Full wwPDB X-ray Structure Validation Report ⓘ

Aug 9, 2020 – 10:47 AM BST

PDB ID	:	6K79
Title	:	Glycerol kinase form Thermococcus kodakarensis, complex structure with substrate.
Authors	:	Koga, Y.; Angkawidjaja, C.; Matsumura, H.; Hokao, R.
Deposited on	:	2019-06-06
Resolution	:	2.19 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 ①) were used in the production of this report:

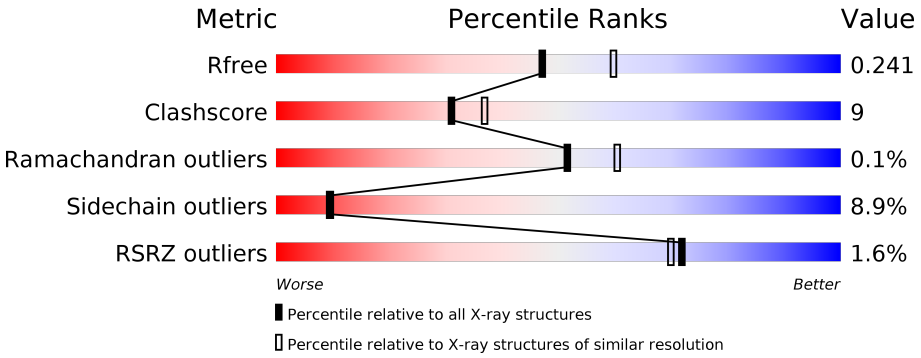
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.13.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.13.1

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 2.19 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	4898 (2.20-2.20)
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (2.20-2.20)

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	B	497	78% 17%
2	A	497	79% 17%
2	C	497	76% 20%
2	D	497	77% 17%

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
4	GOL	A	502	-	-	X	-
4	GOL	D	502	-	-	X	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 16106 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	B	490	Total	C	N	O	S	0	0	0
			3895	2490	657	737	11			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	145	LEU	VAL	conflict	UNP O93623
B	247	GLU	GLN	conflict	UNP O93623
B	271	GLU	LYS	conflict	UNP O93623

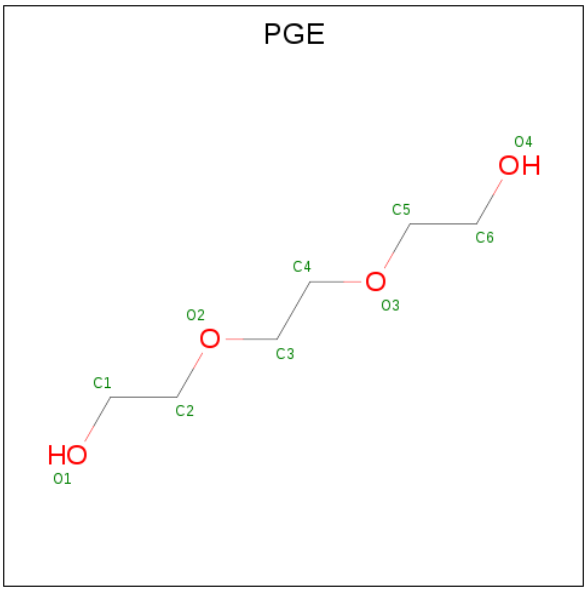
- Molecule 2 is a protein called Glycerol kinase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	490	Total	C	N	O	S	0	0	0
			3894	2489	658	736	11			
2	D	491	Total	C	N	O	S	0	0	0
			3902	2494	659	737	12			
2	A	490	Total	C	N	O	S	0	0	0
			3894	2489	658	736	11			

There are 3 discrepancies between the modelled and reference sequences:

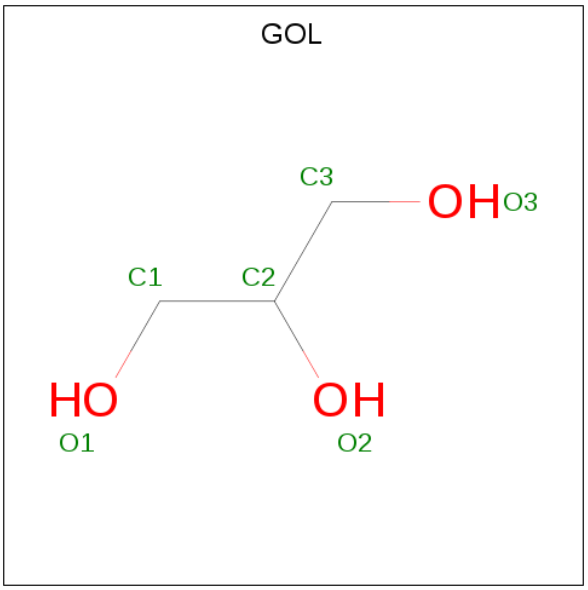
Chain	Residue	Modelled	Actual	Comment	Reference
C	271	GLU	LYS	conflict	UNP O93623
D	271	GLU	LYS	conflict	UNP O93623
A	271	GLU	LYS	conflict	UNP O93623

- Molecule 3 is TRIETHYLENE GLYCOL (three-letter code: PGE) (formula: $C_6H_{14}O_4$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	B	1	Total	C	O	0	0
			10	6	4		
3	C	1	Total	C	O	0	0
			10	6	4		
3	D	1	Total	C	O	0	0
			10	6	4		
3	A	1	Total	C	O	0	0
			10	6	4		

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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

- Molecule 5 is water.

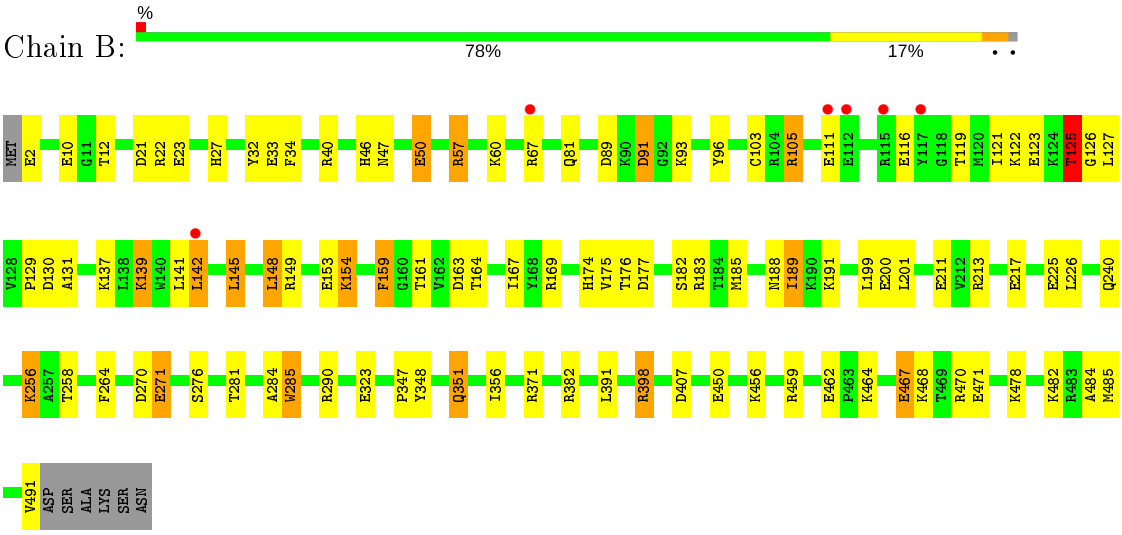
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	B	152	Total O 152 152	0	0
5	C	86	Total O 86 86	0	0
5	D	103	Total O 103 103	0	0
5	A	116	Total O 116 116	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

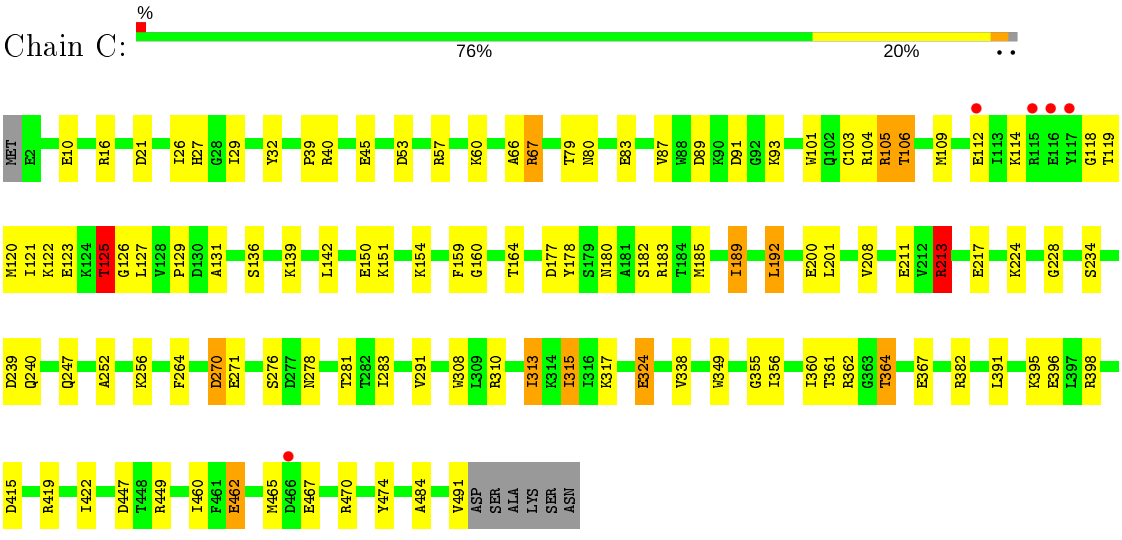
- Molecule 1: Glycerol kinase

Chain B:



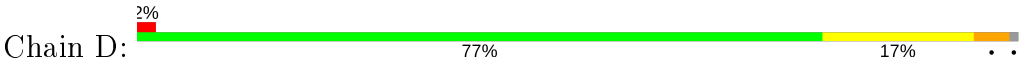
- Molecule 2: Glycerol kinase

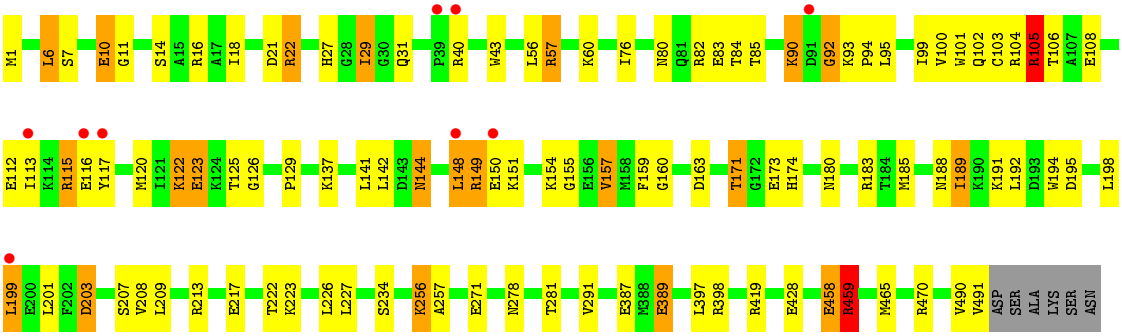
Chain C:



- Molecule 2: Glycerol kinase

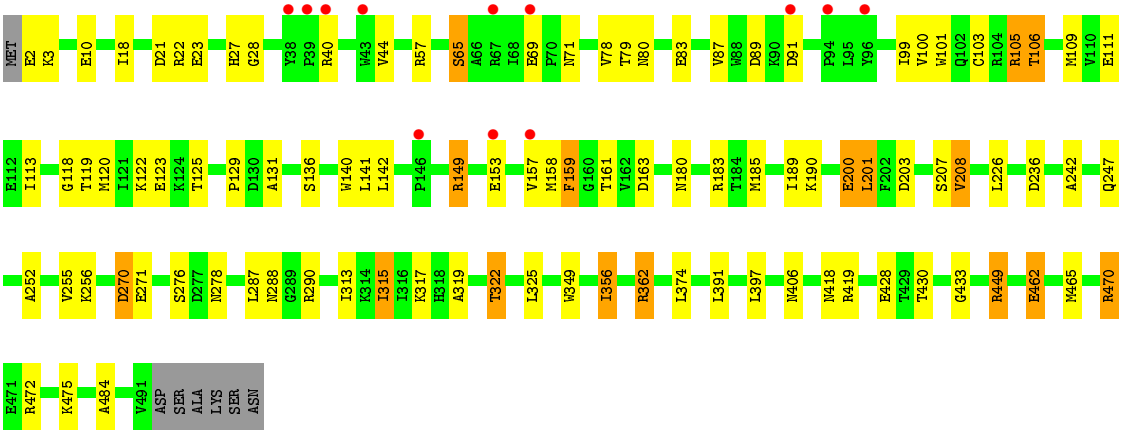
Chain D:





- Molecule 2: Glycerol kinase

Chain A:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	67.04Å 72.13Å 115.99Å 103.43° 94.96° 99.48°	Depositor
Resolution (Å)	46.20 – 2.19 46.20 – 2.19	Depositor EDS
% Data completeness (in resolution range)	98.6 (46.20-2.19) 98.6 (46.20-2.19)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.64 (at 2.18Å)	Xtriage
Refinement program	REFMAC 5.8.0222	Depositor
R, R_{free}	0.185 , 0.238 0.190 , 0.241	Depositor DCC
R_{free} test set	5226 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å^2)	28.2	Xtriage
Anisotropy	0.044	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 42.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	16106	wwPDB-VP
Average B, all atoms (Å^2)	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.56% 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, PGE

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	B	0.62	1/3977 (0.0%)	0.77	3/5388 (0.1%)
2	A	0.56	0/3976	0.72	0/5387
2	C	0.53	0/3976	0.71	5/5387 (0.1%)
2	D	0.53	0/3984	0.72	0/5397
All	All	0.56	1/15913 (0.0%)	0.73	8/21559 (0.0%)

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	8
2	A	0	7
2	C	0	5
2	D	0	8
All	All	0	28

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	471	GLU	CD-OE2	5.35	1.31	1.25

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	105	ARG	CB-CA-C	-8.54	93.32	110.40
1	B	371	ARG	NE-CZ-NH2	-6.96	116.82	120.30
1	B	217	GLU	CB-CA-C	-5.74	98.92	110.40
2	C	213	ARG	NE-CZ-NH2	-5.67	117.47	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	16	ARG	CB-CA-C	-5.59	99.22	110.40
1	B	125	THR	C-N-CA	-5.45	110.85	122.30
2	C	125	THR	C-N-CA	-5.45	110.86	122.30
2	C	125	THR	CA-C-N	5.32	126.84	116.20

There are no chirality outliers.

All (28) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	A	105	ARG	Sidechain
2	A	183	ARG	Sidechain
2	A	362	ARG	Sidechain
2	A	419	ARG	Sidechain
2	A	449	ARG	Sidechain
2	A	470	ARG	Sidechain
2	A	472	ARG	Sidechain
1	B	105	ARG	Sidechain
1	B	154	LYS	Peptide
1	B	183	ARG	Sidechain
1	B	213	ARG	Sidechain
1	B	382	ARG	Sidechain
1	B	398	ARG	Sidechain
1	B	40	ARG	Sidechain
1	B	67	ARG	Sidechain
2	C	183	ARG	Sidechain
2	C	213	ARG	Sidechain
2	C	310	ARG	Sidechain
2	C	398	ARG	Sidechain
2	C	419	ARG	Sidechain
2	D	104	ARG	Sidechain
2	D	105	ARG	Sidechain
2	D	149	ARG	Sidechain
2	D	183	ARG	Sidechain
2	D	213	ARG	Sidechain
2	D	40	ARG	Sidechain
2	D	419	ARG	Sidechain
2	D	459	ARG	Sidechain

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	B	3895	0	3864	68	0
2	A	3894	0	3864	72	0
2	C	3894	0	3864	66	0
2	D	3902	0	3876	78	0
3	A	10	0	14	1	0
3	B	10	0	14	1	0
3	C	10	0	14	1	0
3	D	10	0	14	0	0
4	A	6	0	8	5	0
4	B	6	0	8	0	0
4	C	6	0	8	0	0
4	D	6	0	8	6	0
5	A	116	0	0	6	0
5	B	152	0	0	5	0
5	C	86	0	0	2	0
5	D	103	0	0	3	0
All	All	16106	0	15556	283	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 9.

All (283) 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)
2:A:288:ASN:N	5:A:601:HOH:O	1.77	1.14
2:D:459:ARG:HG3	2:D:459:ARG:HH11	1.15	1.11
1:B:121:ILE:HG21	1:B:185:MET:CE	1.83	1.08
2:D:82:ARG:HE	4:D:502:GOL:H31	1.08	1.07
1:B:121:ILE:CG2	1:B:185:MET:HE2	1.89	1.02
1:B:121:ILE:HG21	1:B:185:MET:HE2	1.42	0.96
2:A:322:THR:HG23	2:A:374:LEU:HD11	1.52	0.89
2:C:462:GLU:CD	2:C:462:GLU:H	1.77	0.88
1:B:96:TYR:CD1	1:B:145:LEU:HD21	2.10	0.87
2:C:192:LEU:HD21	2:C:291:VAL:HG21	1.57	0.86
1:B:103:CYS:SG	1:B:105:ARG:HD2	2.15	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:467:GLU:HG2	1:B:470:ARG:NH2	1.92	0.85
2:C:151:LYS:O	2:C:154:LYS:O	1.95	0.84
2:C:106:THR:HG22	2:C:131:ALA:CB	2.07	0.83
1:B:182:SER:HB2	1:B:189:ILE:HD11	1.57	0.83
2:D:129:PRO:HA	2:D:185:MET:CE	2.08	0.83
2:D:82:ARG:NE	4:D:502:GOL:H31	1.93	0.82
2:A:278:ASN:ND2	2:A:349:TRP:HE1	1.78	0.82
2:C:80:ASN:HD21	2:C:180:ASN:HD21	1.25	0.81
2:A:18:ILE:CD1	2:A:428:GLU:HG2	2.10	0.81
2:A:462:GLU:CD	2:A:462:GLU:H	1.85	0.80
1:B:164:THR:HG22	1:B:175:VAL:O	1.80	0.80
2:A:18:ILE:HD13	2:A:428:GLU:HG2	1.63	0.80
2:D:459:ARG:HG3	2:D:459:ARG:NH1	1.91	0.80
2:D:148:LEU:H	2:D:148:LEU:HD12	1.44	0.79
2:D:82:ARG:HE	4:D:502:GOL:C3	1.94	0.79
1:B:121:ILE:HG21	1:B:185:MET:HE1	1.65	0.78
2:A:322:THR:HG21	2:A:374:LEU:HD21	1.64	0.77
2:C:361:THR:H	2:C:364:THR:CG2	1.99	0.76
1:B:32:TYR:CE2	1:B:57:ARG:HG2	2.21	0.76
2:C:106:THR:HG22	2:C:131:ALA:HB1	1.67	0.75
2:A:322:THR:CG2	2:A:374:LEU:HD21	2.16	0.75
2:C:126:GLY:HA3	2:C:281:THR:O	1.86	0.75
2:A:101:TRP:CD2	4:A:502:GOL:H32	2.22	0.74
2:A:278:ASN:HD22	2:A:349:TRP:HE1	1.35	0.74
1:B:161:THR:O	1:B:164:THR:OG1	2.06	0.74
2:D:199:LEU:HD21	2:D:209:LEU:HD11	1.70	0.73
2:D:80:ASN:HD21	2:D:180:ASN:HD21	1.36	0.73
2:D:458:GLU:OE2	2:D:459:ARG:HB2	1.88	0.73
2:C:53:ASP:HB2	5:C:664:HOH:O	1.89	0.72
1:B:141:LEU:O	1:B:145:LEU:HB2	1.89	0.72
2:C:106:THR:HG21	2:C:136:SER:OG	1.89	0.72
2:C:360:ILE:HA	2:C:364:THR:HG21	1.71	0.72
1:B:351:GLN:HG3	5:B:688:HOH:O	1.90	0.72
2:D:459:ARG:CG	2:D:459:ARG:HH11	1.99	0.72
2:D:57:ARG:HH11	2:D:57:ARG:HG3	1.55	0.72
2:A:21:ASP:OD2	2:A:27:HIS:HE1	1.73	0.71
1:B:129:PRO:HA	1:B:185:MET:HE3	1.73	0.70
2:A:129:PRO:HA	2:A:185:MET:CE	2.21	0.70
2:D:129:PRO:HA	2:D:185:MET:HE1	1.74	0.69
2:D:83:GLU:OE1	4:D:502:GOL:H2	1.93	0.69
2:A:80:ASN:HD21	2:A:180:ASN:HD21	1.40	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:456:LYS:HE3	5:B:658:HOH:O	1.93	0.69
2:C:240:GLN:HE22	2:C:256:LYS:NZ	1.91	0.69
2:A:106:THR:HG21	2:A:136:SER:OG	1.92	0.68
2:C:361:THR:H	2:C:364:THR:HG23	1.58	0.68
1:B:129:PRO:HA	1:B:185:MET:CE	2.23	0.68
2:A:129:PRO:HA	2:A:185:MET:HE1	1.76	0.68
2:C:45:GLU:OE2	2:C:105:ARG:NH2	2.19	0.67
1:B:145:LEU:HB3	1:B:148:LEU:HB2	1.77	0.66
2:A:109:MET:O	2:A:113:ILE:HG12	1.95	0.66
2:D:222:THR:HG21	2:D:227:LEU:HD12	1.76	0.66
2:A:319:ALA:O	2:A:322:THR:HB	1.95	0.65
2:C:462:GLU:CD	2:C:462:GLU:N	2.48	0.65
2:A:149:ARG:HH11	2:A:149:ARG:CG	2.10	0.64
2:A:101:TRP:CE2	4:A:502:GOL:H31	2.33	0.63
2:A:122:LYS:O	2:A:125:THR:O	2.17	0.63
2:D:21:ASP:OD2	2:D:27:HIS:HE1	1.80	0.63
2:A:322:THR:CG2	2:A:374:LEU:HD11	2.26	0.62
1:B:270:ASP:OD1	1:B:290:ARG:NH2	2.30	0.62
1:B:163:ASP:O	1:B:167:ILE:HG12	2.00	0.62
2:A:322:THR:HG23	2:A:374:LEU:CD1	2.29	0.62
2:C:278:ASN:HD22	2:C:349:TRP:HE1	1.44	0.62
2:C:356:ILE:HD11	2:C:484:ALA:HA	1.80	0.61
2:D:57:ARG:NH1	2:D:57:ARG:HG3	2.14	0.61
1:B:121:ILE:HG23	1:B:185:MET:HE2	1.83	0.61
2:C:313:ILE:HG23	2:C:315:ILE:HG12	1.82	0.61
2:D:115:ARG:HA	5:D:697:HOH:O	2.00	0.61
2:A:18:ILE:CD1	2:A:428:GLU:CG	2.78	0.60
1:B:21:ASP:OD2	1:B:27:HIS:HE1	1.83	0.60
1:B:188:ASN:O	1:B:191:LYS:O	2.20	0.60
2:D:148:LEU:HD12	2:D:148:LEU:N	2.10	0.59
2:D:80:ASN:ND2	2:D:163:ASP:HB3	2.17	0.59
2:A:149:ARG:O	2:A:153:GLU:HG2	2.03	0.59
2:D:222:THR:HG21	2:D:227:LEU:CD1	2.33	0.59
2:C:122:LYS:O	2:C:125:THR:O	2.21	0.58
2:D:159:PHE:O	2:D:174:HIS:HE1	1.85	0.58
2:D:103:CYS:SG	2:D:105:ARG:HD2	2.43	0.58
1:B:149:ARG:O	1:B:153:GLU:HG2	2.03	0.58
2:D:194:TRP:CG	2:D:209:LEU:HD13	2.39	0.57
2:D:465:MET:HE3	2:D:470:ARG:HA	1.86	0.57
1:B:142:LEU:C	1:B:142:LEU:HD23	2.24	0.57
2:D:188:ASN:O	2:D:191:LYS:O	2.23	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:462:GLU:CD	2:A:462:GLU:N	2.56	0.57
1:B:121:ILE:CG2	1:B:185:MET:CE	2.59	0.57
1:B:96:TYR:CG	1:B:145:LEU:HD21	2.39	0.57
2:D:99:ILE:HD12	2:D:141:LEU:CD2	2.35	0.56
2:A:149:ARG:HH22	2:A:203:ASP:HB3	1.70	0.56
1:B:211:GLU:HG2	2:C:211:GLU:CD	2.25	0.56
2:C:129:PRO:HA	2:C:185:MET:CE	2.36	0.56
2:D:129:PRO:CA	2:D:185:MET:HE1	2.35	0.56
2:C:182:SER:HB2	2:C:189:ILE:HD11	1.87	0.55
2:C:21:ASP:OD2	2:C:27:HIS:HE1	1.89	0.55
2:A:44:VAL:HG12	2:A:100:VAL:HG21	1.89	0.55
2:D:99:ILE:HG22	2:D:137:LYS:HD3	1.89	0.55
2:D:129:PRO:HA	2:D:185:MET:HE3	1.87	0.55
1:B:2:GLU:CD	5:A:603:HOH:O	2.44	0.55
2:C:129:PRO:HA	2:C:185:MET:HE1	1.89	0.55
2:C:367:GLU:H	2:C:367:GLU:CD	2.10	0.55
2:C:32:TYR:CE2	2:C:57:ARG:HG2	2.42	0.54
2:A:101:TRP:CD2	4:A:502:GOL:C3	2.90	0.54
1:B:122:LYS:O	1:B:125:THR:O	2.25	0.54
2:A:271:GLU:CD	2:A:290:ARG:HH11	2.12	0.53
2:C:467:GLU:CD	2:C:470:ARG:NH1	2.62	0.53
2:D:155:GLY:HA2	2:D:207:SER:OG	2.09	0.53
2:A:149:ARG:NH2	2:A:203:ASP:HB3	2.23	0.53
2:C:308:TRP:CZ2	2:C:313:ILE:HD12	2.44	0.53
2:D:149:ARG:HH22	2:D:203:ASP:HB3	1.73	0.52
2:C:109:MET:SD	2:C:139:LYS:HD3	2.50	0.52
2:D:123:GLU:HG2	5:D:700:HOH:O	2.08	0.52
1:B:240:GLN:HE22	1:B:256:LYS:HZ3	1.57	0.52
2:C:247:GLN:HG3	2:C:256:LYS:HG3	1.90	0.52
1:B:47:ASN:HB3	1:B:50:GLU:CG	2.39	0.52
2:A:125:THR:HA	2:A:189:ILE:HG12	1.92	0.52
2:C:395:LYS:HG2	2:C:396:GLU:HG2	1.91	0.52
2:D:159:PHE:CG	2:D:160:GLY:N	2.78	0.52
2:D:155:GLY:HA2	2:D:207:SER:HG	1.75	0.52
2:D:465:MET:O	2:D:470:ARG:NH2	2.36	0.52
2:C:264:PHE:CZ	3:C:501:PGE:H2	2.45	0.52
2:A:101:TRP:CE2	4:A:502:GOL:C3	2.93	0.51
2:C:125:THR:HG22	2:C:127:LEU:H	1.75	0.51
2:C:26:ILE:HG21	2:C:29:ILE:HD11	1.92	0.51
2:C:308:TRP:CH2	2:C:313:ILE:HD12	2.45	0.51
1:B:240:GLN:HE22	1:B:256:LYS:NZ	2.08	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:57:ARG:HD2	5:C:669:HOH:O	2.11	0.50
2:D:144:ASN:N	2:D:144:ASN:OD1	2.44	0.50
2:D:126:GLY:HA3	2:D:281:THR:HB	1.92	0.50
2:D:389:GLU:O	2:D:389:GLU:HG2	2.11	0.50
2:A:149:ARG:NH1	2:A:149:ARG:CG	2.73	0.50
1:B:2:GLU:HB2	2:A:290:ARG:NH2	2.26	0.50
2:C:39:PRO:O	2:C:40:ARG:HG3	2.11	0.50
2:D:82:ARG:HH21	4:D:502:GOL:H12	1.76	0.50
1:B:482:LYS:HA	1:B:485:MET:CE	2.42	0.50
2:D:93:LYS:HD2	2:D:94:PRO:HD2	1.94	0.50
2:A:255:VAL:HB	2:A:397:LEU:HD12	1.94	0.49
2:D:99:ILE:HD12	2:D:141:LEU:HD22	1.93	0.49
1:B:131:ALA:O	1:B:137:LYS:HE2	2.13	0.49
1:B:264:PHE:CZ	3:B:501:PGE:H3	2.48	0.49
2:A:149:ARG:HG3	2:A:149:ARG:NH1	2.27	0.49
2:A:106:THR:HG22	2:A:131:ALA:HB1	1.95	0.48
2:A:23:GLU:OE2	5:A:602:HOH:O	2.20	0.48
1:B:126:GLY:HA3	1:B:281:THR:O	2.13	0.48
2:C:447:ASP:OD2	2:C:449:ARG:NH2	2.46	0.48
2:D:105:ARG:HG2	2:D:106:THR:N	2.28	0.48
2:A:271:GLU:HG2	2:A:290:ARG:NH1	2.28	0.48
2:A:89:ASP:C	2:A:89:ASP:OD1	2.52	0.48
1:B:96:TYR:CD1	1:B:145:LEU:CD2	2.89	0.48
2:D:82:ARG:HB2	4:D:502:GOL:H2	1.95	0.48
1:B:89:ASP:HB3	1:B:91:ASP:H	1.79	0.48
1:B:142:LEU:O	1:B:149:ARG:HB2	2.13	0.48
1:B:284:ALA:O	1:B:285:TRP:CD1	2.67	0.48
2:A:79:THR:HG21	2:A:430:THR:HG22	1.95	0.48
2:D:157:VAL:CG2	2:D:208:VAL:HG12	2.44	0.48
2:A:99:ILE:HD13	2:A:105:ARG:HD3	1.95	0.47
2:A:157:VAL:O	2:A:208:VAL:HG23	2.14	0.47
2:C:178:TYR:HB3	2:C:283:ILE:HG21	1.97	0.47
2:A:149:ARG:HG3	2:A:149:ARG:HH11	1.79	0.47
1:B:47:ASN:HB3	1:B:50:GLU:HG3	1.96	0.47
2:A:27:HIS:HD2	5:A:672:HOH:O	1.97	0.47
2:A:101:TRP:CG	4:A:502:GOL:H32	2.49	0.47
1:B:33:GLU:HG3	1:B:34:PHE:N	2.28	0.47
2:D:278:ASN:ND2	2:D:387:GLU:OE2	2.35	0.47
1:B:159:PHE:O	1:B:174:HIS:HE1	1.98	0.47
2:D:85:THR:HG23	2:D:159:PHE:HE1	1.79	0.47
2:D:90:LYS:NZ	2:D:90:LYS:CB	2.75	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:125:THR:CG2	2:C:127:LEU:HB2	2.44	0.47
2:D:142:LEU:HA	2:D:148:LEU:CD1	2.45	0.47
2:D:6:LEU:O	2:D:76:ILE:HA	2.15	0.47
2:A:103:CYS:SG	2:A:105:ARG:HD2	2.55	0.47
2:A:252:ALA:HB2	2:A:270:ASP:HB2	1.97	0.47
2:A:28:GLY:HA2	2:A:65:SER:HB3	1.96	0.47
2:A:465:MET:O	2:A:470:ARG:NH2	2.48	0.47
1:B:22:ARG:NH1	1:B:450:GLU:OE2	2.37	0.47
2:A:140:TRP:HE3	2:A:141:LEU:HD12	1.80	0.46
2:C:338:VAL:O	2:C:355:GLY:HA2	2.15	0.46
2:D:122:LYS:O	2:D:125:THR:O	2.33	0.46
1:B:347:PRO:HD2	1:B:348:TYR:CE2	2.50	0.46
1:B:164:THR:CG2	1:B:176:THR:HB	2.46	0.46
2:C:125:THR:HG23	2:C:127:LEU:CG	2.46	0.46
2:C:276:SER:HB2	2:C:391:LEU:CD1	2.46	0.46
2:A:322:THR:HG22	2:A:406:ASN:HD21	1.81	0.46
2:A:418:ASN:HB2	2:A:470:ARG:CZ	2.46	0.45
2:A:313:ILE:HG23	2:A:315:ILE:HD13	1.98	0.45
1:B:46:HIS:HD1	1:B:81:GLN:HE22	1.65	0.45
2:C:121:ILE:O	2:C:125:THR:HB	2.17	0.45
1:B:271:GLU:CD	1:B:271:GLU:H	2.18	0.45
2:D:100:VAL:HG12	2:D:102:GLN:H	1.82	0.45
1:B:256:LYS:HE2	1:B:258:THR:OG1	2.17	0.45
2:D:257:ALA:HB2	2:D:397:LEU:HD11	1.98	0.45
2:C:240:GLN:HE22	2:C:256:LYS:HZ1	1.63	0.45
2:D:159:PHE:CD1	2:D:160:GLY:N	2.84	0.45
2:C:79:THR:OG1	2:C:239:ASP:HA	2.16	0.45
2:D:6:LEU:HD13	2:D:76:ILE:HG12	1.99	0.45
2:A:200:GLU:O	2:A:201:LEU:C	2.53	0.45
2:D:149:ARG:NH2	2:D:203:ASP:HB3	2.31	0.45
2:D:22:ARG:NH1	5:D:612:HOH:O	2.49	0.44
2:A:159:PHE:HB3	2:A:208:VAL:HG13	1.99	0.44
2:C:422:ILE:HG13	2:C:460:ILE:HG23	2.00	0.44
1:B:125:THR:HG23	1:B:127:LEU:H	1.81	0.44
1:B:478:LYS:CG	5:B:611:HOH:O	2.66	0.44
1:B:125:THR:CG2	1:B:127:LEU:H	2.31	0.44
1:B:276:SER:HB2	1:B:391:LEU:HD11	2.00	0.44
2:D:43:TRP:CE2	2:D:105:ARG:HB2	2.53	0.44
2:D:171:THR:HG22	2:D:173:GLU:H	1.83	0.44
2:A:356:ILE:HD11	2:A:484:ALA:HA	2.00	0.43
2:A:276:SER:HB2	2:A:391:LEU:HD11	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:171:THR:CG2	2:D:173:GLU:H	2.31	0.43
2:A:247:GLN:HG3	2:A:256:LYS:HG3	2.01	0.43
1:B:468:LYS:HE3	1:B:468:LYS:HB3	1.79	0.43
2:D:85:THR:HG23	2:D:159:PHE:CE1	2.53	0.43
1:B:323:GLU:OE2	1:B:407:ASP:HB2	2.18	0.43
2:A:118:GLY:HA2	2:A:129:PRO:HG2	2.01	0.43
2:A:322:THR:HG22	2:A:406:ASN:ND2	2.33	0.43
2:A:242:ALA:O	2:A:433:GLY:HA3	2.19	0.43
2:C:66:ALA:O	2:C:67:ARG:CB	2.66	0.43
1:B:139:LYS:O	1:B:142:LEU:HD22	2.18	0.43
1:B:467:GLU:HG2	1:B:470:ARG:HH22	1.76	0.43
2:C:415:ASP:HB3	2:C:465:MET:CB	2.49	0.43
2:C:415:ASP:HB3	2:C:465:MET:HB2	1.99	0.43
2:D:83:GLU:HB2	2:D:101:TRP:HB3	2.01	0.43
1:B:478:LYS:HG2	5:B:611:HOH:O	2.18	0.43
2:C:382:ARG:HG2	2:C:474:TYR:CZ	2.53	0.43
2:D:217:GLU:O	2:D:234:SER:HA	2.18	0.43
2:A:44:VAL:HG12	2:A:100:VAL:CG2	2.49	0.43
2:D:16:ARG:HG2	2:D:31:GLN:HB3	2.01	0.43
2:C:106:THR:CG2	2:C:136:SER:OG	2.62	0.42
2:D:10:GLU:OE1	2:D:11:GLY:O	2.37	0.42
2:D:256:LYS:HA	2:D:398:ARG:O	2.18	0.42
1:B:226:LEU:HD12	1:B:226:LEU:HA	1.91	0.42
2:C:252:ALA:HB2	2:C:270:ASP:HB2	2.01	0.42
2:D:188:ASN:HB2	2:D:195:ASP:HB2	2.02	0.42
2:A:287:LEU:CA	5:A:601:HOH:O	2.67	0.42
2:C:106:THR:CG2	2:C:131:ALA:HA	2.49	0.42
2:D:201:LEU:O	2:D:201:LEU:HD12	2.19	0.42
2:A:111:GLU:OE2	2:A:111:GLU:HA	2.20	0.42
2:C:89:ASP:C	2:C:89:ASP:OD1	2.57	0.42
2:D:125:THR:HA	2:D:189:ILE:HG12	2.00	0.42
2:D:6:LEU:C	2:D:6:LEU:CD2	2.88	0.42
2:D:83:GLU:O	2:D:84:THR:C	2.58	0.42
2:C:240:GLN:HE22	2:C:256:LYS:HZ3	1.64	0.42
2:D:18:ILE:HG12	2:D:29:ILE:HG22	2.02	0.42
2:C:177:ASP:HA	2:C:213:ARG:O	2.19	0.42
2:D:157:VAL:HG22	2:D:208:VAL:HG12	2.01	0.42
3:A:501:PGE:H42	5:A:700:HOH:O	2.18	0.42
1:B:276:SER:HB2	1:B:391:LEU:CD1	2.49	0.42
2:C:324:GLU:HG2	2:C:324:GLU:H	1.65	0.41
2:C:278:ASN:ND2	2:C:349:TRP:HE1	2.15	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:129:PRO:CA	1:B:185:MET:HE3	2.47	0.41
2:D:142:LEU:HD23	2:D:148:LEU:HD13	2.01	0.41
2:A:103:CYS:SG	2:A:105:ARG:NH1	2.84	0.41
2:C:217:GLU:O	2:C:234:SER:HA	2.20	0.41
2:A:99:ILE:CD1	2:A:141:LEU:CD1	2.98	0.41
2:D:6:LEU:HD23	2:D:7:SER:N	2.36	0.41
1:B:240:GLN:NE2	1:B:256:LYS:NZ	2.69	0.41
2:C:118:GLY:HA2	2:C:129:PRO:HG2	2.03	0.41
2:C:356:ILE:CD1	2:C:484:ALA:HA	2.50	0.41
2:A:80:ASN:ND2	2:A:163:ASP:HB3	2.36	0.41
1:B:356:ILE:CG2	1:B:484:ALA:HB2	2.51	0.41
2:C:83:GLU:HB2	2:C:101:TRP:HB3	2.03	0.41
2:D:92:GLY:O	2:D:93:LYS:C	2.53	0.41
1:B:464:LYS:CE	5:B:604:HOH:O	2.69	0.41
2:A:78:VAL:O	2:A:236:ASP:HA	2.21	0.40
2:C:103:CYS:SG	2:C:105:ARG:HG3	2.61	0.40
1:B:121:ILE:O	1:B:125:THR:HG22	2.21	0.40
1:B:126:GLY:HA3	1:B:281:THR:HB	2.02	0.40
2:C:160:GLY:HA3	2:C:164:THR:HB	2.04	0.40
2:A:83:GLU:HB2	2:A:101:TRP:HB3	2.03	0.40
2:A:87:VAL:HG22	2:A:141:LEU:HD23	2.03	0.40
2:A:87:VAL:HA	2:A:158:MET:O	2.21	0.40
1:B:256:LYS:HA	1:B:398:ARG:O	2.21	0.40
2:C:224:LYS:O	2:C:228:GLY:N	2.48	0.40
2:D:56:LEU:HD12	2:D:56:LEU:HA	1.95	0.40
2:D:199:LEU:HD12	2:D:199:LEU:HA	1.90	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	B	488/497 (98%)	473 (97%)	15 (3%)	0	100 100
2	A	488/497 (98%)	470 (96%)	18 (4%)	0	100 100
2	C	488/497 (98%)	464 (95%)	24 (5%)	0	100 100
2	D	489/497 (98%)	465 (95%)	23 (5%)	1 (0%)	47 55
All	All	1953/1988 (98%)	1872 (96%)	80 (4%)	1 (0%)	51 60

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	D	92	GLY

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	B	403/409 (98%)	368 (91%)	35 (9%)	10 10
2	A	403/409 (98%)	369 (92%)	34 (8%)	11 11
2	C	403/409 (98%)	371 (92%)	32 (8%)	12 12
2	D	404/409 (99%)	361 (89%)	43 (11%)	6 6
All	All	1613/1636 (99%)	1469 (91%)	144 (9%)	9 9

All (144) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	10	GLU
1	B	12	THR
1	B	23	GLU
1	B	50	GLU
1	B	57	ARG
1	B	60	LYS
1	B	91	ASP
1	B	93	LYS
1	B	111	GLU
1	B	116	GLU

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Mol	Chain	Res	Type
1	B	119	THR
1	B	123	GLU
1	B	125	THR
1	B	130	ASP
1	B	139	LYS
1	B	142	LEU
1	B	145	LEU
1	B	148	LEU
1	B	154	LYS
1	B	159	PHE
1	B	169	ARG
1	B	177	ASP
1	B	189	ILE
1	B	199	LEU
1	B	200	GLU
1	B	201	LEU
1	B	225	GLU
1	B	256	LYS
1	B	271	GLU
1	B	285	TRP
1	B	351	GLN
1	B	459	ARG
1	B	462	GLU
1	B	467	GLU
1	B	491	VAL
2	C	10	GLU
2	C	60	LYS
2	C	67	ARG
2	C	87	VAL
2	C	91	ASP
2	C	93	LYS
2	C	104	ARG
2	C	106	THR
2	C	112	GLU
2	C	114	LYS
2	C	119	THR
2	C	120	MET
2	C	123	GLU
2	C	125	THR
2	C	142	LEU
2	C	150	GLU
2	C	159	PHE

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Mol	Chain	Res	Type
2	C	189	ILE
2	C	192	LEU
2	C	200	GLU
2	C	201	LEU
2	C	208	VAL
2	C	270	ASP
2	C	271	GLU
2	C	313	ILE
2	C	315	ILE
2	C	317	LYS
2	C	324	GLU
2	C	362	ARG
2	C	364	THR
2	C	462	GLU
2	C	491	VAL
2	D	1	MET
2	D	6	LEU
2	D	10	GLU
2	D	14	SER
2	D	22	ARG
2	D	29	ILE
2	D	57	ARG
2	D	60	LYS
2	D	90	LYS
2	D	95	LEU
2	D	105	ARG
2	D	108	GLU
2	D	112	GLU
2	D	113	ILE
2	D	115	ARG
2	D	116	GLU
2	D	117	TYR
2	D	120	MET
2	D	122	LYS
2	D	123	GLU
2	D	144	ASN
2	D	148	LEU
2	D	150	GLU
2	D	151	LYS
2	D	154	LYS
2	D	157	VAL
2	D	171	THR

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Mol	Chain	Res	Type
2	D	189	ILE
2	D	192	LEU
2	D	198	LEU
2	D	199	LEU
2	D	203	ASP
2	D	223	LYS
2	D	226	LEU
2	D	256	LYS
2	D	271	GLU
2	D	291	VAL
2	D	389	GLU
2	D	428	GLU
2	D	458	GLU
2	D	459	ARG
2	D	490	VAL
2	D	491	VAL
2	A	2	GLU
2	A	3	LYS
2	A	10	GLU
2	A	22	ARG
2	A	40	ARG
2	A	57	ARG
2	A	65	SER
2	A	69	GLU
2	A	71	ASN
2	A	91	ASP
2	A	106	THR
2	A	119	THR
2	A	120	MET
2	A	123	GLU
2	A	142	LEU
2	A	149	ARG
2	A	159	PHE
2	A	161	THR
2	A	190	LYS
2	A	200	GLU
2	A	201	LEU
2	A	207	SER
2	A	208	VAL
2	A	226	LEU
2	A	270	ASP
2	A	315	ILE

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Mol	Chain	Res	Type
2	A	317	LYS
2	A	322	THR
2	A	325	LEU
2	A	356	ILE
2	A	362	ARG
2	A	449	ARG
2	A	462	GLU
2	A	475	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	27	HIS
1	B	36	GLN
1	B	174	HIS
1	B	240	GLN
2	C	27	HIS
2	C	36	GLN
2	C	80	ASN
2	C	144	ASN
2	C	240	GLN
2	C	278	ASN
2	D	27	HIS
2	D	36	GLN
2	D	80	ASN
2	D	174	HIS
2	D	247	GLN
2	A	27	HIS
2	A	36	GLN
2	A	80	ASN
2	A	240	GLN
2	A	278	ASN

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 (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

8 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	$\#\|Z\|>2$
4	GOL	C	502	-	5,5,5	0.18	0	5,5,5	0.74	0
3	PGE	C	501	-	9,9,9	0.41	0	8,8,8	0.57	0
3	PGE	B	501	-	9,9,9	0.38	0	8,8,8	0.52	0
3	PGE	D	501	-	9,9,9	0.57	0	8,8,8	0.68	0
3	PGE	A	501	-	9,9,9	0.48	0	8,8,8	0.59	0
4	GOL	B	502	-	5,5,5	0.35	0	5,5,5	0.82	0
4	GOL	D	502	-	5,5,5	0.59	0	5,5,5	0.95	0
4	GOL	A	502	-	5,5,5	0.68	0	5,5,5	1.52	1 (20%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	GOL	C	502	-	-	2/4/4/4	-
3	PGE	C	501	-	-	3/7/7/7	-
3	PGE	B	501	-	-	3/7/7/7	-
3	PGE	D	501	-	-	3/7/7/7	-
3	PGE	A	501	-	-	4/7/7/7	-
4	GOL	B	502	-	-	2/4/4/4	-
4	GOL	D	502	-	-	2/4/4/4	-
4	GOL	A	502	-	-	0/4/4/4	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	502	GOL	O2-C2-C1	2.38	119.60	109.12

There are no chirality outliers.

All (19) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	D	502	GOL	C1-C2-C3-O3
3	C	501	PGE	O1-C1-C2-O2
3	B	501	PGE	O3-C5-C6-O4
3	D	501	PGE	O3-C5-C6-O4
3	B	501	PGE	O2-C3-C4-O3
3	A	501	PGE	O1-C1-C2-O2
4	C	502	GOL	O1-C1-C2-C3
4	B	502	GOL	O1-C1-C2-C3
4	D	502	GOL	O2-C2-C3-O3
3	C	501	PGE	O2-C3-C4-O3
4	C	502	GOL	O1-C1-C2-O2
3	A	501	PGE	O3-C5-C6-O4
3	A	501	PGE	O2-C3-C4-O3
3	D	501	PGE	C3-C4-O3-C5
3	B	501	PGE	C3-C4-O3-C5
3	A	501	PGE	C4-C3-O2-C2
3	D	501	PGE	O2-C3-C4-O3
3	C	501	PGE	O3-C5-C6-O4
4	B	502	GOL	O1-C1-C2-O2

There are no ring outliers.

5 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	501	PGE	1	0
3	B	501	PGE	1	0
3	A	501	PGE	1	0
4	D	502	GOL	6	0
4	A	502	GOL	5	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues

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	B	490/497 (98%)	-0.24	6 (1%) 79 77	15, 27, 52, 77	0
2	A	490/497 (98%)	-0.06	12 (2%) 59 56	15, 31, 63, 88	0
2	C	490/497 (98%)	-0.14	5 (1%) 82 81	19, 32, 56, 84	0
2	D	491/497 (98%)	-0.03	9 (1%) 68 66	17, 32, 65, 112	0
All	All	1961/1988 (98%)	-0.12	32 (1%) 72 70	15, 31, 60, 112	0

All (32) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	117	TYR	8.7
2	A	40	ARG	3.4
2	D	91	ASP	3.4
2	D	40	ARG	3.3
2	C	115	ARG	3.2
2	D	39	PRO	2.9
2	D	148	LEU	2.9
2	A	96	TYR	2.9
2	A	43	TRP	2.9
1	B	117	TYR	2.9
2	A	91	ASP	2.8
1	B	112	GLU	2.7
2	C	112	GLU	2.7
2	A	94	PRO	2.6
1	B	142	LEU	2.5
2	A	38	TYR	2.4
2	A	39	PRO	2.4
2	D	113	ILE	2.4
2	D	199	LEU	2.3
1	B	115	ARG	2.3
2	C	116	GLU	2.3

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Mol	Chain	Res	Type	RSRZ
2	A	153	GLU	2.3
2	A	157	VAL	2.3
2	C	466	ASP	2.3
1	B	67	ARG	2.2
2	D	116	GLU	2.2
2	C	117	TYR	2.2
2	A	146	PRO	2.2
2	A	69	GLU	2.2
1	B	111	GLU	2.2
2	D	150	GLU	2.1
2	A	67	ARG	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 monosaccharides 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, 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
4	GOL	D	502	6/6	0.81	0.34	46,52,61,61	0
4	GOL	C	502	6/6	0.90	0.23	30,35,39,56	0
3	PGE	D	501	10/10	0.91	0.19	42,45,46,47	0
4	GOL	A	502	6/6	0.91	0.26	36,45,49,57	0
3	PGE	A	501	10/10	0.92	0.16	33,37,41,46	0
3	PGE	B	501	10/10	0.92	0.13	34,38,40,41	0
3	PGE	C	501	10/10	0.92	0.12	38,42,47,48	0
4	GOL	B	502	6/6	0.93	0.22	28,32,44,58	0

6.5 Other polymers (i)

There are no such residues in this entry.