Full wwPDB X-ray Structure Validation Report (i)

May 21, 2020 – 03:02 am BST

PDB ID	:	4E1J
Title	:	Crystal structure of glycerol kinase in complex with glycerol from Sinorhizobium meliloti 1021
Authors	:	Agarwal, R.; Chamala, S.; Evans, B.; Foti, R.; Gizzi, A.; Hillerich, B.; Kar, A.; Lafleur, J.; Siedel, R.; Villigas, G.; Zencheck, W.; Almo, S.C.; Swaminathan, S.; New York Structural Genomics Research Consortium (NYSGRC)
Deposited on	:	2012-03-06
Resolution	:	2.33 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 (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

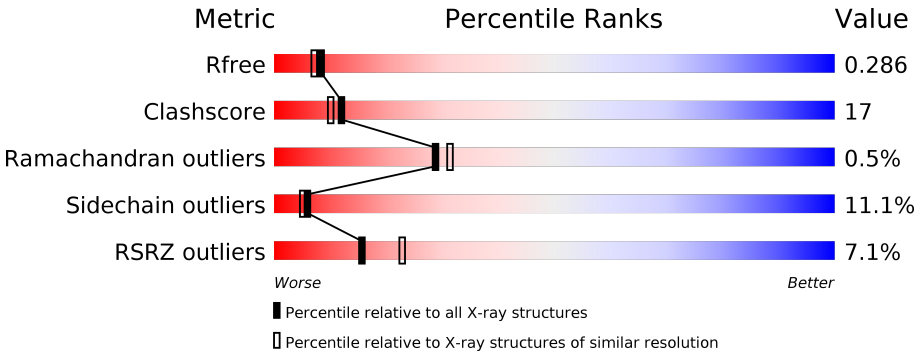
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA,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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.33 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	2096 (2.36-2.32)
Clashscore	141614	2193 (2.36-2.32)
Ramachandran outliers	138981	2159 (2.36-2.32)
Sidechain outliers	138945	2160 (2.36-2.32)
RSRZ outliers	127900	2067 (2.36-2.32)

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 <=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	520	2% 72% 18% 6%
1	B	520	% 65% 23% 6% 7%
1	C	520	3% 68% 25%
1	D	520	20% 60% 21% 16%

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 14333 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 Glycerol kinase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	498	Total	C	N	O	S	Se	0	0	0
			3754	2382	650	706	8	8			
1	B	484	Total	C	N	O	S	Se	0	0	0
			3678	2332	642	688	8	8			
1	C	503	Total	C	N	O	S	Se	0	0	0
			3774	2387	654	716	8	9			
1	D	437	Total	C	N	O	S	Se	0	0	0
			3009	1875	533	587	8	6			

There are 92 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MSE	-	EXPRESSION TAG	UNP O86033
A	2	HIS	-	EXPRESSION TAG	UNP O86033
A	3	HIS	-	EXPRESSION TAG	UNP O86033
A	4	HIS	-	EXPRESSION TAG	UNP O86033
A	5	HIS	-	EXPRESSION TAG	UNP O86033
A	6	HIS	-	EXPRESSION TAG	UNP O86033
A	7	HIS	-	EXPRESSION TAG	UNP O86033
A	8	SER	-	EXPRESSION TAG	UNP O86033
A	9	SER	-	EXPRESSION TAG	UNP O86033
A	10	GLY	-	EXPRESSION TAG	UNP O86033
A	11	VAL	-	EXPRESSION TAG	UNP O86033
A	12	ASP	-	EXPRESSION TAG	UNP O86033
A	13	LEU	-	EXPRESSION TAG	UNP O86033
A	14	GLY	-	EXPRESSION TAG	UNP O86033
A	15	THR	-	EXPRESSION TAG	UNP O86033
A	16	GLU	-	EXPRESSION TAG	UNP O86033
A	17	ASN	-	EXPRESSION TAG	UNP O86033
A	18	LEU	-	EXPRESSION TAG	UNP O86033
A	19	TYR	-	EXPRESSION TAG	UNP O86033
A	20	PHE	-	EXPRESSION TAG	UNP O86033
A	21	GLN	-	EXPRESSION TAG	UNP O86033

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Chain	Residue	Modelled	Actual	Comment	Reference
A	22	SER	-	EXPRESSION TAG	UNP O86033
A	23	MSE	-	EXPRESSION TAG	UNP O86033
B	1	MSE	-	EXPRESSION TAG	UNP O86033
B	2	HIS	-	EXPRESSION TAG	UNP O86033
B	3	HIS	-	EXPRESSION TAG	UNP O86033
B	4	HIS	-	EXPRESSION TAG	UNP O86033
B	5	HIS	-	EXPRESSION TAG	UNP O86033
B	6	HIS	-	EXPRESSION TAG	UNP O86033
B	7	HIS	-	EXPRESSION TAG	UNP O86033
B	8	SER	-	EXPRESSION TAG	UNP O86033
B	9	SER	-	EXPRESSION TAG	UNP O86033
B	10	GLY	-	EXPRESSION TAG	UNP O86033
B	11	VAL	-	EXPRESSION TAG	UNP O86033
B	12	ASP	-	EXPRESSION TAG	UNP O86033
B	13	LEU	-	EXPRESSION TAG	UNP O86033
B	14	GLY	-	EXPRESSION TAG	UNP O86033
B	15	THR	-	EXPRESSION TAG	UNP O86033
B	16	GLU	-	EXPRESSION TAG	UNP O86033
B	17	ASN	-	EXPRESSION TAG	UNP O86033
B	18	LEU	-	EXPRESSION TAG	UNP O86033
B	19	TYR	-	EXPRESSION TAG	UNP O86033
B	20	PHE	-	EXPRESSION TAG	UNP O86033
B	21	GLN	-	EXPRESSION TAG	UNP O86033
B	22	SER	-	EXPRESSION TAG	UNP O86033
B	23	MSE	-	EXPRESSION TAG	UNP O86033
C	1	MSE	-	EXPRESSION TAG	UNP O86033
C	2	HIS	-	EXPRESSION TAG	UNP O86033
C	3	HIS	-	EXPRESSION TAG	UNP O86033
C	4	HIS	-	EXPRESSION TAG	UNP O86033
C	5	HIS	-	EXPRESSION TAG	UNP O86033
C	6	HIS	-	EXPRESSION TAG	UNP O86033
C	7	HIS	-	EXPRESSION TAG	UNP O86033
C	8	SER	-	EXPRESSION TAG	UNP O86033
C	9	SER	-	EXPRESSION TAG	UNP O86033
C	10	GLY	-	EXPRESSION TAG	UNP O86033
C	11	VAL	-	EXPRESSION TAG	UNP O86033
C	12	ASP	-	EXPRESSION TAG	UNP O86033
C	13	LEU	-	EXPRESSION TAG	UNP O86033
C	14	GLY	-	EXPRESSION TAG	UNP O86033
C	15	THR	-	EXPRESSION TAG	UNP O86033
C	16	GLU	-	EXPRESSION TAG	UNP O86033
C	17	ASN	-	EXPRESSION TAG	UNP O86033

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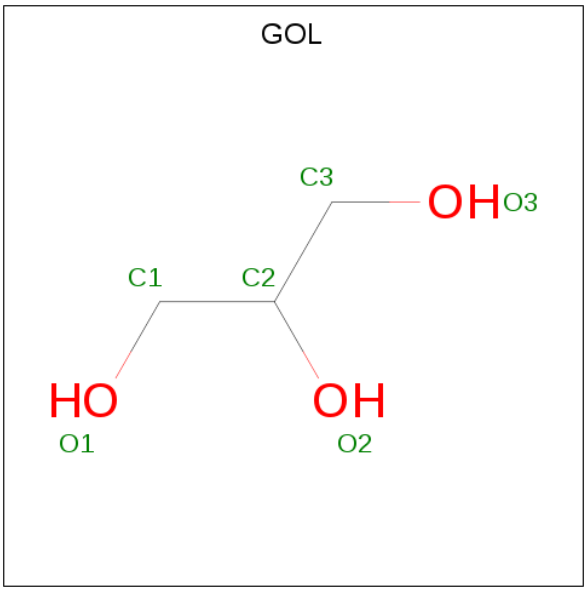
Chain	Residue	Modelled	Actual	Comment	Reference
C	18	LEU	-	EXPRESSION TAG	UNP O86033
C	19	TYR	-	EXPRESSION TAG	UNP O86033
C	20	PHE	-	EXPRESSION TAG	UNP O86033
C	21	GLN	-	EXPRESSION TAG	UNP O86033
C	22	SER	-	EXPRESSION TAG	UNP O86033
C	23	MSE	-	EXPRESSION TAG	UNP O86033
D	1	MSE	-	EXPRESSION TAG	UNP O86033
D	2	HIS	-	EXPRESSION TAG	UNP O86033
D	3	HIS	-	EXPRESSION TAG	UNP O86033
D	4	HIS	-	EXPRESSION TAG	UNP O86033
D	5	HIS	-	EXPRESSION TAG	UNP O86033
D	6	HIS	-	EXPRESSION TAG	UNP O86033
D	7	HIS	-	EXPRESSION TAG	UNP O86033
D	8	SER	-	EXPRESSION TAG	UNP O86033
D	9	SER	-	EXPRESSION TAG	UNP O86033
D	10	GLY	-	EXPRESSION TAG	UNP O86033
D	11	VAL	-	EXPRESSION TAG	UNP O86033
D	12	ASP	-	EXPRESSION TAG	UNP O86033
D	13	LEU	-	EXPRESSION TAG	UNP O86033
D	14	GLY	-	EXPRESSION TAG	UNP O86033
D	15	THR	-	EXPRESSION TAG	UNP O86033
D	16	GLU	-	EXPRESSION TAG	UNP O86033
D	17	ASN	-	EXPRESSION TAG	UNP O86033
D	18	LEU	-	EXPRESSION TAG	UNP O86033
D	19	TYR	-	EXPRESSION TAG	UNP O86033
D	20	PHE	-	EXPRESSION TAG	UNP O86033
D	21	GLN	-	EXPRESSION TAG	UNP O86033
D	22	SER	-	EXPRESSION TAG	UNP O86033
D	23	MSE	-	EXPRESSION TAG	UNP O86033

- Molecule 2 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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

- Molecule 3 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Na 1 1	0	0
3	C	1	Total Na 1 1	0	0

- Molecule 4 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	C	1	Total Cl 1 1	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	21	Total O 21 21	0	0

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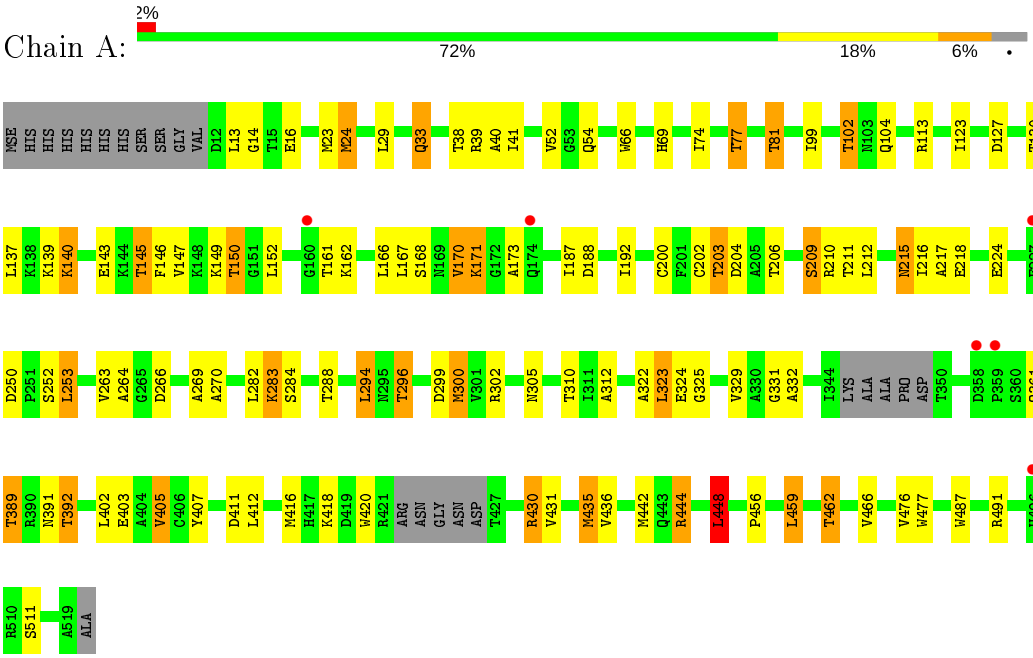
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	B	28	Total O 28 28	0	0
5	C	24	Total O 24 24	0	0
5	D	24	Total O 24 24	0	0

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.

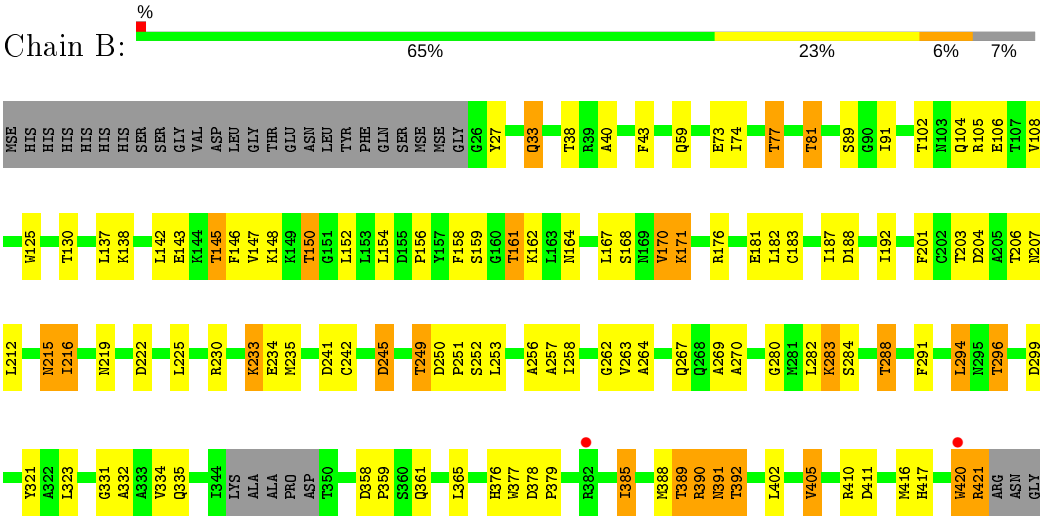
- Molecule 1: Glycerol kinase

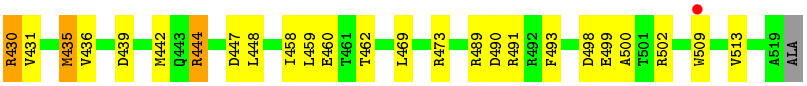
Chain A:



- Molecule 1: Glycerol kinase

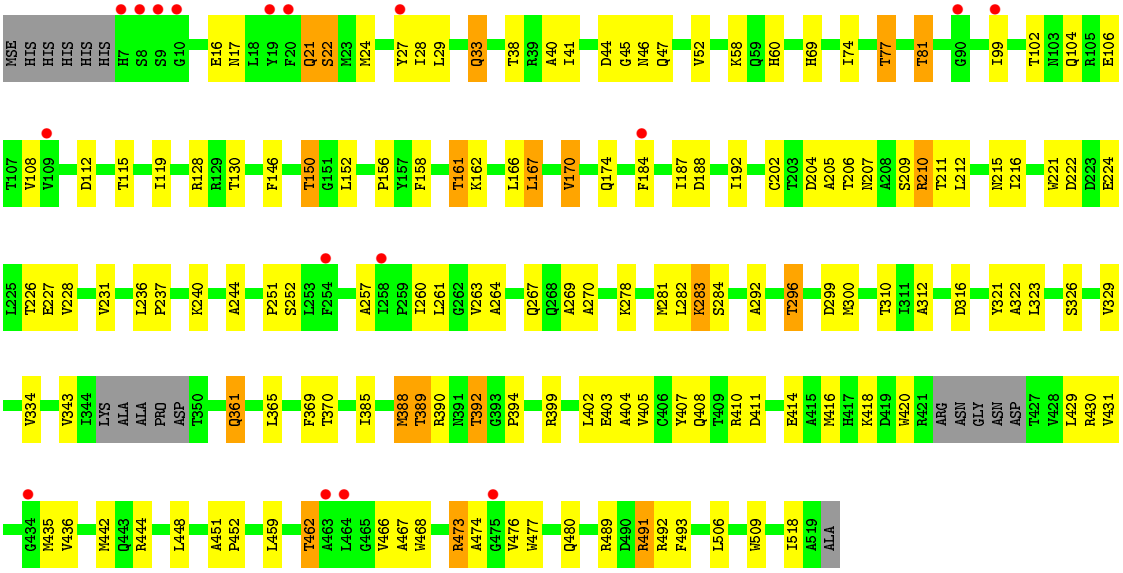
Chain B:





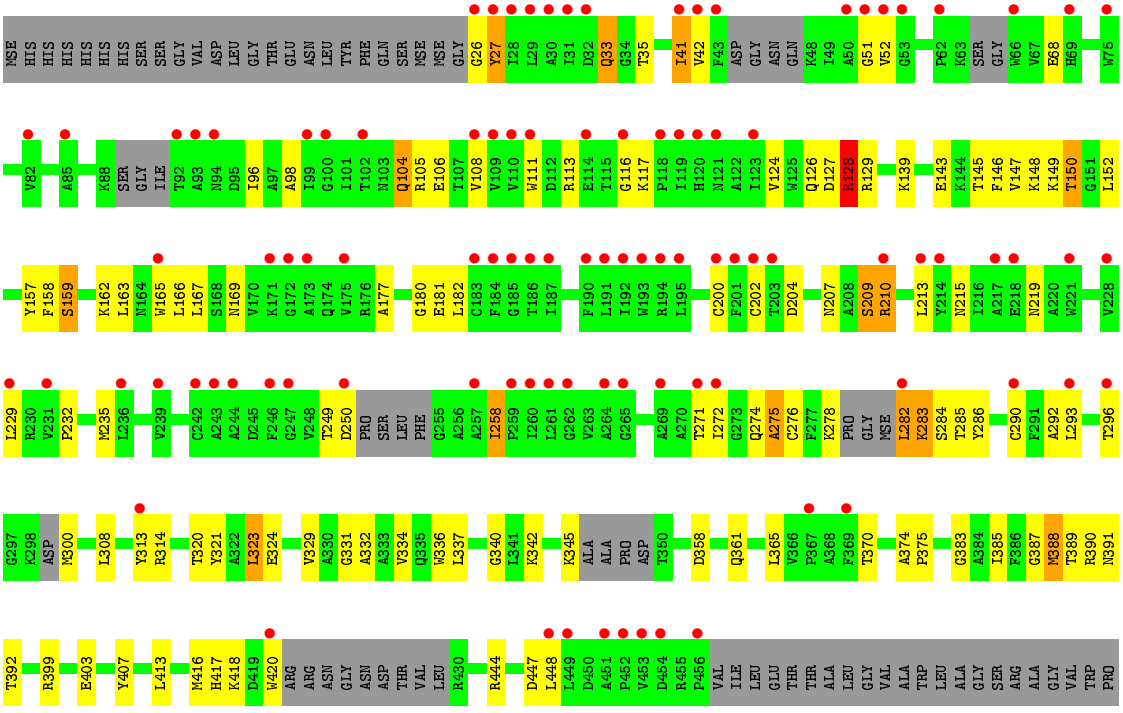
• Molecule 1: Glycerol kinase

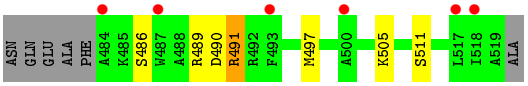
Chain C:



• Molecule 1: Glycerol kinase

Chain D:




ASN
GLN
GLU
ALA
PHE
A484
K485
S486
W487
A488
R489
D490
R491
R492
F493
M497
A500
K505
S511
L517
I518
A519
ALA

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	93.22Å 101.97Å 107.55Å 90.00° 90.03° 90.00°	Depositor
Resolution (Å)	47.57 – 2.33 47.57 – 2.33	Depositor EDS
% Data completeness (in resolution range)	99.9 (47.57-2.33) 99.8 (47.57-2.33)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.95 (at 2.34Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.230 , 0.290 0.229 , 0.286	Depositor DCC
R_{free} test set	4303 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å^2)	47.3	Xtriage
Anisotropy	0.042	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 24.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.29$	Xtriage
Estimated twinning fraction	0.125 for h,-k,-l	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	14333	wwPDB-VP
Average B, all atoms (Å^2)	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.39% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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, CL, NA

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	0.87	0/3824	0.88	5/5191 (0.1%)
1	B	0.88	1/3748 (0.0%)	0.87	3/5085 (0.1%)
1	C	0.75	0/3844	0.80	1/5220 (0.0%)
1	D	0.59	0/3057	0.71	1/4169 (0.0%)
All	All	0.79	1/14473 (0.0%)	0.82	10/19665 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	209	SER	CB-OG	-5.24	1.35	1.42

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	410	ARG	NE-CZ-NH2	-5.78	117.41	120.30
1	B	241	ASP	CB-CG-OD1	5.69	123.42	118.30
1	A	448	LEU	CB-CG-CD1	5.60	120.51	111.00
1	A	209	SER	CB-CA-C	-5.43	99.78	110.10
1	B	430	ARG	NE-CZ-NH1	5.42	123.01	120.30
1	A	405	VAL	CG1-CB-CG2	-5.32	102.39	110.90
1	D	128	ARG	NE-CZ-NH2	-5.22	117.69	120.30
1	A	323	LEU	CA-CB-CG	5.15	127.14	115.30
1	A	300	MSE	CB-CG-SE	-5.07	97.50	112.70
1	C	399	ARG	NE-CZ-NH1	5.03	122.82	120.30

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	3754	0	3611	122	0
1	B	3678	0	3575	136	0
1	C	3774	0	3582	120	0
1	D	3009	0	2539	101	0
2	A	6	0	8	0	0
2	B	6	0	8	2	0
2	C	6	0	7	1	0
3	A	1	0	0	0	0
3	C	1	0	0	0	0
4	C	1	0	0	0	0
5	A	21	0	0	2	0
5	B	28	0	0	3	0
5	C	24	0	0	1	0
5	D	24	0	0	1	0
All	All	14333	0	13330	473	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 17.

All (473) 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:171:LYS:HE2	1:B:171:LYS:H	1.07	1.11
1:B:282:LEU:CD1	1:B:416:MSE:HE1	1.80	1.11
1:C:402:LEU:O	1:C:405:VAL:HG12	1.52	1.10
1:D:361:GLN:HE22	1:D:392:THR:HG22	1.07	1.09
1:A:402:LEU:O	1:A:405:VAL:HG12	1.54	1.08
1:D:361:GLN:NE2	1:D:392:THR:HG22	1.70	1.06
1:B:411:ASP:OD2	1:B:509:TRP:HZ3	1.45	0.98
1:C:473:ARG:HG2	1:C:473:ARG:HH11	1.28	0.97
1:A:270:ALA:HB2	1:A:462:THR:HG22	1.44	0.95
1:B:270:ALA:HB2	1:B:462:THR:HG22	1.44	0.95
1:C:146:PHE:O	1:C:150:THR:HB	1.65	0.95
1:B:150:THR:HG22	1:B:152:LEU:H	1.31	0.94
1:B:411:ASP:OD2	1:B:509:TRP:CZ3	2.21	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:224:GLU:O	1:C:228:VAL:HG23	1.68	0.93
1:D:276:CYS:HA	1:D:278:LYS:HE3	1.52	0.92
1:B:282:LEU:HD12	1:B:416:MSE:HE1	1.48	0.92
1:B:74:ILE:O	1:B:77:THR:HG22	1.70	0.92
1:B:282:LEU:HD13	1:B:416:MSE:HE1	1.53	0.91
1:A:389:THR:H	1:A:392:THR:CG2	1.84	0.91
1:A:171:LYS:HE2	1:A:171:LYS:H	1.36	0.90
1:C:99:ILE:HG22	1:C:260:ILE:HG23	1.54	0.89
1:C:389:THR:H	1:C:392:THR:HG23	1.37	0.89
1:B:365:LEU:HD13	1:B:385:ILE:CD1	2.05	0.86
1:D:388:MSE:HA	1:D:392:THR:HG21	1.57	0.86
1:D:389:THR:H	1:D:392:THR:HG23	1.39	0.86
1:C:411:ASP:OD2	1:C:509:TRP:HZ3	1.59	0.85
1:A:170:VAL:HG22	1:A:173:ALA:HB2	1.58	0.84
1:A:77:THR:O	1:A:81:THR:HB	1.76	0.84
1:C:77:THR:O	1:C:81:THR:HB	1.78	0.84
1:B:365:LEU:HD13	1:B:385:ILE:HD13	1.60	0.83
1:B:171:LYS:HE2	1:B:171:LYS:N	1.91	0.83
1:B:33:GLN:HE22	1:B:104:GLN:HE21	1.23	0.83
1:A:150:THR:HG22	1:A:152:LEU:H	1.44	0.82
1:C:58:LYS:HD3	1:C:60:HIS:CE1	2.15	0.81
1:D:361:GLN:HE22	1:D:392:THR:CG2	1.92	0.79
1:D:105:ARG:HD2	1:D:210:ARG:HD3	1.64	0.79
1:D:163:LEU:HD12	1:D:166:LEU:HD12	1.65	0.79
1:B:389:THR:H	1:B:392:THR:CG2	1.96	0.79
1:C:206:THR:O	1:C:209:SER:HB3	1.83	0.78
1:D:249:THR:HG22	1:D:258:ILE:H	1.45	0.78
1:D:389:THR:H	1:D:392:THR:CG2	1.96	0.78
1:D:111:TRP:HD1	1:D:116:GLY:HA2	1.48	0.78
1:A:206:THR:O	1:A:209:SER:HB2	1.84	0.78
1:C:33:GLN:HE22	1:C:104:GLN:HE21	1.30	0.77
1:B:146:PHE:O	1:B:150:THR:HB	1.84	0.77
1:D:146:PHE:O	1:D:150:THR:HB	1.84	0.77
1:A:33:GLN:HE22	1:A:104:GLN:HE21	1.33	0.77
1:A:411:ASP:OD2	1:A:509:TRP:HZ3	1.69	0.76
1:B:431:VAL:HG12	1:B:436:VAL:HG11	1.66	0.76
1:C:150:THR:HG22	1:C:152:LEU:H	1.49	0.76
1:D:282:LEU:HA	1:D:293:LEU:O	1.86	0.76
1:B:389:THR:H	1:B:392:THR:HG23	1.49	0.76
1:C:282:LEU:CD1	1:C:416:MSE:HE1	2.16	0.75
1:B:288:THR:HG22	1:B:332:ALA:HB2	1.68	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:282:LEU:HD13	1:C:416:MSE:CE	2.16	0.75
1:D:283:LYS:HE2	1:D:293:LEU:HD13	1.67	0.75
1:C:38:THR:HB	1:C:77:THR:HG23	1.68	0.75
1:B:171:LYS:CE	1:B:171:LYS:H	1.95	0.74
1:D:274:GLN:HE21	1:D:283:LYS:HB2	1.51	0.74
1:A:491:ARG:HD2	5:A:707:HOH:O	1.86	0.74
1:B:282:LEU:HD13	1:B:416:MSE:CE	2.16	0.74
1:B:421:ARG:NE	1:B:421:ARG:HA	2.03	0.73
1:D:128:ARG:HD3	1:D:370:THR:O	1.88	0.73
1:A:389:THR:HG23	1:A:391:ASN:H	1.53	0.73
1:D:300:MSE:HG3	1:D:321:TYR:CE2	2.23	0.72
1:B:156:PRO:O	1:B:162:LYS:HE3	1.88	0.72
1:C:296:THR:HG23	1:C:299:ASP:O	1.88	0.72
1:D:145:THR:HA	1:D:148:LYS:HE2	1.71	0.72
1:D:491:ARG:HH11	1:D:491:ARG:CG	2.02	0.72
1:A:382:ARG:HD2	1:D:387:GLY:HA2	1.72	0.71
1:C:282:LEU:HD12	1:C:416:MSE:HE1	1.71	0.71
1:B:145:THR:HG22	1:B:148:LYS:NZ	2.05	0.71
1:D:389:THR:HG22	1:D:391:ASN:H	1.56	0.71
1:A:192:ILE:HD11	1:A:263:VAL:HG21	1.73	0.71
1:C:211:THR:O	1:C:212:LEU:HB2	1.89	0.70
1:D:148:LYS:HE3	1:D:149:LYS:HG3	1.73	0.70
1:B:150:THR:HG23	1:B:152:LEU:HG	1.74	0.70
1:C:102:THR:HG22	1:C:264:ALA:O	1.91	0.70
1:A:325:GLY:HA3	1:A:412:LEU:HD13	1.74	0.70
1:C:270:ALA:HB2	1:C:462:THR:HG22	1.75	0.69
1:C:361:GLN:HE21	1:C:392:THR:HG22	1.57	0.69
1:A:296:THR:HG23	1:A:299:ASP:O	1.91	0.69
1:A:215:ASN:HD22	1:A:217:ALA:H	1.40	0.69
1:A:171:LYS:N	1:A:171:LYS:HE2	2.07	0.69
1:C:40:ALA:CB	1:C:81:THR:HG23	2.24	0.68
1:B:431:VAL:CG1	1:B:436:VAL:HG11	2.23	0.68
1:A:38:THR:CB	1:A:77:THR:HG23	2.24	0.68
1:D:113:ARG:HH21	1:D:180:GLY:HA3	1.57	0.68
1:C:369:PHE:O	1:C:370:THR:HG23	1.94	0.68
1:D:271:THR:HG22	1:D:276:CYS:HB2	1.76	0.67
1:A:296:THR:HG21	5:A:713:HOH:O	1.93	0.67
1:A:361:GLN:HE22	1:A:392:THR:HB	1.59	0.67
1:C:221:TRP:CZ2	1:C:237:PRO:HD2	2.29	0.67
1:C:431:VAL:HG13	1:C:436:VAL:HG11	1.77	0.67
1:C:410:ARG:HE	1:C:506:LEU:HD22	1.60	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:40:ALA:HB2	1:B:81:THR:HG23	1.77	0.66
1:A:361:GLN:NE2	1:A:392:THR:HB	2.11	0.66
1:C:166:LEU:O	1:C:170:VAL:HG13	1.96	0.66
1:C:473:ARG:NH1	1:C:473:ARG:HG2	2.06	0.66
1:B:296:THR:CG2	1:B:299:ASP:O	2.44	0.65
1:C:119:ILE:HG23	1:C:170:VAL:HG21	1.76	0.65
1:C:17:ASN:O	1:C:21:GLN:HB2	1.96	0.65
1:C:150:THR:CG2	1:C:152:LEU:HB2	2.27	0.65
1:B:296:THR:HG23	1:B:299:ASP:O	1.97	0.65
1:D:33:GLN:HE22	1:D:104:GLN:HE21	1.43	0.65
1:A:74:ILE:O	1:A:77:THR:HG22	1.96	0.65
1:D:150:THR:HG22	1:D:152:LEU:H	1.61	0.64
1:B:365:LEU:HD13	1:B:385:ILE:HD11	1.79	0.64
1:C:22:SER:O	1:C:45:GLY:HA3	1.98	0.64
1:A:389:THR:CG2	1:A:391:ASN:OD1	2.46	0.64
1:B:389:THR:HG21	1:B:391:ASN:ND2	2.12	0.64
1:D:165:TRP:O	1:D:169:ASN:HB2	1.97	0.64
1:A:283:LYS:HG2	1:A:284:SER:N	2.13	0.64
1:B:458:ILE:HG23	1:B:460:GLU:OE1	1.98	0.64
1:B:365:LEU:CD1	1:B:385:ILE:HD13	2.28	0.64
1:A:296:THR:CG2	1:A:299:ASP:O	2.46	0.63
1:C:38:THR:CB	1:C:77:THR:HG23	2.27	0.63
1:A:102:THR:HG21	1:A:269:ALA:HB3	1.81	0.63
1:D:200:CYS:HG	1:D:202:CYS:HG	1.46	0.63
1:D:111:TRP:CD1	1:D:116:GLY:HA2	2.33	0.63
1:B:203:THR:HG21	5:B:716:HOH:O	1.98	0.63
1:D:491:ARG:HH11	1:D:491:ARG:HG3	1.63	0.63
1:A:166:LEU:O	1:A:170:VAL:HG13	1.99	0.63
1:C:411:ASP:OD2	1:C:509:TRP:CZ3	2.47	0.62
1:B:211:THR:O	1:B:212:LEU:HB2	1.98	0.62
1:C:389:THR:H	1:C:392:THR:CG2	2.10	0.62
1:C:40:ALA:HB2	1:C:81:THR:HG23	1.82	0.62
1:A:150:THR:CG2	1:A:152:LEU:HB2	2.29	0.62
1:C:33:GLN:HE21	1:C:187:ILE:HG21	1.63	0.62
1:A:282:LEU:CD1	1:A:416:MSE:HE1	2.29	0.62
1:B:390:ARG:HH22	1:C:370:THR:HG21	1.65	0.62
1:B:33:GLN:HE21	1:B:187:ILE:HG21	1.65	0.62
1:C:150:THR:HG22	1:C:152:LEU:N	2.14	0.62
1:C:251:PRO:HG3	1:C:257:ALA:HB2	1.81	0.62
1:B:188:ASP:OD2	1:B:203:THR:HG23	2.00	0.61
1:D:489:ARG:HG2	1:D:490:ASP:N	2.14	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:102:THR:HG22	1:B:264:ALA:O	2.01	0.61
1:A:389:THR:HG22	1:A:392:THR:HG22	1.83	0.61
1:B:130:THR:OG1	1:B:161:THR:CG2	2.48	0.61
1:B:361:GLN:HE22	1:B:392:THR:HG22	1.66	0.61
1:A:431:VAL:HG11	1:A:442:MSE:SE	2.50	0.61
1:A:38:THR:HB	1:A:77:THR:HG23	1.83	0.60
1:B:119:ILE:HD11	1:B:182:LEU:CD2	2.30	0.60
1:A:145:THR:HG21	1:A:224:GLU:OE1	2.01	0.60
1:D:389:THR:HG22	1:D:390:ARG:N	2.16	0.60
1:A:389:THR:HG23	1:A:391:ASN:OD1	2.00	0.60
1:D:105:ARG:NH2	1:D:324:GLU:OE2	2.27	0.60
1:B:389:THR:HG22	1:B:391:ASN:H	1.66	0.60
1:B:102:THR:HG21	1:B:269:ALA:CB	2.32	0.60
1:B:389:THR:CG2	1:B:391:ASN:ND2	2.64	0.60
1:D:163:LEU:CD1	1:D:166:LEU:HD12	2.32	0.60
1:A:389:THR:H	1:A:392:THR:HG21	1.65	0.60
1:B:389:THR:CG2	1:B:391:ASN:HD22	2.14	0.59
1:A:38:THR:OG1	1:A:77:THR:CG2	2.51	0.59
1:A:40:ALA:CB	1:A:81:THR:HG23	2.32	0.59
1:A:41:ILE:HG12	1:A:52:VAL:HG22	1.84	0.59
1:B:498:ASP:OD2	1:B:500:ALA:HB3	2.02	0.59
1:D:286:TYR:CE1	1:D:290:CYS:SG	2.90	0.59
1:A:250:ASP:HB3	1:A:253:LEU:HD22	1.83	0.59
1:C:102:THR:HG21	1:C:269:ALA:CB	2.33	0.59
1:A:411:ASP:OD2	1:A:509:TRP:CZ3	2.55	0.59
1:A:145:THR:O	1:A:149:LYS:HG2	2.02	0.59
1:C:312:ALA:HB2	1:C:322:ALA:HB2	1.85	0.59
1:A:102:THR:HG21	1:A:269:ALA:CB	2.33	0.58
1:D:447:ASP:HB3	1:D:497:MSE:HE3	1.84	0.58
1:A:40:ALA:HB2	1:A:81:THR:HG23	1.84	0.58
1:A:14:GLY:HA2	1:A:16:GLU:OE1	2.03	0.58
1:A:209:SER:HA	1:A:216:ILE:HD11	1.84	0.58
1:D:403:GLU:HB3	1:D:407:TYR:CE2	2.39	0.58
1:A:102:THR:HG22	1:A:264:ALA:O	2.04	0.58
1:C:388:MSE:HA	1:C:392:THR:HG21	1.84	0.58
1:D:403:GLU:OE1	1:D:505:LYS:NZ	2.36	0.57
1:A:188:ASP:OD2	1:A:203:THR:HG22	2.04	0.57
1:B:431:VAL:HG11	1:B:442:MSE:SE	2.54	0.57
1:B:209:SER:HA	1:B:216:ILE:HD11	1.85	0.57
1:B:249:THR:CG2	1:B:256:ALA:O	2.52	0.57
1:B:361:GLN:NE2	1:B:392:THR:HG22	2.18	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:113:ARG:HH21	1:D:180:GLY:CA	2.18	0.57
1:D:365:LEU:HD13	1:D:385:ILE:HG12	1.86	0.57
1:A:305:ASN:ND2	1:A:418:LYS:HE2	2.20	0.57
1:B:192:ILE:HD11	1:B:263:VAL:HG21	1.87	0.57
1:C:38:THR:OG1	1:C:77:THR:CG2	2.53	0.57
1:A:171:LYS:CE	1:A:171:LYS:H	2.15	0.57
1:D:337:LEU:O	1:D:342:LYS:N	2.38	0.57
1:C:216:ILE:HG23	1:C:321:TYR:HE1	1.69	0.57
1:A:300:MSE:HE2	1:A:302:ARG:HH22	1.69	0.56
1:C:108:VAL:HG13	1:C:184:PHE:HE1	1.70	0.56
1:C:267:GLN:HE21	2:C:602:GOL:H12	1.70	0.56
1:D:213:LEU:HD23	1:D:229:LEU:HD12	1.87	0.56
1:B:73:GLU:O	1:B:77:THR:HB	2.06	0.56
1:B:38:THR:HB	1:B:77:THR:HG23	1.87	0.56
1:A:130:THR:OG1	1:A:161:THR:CG2	2.54	0.56
1:B:206:THR:O	1:B:209:SER:HB2	2.06	0.56
1:B:245:ASP:OD1	1:B:473:ARG:NH2	2.35	0.56
1:C:150:THR:HG21	1:C:152:LEU:HB2	1.87	0.56
1:C:38:THR:OG1	1:C:77:THR:HG21	2.06	0.56
1:A:200:CYS:SG	1:A:202:CYS:SG	3.00	0.56
1:A:361:GLN:OE1	1:A:391:ASN:ND2	2.39	0.56
1:C:361:GLN:NE2	1:C:392:THR:HA	2.20	0.56
1:B:439:ASP:OD2	1:B:491:ARG:NH1	2.40	0.55
1:A:215:ASN:ND2	1:A:217:ALA:H	2.03	0.55
1:A:294:LEU:HB2	1:A:416:MSE:HE3	1.88	0.55
1:B:388:MSE:HA	1:B:392:THR:HG21	1.88	0.55
1:D:249:THR:HG22	1:D:258:ILE:N	2.19	0.55
1:A:152:LEU:HD11	1:A:209:SER:O	2.06	0.55
1:C:156:PRO:O	1:C:162:LYS:HE3	2.07	0.55
1:D:180:GLY:HA2	5:D:607:HOH:O	2.05	0.55
1:D:108:VAL:HG21	1:D:162:LYS:HB2	1.88	0.55
1:D:271:THR:CG2	1:D:276:CYS:HB2	2.37	0.55
1:C:150:THR:HG23	1:C:152:LEU:HD12	1.88	0.55
1:C:491:ARG:HG3	1:C:492:ARG:N	2.22	0.55
1:A:211:THR:O	1:A:212:LEU:HB2	2.07	0.55
1:C:192:ILE:HD11	1:C:263:VAL:HG21	1.87	0.55
1:D:111:TRP:HA	1:D:117:LYS:O	2.07	0.55
1:D:416:MSE:C	1:D:418:LYS:H	2.11	0.55
1:B:38:THR:CB	1:B:77:THR:HG23	2.36	0.54
1:B:38:THR:HG22	1:B:81:THR:HG21	1.89	0.54
1:A:146:PHE:O	1:A:150:THR:HB	2.06	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:296:THR:O	1:B:296:THR:HG23	2.07	0.54
1:A:430:ARG:HD2	1:A:487:TRP:CZ2	2.42	0.54
1:C:474:ALA:HB3	1:C:476:VAL:HG22	1.89	0.54
1:B:249:THR:HG22	1:B:256:ALA:O	2.06	0.54
1:C:410:ARG:O	1:C:414:GLU:HG2	2.07	0.54
1:A:29:LEU:HD23	1:A:99:ILE:HG12	1.90	0.54
1:A:33:GLN:HE21	1:A:187:ILE:HG21	1.72	0.54
1:C:29:LEU:HD23	1:C:99:ILE:HD11	1.90	0.54
1:D:300:MSE:HG3	1:D:321:TYR:CD2	2.43	0.54
1:D:283:LYS:O	1:D:292:ALA:HA	2.08	0.54
1:A:431:VAL:HG13	1:A:436:VAL:HG11	1.89	0.54
1:D:389:THR:CG2	1:D:390:ARG:N	2.71	0.54
1:B:294:LEU:HD13	1:B:416:MSE:HE3	1.90	0.53
1:C:130:THR:OG1	1:C:161:THR:CG2	2.56	0.53
1:A:444:ARG:HD2	1:A:448:LEU:HD22	1.90	0.53
1:D:283:LYS:CE	1:D:293:LEU:HD13	2.35	0.53
1:C:403:GLU:HB3	1:C:407:TYR:CE2	2.43	0.53
1:A:113:ARG:O	1:A:113:ARG:HG3	2.07	0.53
1:A:170:VAL:HA	1:A:171:LYS:HE2	1.90	0.53
1:B:145:THR:HG22	1:B:148:LYS:HZ3	1.72	0.53
1:C:343:VAL:O	1:C:394:PRO:HB3	2.07	0.53
1:C:296:THR:CG2	1:C:299:ASP:O	2.56	0.53
1:C:46:ASN:O	1:C:47:GLN:HB2	2.08	0.53
1:D:33:GLN:NE2	1:D:104:GLN:HE21	2.07	0.53
1:A:282:LEU:HD13	1:A:416:MSE:CE	2.38	0.53
1:A:130:THR:CB	1:A:161:THR:CG2	2.86	0.53
1:A:133:PHE:CE2	1:A:137:LEU:HD11	2.45	0.52
1:C:205:ALA:O	1:C:209:SER:HB2	2.09	0.52
1:B:130:THR:CB	1:B:161:THR:CG2	2.87	0.52
1:C:278:LYS:HB2	1:C:281:MSE:SE	2.60	0.52
1:C:410:ARG:NE	1:C:506:LEU:HD22	2.23	0.52
1:B:150:THR:HG22	1:B:152:LEU:N	2.11	0.52
1:A:294:LEU:HD13	1:A:416:MSE:HE3	1.91	0.52
1:B:417:HIS:CD2	1:B:421:ARG:HH11	2.28	0.52
1:B:291:PHE:CE1	2:B:601:GOL:H32	2.45	0.52
1:A:140:LYS:HE3	1:A:140:LYS:HA	1.91	0.52
1:B:143:GLU:O	1:B:147:VAL:HG23	2.10	0.52
1:D:329:VAL:HG13	1:D:332:ALA:HB3	1.91	0.52
1:A:431:VAL:O	1:A:456:PRO:HD3	2.10	0.51
1:B:106:GLU:HB2	1:B:125:TRP:HB3	1.91	0.51
1:B:249:THR:HB	1:B:258:ILE:H	1.75	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:282:LEU:HD23	1:D:282:LEU:N	2.25	0.51
1:C:404:ALA:O	1:C:408:GLN:HG3	2.11	0.51
1:A:23:MSE:O	1:A:24:MSE:CB	2.57	0.51
1:B:119:ILE:HG23	1:B:170:VAL:HG21	1.92	0.51
1:D:399:ARG:HG2	1:D:403:GLU:HG3	1.93	0.51
1:C:150:THR:HG22	1:C:152:LEU:CB	2.41	0.51
1:C:202:CYS:SG	1:C:240:LYS:HE2	2.51	0.51
1:C:282:LEU:CD1	1:C:416:MSE:CE	2.79	0.51
1:C:473:ARG:CG	1:C:473:ARG:HH11	2.10	0.51
1:A:300:MSE:HE2	1:A:302:ARG:NH2	2.25	0.50
1:C:106:GLU:OE2	1:C:210:ARG:HD3	2.11	0.50
1:C:74:ILE:O	1:C:77:THR:HG22	2.11	0.50
1:D:274:GLN:NE2	1:D:283:LYS:HB2	2.23	0.50
1:B:102:THR:HG21	1:B:269:ALA:HB2	1.94	0.50
1:B:389:THR:O	1:B:392:THR:HG23	2.11	0.50
1:B:119:ILE:CD1	1:B:182:LEU:HD22	2.41	0.50
1:C:388:MSE:SE	1:C:388:MSE:H	2.44	0.50
1:C:69:HIS:HD1	1:C:104:GLN:HE22	1.60	0.50
1:B:267:GLN:O	1:B:283:LYS:HE2	2.11	0.50
1:A:388:MSE:HE2	1:D:383:GLY:C	2.32	0.50
1:A:331:GLY:HA3	1:A:435:MSE:HE1	1.94	0.50
1:C:150:THR:CG2	1:C:152:LEU:CB	2.89	0.50
1:A:282:LEU:HD13	1:A:416:MSE:HE1	1.93	0.50
1:C:112:ASP:HB3	1:C:115:THR:OG1	2.12	0.50
1:C:38:THR:CB	1:C:77:THR:CG2	2.89	0.50
1:B:130:THR:CB	1:B:161:THR:HG23	2.42	0.49
1:D:313:TYR:CE1	1:D:320:THR:CB	2.95	0.49
1:D:413:LEU:HA	1:D:416:MSE:HE2	1.93	0.49
1:B:145:THR:HG22	1:B:148:LYS:HZ1	1.74	0.49
1:D:152:LEU:HB3	1:D:158:PHE:CE2	2.46	0.49
1:D:219:ASN:ND2	1:D:314:ARG:HH11	2.09	0.49
1:D:388:MSE:CA	1:D:392:THR:HG21	2.37	0.49
1:A:389:THR:H	1:A:392:THR:HG22	1.72	0.49
1:B:219:ASN:ND2	1:B:314:ARG:HH11	2.10	0.49
1:B:491:ARG:HG2	1:B:493:PHE:CE1	2.47	0.49
1:A:456:PRO:HD2	1:A:459:LEU:HD12	1.93	0.49
1:A:66:TRP:HA	1:A:127:ASP:OD2	2.12	0.49
1:B:431:VAL:CG1	1:B:436:VAL:CG1	2.90	0.49
1:D:336:TRP:O	1:D:340:GLY:N	2.46	0.49
1:A:102:THR:CG2	1:A:269:ALA:CB	2.91	0.49
1:C:130:THR:CB	1:C:161:THR:HG23	2.43	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:150:THR:CG2	1:C:152:LEU:CG	2.91	0.49
1:B:40:ALA:CB	1:B:81:THR:HG23	2.41	0.48
1:C:216:ILE:HG22	1:C:300:MSE:SE	2.63	0.48
1:D:177:ALA:HB2	1:D:182:LEU:HD12	1.94	0.48
1:D:308:LEU:HB2	1:D:324:GLU:HB3	1.95	0.48
1:B:119:ILE:HD11	1:B:182:LEU:HD22	1.94	0.48
1:B:509:TRP:CZ3	1:B:513:VAL:HG21	2.47	0.48
1:B:188:ASP:OD2	1:B:203:THR:CG2	2.61	0.48
1:C:284:SER:HB2	1:C:292:ALA:HB2	1.94	0.48
1:D:108:VAL:HG22	1:D:159:SER:HB3	1.95	0.48
1:A:145:THR:HG22	1:A:149:LYS:HE2	1.95	0.48
1:D:399:ARG:O	1:D:403:GLU:HG3	2.12	0.48
1:B:119:ILE:HD11	1:B:182:LEU:HD21	1.93	0.48
1:B:280:GLY:HA2	1:B:420:TRP:CZ3	2.49	0.48
1:A:150:THR:HG23	1:A:152:LEU:HB2	1.96	0.48
1:B:390:ARG:HH22	1:C:370:THR:CG2	2.27	0.48
1:D:113:ARG:NH2	1:D:180:GLY:HA3	2.28	0.47
1:D:489:ARG:HG2	1:D:490:ASP:C	2.35	0.47
1:A:403:GLU:HB3	1:A:407:TYR:CE2	2.50	0.47
1:A:294:LEU:CD1	1:A:416:MSE:HE3	2.44	0.47
1:C:244:ALA:O	1:C:261:LEU:HA	2.14	0.47
1:C:24:MSE:HA	1:C:27:TYR:CE2	2.49	0.47
1:C:222:ASP:O	1:C:226:THR:HG23	2.15	0.47
1:D:41:ILE:HA	1:D:51:GLY:O	2.14	0.47
1:A:130:THR:HG21	1:A:161:THR:HG22	1.97	0.47
1:B:106:GLU:OE1	2:B:601:GOL:O3	2.28	0.47
1:C:161:THR:HB	5:C:702:HOH:O	2.14	0.47
1:A:188:ASP:OD2	1:A:203:THR:CG2	2.62	0.46
1:B:280:GLY:CA	1:B:420:TRP:CZ3	2.98	0.46
1:C:44:ASP:OD1	1:C:46:ASN:N	2.49	0.46
1:A:33:GLN:NE2	1:A:104:GLN:HE21	2.08	0.46
1:A:282:LEU:HD12	1:A:416:MSE:HE1	1.97	0.46
1:C:166:LEU:O	1:C:170:VAL:CG1	2.63	0.46
1:C:365:LEU:HD13	1:C:385:ILE:HG12	1.98	0.46
1:B:154:LEU:HD23	1:B:154:LEU:HA	1.82	0.46
1:C:150:THR:CG2	1:C:152:LEU:HD12	2.45	0.46
1:B:389:THR:CG2	1:B:391:ASN:H	2.29	0.46
1:D:124:VAL:O	1:D:162:LYS:HE2	2.16	0.46
1:C:28:ILE:HG21	1:C:467:ALA:HA	1.97	0.46
1:C:361:GLN:NE2	1:C:392:THR:HG22	2.30	0.46
1:B:509:TRP:CH2	1:B:513:VAL:HG21	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:361:GLN:HE22	1:A:392:THR:CB	2.27	0.45
1:B:27:TYR:HA	1:B:43:PHE:O	2.16	0.45
1:B:242:CYS:HB3	1:B:469:LEU:HD13	1.98	0.45
1:C:150:THR:CG2	1:C:152:LEU:HG	2.46	0.45
1:D:272:ILE:HG22	1:D:272:ILE:O	2.16	0.45
1:A:123:ILE:HG21	1:A:162:LYS:HG2	1.98	0.45
1:A:389:THR:HG21	1:A:391:ASN:OD1	2.16	0.45
1:B:130:THR:HG21	1:B:161:THR:CG2	2.45	0.45
1:B:181:GLU:O	1:B:182:LEU:HD23	2.16	0.45
1:C:329:VAL:HG11	1:C:369:PHE:CD2	2.52	0.45
1:D:157:TYR:O	1:D:162:LYS:NZ	2.49	0.45
1:A:282:LEU:HB3	1:A:294:LEU:HD12	1.98	0.45
1:C:40:ALA:HB3	1:C:81:THR:HG23	1.96	0.45
1:A:102:THR:CG2	1:A:266:ASP:HA	2.45	0.45
1:C:108:VAL:HG13	1:C:184:PHE:CE1	2.51	0.45
1:D:181:GLU:O	1:D:182:LEU:HD23	2.16	0.45
1:B:137:LEU:HD22	1:B:142:LEU:HD12	1.98	0.45
1:B:296:THR:HG22	1:B:321:TYR:HB2	1.98	0.45
1:C:167:LEU:HG	1:C:174:GLN:HG2	1.99	0.45
1:C:361:GLN:HE21	1:C:392:THR:HA	1.82	0.45
1:C:491:ARG:HG2	1:C:493:PHE:CE1	2.51	0.45
1:B:77:THR:O	1:B:81:THR:HB	2.16	0.44
1:D:358:ASP:HB3	1:D:361:GLN:HG3	1.98	0.44
1:A:13:LEU:HA	1:A:14:GLY:HA2	1.84	0.44
1:A:38:THR:OG1	1:A:77:THR:HG21	2.17	0.44
1:A:361:GLN:HE22	1:A:392:THR:HA	1.82	0.44
1:A:102:THR:CG2	1:A:269:ALA:HB2	2.47	0.44
1:A:39:ARG:HD2	1:A:54:GLN:OE1	2.17	0.44
1:B:215:ASN:HD22	1:B:215:ASN:C	2.21	0.44
1:D:98:ALA:HA	1:D:258:ILE:HG22	1.99	0.44
1:C:221:TRP:HZ2	1:C:237:PRO:HD2	1.77	0.44
1:D:127:ASP:OD2	1:D:129:ARG:NH2	2.42	0.44
1:D:26:GLY:HA2	1:D:27:TYR:HA	1.74	0.44
1:D:293:LEU:HA	1:D:323:LEU:O	2.17	0.44
1:B:89:SER:HB3	1:B:91:ILE:HG12	1.99	0.44
1:A:389:THR:O	1:A:392:THR:HG23	2.18	0.44
1:B:146:PHE:CE1	1:B:225:LEU:HD22	2.52	0.44
1:B:249:THR:HG22	1:B:257:ALA:HA	1.98	0.44
1:C:431:VAL:HG11	1:C:442:MSE:SE	2.68	0.44
1:C:210:ARG:HH21	1:C:310:THR:HB	1.83	0.43
1:A:329:VAL:HG13	1:A:332:ALA:HB3	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:410:ARG:HH21	1:C:506:LEU:HD22	1.83	0.43
1:A:143:GLU:O	1:A:147:VAL:HG23	2.18	0.43
1:A:40:ALA:HB2	1:A:81:THR:CG2	2.48	0.43
1:B:105:ARG:HD2	1:B:210:ARG:HD2	2.00	0.43
1:B:215:ASN:HB2	1:B:222:ASP:HB2	2.00	0.43
1:C:40:ALA:HB2	1:C:81:THR:CG2	2.48	0.43
1:B:402:LEU:O	1:B:405:VAL:HG12	2.19	0.43
1:B:444:ARG:HA	1:B:444:ARG:HD3	1.66	0.43
1:B:242:CYS:O	1:B:262:GLY:HA2	2.19	0.43
1:C:29:LEU:HD23	1:C:99:ILE:CD1	2.49	0.43
1:B:130:THR:OG1	1:B:161:THR:HG21	2.17	0.43
1:B:150:THR:CG2	1:B:152:LEU:HB2	2.48	0.43
1:D:27:TYR:HB3	1:D:96:ILE:HA	2.00	0.43
1:B:282:LEU:HB3	1:B:294:LEU:HD12	2.00	0.43
1:B:431:VAL:HG12	1:B:436:VAL:CG1	2.41	0.43
1:A:38:THR:OG1	1:A:77:THR:HG23	2.16	0.43
1:D:105:ARG:HH22	1:D:324:GLU:CD	2.18	0.43
1:D:143:GLU:O	1:D:147:VAL:HG23	2.19	0.43
1:D:207:ASN:HA	1:D:210:ARG:HG3	2.00	0.43
1:A:13:LEU:O	1:B:164:ASN:ND2	2.32	0.42
1:A:150:THR:CG2	1:A:152:LEU:H	2.23	0.42
1:A:102:THR:CG2	1:A:264:ALA:O	2.65	0.42
1:C:216:ILE:HG23	1:C:321:TYR:CE1	2.52	0.42
1:A:210:ARG:HA	1:A:210:ARG:HD2	1.79	0.42
1:A:403:GLU:OE2	1:A:444:ARG:NE	2.49	0.42
1:B:130:THR:HG21	1:B:161:THR:HG22	2.01	0.42
1:B:201:PHE:HA	5:B:723:HOH:O	2.19	0.42
1:B:358:ASP:OD1	1:B:361:GLN:HG2	2.19	0.42
1:C:451:ALA:HB1	1:C:452:PRO:HD2	2.02	0.42
1:D:105:ARG:CZ	1:D:210:ARG:HE	2.31	0.42
1:D:274:GLN:O	1:D:275:ALA:C	2.57	0.42
1:C:130:THR:HG21	1:C:161:THR:HG23	2.02	0.42
1:A:476:VAL:HG23	1:A:477:TRP:CD1	2.55	0.42
1:B:421:ARG:HA	1:B:421:ARG:HE	1.83	0.42
1:B:183:CYS:HB3	1:B:201:PHE:CE1	2.55	0.42
1:D:272:ILE:HD11	1:D:313:TYR:CD2	2.54	0.42
1:A:215:ASN:ND2	1:A:218:GLU:H	2.18	0.42
1:D:345:LYS:HA	1:D:345:LYS:HD3	1.83	0.42
1:B:146:PHE:CD1	1:B:225:LEU:HD22	2.55	0.42
1:A:130:THR:HG21	1:A:161:THR:CG2	2.49	0.42
1:D:403:GLU:CD	1:D:505:LYS:HZ1	2.21	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:283:LYS:HA	1:C:430:ARG:O	2.19	0.41
1:D:413:LEU:HD12	1:D:416:MSE:HE2	2.01	0.41
1:A:312:ALA:HB2	1:A:322:ALA:HB2	2.02	0.41
1:A:210:ARG:NH2	1:A:324:GLU:OE2	2.53	0.41
1:B:358:ASP:HA	1:B:359:PRO:HD3	1.76	0.41
1:B:59:GLN:NE2	5:B:707:HOH:O	2.52	0.41
1:C:188:ASP:CG	1:C:207:ASN:ND2	2.73	0.41
1:C:468:TRP:HA	1:C:477:TRP:CE3	2.55	0.41
1:D:331:GLY:O	1:D:334:VAL:HG22	2.20	0.41
1:B:106:GLU:HG2	1:B:158:PHE:HA	2.02	0.41
1:B:283:LYS:HG2	1:B:284:SER:N	2.30	0.41
1:D:416:MSE:C	1:D:418:LYS:N	2.73	0.41
1:A:210:ARG:HH22	1:A:324:GLU:CD	2.24	0.41
1:C:429:LEU:HG	1:C:431:VAL:HG23	2.01	0.41
1:A:69:HIS:HD1	1:A:104:GLN:HE22	1.68	0.41
1:B:108:VAL:CG2	1:B:159:SER:HB3	2.50	0.41
1:C:44:ASP:OD1	1:C:46:ASN:HB2	2.21	0.41
1:A:145:THR:O	1:A:149:LYS:CG	2.68	0.41
1:D:285:THR:O	1:D:290:CYS:HA	2.21	0.41
1:B:331:GLY:HA3	1:B:435:MSE:HE1	2.02	0.41
1:C:389:THR:N	1:C:392:THR:HG23	2.19	0.41
1:C:473:ARG:CG	1:C:473:ARG:NH1	2.73	0.41
1:D:152:LEU:HD11	1:D:209:SER:O	2.20	0.41
1:B:250:ASP:HA	1:B:251:PRO:HD3	1.94	0.41
1:C:41:ILE:HG12	1:C:52:VAL:HG22	2.03	0.41
1:D:282:LEU:N	1:D:282:LEU:CD2	2.83	0.41
1:A:130:THR:OG1	1:A:161:THR:HG21	2.20	0.41
1:A:389:THR:CG2	1:A:391:ASN:H	2.29	0.41
1:B:447:ASP:O	1:B:502:ARG:NE	2.46	0.41
1:C:128:ARG:HG3	1:C:370:THR:HB	2.01	0.41
1:D:68:GLU:HA	1:D:124:VAL:HG23	2.02	0.41
1:B:130:THR:HB	1:B:161:THR:HG23	2.02	0.41
1:B:376:HIS:O	1:B:377:TRP:C	2.57	0.41
1:B:378:ASP:HA	1:B:379:PRO:HD2	1.87	0.41
1:A:14:GLY:N	1:B:230:ARG:HG3	2.36	0.41
1:C:106:GLU:HG2	1:C:158:PHE:HA	2.02	0.41
1:C:435:MSE:HB2	1:C:435:MSE:HE3	1.74	0.41
1:D:491:ARG:CG	1:D:491:ARG:NH1	2.69	0.41
1:B:119:ILE:CD1	1:B:182:LEU:HD13	2.51	0.40
1:A:215:ASN:HD22	1:A:217:ALA:N	2.14	0.40
1:D:389:THR:H	1:D:392:THR:HG21	1.82	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:203:THR:HG22	1:B:207:ASN:HB2	2.02	0.40
1:B:233:LYS:HE2	1:B:234:GLU:OE2	2.22	0.40
1:D:374:ALA:HA	1:D:375:PRO:HA	1.77	0.40
1:A:130:THR:CB	1:A:161:THR:HG23	2.51	0.40
1:B:148:LYS:HE2	1:B:148:LYS:HB3	1.91	0.40
1:C:231:VAL:HG11	1:C:236:LEU:HD21	2.03	0.40
1:B:150:THR:HG23	1:B:152:LEU:CG	2.46	0.40
1:D:35:THR:HG21	1:D:126:GLN:OE1	2.21	0.40
1:D:232:PRO:O	1:D:235:MSE:HB2	2.21	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	492/520 (95%)	466 (95%)	25 (5%)	1 (0%)	47	55
1	B	478/520 (92%)	458 (96%)	19 (4%)	1 (0%)	47	55
1	C	497/520 (96%)	470 (95%)	26 (5%)	1 (0%)	47	55
1	D	417/520 (80%)	370 (89%)	40 (10%)	7 (2%)	9	6
All	All	1884/2080 (91%)	1764 (94%)	110 (6%)	10 (0%)	29	31

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	24	MSE
1	C	518	ILE
1	D	52	VAL
1	D	417	HIS
1	B	499	GLU
1	D	486	SER

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Mol	Chain	Res	Type
1	D	42	VAL
1	D	106	GLU
1	D	275	ALA
1	D	41	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	371/405 (92%)	331 (89%)	40 (11%)	6 5
1	B	367/405 (91%)	320 (87%)	47 (13%)	4 3
1	C	368/405 (91%)	331 (90%)	37 (10%)	7 6
1	D	242/405 (60%)	217 (90%)	25 (10%)	7 6
All	All	1348/1620 (83%)	1199 (89%)	149 (11%)	6 5

All (149) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	33	GLN
1	A	77	THR
1	A	81	THR
1	A	102	THR
1	A	136	LYS
1	A	139	LYS
1	A	140	LYS
1	A	145	THR
1	A	150	THR
1	A	167	LEU
1	A	168	SER
1	A	170	VAL
1	A	171	LYS
1	A	203	THR
1	A	204	ASP
1	A	215	ASN
1	A	249	THR

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Mol	Chain	Res	Type
1	A	252	SER
1	A	253	LEU
1	A	283	LYS
1	A	288	THR
1	A	294	LEU
1	A	296	THR
1	A	310	THR
1	A	323	LEU
1	A	382	ARG
1	A	388	MSE
1	A	389	THR
1	A	392	THR
1	A	420	TRP
1	A	430	ARG
1	A	435	MSE
1	A	444	ARG
1	A	448	LEU
1	A	459	LEU
1	A	462	THR
1	A	466	VAL
1	A	499	GLU
1	A	509	TRP
1	A	511	SER
1	B	33	GLN
1	B	77	THR
1	B	81	THR
1	B	113	ARG
1	B	138	LYS
1	B	145	THR
1	B	150	THR
1	B	161	THR
1	B	167	LEU
1	B	168	SER
1	B	170	VAL
1	B	171	LYS
1	B	176	ARG
1	B	204	ASP
1	B	209	SER
1	B	210	ARG
1	B	215	ASN
1	B	216	ILE
1	B	233	LYS

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Mol	Chain	Res	Type
1	B	235	MSE
1	B	245	ASP
1	B	249	THR
1	B	252	SER
1	B	253	LEU
1	B	283	LYS
1	B	288	THR
1	B	294	LEU
1	B	296	THR
1	B	310	THR
1	B	323	LEU
1	B	334	VAL
1	B	335	GLN
1	B	385	ILE
1	B	389	THR
1	B	390	ARG
1	B	391	ASN
1	B	392	THR
1	B	405	VAL
1	B	420	TRP
1	B	421	ARG
1	B	430	ARG
1	B	435	MSE
1	B	444	ARG
1	B	448	LEU
1	B	459	LEU
1	B	489	ARG
1	B	490	ASP
1	C	16	GLU
1	C	21	GLN
1	C	22	SER
1	C	33	GLN
1	C	77	THR
1	C	81	THR
1	C	150	THR
1	C	161	THR
1	C	167	LEU
1	C	170	VAL
1	C	204	ASP
1	C	210	ARG
1	C	215	ASN
1	C	227	GLU

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Mol	Chain	Res	Type
1	C	252	SER
1	C	283	LYS
1	C	296	THR
1	C	316	ASP
1	C	323	LEU
1	C	326	SER
1	C	334	VAL
1	C	361	GLN
1	C	388	MSE
1	C	389	THR
1	C	390	ARG
1	C	392	THR
1	C	418	LYS
1	C	420	TRP
1	C	444	ARG
1	C	448	LEU
1	C	459	LEU
1	C	462	THR
1	C	466	VAL
1	C	473	ARG
1	C	480	GLN
1	C	489	ARG
1	C	491	ARG
1	D	27	TYR
1	D	33	GLN
1	D	104	GLN
1	D	128	ARG
1	D	139	LYS
1	D	150	THR
1	D	159	SER
1	D	167	LEU
1	D	204	ASP
1	D	209	SER
1	D	210	ARG
1	D	215	ASN
1	D	250	ASP
1	D	258	ILE
1	D	282	LEU
1	D	283	LYS
1	D	284	SER
1	D	296	THR
1	D	323	LEU

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Mol	Chain	Res	Type
1	D	388	MSE
1	D	420	TRP
1	D	444	ARG
1	D	448	LEU
1	D	491	ARG
1	D	511	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	33	GLN
1	A	59	GLN
1	A	60	HIS
1	A	76	GLN
1	A	215	ASN
1	A	305	ASN
1	A	361	GLN
1	A	391	ASN
1	A	496	HIS
1	B	33	GLN
1	B	59	GLN
1	B	215	ASN
1	B	305	ASN
1	B	361	GLN
1	B	391	ASN
1	B	417	HIS
1	B	443	GLN
1	B	496	HIS
1	C	33	GLN
1	C	59	GLN
1	C	60	HIS
1	C	215	ASN
1	C	361	GLN
1	D	33	GLN
1	D	215	ASN
1	D	219	ASN
1	D	274	GLN
1	D	361	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 carbohydrates in this entry.

5.6 Ligand geometry

Of 6 ligands modelled in this entry, 3 are monoatomic - leaving 3 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	$\#\|Z\| > 2$
2	GOL	C	602	-	5,5,5	0.51	0	5,5,5	1.99	2 (40%)
2	GOL	B	601	-	5,5,5	0.63	0	5,5,5	0.47	0
2	GOL	A	601	-	5,5,5	0.25	0	5,5,5	0.61	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
2	GOL	C	602	-	-	2/4/4/4	-
2	GOL	B	601	-	-	2/4/4/4	-
2	GOL	A	601	-	-	0/4/4/4	-

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	602	GOL	O2-C2-C1	3.00	122.33	109.12
2	C	602	GOL	O2-C2-C3	2.15	118.58	109.12

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	602	GOL	O1-C1-C2-C3
2	C	602	GOL	C1-C2-C3-O3
2	B	601	GOL	C1-C2-C3-O3
2	B	601	GOL	O2-C2-C3-O3

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	602	GOL	1	0
2	B	601	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

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, 95^{th} 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	488/520 (93%)	0.15	9 (1%) 68 76	24, 39, 57, 64	0
1	B	476/520 (91%)	0.12	3 (0%) 89 93	25, 38, 55, 66	0
1	C	493/520 (94%)	0.38	17 (3%) 45 55	30, 50, 69, 73	0
1	D	430/520 (82%)	1.36	105 (24%) 0 1	42, 81, 105, 111	0
All	All	1887/2080 (90%)	0.48	134 (7%) 16 23	24, 47, 93, 111	0

All (134) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	184	PHE	10.2
1	D	257	ALA	8.9
1	D	31	ILE	8.4
1	D	244	ALA	8.2
1	D	108	VAL	7.7
1	D	272	ILE	7.3
1	D	262	GLY	7.1
1	D	190	PHE	7.0
1	D	109	VAL	6.5
1	D	120	HIS	6.2
1	D	452	PRO	5.9
1	D	116	GLY	5.7
1	D	221	TRP	5.3
1	D	261	LEU	5.2
1	D	271	THR	5.0
1	D	110	VAL	5.0
1	D	43	PHE	4.7
1	D	41	ILE	4.7
1	D	119	ILE	4.7
1	D	453	VAL	4.6
1	D	448	LEU	4.6

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Mol	Chain	Res	Type	RSRZ
1	D	32	ASP	4.6
1	D	213	LEU	4.3
1	D	243	ALA	4.2
1	D	229	LEU	4.2
1	D	173	ALA	4.2
1	D	92	THR	4.2
1	D	52	VAL	4.2
1	D	102	THR	4.1
1	D	313	TYR	4.1
1	D	487	TRP	4.1
1	D	200	CYS	4.0
1	C	19	TYR	3.9
1	D	30	ALA	3.9
1	C	258	ILE	3.9
1	C	464	LEU	3.9
1	D	165	TRP	3.8
1	D	454	ASP	3.8
1	D	75	TRP	3.7
1	D	217	ALA	3.7
1	A	496	HIS	3.7
1	C	7	HIS	3.6
1	D	449	LEU	3.6
1	C	90	GLY	3.6
1	D	201	PHE	3.5
1	C	99	ILE	3.5
1	D	82	VAL	3.4
1	D	186	THR	3.4
1	C	463	ALA	3.4
1	D	369	PHE	3.4
1	D	51	GLY	3.3
1	C	20	PHE	3.3
1	D	250	ASP	3.3
1	D	99	ILE	3.2
1	D	26	GLY	3.1
1	D	260	ILE	3.1
1	C	109	VAL	3.0
1	D	27	TYR	3.0
1	D	242	CYS	3.0
1	A	229	LEU	3.0
1	D	29	LEU	3.0
1	D	187	ILE	3.0
1	D	85	ALA	3.0

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Mol	Chain	Res	Type	RSRZ
1	D	53	GLY	3.0
1	D	42	VAL	3.0
1	D	282	LEU	2.9
1	D	247	GLY	2.9
1	D	66	TRP	2.9
1	C	184	PHE	2.9
1	D	202	CYS	2.9
1	D	111	TRP	2.9
1	C	254	PHE	2.8
1	D	121	ASN	2.8
1	C	27	TYR	2.8
1	C	9	SER	2.8
1	D	28	ILE	2.8
1	C	8	SER	2.7
1	D	93	ALA	2.7
1	B	420	TRP	2.7
1	A	359	PRO	2.7
1	D	94	ASN	2.7
1	D	290	CYS	2.7
1	D	228	VAL	2.7
1	D	456	PRO	2.6
1	D	367	PRO	2.6
1	D	517	LEU	2.6
1	D	183	CYS	2.6
1	D	269	ALA	2.6
1	D	175	VAL	2.5
1	D	171	LYS	2.5
1	D	239	VAL	2.5
1	D	293	LEU	2.5
1	D	191	LEU	2.4
1	D	218	GLU	2.4
1	A	228	VAL	2.4
1	C	475	GLY	2.4
1	D	484	ALA	2.4
1	D	50	ALA	2.4
1	D	118	PRO	2.3
1	D	231	VAL	2.3
1	D	493	PHE	2.3
1	B	509	TRP	2.3
1	D	194	ARG	2.3
1	D	100	GLY	2.3
1	A	509	TRP	2.3

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Mol	Chain	Res	Type	RSRZ
1	D	114	GLU	2.3
1	D	172	GLY	2.3
1	D	193	TRP	2.3
1	D	236	LEU	2.2
1	D	265	GLY	2.2
1	D	296	THR	2.2
1	A	227	GLU	2.2
1	C	10	GLY	2.2
1	D	210	ARG	2.2
1	D	192	ILE	2.2
1	D	246	PHE	2.2
1	D	518	ILE	2.2
1	D	214	TYR	2.2
1	D	500	ALA	2.2
1	D	69	HIS	2.1
1	D	123	ILE	2.1
1	A	358	ASP	2.1
1	D	264	ALA	2.1
1	D	420	TRP	2.1
1	D	185	GLY	2.1
1	B	382	ARG	2.1
1	D	259	PRO	2.1
1	D	451	ALA	2.1
1	D	62	PRO	2.1
1	A	174	GLN	2.0
1	A	160	GLY	2.0
1	C	434	GLY	2.0
1	D	195	LEU	2.0
1	D	203	THR	2.0

6.2 Non-standard residues in protein, DNA, RNA chains (i)

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

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands

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, 95^{th} 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	NA	A	602	1/1	0.89	0.24	56,56,56,56	0
4	CL	C	601	1/1	0.91	0.16	51,51,51,51	0
3	NA	C	603	1/1	0.92	0.36	37,37,37,37	0
2	GOL	C	602	6/6	0.94	0.20	34,37,41,44	0
2	GOL	B	601	6/6	0.98	0.11	26,28,31,32	0
2	GOL	A	601	6/6	0.98	0.12	25,28,29,30	0

6.5 Other polymers

There are no such residues in this entry.