



Full wwPDB X-ray Structure Validation Report

May 28, 2020 – 12:37 am BST

PDB ID : 4LRY
Title : Crystal Structure of the E.coli DhaR(N)-DhaK(T79L) complex
Authors : Shi, R.; McDonald, L.; Cygler, M.; Ekiel, I.
Deposited on : 2013-07-21
Resolution : 2.83 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 following versions of software and data (see [references](#) ) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

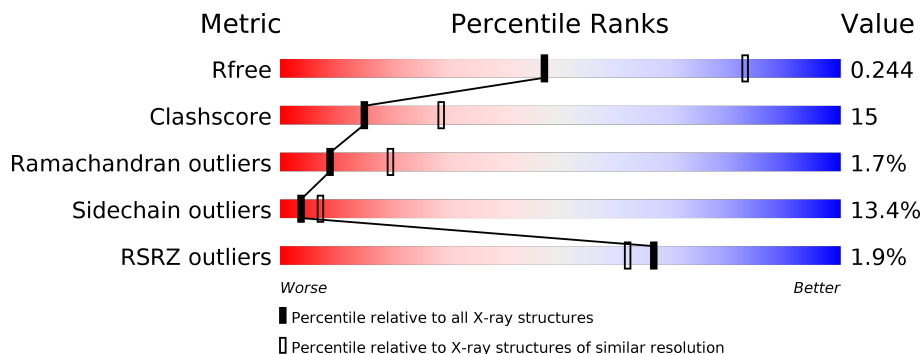
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.83 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}	130704	1031 (2.86-2.82)
Clashscore	141614	1078 (2.86-2.82)
Ramachandran outliers	138981	1050 (2.86-2.82)
Sidechain outliers	138945	1051 (2.86-2.82)
RSRZ outliers	127900	1019 (2.86-2.82)

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 on 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	 2% 68% 29%
1	B	356	 2% 68% 27%
2	C	318	 2% 54% 29% 8% 8%
2	D	318	 2% 61% 22% 8% 8%

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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	GOL	A	401	-	-	X	-
3	GOL	B	401	-	-	X	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 9942 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
			Total	C	N	O	S			
1	A	356	Total	C	N	O	S	0	0	0
			2682	1681	460	528	13			
1	B	356	Total	C	N	O	S	0	1	0
			2690	1689	460	528	13			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	79	LEU	THR	engineered mutation	UNP P76015
B	79	LEU	THR	engineered mutation	UNP P76015

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	C	294	Total	C	N	O	S	0	0	0
			2264	1435	392	425	12			
2	D	294	Total	C	N	O	S	0	0	0
			2264	1435	392	425	12			

- Molecule 3 is GLYCEROL (three-letter code: 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	13	Total O 13 13	0	0
4	B	6	Total O 6 6	0	0
4	C	6	Total O 6 6	0	0
4	D	5	Total O 5 5	0	0

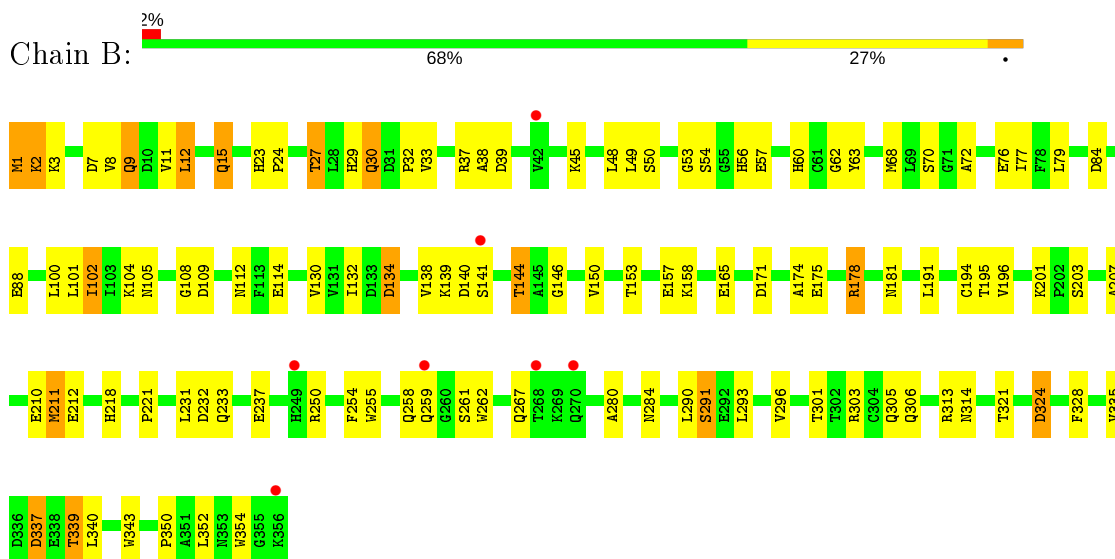
3 Residue-property plots i

These plots are drawn for all protein, RNA and DNA 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.

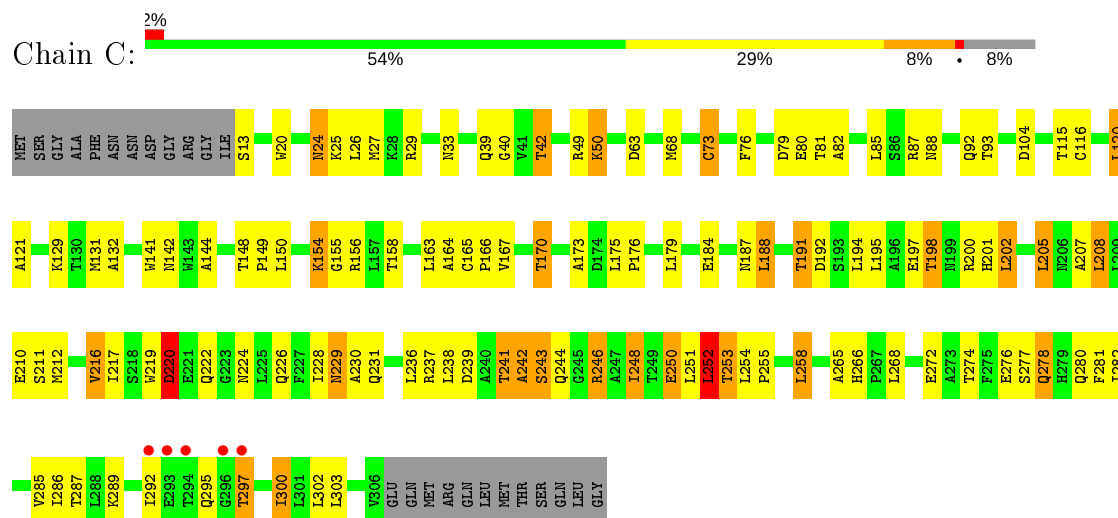
- Molecule 1: PTS-dependent dihydroxyacetone kinase, dihydroxyacetone-binding subunit DhaK



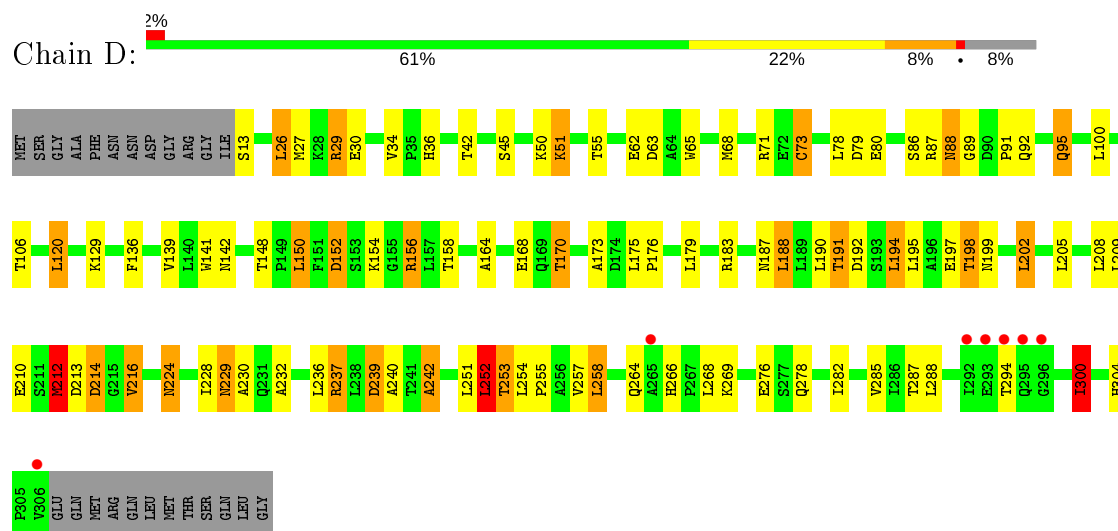
- Molecule 1: PTS-dependent dihydroxyacetone kinase, dihydroxyacetone-binding subunit DhaK



- 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	231.40 Å 231.40 Å 79.76 Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	50.00 – 2.83 46.83 – 2.83	Depositor EDS
% Data completeness (in resolution range)	96.9 (50.00-2.83) 96.9 (46.83-2.83)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.91 (at 2.81 Å)	Xtrriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.201 , 0.241 0.203 , 0.244	Depositor DCC
R_{free} test set	2860 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å ²)	53.8	Xtrriage
Anisotropy	0.111	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 45.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtrriage
Estimated twinning fraction	0.046 for h,-h-k,-l	Xtrriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	9942	wwPDB-VP
Average B, all atoms (Å ²)	59.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.10% 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

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	0.81	0/2731	0.90	4/3711 (0.1%)
1	B	0.80	0/2743	0.88	1/3727 (0.0%)
2	C	0.83	1/2306 (0.0%)	0.96	2/3140 (0.1%)
2	D	0.86	1/2306 (0.0%)	0.98	6/3140 (0.2%)
All	All	0.82	2/10086 (0.0%)	0.93	13/13718 (0.1%)

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
1	B	0	1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	73	CYS	CB-SG	-6.39	1.71	1.82
2	D	73	CYS	CB-SG	-5.33	1.73	1.81

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	26	LEU	CA-CB-CG	7.17	131.80	115.30
1	A	69	LEU	CA-CB-CG	6.76	130.84	115.30
1	A	69	LEU	CB-CG-CD1	-6.32	100.25	111.00
1	B	324	ASP	CB-CG-OD1	5.87	123.58	118.30
2	D	252	LEU	CA-CB-CG	5.70	128.41	115.30
2	C	252	LEU	CA-CB-CG	5.66	128.32	115.30
2	D	27	MET	N-CA-CB	-5.65	100.44	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^o)	Ideal(^o)
1	A	4	LEU	CA-CB-CG	-5.62	102.38	115.30
1	A	140	ASP	CB-CG-OD1	5.40	123.16	118.30
2	C	300	ILE	CB-CA-C	-5.28	101.03	111.60
2	D	27	MET	CA-CB-CG	5.28	122.28	113.30
2	D	152	ASP	N-CA-CB	-5.20	101.24	110.60
2	D	300	ILE	CB-CA-C	-5.07	101.46	111.60

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	1	MET	Peptide

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	2682	0	2641	71	0
1	B	2690	0	2650	81	0
2	C	2264	0	2280	102	0
2	D	2264	0	2280	83	0
3	A	6	0	8	4	0
3	B	6	0	8	4	0
4	A	13	0	0	3	0
4	B	6	0	0	3	0
4	C	6	0	0	1	0
4	D	5	0	0	0	0
All	All	9942	0	9867	299	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 15.

All (299) 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	1.30	1.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:218:HIS:NE2	3:A:401:GOL:H2	1.47	1.27
1:A:209:ASN:HD21	1:B:1:MET:CG	1.60	1.13
1:A:248:TYR:CE2	1:A:250:ARG:HD2	1.87	1.10
1:A:218:HIS:CE1	3:A:401:GOL:H2	1.87	1.09
1:B:218:HIS:CE1	3:B:401:GOL:H2	1.88	1.07
2:C:211:SER:HB3	2:D:300:ILE:HD11	1.14	1.07
2:C:211:SER:CB	2:D:300:ILE:HD11	1.85	1.07
1:B:218:HIS:NE2	3:B:401:GOL:C2	2.20	1.05
2:C:253:THR:HG23	2:C:276:GLU:HB3	1.41	1.03
1:A:218:HIS:NE2	3:A:401:GOL:C2	2.23	1.01
1:B:12:LEU:HD11	1:B:77:ILE:HG13	1.45	0.98
2:D:216:VAL:H	2:D:229:ASN:HD21	0.98	0.96
1:A:209:ASN:ND2	1:B:1:MET:CG	2.32	0.91
2:D:216:VAL:H	2:D:229:ASN:ND2	1.68	0.90
1:A:153:THR:O	1:A:157:GLU:HG3	1.71	0.90
1:A:352:LEU:HD22	1:A:354:TRP:HZ3	1.37	0.89
1:A:88:GLU:OE2	2:C:42:THR:HG21	1.76	0.86
1:A:152:ASN:ND2	1:A:184:GLY:HA3	1.92	0.85
2:C:173:ALA:HB3	2:D:173:ALA:HB3	1.59	0.85
1:A:352:LEU:HD22	1:A:354:TRP:CZ3	2.11	0.84
1:A:284:ASN:HB2	1:A:293:LEU:HD11	1.60	0.83
2:D:152:ASP:HB2	2:D:156:ARG:O	1.78	0.81
2:D:51:LYS:O	2:D:55:THR:HG23	1.80	0.81
2:C:211:SER:HB3	2:D:300:ILE:CD1	2.04	0.81
2:D:216:VAL:N	2:D:229:ASN:HD21	1.79	0.80
2:C:121:ALA:HB1	2:C:149:PRO:HD3	1.64	0.78
1:A:248:TYR:HE2	1:A:250:ARG:HD2	1.47	0.78
1:A:80:SER:HB2	1:A:109:ASP:OD1	1.84	0.78
2:C:188:LEU:HD13	2:D:188:LEU:HD13	1.66	0.78
1:A:3:LYS:HB3	1:A:5:ILE:HG12	1.68	0.74
1:B:30:GLN:HA	1:B:30:GLN:HE21	1.51	0.74
1:A:31:ASP:HB3	2:C:39:GLN:OE1	1.88	0.74
2:C:220:ASP:OD1	2:C:226:GLN:NE2	2.21	0.74
2:C:187:ASN:O	2:C:191:THR:HG23	1.89	0.73
1:B:2:LYS:HG2	1:B:2:LYS:O	1.89	0.72
2:C:216:VAL:H	2:C:229:ASN:ND2	1.88	0.72
1:B:153:THR:O	1:B:157:GLU:HG3	1.90	0.71
2:D:187:ASN:O	2:D:191:THR:HG23	1.90	0.71
1:B:76:GLU:HB3	4:B:501:HOH:O	1.91	0.70
2:C:201:HIS:CD2	2:D:202:LEU:HD11	2.27	0.70
2:C:212:MET:HE2	2:D:212:MET:HE2	1.74	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:258:LEU:HD21	2:D:288:LEU:HD13	1.75	0.69
2:C:216:VAL:H	2:C:229:ASN:HD21	1.38	0.69
2:C:212:MET:CE	2:D:212:MET:CE	2.71	0.68
2:C:237:ARG:HE	2:C:282:ILE:HD11	1.57	0.68
2:C:253:THR:CG2	2:C:276:GLU:HB3	2.20	0.68
1:B:352:LEU:HD22	1:B:354:TRP:CZ3	2.29	0.68
2:C:212:MET:HE3	2:D:212:MET:HG3	1.77	0.66
2:D:229:ASN:HD22	2:D:229:ASN:H	1.42	0.66
1:B:284:ASN:HB2	1:B:293:LEU:HD11	1.78	0.66
1:A:191:LEU:HD23	1:A:211:MET:HB3	1.77	0.66
1:B:105:ASN:O	1:B:144:THR:OG1	2.13	0.66
1:B:335:VAL:HG21	1:B:340:LEU:HD21	1.78	0.66
2:D:253:THR:CG2	2:D:276:GLU:HB3	2.26	0.66
1:B:171:ASP:O	1:B:175:GLU:HG2	1.96	0.65
1:B:255:TRP:CZ3	1:B:261:SER:HA	2.32	0.65
1:B:313:ARG:HG3	1:B:343:TRP:CD1	2.31	0.65
2:D:210:GLU:OE2	2:D:229:ASN:HB2	1.97	0.65
2:C:212:MET:HE3	2:D:212:MET:CE	2.26	0.65
2:C:87:ARG:HD3	2:C:104:ASP:OD2	1.98	0.63
2:C:76:PHE:CE1	2:C:87:ARG:HG2	2.34	0.63
2:C:219:TRP:CE3	2:C:248:ILE:HD13	2.33	0.63
1:A:203:SER:O	2:C:25:LYS:HE3	1.98	0.62
1:B:3:LYS:NZ	1:B:195:THR:O	2.33	0.62
2:D:236:LEU:HD13	2:D:252:LEU:HD11	1.81	0.62
2:C:68:MET:CE	2:D:173:ALA:HA	2.29	0.62
2:C:212:MET:CE	2:D:212:MET:HE2	2.30	0.61
1:A:233:GLN:O	1:A:237:GLU:HG2	1.99	0.61
2:D:150:LEU:O	2:D:158:THR:HG22	2.01	0.61
2:D:239:ASP:OD2	2:D:242:ALA:HB3	2.00	0.61
2:D:92:GLN:HA	2:D:95:GLN:HG3	1.83	0.61
2:C:212:MET:HE3	2:D:212:MET:HE3	1.83	0.60
2:D:29:ARG:HG2	2:D:136:PHE:O	2.00	0.60
1:A:48:LEU:HD12	1:A:100:LEU:HB3	1.83	0.60
1:A:4:LEU:HD22	1:B:328:PHE:CE2	2.37	0.59
1:A:301:THR:HG22	1:A:311:ILE:HD12	1.84	0.59
2:C:212:MET:CE	2:D:212:MET:HE3	2.32	0.58
1:B:174:ALA:O	1:B:178:ARG:HG3	2.04	0.58
2:C:132:ALA:HA	2:C:141:TRP:O	2.03	0.58
2:D:100:LEU:HD22	2:D:139:VAL:HG11	1.86	0.58
1:A:56:HIS:HA	1:A:321:THR:O	2.04	0.57
2:C:81:THR:O	2:C:82:ALA:HB3	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:49:LEU:HD22	1:B:101:LEU:HD22	1.86	0.56
1:B:49:LEU:C	1:B:49:LEU:HD23	2.26	0.56
2:C:217:ILE:HG12	2:C:228:ILE:HG13	1.85	0.56
2:D:152:ASP:HB3	2:D:156:ARG:H	1.70	0.56
2:D:91:PRO:O	2:D:95:GLN:HG2	2.04	0.56
2:D:210:GLU:OE2	2:D:229:ASN:CB	2.53	0.56
1:A:231:LEU:HD11	1:A:296:VAL:HG22	1.88	0.56
2:C:241:THR:O	2:C:243:SER:N	2.38	0.56
2:C:252:LEU:HD21	2:C:254:LEU:HD21	1.88	0.56
2:C:187:ASN:HB3	2:D:188:LEU:HD21	1.87	0.56
2:C:280:GLN:HG2	2:C:281:PHE:N	2.20	0.56
2:D:152:ASP:CB	2:D:156:ARG:O	2.52	0.55
1:A:17:ALA:O	1:A:21:LYS:HG3	2.07	0.55
1:B:191:LEU:HD23	1:B:211:MET:HB3	1.88	0.55
2:D:68:MET:HE1	2:D:71:ARG:HH11	1.72	0.55
1:A:9:GLN:H	1:A:9:GLN:NE2	2.04	0.55
2:C:173:ALA:O	2:C:176:PRO:HD2	2.07	0.54
2:C:220:ASP:HB3	2:C:222:GLN:H	1.72	0.54
1:B:37:ARG:HB3	1:B:39:ASP:OD1	2.08	0.54
1:A:76:GLU:HB2	1:A:79:LEU:HB2	1.90	0.54
1:B:62:GLY:O	1:B:350:PRO:HD2	2.07	0.54
2:C:255:PRO:HG3	2:C:274:THR:O	2.08	0.54
2:C:68:MET:HE3	2:D:173:ALA:HA	1.89	0.54
2:C:205:LEU:HD23	2:D:205:LEU:HB3	1.90	0.54
2:C:229:ASN:HD22	2:C:229:ASN:H	1.55	0.53
2:C:286:ILE:HA	2:C:302:LEU:O	2.08	0.53
1:B:11:VAL:O	1:B:15:GLN:HG3	2.09	0.53
1:B:165:GLU:OE1	1:B:165:GLU:HA	2.07	0.53
1:A:313:ARG:HG3	1:A:343:TRP:CD1	2.44	0.53
2:D:229:ASN:HD22	2:D:229:ASN:N	2.04	0.52
1:B:191:LEU:CD2	1:B:211:MET:HB3	2.39	0.52
1:A:156:ILE:HG12	1:A:180:LEU:HB3	1.91	0.52
1:B:134:ASP:OD1	1:B:134:ASP:N	2.42	0.52
2:C:163:LEU:C	2:C:163:LEU:HD23	2.30	0.52
1:A:4:LEU:HD22	1:B:328:PHE:HE2	1.73	0.52
2:C:278:GLN:O	2:C:278:GLN:CG	2.57	0.52
1:A:6:ASN:OD1	1:B:232:ASP:HB2	2.10	0.52
2:C:188:LEU:CD1	2:D:188:LEU:HD13	2.38	0.52
1:B:114:GLU:HG2	1:B:262:TRP:CH2	2.45	0.52
2:C:188:LEU:O	2:C:192:ASP:HB2	2.10	0.51
2:D:87:ARG:O	2:D:88:ASN:HB3	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:129:LYS:NZ	2:C:170:THR:HB	2.24	0.51
2:C:194:LEU:O	2:C:198:THR:CG2	2.57	0.51
1:A:40:ALA:HA	1:A:41:PRO:C	2.31	0.51
1:B:48:LEU:HD11	1:B:102:ILE:HD11	1.90	0.51
2:C:219:TRP:HB2	2:C:224:ASN:O	2.11	0.51
2:D:68:MET:CE	2:D:71:ARG:HH11	2.23	0.51
2:C:280:GLN:HG2	2:C:281:PHE:H	1.75	0.51
2:D:194:LEU:O	2:D:198:THR:HG23	2.11	0.51
1:B:53:GLY:HA2	1:B:79:LEU:O	2.11	0.51
1:A:152:ASN:HD21	1:A:184:GLY:HA3	1.72	0.51
1:B:231:LEU:HD11	1:B:296:VAL:HG22	1.93	0.51
1:A:56:HIS:CE1	1:A:217:ILE:HD12	2.46	0.50
1:B:203:SER:HB3	4:B:502:HOH:O	2.10	0.50
2:C:217:ILE:HD11	2:C:236:LEU:HD12	1.93	0.50
2:D:194:LEU:O	2:D:198:THR:CG2	2.59	0.50
2:D:65:TRP:CD2	2:D:89:GLY:HA2	2.45	0.50
1:A:83:PRO:HD3	1:A:112:ASN:OD1	2.11	0.50
2:C:278:GLN:O	2:C:278:GLN:HG2	2.10	0.50
2:D:50:LYS:HE3	2:D:79:ASP:HB2	1.92	0.50
1:A:196:VAL:HG13	4:A:501:HOH:O	2.10	0.50
2:C:194:LEU:O	2:C:198:THR:HG22	2.11	0.50
2:C:79:ASP:OD1	2:C:79:ASP:C	2.48	0.50
2:D:253:THR:HG22	2:D:276:GLU:HB3	1.93	0.50
2:C:208:LEU:HB3	2:D:209:LEU:HD21	1.93	0.50
1:B:335:VAL:HG12	1:B:339:THR:HG21	1.93	0.50
1:B:84:ASP:O	1:B:88:GLU:HG3	2.11	0.50
2:C:29:ARG:NH1	2:C:141:TRP:HZ2	2.10	0.50
1:A:4:LEU:CD2	1:B:328:PHE:HE2	2.25	0.49
1:A:315:LEU:HD11	1:A:352:LEU:HD21	1.94	0.49
1:B:212:GLU:OE2	1:B:221:PRO:HA	2.11	0.49
1:B:337:ASP:N	1:B:337:ASP:OD1	2.45	0.49
1:B:50:SER:O	1:B:72:ALA:HA	2.12	0.49
2:D:29:ARG:NH1	2:D:141:TRP:HZ2	2.10	0.49
1:A:84:ASP:O	1:A:88:GLU:HG3	2.12	0.49
2:C:144:ALA:CB	2:C:170:THR:HG23	2.43	0.49
2:C:76:PHE:CD1	2:C:87:ARG:HG2	2.47	0.49
2:D:152:ASP:HB3	2:D:156:ARG:N	2.28	0.49
1:A:253:ARG:HD2	1:A:262:TRP:HB3	1.95	0.49
2:D:175:LEU:HB3	2:D:176:PRO:CD	2.43	0.49
2:C:131:MET:HB2	2:C:167:VAL:HG23	1.94	0.48
1:B:63:TYR:O	1:B:68:MET:HB3	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:191:LEU:CD2	1:A:211:MET:HB3	2.44	0.48
1:B:108:GLY:O	1:B:112:ASN:ND2	2.46	0.48
1:B:48:LEU:O	1:B:70:SER:HB2	2.13	0.48
2:C:80:GLU:HG3	2:C:158:THR:HA	1.95	0.48
1:B:231:LEU:HD11	1:B:296:VAL:CG2	2.44	0.48
2:C:144:ALA:HB3	2:C:170:THR:HG23	1.96	0.48
1:B:29:HIS:O	1:B:33:VAL:HA	2.14	0.48
1:B:27:THR:OG1	1:B:38:ALA:HA	2.13	0.48
1:B:60:HIS:NE2	1:B:104:LYS:NZ	2.49	0.48
2:C:68:MET:HE3	2:D:176:PRO:HG2	1.95	0.48
1:A:86:ILE:HD13	1:A:113:PHE:CD2	2.49	0.48
2:C:13:SER:N	4:C:406:HOH:O	2.47	0.48
2:D:224:ASN:N	2:D:224:ASN:ND2	2.62	0.48
1:B:9:GLN:HE21	1:B:9:GLN:H	1.61	0.47
2:C:175:LEU:HB3	2:C:176:PRO:HD3	1.96	0.47
1:A:218:HIS:CE1	3:A:401:GOL:C2	2.79	0.47
2:C:144:ALA:CB	2:C:170:THR:CG2	2.93	0.47
1:A:1:MET:HA	4:A:509:HOH:O	2.14	0.47
1:B:29:HIS:HD2	1:B:32:PRO:O	1.96	0.47
2:C:286:ILE:HG22	2:C:303:LEU:HD23	1.95	0.47
1:B:12:LEU:HD21	1:B:54:SER:CB	2.45	0.47
1:A:293:LEU:HA	1:A:293:LEU:HD23	1.61	0.47
1:B:100:LEU:HD11	1:B:130:VAL:HG23	1.97	0.47
2:C:154:LYS:HD2	2:C:154:LYS:H	1.79	0.47
1:B:11:VAL:HB	4:B:505:HOH:O	2.14	0.47
1:B:30:GLN:HA	1:B:30:GLN:NE2	2.24	0.47
2:C:148:THR:HG21	2:C:179:LEU:HD13	1.97	0.47
1:B:290:LEU:O	1:B:293:LEU:HB2	2.15	0.47
2:C:73:CYS:HA	2:C:93:THR:HG21	1.96	0.47
2:D:188:LEU:O	2:D:192:ASP:HB2	2.15	0.47
2:D:68:MET:HE1	2:D:71:ARG:NH1	2.30	0.47
1:B:132:ILE:HA	1:B:181:ASN:OD1	2.14	0.46
2:C:184:GLU:HG3	2:C:188:LEU:HD22	1.97	0.46
2:D:229:ASN:H	2:D:229:ASN:ND2	2.12	0.46
2:C:241:THR:C	2:C:243:SER:H	2.18	0.46
2:D:268:LEU:O	2:D:287:THR:HA	2.15	0.46
1:B:45:LYS:HD3	1:B:165:GLU:OE1	2.15	0.46
2:C:268:LEU:O	2:C:287:THR:HG23	2.16	0.46
1:B:194:CYS:HA	1:B:324:ASP:OD1	2.15	0.46
1:A:231:LEU:CD1	1:A:296:VAL:HG22	2.45	0.46
2:D:175:LEU:HB3	2:D:176:PRO:HD3	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:254:PHE:CZ	1:A:263:GLN:HG2	2.50	0.46
1:A:92:GLN:OE1	1:A:92:GLN:HA	2.15	0.46
2:C:292:ILE:HA	2:C:297:THR:HG23	1.98	0.46
2:C:211:SER:HB2	2:D:300:ILE:HD11	1.89	0.46
1:A:255:TRP:HB2	1:A:262:TRP:CZ3	2.51	0.46
2:C:208:LEU:HD12	2:C:208:LEU:HA	1.78	0.46
1:A:194:CYS:HA	1:A:324:ASP:OD1	2.17	0.45
1:A:280:ALA:O	1:A:314:ASN:HA	2.16	0.45
1:A:335:VAL:HG12	1:A:339:THR:HG21	1.98	0.45
1:B:23:HIS:CE1	1:B:350:PRO:HB3	2.51	0.45
2:C:129:LYS:HZ1	2:C:170:THR:HB	1.82	0.45
2:C:187:ASN:CB	2:D:188:LEU:HD21	2.47	0.45
2:D:95:GLN:H	2:D:95:GLN:HG2	1.60	0.45
2:C:241:THR:HG22	2:C:242:ALA:N	2.30	0.45
2:D:237:ARG:HD2	2:D:278:GLN:NE2	2.32	0.45
1:A:57:GLU:H	1:A:57:GLU:CD	2.19	0.44
2:C:116:CYS:O	2:C:120:LEU:HB2	2.17	0.44
1:B:2:LYS:CG	1:B:2:LYS:O	2.61	0.44
2:C:154:LYS:HD2	2:C:154:LYS:N	2.33	0.44
2:D:264:GLN:HG2	2:D:266:HIS:CE1	2.52	0.44
2:C:238:LEU:HD22	2:C:251:LEU:HD22	1.99	0.44
2:C:73:CYS:HB2	2:C:164:ALA:O	2.18	0.44
1:A:356:LYS:O	1:A:356:LYS:HG3	2.17	0.44
1:A:244:VAL:HG12	1:A:245:ASN:OD1	2.18	0.44
2:D:212:MET:HB3	2:D:213:ASP:H	1.41	0.44
1:A:336:ASP:C	1:A:336:ASP:OD1	2.56	0.44
2:D:214:ASP:N	2:D:214:ASP:OD2	2.50	0.44
1:B:7:ASP:CG	1:B:9:GLN:HE22	2.21	0.43
2:D:129:LYS:NZ	2:D:170:THR:HG21	2.33	0.43
2:C:211:SER:CB	2:D:300:ILE:CD1	2.76	0.43
2:D:228:ILE:HG13	2:D:232:ALA:HB3	2.00	0.43
1:B:174:ALA:O	1:B:178:ARG:CG	2.66	0.43
1:B:56:HIS:HB3	1:B:321:THR:O	2.18	0.43
2:C:212:MET:HE3	2:D:212:MET:CG	2.47	0.43
2:D:73:CYS:HB2	2:D:164:ALA:O	2.18	0.43
2:C:255:PRO:HD2	2:C:258:LEU:HB2	1.99	0.43
1:A:36:THR:HG22	1:A:93:VAL:CG1	2.48	0.43
2:C:29:ARG:NH1	2:C:141:TRP:CZ2	2.86	0.43
2:C:229:ASN:O	2:C:230:ALA:C	2.57	0.43
2:C:300:ILE:HG21	2:C:300:ILE:HD13	1.74	0.43
2:D:254:LEU:HA	2:D:255:PRO:HD2	1.80	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:200:ARG:HD2	2:C:200:ARG:HA	1.87	0.43
2:C:207:ALA:HA	2:C:210:GLU:HB2	2.00	0.43
1:A:86:ILE:HD13	1:A:113:PHE:CG	2.54	0.43
1:A:140:ASP:HA	1:A:144:THR:O	2.19	0.43
1:A:201:LYS:HE2	1:A:201:LYS:HB3	1.70	0.43
1:B:280:ALA:O	1:B:314:ASN:HA	2.19	0.43
2:D:51:LYS:HE3	2:D:51:LYS:HB3	1.64	0.43
1:B:178:ARG:HD3	1:B:254[A]:PHE:CE1	2.54	0.42
4:A:505:HOH:O	1:B:291:SER:HB3	2.19	0.42
2:C:79:ASP:HB3	2:C:85:LEU:HD11	2.01	0.42
1:A:180:LEU:HA	1:A:180:LEU:HD23	1.86	0.42
1:B:158:LYS:HG2	1:B:343:TRP:CZ3	2.54	0.42
1:B:178:ARG:HD3	1:B:254[A]:PHE:CZ	2.54	0.42
1:B:254[A]:PHE:HZ	1:B:267:GLN:HE22	1.67	0.42
1:A:338:GLU:OE1	1:A:338:GLU:N	2.42	0.42
1:B:233:GLN:O	1:B:237:GLU:HG2	2.20	0.42
1:B:29:HIS:CD2	1:B:30:GLN:O	2.73	0.42
2:C:212:MET:HE2	2:D:212:MET:CE	2.40	0.42
1:A:174:ALA:HB1	1:A:178:ARG:NH2	2.35	0.42
1:A:44:GLY:C	1:A:97:GLU:HG3	2.40	0.42
1:B:255:TRP:CZ3	1:B:261:SER:CA	3.02	0.42
2:D:214:ASP:OD1	2:D:304:HIS:ND1	2.39	0.42
2:C:277:SER:O	2:C:278:GLN:C	2.58	0.42
2:D:148:THR:HG21	2:D:179:LEU:HA	2.02	0.42
2:C:202:LEU:HD22	2:D:205:LEU:HD22	2.02	0.42
1:B:303:ARG:HA	1:B:303:ARG:HD2	1.77	0.41
2:D:129:LYS:HE3	2:D:170:THR:HG21	2.02	0.41
1:A:278:VAL:HG12	1:A:334:LYS:HA	2.02	0.41
1:A:134:ASP:N	1:A:134:ASP:OD1	2.53	0.41
1:A:48:LEU:HA	1:A:48:LEU:HD12	1.92	0.41
2:C:49:ARG:NH1	2:C:50:LYS:HE3	2.35	0.41
1:B:23:HIS:HA	1:B:24:PRO:HD2	1.90	0.41
1:B:30:GLN:HE21	1:B:30:GLN:CA	2.27	0.41
2:C:165:CYS:HB2	2:C:166:PRO:HD2	2.02	0.41
1:B:140:ASP:OD1	1:B:146:GLY:N	2.53	0.41
2:C:246:ARG:HG2	2:C:250:GLU:OE1	2.20	0.41
2:C:212:MET:HG3	2:D:212:MET:HE3	2.01	0.41
2:D:183:ARG:O	2:D:187:ASN:HB2	2.21	0.41
1:A:347:VAL:O	1:A:353:ASN:HA	2.21	0.41
2:C:175:LEU:HA	2:C:175:LEU:HD12	1.83	0.40
1:B:207:ALA:HB3	1:B:210:GLU:OE1	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:20:TRP:O	2:C:24:ASN:HB2	2.22	0.40
2:D:36:HIS:O	2:D:106:THR:HA	2.20	0.40
2:C:205:LEU:HG	2:D:209:LEU:CD1	2.51	0.40
1:A:58:PRO:HD2	1:A:319:TYR:O	2.21	0.40
2:C:173:ALA:HA	2:D:68:MET:HE3	2.03	0.40
1:A:65:GLY:N	1:A:349:THR:HG22	2.36	0.40
2:D:120:LEU:HD23	2:D:120:LEU:HA	1.92	0.40
1:A:26:LEU:HD22	1:A:64:ILE:CG2	2.51	0.40
1:B:102:ILE:HG23	1:B:132:ILE:HD11	2.04	0.40
1:B:218:HIS:NE2	3:B:401:GOL:O2	2.52	0.40
1:B:56:HIS:O	1:B:57:GLU:C	2.59	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%)	312 (88%)	34 (10%)	8 (2%)	6	13
1	B	355/356 (100%)	315 (89%)	38 (11%)	2 (1%)	25	46
2	C	292/318 (92%)	262 (90%)	22 (8%)	8 (3%)	5	11
2	D	292/318 (92%)	269 (92%)	19 (6%)	4 (1%)	11	24
All	All	1293/1348 (96%)	1158 (90%)	113 (9%)	22 (2%)	9	20

All (22) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	C	220	ASP
2	D	212	MET
1	A	105	ASN
1	A	107	THR

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Mol	Chain	Res	Type
1	A	140	ASP
2	C	40	GLY
2	C	241	THR
2	C	242	ALA
2	C	265	ALA
2	D	242	ALA
1	B	141	SER
2	C	155	GLY
2	D	240	ALA
2	D	230	ALA
1	A	46	VAL
1	A	135	ASP
1	A	166	ARG
1	A	323	LEU
2	C	231	GLN
2	C	115	THR
1	A	150	VAL
1	B	150	VAL

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	287/288 (100%)	262 (91%)	25 (9%)	10	21
1	B	288/288 (100%)	262 (91%)	26 (9%)	9	19
2	C	241/260 (93%)	199 (83%)	42 (17%)	2	2
2	D	241/260 (93%)	192 (80%)	49 (20%)	1	1
All	All	1057/1096 (96%)	915 (87%)	142 (13%)	4	7

All (142) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	LYS
1	A	7	ASP
1	A	9	GLN

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Mol	Chain	Res	Type
1	A	12	LEU
1	A	31	ASP
1	A	33	VAL
1	A	45	LYS
1	A	77	ILE
1	A	92	GLN
1	A	130	VAL
1	A	141	SER
1	A	142	LEU
1	A	158	LYS
1	A	201	LYS
1	A	205	THR
1	A	229	SER
1	A	233	GLN
1	A	250	ARG
1	A	253	ARG
1	A	274	SER
1	A	289	PRO
1	A	291	SER
1	A	302	THR
1	A	310	THR
1	A	339	THR
1	B	2	LYS
1	B	8	VAL
1	B	9	GLN
1	B	12	LEU
1	B	15	GLN
1	B	27	THR
1	B	30	GLN
1	B	102	ILE
1	B	109	ASP
1	B	134	ASP
1	B	138	VAL
1	B	139	LYS
1	B	144	THR
1	B	178	ARG
1	B	196	VAL
1	B	201	LYS
1	B	211	MET
1	B	250	ARG
1	B	258	GLN
1	B	259	GLN

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Mol	Chain	Res	Type
1	B	291	SER
1	B	301	THR
1	B	305	GLN
1	B	306	GLN
1	B	337	ASP
1	B	339	THR
2	C	24	ASN
2	C	26	LEU
2	C	27	MET
2	C	33	ASN
2	C	42	THR
2	C	50	LYS
2	C	63	ASP
2	C	88	ASN
2	C	92	GLN
2	C	120	LEU
2	C	142	ASN
2	C	150	LEU
2	C	154	LYS
2	C	156	ARG
2	C	170	THR
2	C	188	LEU
2	C	191	THR
2	C	195	LEU
2	C	197	GLU
2	C	198	THR
2	C	202	LEU
2	C	205	LEU
2	C	208	LEU
2	C	216	VAL
2	C	220	ASP
2	C	229	ASN
2	C	239	ASP
2	C	243	SER
2	C	244	GLN
2	C	246	ARG
2	C	248	ILE
2	C	250	GLU
2	C	252	LEU
2	C	253	THR
2	C	258	LEU
2	C	266	HIS

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Mol	Chain	Res	Type
2	C	272	GLU
2	C	278	GLN
2	C	285	VAL
2	C	289	LYS
2	C	295	GLN
2	C	297	THR
2	D	13	SER
2	D	26	LEU
2	D	29	ARG
2	D	30	GLU
2	D	34	VAL
2	D	42	THR
2	D	45	SER
2	D	51	LYS
2	D	62	GLU
2	D	63	ASP
2	D	78	LEU
2	D	80	GLU
2	D	86	SER
2	D	88	ASN
2	D	95	GLN
2	D	120	LEU
2	D	142	ASN
2	D	150	LEU
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	202	LEU
2	D	208	LEU
2	D	212	MET
2	D	214	ASP
2	D	216	VAL
2	D	224	ASN

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Mol	Chain	Res	Type
2	D	229	ASN
2	D	237	ARG
2	D	239	ASP
2	D	251	LEU
2	D	252	LEU
2	D	253	THR
2	D	257	VAL
2	D	258	LEU
2	D	269	LYS
2	D	282	ILE
2	D	285	VAL
2	D	294	THR
2	D	300	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	9	GLN
1	A	183	GLN
1	A	185	HIS
1	A	209	ASN
1	B	9	GLN
1	B	29	HIS
1	B	30	GLN
1	B	183	GLN
1	B	185	HIS
1	B	249	HIS
1	B	267	GLN
1	B	305	GLN
1	B	314	ASN
2	C	88	ASN
2	C	201	HIS
2	C	229	ASN
2	D	58	GLN
2	D	88	ASN
2	D	224	ASN
2	D	229	ASN
2	D	266	HIS
2	D	278	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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

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	B	401	-	5,5,5	0.37	0	5,5,5	1.08	0
3	GOL	A	401	-	5,5,5	0.56	0	5,5,5	0.63	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	401	-	-	1/4/4/4	-
3	GOL	A	401	-	-	2/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (3) torsion outliers are listed below:

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

There are no ring outliers.

2 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	401	GOL	4	0
3	A	401	GOL	4	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	356/356 (100%)	-0.12	6 (1%) 70 66	40, 59, 78, 87	0
1	B	356/356 (100%)	-0.09	7 (1%) 65 60	42, 58, 78, 92	0
2	C	294/318 (92%)	-0.13	5 (1%) 70 66	35, 54, 93, 120	0
2	D	294/318 (92%)	-0.12	7 (2%) 59 54	35, 53, 92, 113	0
All	All	1300/1348 (96%)	-0.11	25 (1%) 66 62	35, 57, 85, 120	0

All (25) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	C	296	GLY	4.6
1	A	258	GLN	3.8
2	C	292	ILE	3.7
2	D	294	THR	3.3
2	C	294	THR	3.0
2	C	293	GLU	3.0
2	C	297	THR	2.9
1	B	356	LYS	2.9
1	B	270	GLN	2.9
2	D	292	ILE	2.8
2	D	296	GLY	2.8
1	B	259	GLN	2.8
1	B	249	HIS	2.6
1	B	141	SER	2.4
1	A	336	ASP	2.4
1	A	98	GLY	2.4
1	B	42	VAL	2.3
1	A	339	THR	2.3
2	D	306	VAL	2.2
1	B	268	THR	2.2
1	A	259	GLN	2.2

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Mol	Chain	Res	Type	RSRZ
2	D	265	ALA	2.1
2	D	295	GLN	2.1
2	D	293	GLU	2.1
1	A	95	GLY	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 carbohydrates 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	0.96	0.23	64,67,68,69	0
3	GOL	A	401	6/6	0.96	0.17	58,59,60,62	0

6.5 Other polymers [i](#)

There are no such residues in this entry.