49	0.94
2:D:68:MET:HE2	2:D:71:ARG:HH11	1.31	0.94
1:A:218:HIS:NE2	3:A:401:GOL:C2	2.31	0.93
2:D:216:VAL:N	2:D:229:ASN:HD21	1.67	0.92
2:C:212:MET:HE3	2:D:212:MET:CE	2.01	0.89
1:A:153:THR:O	1:A:157:GLU:HG3	1.73	0.89
2:C:211:SER:HB3	2:D:300:ILE:CD1	2.00	0.86
2:C:131:MET:O	2:C:134:GLN:HG3	1.76	0.84
2:D:68:MET:CE	2:D:71:ARG:HH11	1.92	0.83
2:D:150:LEU:O	2:D:158:THR:HG22	1.79	0.83
2:C:212:MET:CE	2:D:212:MET:HE3	2.09	0.81
2:C:220:ASP:OD1	2:C:226:GLN:NE2	2.15	0.79
2:D:216:VAL:H	2:D:229:ASN:HD21	0.84	0.78
1:A:284:ASN:HB2	1:A:293:LEU:HD11	1.64	0.77
2:D:92:GLN:HA	2:D:95:GLN:HG3	1.67	0.76
2:C:235:VAL:O	2:C:282:ILE:HD12	1.87	0.74
1:B:9:GLN:H	1:B:9:GLN:HE21	1.36	0.71
2:C:29:ARG:HG2	2:C:136:PHE:O	1.91	0.71
2:C:29:ARG:NH1	2:C:141:TRP:HZ2	1.88	0.70
2:D:214:ASP:OD1	2:D:304:HIS:ND1	2.22	0.70
2:C:68:MET:HE3	2:D:173:ALA:HA	1.75	0.69
1:A:233:GLN:O	1:A:237:GLU:HG2	1.94	0.67
2:D:79:ASP:HB3	2:D:85:LEU:HD11	1.76	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:218:HIS:NE2	3:B:401:GOL:O2	2.28	0.66
1:B:12:LEU:HD11	1:B:77:ILE:HG13	1.79	0.65
1:B:284:ASN:HB2	1:B:293:LEU:HD11	1.80	0.64
2:D:152:ASP:HB2	2:D:156:ARG:O	1.98	0.63
2:C:217:ILE:CG1	2:C:228:ILE:HG13	2.28	0.62
2:D:210:GLU:OE2	2:D:229:ASN:HB2	2.00	0.62
1:A:31:ASP:HB3	2:C:39:GLN:OE1	1.99	0.62
2:D:32:TRP:HB2	2:D:139:VAL:HG21	1.80	0.62
2:D:239:ASP:OD2	2:D:242:ALA:HB3	1.99	0.62
2:C:71:ARG:HG2	2:C:72:GLU:N	2.14	0.61
1:A:23:HIS:CE1	1:A:350:PRO:HB3	2.34	0.61
1:B:48:LEU:HD11	1:B:102:ILE:HD11	1.82	0.61
1:A:219:GLY:O	2:C:25:LYS:HE2	2.00	0.61
1:A:44:GLY:O	1:A:97:GLU:HG3	2.01	0.61
2:D:201:HIS:HD2	2:D:205:LEU:HD13	1.66	0.61
2:C:194:LEU:O	2:C:198:THR:HG23	2.01	0.60
2:D:194:LEU:O	2:D:198:THR:HG23	2.00	0.60
1:B:231:LEU:HD11	1:B:296:VAL:CG2	2.32	0.60
2:C:173:ALA:HB3	2:D:173:ALA:HB3	1.84	0.60
1:B:11:VAL:O	1:B:15:GLN:HG3	2.01	0.60
2:C:173:ALA:O	2:C:176:PRO:HD2	2.03	0.59
1:B:231:LEU:CD1	1:B:296:VAL:HG22	2.33	0.59
2:C:29:ARG:NH1	2:C:141:TRP:CZ2	2.70	0.59
1:A:218:HIS:NE2	3:A:401:GOL:O2	2.36	0.58
1:A:56:HIS:HA	1:A:321:THR:O	2.04	0.58
2:C:237:ARG:HE	2:C:282:ILE:HD11	1.70	0.57
2:D:227:PHE:HE2	2:D:229:ASN:HB3	1.69	0.57
2:D:29:ARG:NH1	2:D:141:TRP:HZ2	2.03	0.56
1:B:37:ARG:NH2	1:B:66:GLN:HA	2.20	0.56
1:A:32:PRO:HB2	1:A:85:LYS:HG2	1.88	0.55
2:C:200:ARG:HH12	2:D:295:GLN:NE2	2.04	0.55
2:C:173:ALA:HA	2:D:68:MET:HE3	1.87	0.55
1:B:231:LEU:HD11	1:B:296:VAL:HG22	1.88	0.54
2:D:32:TRP:CB	2:D:139:VAL:HG21	2.37	0.54
2:D:68:MET:CE	2:D:71:ARG:NH1	2.68	0.54
1:A:301:THR:HG22	1:A:311:ILE:HD12	1.90	0.54
2:D:129:LYS:HG3	2:D:146:CYS:SG	2.48	0.54
1:B:313:ARG:HG3	1:B:343:TRP:CD1	2.43	0.54
2:D:201:HIS:CD2	2:D:205:LEU:HD13	2.43	0.54
2:C:81:THR:O	2:C:82:ALA:HB3	2.08	0.54
1:A:174:ALA:O	1:A:178:ARG:HB2	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:254:PHE:CZ	1:A:263:GLN:HG2	2.43	0.54
2:C:68:MET:HB2	2:D:176:PRO:HG3	1.89	0.53
1:B:231:LEU:CD1	1:B:296:VAL:CG2	2.86	0.53
2:C:79:ASP:OD1	2:C:79:ASP:C	2.50	0.53
2:D:76:PHE:CD1	2:D:87:ARG:HB3	2.43	0.53
1:A:191:LEU:HD23	1:A:211:MET:HB3	1.90	0.53
2:D:229:ASN:HD22	2:D:229:ASN:H	1.57	0.53
1:A:4:LEU:HD21	1:B:328:PHE:HE2	1.74	0.52
2:C:76:PHE:CE1	2:C:87:ARG:HG2	2.44	0.52
2:D:227:PHE:CE2	2:D:229:ASN:HB3	2.43	0.52
1:A:4:LEU:CD2	1:B:328:PHE:HE2	2.22	0.52
1:B:48:LEU:CD1	1:B:100:LEU:HD23	2.39	0.52
1:B:30:GLN:HE21	1:B:30:GLN:HA	1.74	0.52
2:C:216:VAL:H	2:C:229:ASN:ND2	2.08	0.52
2:C:132:ALA:HA	2:C:141:TRP:O	2.10	0.52
2:C:68:MET:CE	2:D:173:ALA:HA	2.38	0.51
1:A:218:HIS:CE1	3:A:401:GOL:C2	2.80	0.51
2:D:140:LEU:HD22	2:D:145:PHE:HE2	1.76	0.51
1:A:142:LEU:HD22	2:C:22:ARG:HG2	1.93	0.50
1:A:114:GLU:HG2	1:A:262:TRP:CH2	2.45	0.50
1:B:153:THR:O	1:B:157:GLU:HG3	2.11	0.50
2:D:26:LEU:O	2:D:27:MET:HB2	2.09	0.50
1:A:17:ALA:O	1:A:21:LYS:HG3	2.12	0.50
2:C:173:ALA:C	2:C:176:PRO:HD2	2.37	0.50
2:C:278:GLN:O	2:C:279:HIS:HB2	2.10	0.50
2:D:168:GLU:CD	2:D:168:GLU:H	2.20	0.49
1:B:9:GLN:H	1:B:9:GLN:NE2	2.08	0.49
1:B:23:HIS:CE1	1:B:350:PRO:HB3	2.47	0.49
1:B:56:HIS:CE1	1:B:217:ILE:HD12	2.47	0.49
1:A:198:ALA:O	2:C:28:LYS:HG3	2.12	0.49
2:C:254:LEU:HD22	2:C:258:LEU:HD13	1.95	0.48
2:D:236:LEU:HD13	2:D:252:LEU:HD11	1.96	0.48
2:D:188:LEU:O	2:D:192:ASP:HB2	2.13	0.48
1:B:208:ASP:O	1:B:209:ASN:C	2.55	0.48
2:D:73:CYS:HB2	2:D:164:ALA:O	2.14	0.48
2:C:87:ARG:HD3	2:C:104:ASP:OD2	2.14	0.48
2:C:146:CYS:O	2:C:162:ALA:HA	2.14	0.48
2:C:187:ASN:HB3	2:D:188:LEU:HD21	1.96	0.47
2:D:53:MET:HE3	2:D:77:ILE:CG2	2.44	0.47
2:C:206:ASN:ND2	2:C:210:GLU:HG2	2.29	0.47
1:A:9:GLN:H	1:A:9:GLN:NE2	2.13	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:134:ASP:OD1	1:B:134:ASP:N	2.44	0.47
2:C:188:LEU:O	2:C:192:ASP:HB2	2.13	0.47
2:D:29:ARG:HG2	2:D:136:PHE:O	2.14	0.47
1:A:209:ASN:HD21	1:B:1:MET:CG	2.27	0.47
1:A:48:LEU:HD12	1:A:100:LEU:HB3	1.96	0.46
1:B:52:GLY:HA3	3:B:401:GOL:O1	2.15	0.46
1:A:152:ASN:ND2	1:A:184:GLY:HA3	2.31	0.46
1:A:231:LEU:HD11	1:A:296:VAL:HG22	1.98	0.46
2:C:183:ARG:O	2:C:187:ASN:HB2	2.16	0.46
2:C:188:LEU:HD13	2:D:188:LEU:HD13	1.98	0.46
2:D:187:ASN:O	2:D:191:THR:HG23	2.16	0.46
1:A:105:ASN:ND2	1:A:147:ARG:O	2.47	0.46
2:C:175:LEU:HD12	2:C:175:LEU:HA	1.72	0.46
2:D:91:PRO:O	2:D:95:GLN:HG2	2.16	0.46
1:B:30:GLN:HA	1:B:30:GLN:NE2	2.31	0.45
1:B:276:ASP:OD1	1:B:334:LYS:HD2	2.15	0.45
1:A:4:LEU:HB2	1:B:292:GLU:OE1	2.15	0.45
1:B:215:VAL:HG22	1:B:216:GLY:N	2.31	0.45
2:D:119:SER:O	2:D:123:ILE:HD12	2.16	0.45
2:D:188:LEU:HD12	2:D:188:LEU:HA	1.87	0.45
1:A:183:GLN:HB3	1:A:334:LYS:HB3	1.97	0.45
2:D:29:ARG:HH12	2:D:141:TRP:HZ2	1.64	0.45
1:B:10:ASP:O	1:B:11:VAL:C	2.59	0.45
2:D:277:SER:C	2:D:278:GLN:HG3	2.42	0.45
1:A:18:GLY:HA3	1:B:294:TYR:O	2.17	0.45
1:A:83:PRO:HG3	2:C:81:THR:HG21	1.99	0.45
1:B:7:ASP:CG	1:B:9:GLN:HE22	2.25	0.45
2:D:76:PHE:CE1	2:D:87:ARG:HB3	2.52	0.45
1:A:76:GLU:HB2	1:A:79:THR:HB	1.99	0.44
1:B:76:GLU:HB2	1:B:79:THR:OG1	2.17	0.44
1:B:194:CYS:HA	1:B:324:ASP:OD1	2.17	0.44
1:A:352:LEU:HD22	1:A:354:TRP:CZ3	2.52	0.44
1:B:108:GLY:O	1:B:112:ASN:ND2	2.50	0.44
1:B:37:ARG:HB3	1:B:39:ASP:OD1	2.18	0.44
1:A:248:TYR:CE2	1:A:250:ARG:HD2	2.52	0.43
2:D:216:VAL:HG13	2:D:229:ASN:ND2	2.33	0.43
2:C:304:HIS:HA	2:C:305:PRO:HD3	1.91	0.43
1:A:68:MET:HA	1:A:161:GLY:HA3	2.01	0.43
2:C:184:GLU:O	2:C:188:LEU:HB2	2.19	0.43
2:C:289:LYS:HA	2:C:290:PRO:HD3	1.86	0.43
2:D:152:ASP:HB3	2:D:156:ARG:N	2.34	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:288:LEU:HD12	2:D:300:ILE:O	2.19	0.43
1:A:99:VAL:O	1:A:127:VAL:HG23	2.18	0.43
1:B:47:ALA:HB3	1:B:99:VAL:HG22	2.01	0.43
2:C:249:THR:HG22	2:C:254:LEU:HD12	2.00	0.43
2:D:50:LYS:HE3	2:D:79:ASP:HB2	1.99	0.43
2:C:151:PHE:CD2	2:C:151:PHE:N	2.87	0.42
1:A:142:LEU:HD13	1:A:143:TYR:CE1	2.54	0.42
1:B:25:SER:O	1:B:26:LEU:HD23	2.19	0.42
1:B:106:TYR:O	1:B:107:THR:C	2.63	0.42
2:D:277:SER:O	2:D:278:GLN:C	2.63	0.42
1:B:251:THR:OG1	1:B:266:GLN:HG2	2.18	0.42
2:C:121:ALA:HB1	2:C:149:PRO:HD3	2.01	0.42
2:C:264:GLN:OE1	2:C:264:GLN:HA	2.20	0.42
2:D:219:TRP:CZ2	2:D:262:ILE:HD11	2.54	0.42
1:B:12:LEU:CD1	1:B:77:ILE:HG13	2.46	0.42
2:C:183:ARG:NH1	2:D:184:GLU:OE1	2.53	0.42
2:D:216:VAL:N	2:D:229:ASN:ND2	2.41	0.42
2:D:258:LEU:HD21	2:D:288:LEU:HD13	2.01	0.42
2:C:18:THR:HG22	2:C:22:ARG:NH1	2.35	0.42
1:A:40:ALA:HA	1:A:41:PRO:C	2.43	0.41
1:A:52:GLY:HA3	3:A:401:GOL:O1	2.19	0.41
1:B:63:TYR:O	1:B:68:MET:HB3	2.20	0.41
1:B:224:ASP:OD1	1:B:224:ASP:C	2.63	0.41
2:C:202:LEU:HD23	2:C:202:LEU:HA	1.90	0.41
1:A:348:HIS:HA	1:A:353:ASN:OD1	2.20	0.41
2:C:201:HIS:CD2	2:D:202:LEU:HD11	2.55	0.41
2:D:248:ILE:HD12	2:D:248:ILE:HA	1.84	0.41
2:D:152:ASP:HB3	2:D:156:ARG:H	1.86	0.41
1:A:56:HIS:CE1	1:A:217:ILE:HD12	2.55	0.41
1:B:114:GLU:HG2	1:B:262:TRP:CH2	2.56	0.41
1:B:199:ALA:O	1:B:201:LYS:HE2	2.20	0.41
1:A:3:LYS:HB3	1:A:5:ILE:HG12	2.01	0.41
2:D:269:LYS:O	2:D:270:HIS:C	2.63	0.41
2:C:144:ALA:CB	2:C:170:THR:HG23	2.51	0.41
2:C:205:LEU:HD23	2:D:205:LEU:HB3	2.03	0.41
2:D:91:PRO:O	2:D:95:GLN:CG	2.69	0.41
1:A:48:LEU:HD22	1:A:161:GLY:HA2	2.03	0.41
2:C:73:CYS:HA	2:C:93:THR:HG21	2.02	0.41
1:B:254:PHE:CE2	1:B:263:GLN:HB3	2.56	0.41
2:C:288:LEU:HA	2:C:300:ILE:O	2.21	0.41
1:B:59:MET:HA	1:B:60:HIS:HA	1.80	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:68:MET:HE1	2:D:71:ARG:NH1	2.36	0.40
2:C:35:PRO:HG2	2:C:106:THR:HG21	2.02	0.40
2:C:76:PHE:CD1	2:C:87:ARG:HG2	2.56	0.40
2:C:255:PRO:O	2:C:256:ALA:C	2.64	0.40
1:B:273:GLN:O	1:B:274:SER:C	2.64	0.40
2:D:268:LEU:O	2:D:287:THR:HA	2.21	0.40
1:B:191:LEU:CD2	1:B:211:MET:HB3	2.52	0.40
2:C:152:ASP:O	2:C:155:GLY:N	2.46	0.40
2:D:68:MET:HE2	2:D:71:ARG:HD2	2.03	0.40
2:D:246:ARG:HG2	2:D:246:ARG:HH11	1.87	0.40
2:D:289:LYS:HA	2:D:290:PRO:HD2	2.00	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	354/356 (99%)	327 (92%)	24 (7%)	3 (1%)	16	44
1	B	354/356 (99%)	322 (91%)	30 (8%)	2 (1%)	21	51
2	C	293/318 (92%)	267 (91%)	19 (6%)	7 (2%)	4	23
2	D	293/318 (92%)	274 (94%)	14 (5%)	5 (2%)	7	29
All	All	1294/1348 (96%)	1190 (92%)	87 (7%)	17 (1%)	9	34

All (17) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	C	220	ASP
1	A	140	ASP
2	C	40	GLY
2	C	230	ALA

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Mol	Chain	Res	Type
2	C	265	ALA
1	A	135	ASP
2	C	153	SER
2	C	242	ALA
2	D	240	ALA
2	C	15	LEU
2	D	278	GLN
1	B	140	ASP
1	A	150	VAL
2	D	27	MET
2	D	118	LEU
1	B	150	VAL
2	D	91	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	287/288 (100%)	261 (91%)	26 (9%)	9	30
1	B	287/288 (100%)	263 (92%)	24 (8%)	10	33
2	C	241/260 (93%)	198 (82%)	43 (18%)	2	7
2	D	241/260 (93%)	194 (80%)	47 (20%)	1	6
All	All	1056/1096 (96%)	916 (87%)	140 (13%)	4	17

All (140) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	LEU
1	A	8	VAL
1	A	9	GLN
1	A	11	VAL
1	A	12	LEU
1	A	30	GLN
1	A	33	VAL
1	A	45	LYS

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Mol	Chain	Res	Type
1	A	82	THR
1	A	91	MET
1	A	102	ILE
1	A	107	THR
1	A	130	VAL
1	A	142	LEU
1	A	185	HIS
1	A	196	VAL
1	A	205	THR
1	A	209	ASN
1	A	247	SER
1	A	253	ARG
1	A	291	SER
1	A	302	THR
1	A	305	GLN
1	A	310	THR
1	A	339	THR
1	A	356	LYS
1	B	2	LYS
1	B	3	LYS
1	B	9	GLN
1	B	12	LEU
1	B	33	VAL
1	B	82	THR
1	B	102	ILE
1	B	132	ILE
1	B	134	ASP
1	B	136	VAL
1	B	138	VAL
1	B	139	LYS
1	B	142	LEU
1	B	144	THR
1	B	196	VAL
1	B	201	LYS
1	B	205	THR
1	B	231	LEU
1	B	233	GLN
1	B	237	GLU
1	B	258	GLN
1	B	339	THR
1	B	347	VAL
1	B	356	LYS

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Mol	Chain	Res	Type
2	C	15	LEU
2	C	16	ILE
2	C	24	ASN
2	C	26	LEU
2	C	33	ASN
2	C	34	VAL
2	C	42	THR
2	C	51	LYS
2	C	58	GLN
2	C	61	LEU
2	C	63	ASP
2	C	80	GLU
2	C	88	ASN
2	C	120	LEU
2	C	126	GLN
2	C	142	ASN
2	C	168	GLU
2	C	170	THR
2	C	188	LEU
2	C	191	THR
2	C	195	LEU
2	C	198	THR
2	C	199	ASN
2	C	205	LEU
2	C	211	SER
2	C	216	VAL
2	C	220	ASP
2	C	225	LEU
2	C	229	ASN
2	C	244	GLN
2	C	246	ARG
2	C	248	ILE
2	C	252	LEU
2	C	253	THR
2	C	258	LEU
2	C	266	HIS
2	C	269	LYS
2	C	272	GLU
2	C	285	VAL
2	C	289	LYS
2	C	293	GLU
2	C	297	THR

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Mol	Chain	Res	Type
2	C	300	ILE
2	D	16	ILE
2	D	21	GLU
2	D	33	ASN
2	D	34	VAL
2	D	42	THR
2	D	45	SER
2	D	51	LYS
2	D	62	GLU
2	D	75	LEU
2	D	80	GLU
2	D	87	ARG
2	D	88	ASN
2	D	91	PRO
2	D	95	GLN
2	D	120	LEU
2	D	142	ASN
2	D	150	LEU
2	D	153	SER
2	D	154	LYS
2	D	156	ARG
2	D	168	GLU
2	D	170	THR
2	D	188	LEU
2	D	190	LEU
2	D	191	THR
2	D	194	LEU
2	D	195	LEU
2	D	197	GLU
2	D	198	THR
2	D	199	ASN
2	D	200	ARG
2	D	202	LEU
2	D	208	LEU
2	D	216	VAL
2	D	225	LEU
2	D	229	ASN
2	D	239	ASP
2	D	241	THR
2	D	252	LEU
2	D	253	THR
2	D	257	VAL

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Mol	Chain	Res	Type
2	D	263	LYS
2	D	269	LYS
2	D	278	GLN
2	D	282	ILE
2	D	285	VAL
2	D	300	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	9	GLN
1	A	152	ASN
1	A	183	GLN
1	A	209	ASN
1	A	249	HIS
1	B	9	GLN
1	B	29	HIS
1	B	66	GLN
1	B	152	ASN
1	B	183	GLN
1	B	185	HIS
1	B	298	ASN
1	B	305	GLN
2	C	58	GLN
2	C	88	ASN
2	C	126	GLN
2	C	201	HIS
2	C	206	ASN
2	C	229	ASN
2	C	278	GLN
2	D	58	GLN
2	D	103	ASN
2	D	201	HIS
2	D	206	ASN
2	D	229	ASN
2	D	295	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 ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

2 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	A	401	-	5,5,5	0.41	0	5,5,5	0.60	0
3	GOL	B	401	-	5,5,5	0.28	0	5,5,5	0.54	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	A	401	-	-	2/4/4/4	-
3	GOL	B	401	-	-	2/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	401	GOL	C1-C2-C3-O3
3	A	401	GOL	O2-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
3	B	401	GOL	C1-C2-C3-O3
3	B	401	GOL	O2-C2-C3-O3

There are no ring outliers.

2 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	401	GOL	6	0
3	B	401	GOL	5	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	356/356 (100%)	-0.33	1 (0%) 90 82	50, 66, 86, 96	0
1	B	356/356 (100%)	-0.28	2 (0%) 85 73	47, 66, 86, 97	0
2	C	295/318 (92%)	-0.08	4 (1%) 73 54	41, 65, 107, 121	0
2	D	295/318 (92%)	-0.16	4 (1%) 73 54	44, 63, 100, 119	0
All	All	1302/1348 (96%)	-0.22	11 (0%) 82 68	41, 65, 94, 121	0

All (11) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	C	306	VAL	3.9
2	D	306	VAL	3.6
2	D	294	THR	3.3
2	D	12	ILE	3.1
2	C	292	ILE	2.6
1	A	1	MET	2.6
1	B	140	ASP	2.5
2	C	257	VAL	2.5
2	C	12	ILE	2.2
2	D	273	ALA	2.1
1	B	1	MET	2.1

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	401	6/6	0.95	0.14	76,79,81,83	0
3	GOL	A	401	6/6	0.97	0.15	69,71,72,75	0

6.5 Other polymers [i](#)

There are no such residues in this entry.