Full wwPDB X-ray Structure Validation Report (i)

May 29, 2020 – 04:26 am BST

PDB ID	:	1GK2
Title	:	Histidine Ammonia-Lyase (HAL) Mutant F329G from Pseudomonas putida
Authors	:	Baedeker, M.; Schulz, G.E.
Deposited on	:	2001-08-07
Resolution	:	1.90 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:

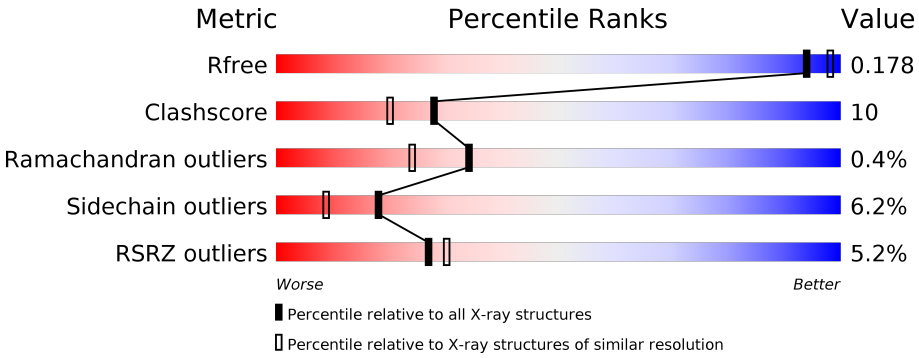
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, 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 1.90 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	6207 (1.90-1.90)
Clashscore	141614	6847 (1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
Sidechain outliers	138945	6760 (1.90-1.90)
RSRZ outliers	127900	6082 (1.90-1.90)

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	509	5% 81% 17%
1	B	509	5% 78% 20%
1	C	509	5% 79% 19%
1	D	509	6% 80% 20%

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
2	GOL	B	1510	-	-	X	-
2	GOL	C	1510	-	-	X	-
2	GOL	D	1510	-	-	X	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 16235 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.

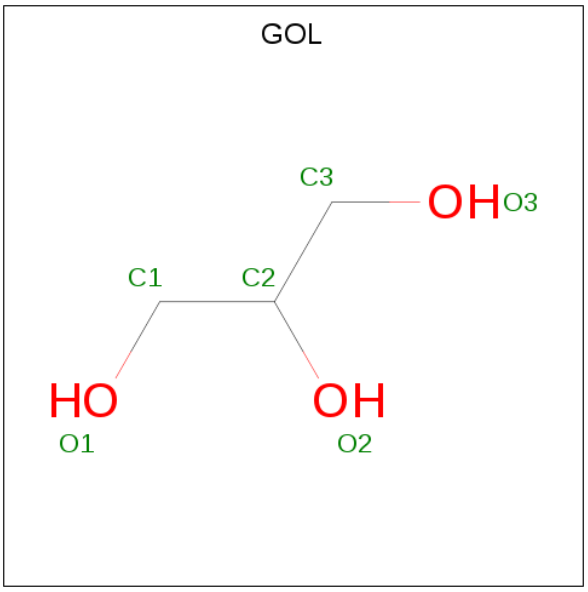
- Molecule 1 is a protein called HISTIDINE AMMONIA-LYASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	509	Total	C	N	O	S	46	0	0
			3757	2353	670	718	16			
1	B	509	Total	C	N	O	S	39	0	0
			3757	2353	670	718	16			
1	C	509	Total	C	N	O	S	39	0	0
			3757	2353	670	718	16			
1	D	509	Total	C	N	O	S	39	0	0
			3757	2353	670	718	16			

There are 8 discrepancies between the modelled and reference sequences:

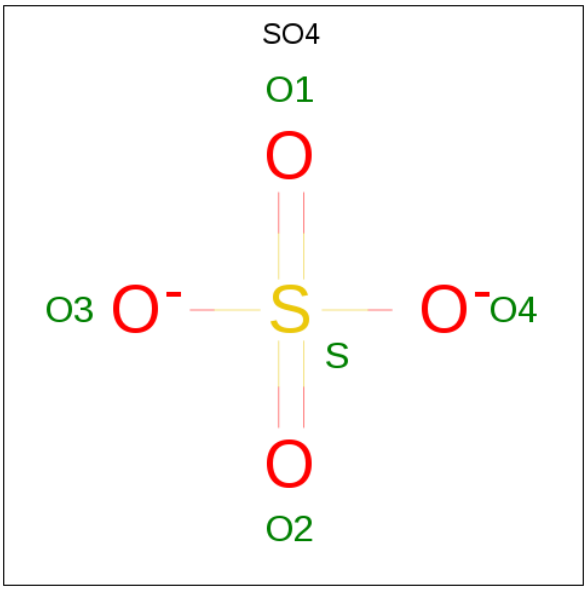
Chain	Residue	Modelled	Actual	Comment	Reference
A	273	ALA	CYS	engineered mutation	UNP P21310
A	329	GLY	PHE	engineered mutation	UNP P21310
B	273	ALA	CYS	engineered mutation	UNP P21310
B	329	GLY	PHE	engineered mutation	UNP P21310
C	273	ALA	CYS	engineered mutation	UNP P21310
C	329	GLY	PHE	engineered mutation	UNP P21310
D	273	ALA	CYS	engineered mutation	UNP P21310
D	329	GLY	PHE	engineered mutation	UNP P21310

- 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
2	D	1	Total C O 6 3 3	0	0

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total O S 5 4 1	0	0
3	C	1	Total O S 5 4 1	0	0
3	C	1	Total O S 5 4 1	0	0
3	D	1	Total O S 5 4 1	0	0

- Molecule 4 is water.

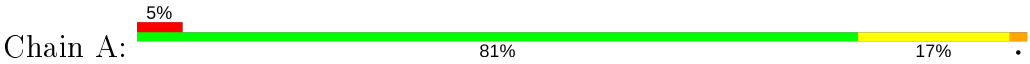
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	289	Total O 289 289	0	0
4	B	298	Total O 298 298	0	0
4	C	286	Total O 286 286	0	0
4	D	290	Total O 290 290	0	0

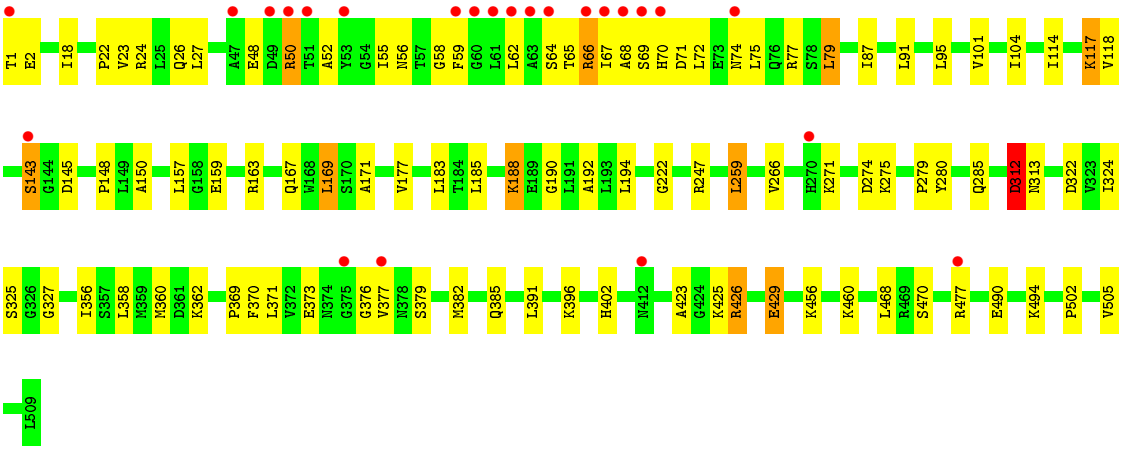
3 Residue-property plots (i)

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: HISTIDINE AMMONIA-LYASE

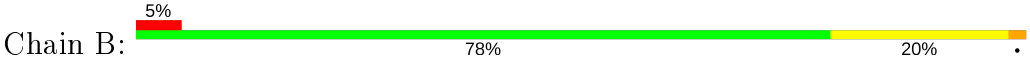
Chain A:

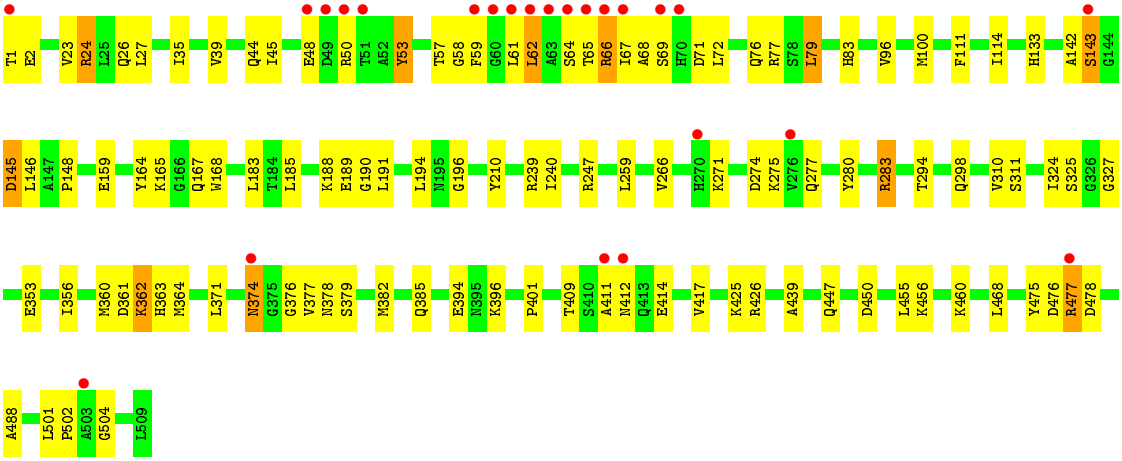




- Molecule 1: HISTIDINE AMMONIA-LYASE

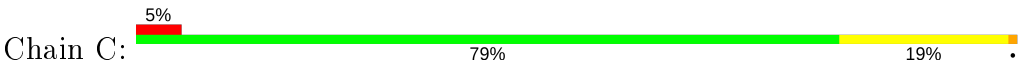
Chain B:

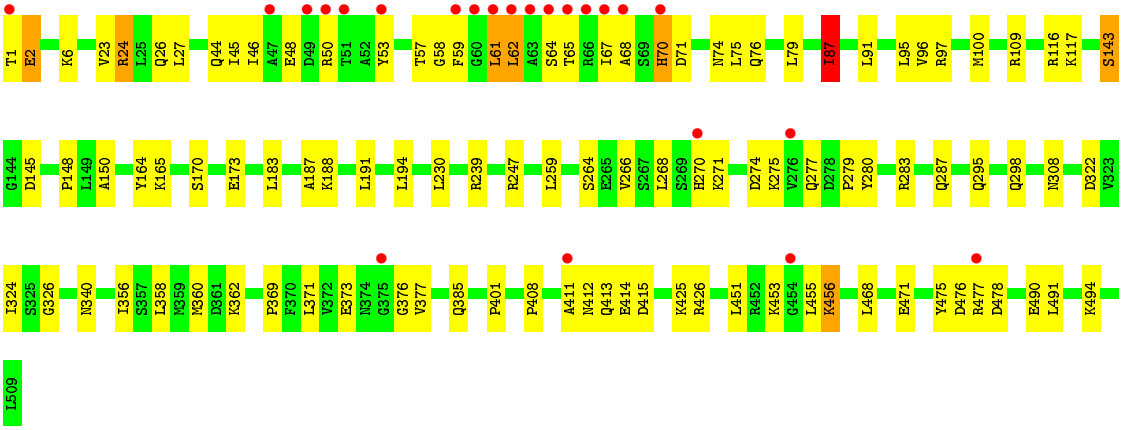




- Molecule 1: HISTIDINE AMMONIA-LYASE

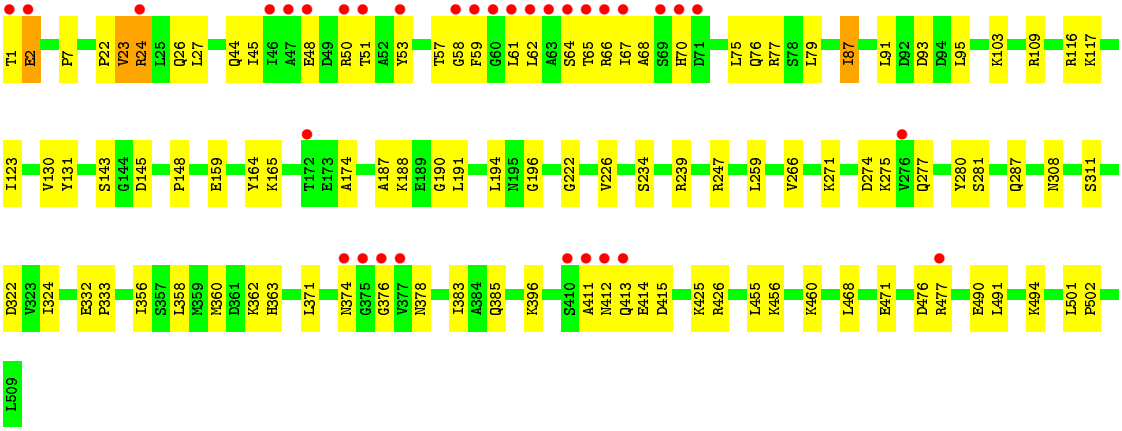
Chain C:





- Molecule 1: HISTIDINE AMMONIA-LYASE

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	77.97Å 130.56Å 115.83Å 90.00° 91.00° 90.00°	Depositor
Resolution (Å)	25.00 – 1.90 25.48 – 1.90	Depositor EDS
% Data completeness (in resolution range)	77.0 (25.00-1.90) 76.9 (25.48-1.90)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	4.44 (at 1.91Å)	Xtriage
Refinement program	SHELX	Depositor
R, R_{free}	0.170 , 0.226 0.178 , 0.178	Depositor DCC
R_{free} test set	6936 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å^2)	12.1	Xtriage
Anisotropy	0.508	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 78.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	0.048 for h,-k,-l	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	16235	wwPDB-VP
Average B, all atoms (Å^2)	19.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.49% 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, SO4

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	0.31	0/3814	0.81	3/5173 (0.1%)
1	B	0.30	0/3814	0.80	3/5173 (0.1%)
1	C	0.30	0/3814	0.79	2/5173 (0.0%)
1	D	0.30	0/3814	0.77	0/5173
All	All	0.30	0/15256	0.79	8/20692 (0.0%)

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	145	ASP	CB-CG-OD2	6.41	124.07	118.30
1	C	97	ARG	NE-CZ-NH2	-5.94	117.33	120.30
1	A	312	ASP	CB-CG-OD2	5.45	123.21	118.30
1	A	79	LEU	CA-CB-CG	5.32	127.55	115.30
1	A	426	ARG	NE-CZ-NH1	-5.30	117.65	120.30
1	C	87	ILE	CA-CB-CG1	5.29	121.05	111.00
1	B	210	TYR	CB-CG-CD2	-5.21	117.88	121.00
1	B	145	ASP	CB-CG-OD1	-5.12	113.69	118.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3757	0	3820	72	0
1	B	3757	0	3820	92	0
1	C	3757	0	3820	82	0
1	D	3757	0	3820	80	0
2	A	6	0	8	0	0
2	B	6	0	8	9	0
2	C	6	0	8	7	0
2	D	6	0	8	7	0
3	A	5	0	0	1	0
3	C	10	0	0	1	0
3	D	5	0	0	0	0
4	A	289	0	0	6	0
4	B	298	0	0	2	0
4	C	286	0	0	4	0
4	D	290	0	0	3	0
All	All	16235	0	15312	296	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 10.

All (296) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:362:LYS:HD2	1:A:369:PRO:HG3	1.52	0.92
1:A:391:LEU:HD11	1:C:87:ILE:HD11	1.51	0.90
1:D:191:LEU:HG	2:D:1510:GOL:H12	1.57	0.87
1:A:377:VAL:HG13	1:C:75:LEU:HD13	1.59	0.85
1:B:376:GLY:HA3	1:D:62:LEU:HD22	1.62	0.80
1:A:117:LYS:HD3	1:A:183:LEU:HD21	1.64	0.79
1:C:279:PRO:HG2	1:C:358:LEU:HD11	1.64	0.79
1:C:471:GLU:HG3	1:C:491:LEU:HD11	1.65	0.77
1:B:62:LEU:HD22	1:D:376:GLY:HA3	1.66	0.77
1:B:48:GLU:HB2	1:B:50:ARG:HE	1.50	0.77
1:A:59:PHE:O	1:C:376:GLY:HA2	1.86	0.76
1:A:66:ARG:O	1:A:67:ILE:HD13	1.87	0.74
1:D:53:TYR:HA	1:D:57:THR:OG1	1.86	0.74
1:B:239:ARG:NH2	1:C:324:ILE:HD11	2.02	0.73
1:D:45:ILE:HA	1:D:50:ARG:NE	2.03	0.72
1:D:490:GLU:HG3	1:D:494:LYS:HE3	1.71	0.72
1:D:44:GLN:O	1:D:48:GLU:HG3	1.90	0.72
1:B:69:SER:HA	1:B:72:LEU:HB2	1.73	0.71
1:B:266:VAL:HG23	1:B:456:LYS:O	1.91	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:377:VAL:HG13	1:D:75:LEU:HD13	1.70	0.71
1:D:1:THR:HG21	1:D:22:PRO:O	1.91	0.70
1:A:279:PRO:HG2	1:A:358:LEU:HD11	1.75	0.68
1:A:266:VAL:HG23	1:A:456:LYS:O	1.94	0.68
1:B:188:LYS:H	2:B:1510:GOL:H32	1.59	0.68
1:B:259:LEU:HD22	1:B:460:LYS:HD3	1.77	0.67
1:A:68:ALA:HB1	1:A:70:HIS:NE2	2.09	0.67
1:C:170:SER:OG	1:C:173:GLU:HG3	1.94	0.67
1:C:266:VAL:HG22	1:C:455:LEU:HB3	1.77	0.67
1:C:53:TYR:HA	1:C:57:THR:OG1	1.94	0.67
1:C:266:VAL:HG23	1:C:456:LYS:O	1.95	0.66
1:C:6:LYS:HB3	4:C:2012:HOH:O	1.93	0.66
1:B:143:SER:HB2	1:C:280:TYR:OH	1.96	0.66
1:A:376:GLY:HA3	1:C:62:LEU:HD22	1.78	0.66
1:B:188:LYS:HA	2:B:1510:GOL:H32	1.78	0.65
1:B:76:GLN:HE22	2:B:1510:GOL:H2	1.62	0.65
1:A:280:TYR:OH	1:D:143:SER:HB2	1.97	0.64
1:B:44:GLN:O	1:B:48:GLU:HG3	1.97	0.64
1:D:190:GLY:O	1:D:194:LEU:HG	1.98	0.64
1:D:360:MET:HE2	1:D:385:GLN:HB2	1.79	0.64
1:A:67:ILE:HB	1:A:72:LEU:HD13	1.79	0.64
1:D:187:ALA:HA	2:D:1510:GOL:O3	1.98	0.64
1:A:59:PHE:CE2	1:A:75:LEU:HD11	2.33	0.64
1:B:409:THR:OG1	1:B:414:GLU:HB2	1.98	0.64
1:A:62:LEU:HA	1:A:65:THR:HB	1.78	0.63
1:D:259:LEU:HD22	1:D:460:LYS:HD3	1.80	0.63
1:B:114:ILE:HG13	1:B:189:GLU:HG2	1.81	0.63
2:C:1510:GOL:H32	4:C:2050:HOH:O	1.99	0.62
1:D:266:VAL:HG23	1:D:456:LYS:O	2.00	0.62
1:A:69:SER:HA	1:A:72:LEU:HB2	1.82	0.62
1:C:96:VAL:O	1:C:100:MET:HG3	2.00	0.61
1:D:2:GLU:HG2	1:D:24:ARG:HB3	1.82	0.61
1:A:490:GLU:HG3	1:A:494:LYS:HE3	1.82	0.60
1:C:59:PHE:CE2	1:C:75:LEU:HD11	2.36	0.60
1:B:277:GLN:HE21	1:B:283:ARG:CZ	2.15	0.60
1:C:490:GLU:HG3	1:C:494:LYS:HE3	1.83	0.60
1:B:280:TYR:OH	1:C:143:SER:HB2	2.03	0.59
1:D:48:GLU:HB2	1:D:50:ARG:HG3	1.83	0.59
1:A:117:LYS:HG2	4:A:2087:HOH:O	2.01	0.59
1:B:142:ALA:O	1:B:143:SER:HB3	2.03	0.59
1:D:2:GLU:HA	1:D:24:ARG:O	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:27:LEU:HD13	1:D:123:ILE:HD11	1.85	0.58
1:C:143:SER:HB2	1:C:414:GLU:OE2	2.02	0.58
1:D:362:LYS:HG3	1:D:363:HIS:N	2.18	0.58
1:C:48:GLU:HB2	1:C:50:ARG:HE	1.67	0.58
1:D:266:VAL:HG22	1:D:455:LEU:HB3	1.85	0.58
1:D:59:PHE:CE2	1:D:75:LEU:HD11	2.37	0.58
1:C:62:LEU:HA	1:C:65:THR:HB	1.85	0.57
1:D:45:ILE:HA	1:D:50:ARG:HE	1.69	0.57
1:A:52:ALA:HB3	1:A:55:ILE:HB	1.86	0.57
1:D:266:VAL:HG22	1:D:455:LEU:CB	2.34	0.57
1:A:70:HIS:H	1:A:70:HIS:CD2	2.23	0.56
1:B:65:THR:HG22	1:B:66:ARG:O	2.04	0.56
1:C:76:GLN:OE1	2:C:1510:GOL:H11	2.05	0.56
1:A:360:MET:HE2	1:A:385:GLN:HB2	1.86	0.56
1:C:70:HIS:H	1:C:70:HIS:CD2	2.24	0.56
2:D:1510:GOL:H32	4:D:2290:HOH:O	2.05	0.56
1:A:490:GLU:CG	1:A:494:LYS:HE3	2.36	0.56
1:A:379:SER:HB3	1:A:382:MET:HE2	1.88	0.56
1:D:76:GLN:HE22	2:D:1510:GOL:C3	2.19	0.56
1:C:68:ALA:HB1	1:C:70:HIS:NE2	2.21	0.55
1:B:240:ILE:HD11	1:C:324:ILE:CG2	2.35	0.55
1:B:188:LYS:N	2:B:1510:GOL:H32	2.22	0.55
1:C:360:MET:HE2	1:C:385:GLN:HB2	1.87	0.55
1:D:188:LYS:HA	2:D:1510:GOL:H2	1.88	0.55
1:B:96:VAL:O	1:B:100:MET:HG3	2.06	0.55
1:A:59:PHE:HE2	1:A:75:LEU:HD11	1.71	0.55
1:A:356:ILE:O	1:A:360:MET:HG2	2.07	0.55
1:A:143:SER:HB2	1:D:280:TYR:OH	2.07	0.54
1:B:377:VAL:CG1	1:D:75:LEU:HD13	2.37	0.54
1:C:356:ILE:O	1:C:360:MET:HG2	2.08	0.54
1:D:48:GLU:HB2	1:D:50:ARG:CG	2.38	0.54
1:B:356:ILE:O	1:B:360:MET:HG2	2.08	0.53
1:B:188:LYS:CA	2:B:1510:GOL:H32	2.38	0.53
1:B:376:GLY:CA	1:D:62:LEU:HD22	2.34	0.53
1:C:67:ILE:HG22	1:C:71:ASP:HB2	1.91	0.53
1:C:164:TYR:CE2	1:C:165:LYS:HG3	2.43	0.53
1:C:266:VAL:HG22	1:C:455:LEU:CB	2.38	0.53
1:B:59:PHE:O	1:D:376:GLY:HA2	2.09	0.53
1:B:324:ILE:HD11	1:C:239:ARG:NH2	2.24	0.52
1:A:157:LEU:HD21	1:A:185:LEU:HG	1.91	0.52
1:B:362:LYS:HG3	1:B:363:HIS:N	2.24	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:143:SER:OG	1:B:146:LEU:HD11	2.09	0.52
1:C:76:GLN:HE22	2:C:1510:GOL:C3	2.22	0.52
1:B:79:LEU:O	1:B:83:HIS:HB2	2.10	0.51
1:D:145:ASP:HB3	1:D:148:PRO:HG2	1.91	0.51
1:D:396:LYS:NZ	4:D:2225:HOH:O	2.43	0.51
1:B:360:MET:HE2	1:B:385:GLN:HB2	1.93	0.51
1:C:362:LYS:HD2	1:C:369:PRO:HG3	1.92	0.51
1:D:411:ALA:O	1:D:412:ASN:HB2	2.11	0.51
1:D:87:ILE:HD11	4:D:2045:HOH:O	2.10	0.51
1:B:48:GLU:CB	1:B:50:ARG:HE	2.22	0.51
1:D:70:HIS:CD2	1:D:70:HIS:H	2.27	0.51
1:A:1:THR:HG22	1:A:1:THR:O	2.11	0.51
1:A:70:HIS:O	1:A:74:ASN:ND2	2.44	0.51
1:C:230:LEU:HD22	1:C:270:HIS:CD2	2.46	0.51
1:C:451:LEU:O	1:C:453:LYS:HD3	2.11	0.50
1:B:165:LYS:O	1:B:167:GLN:OE1	2.30	0.50
1:B:298:GLN:NE2	1:C:298:GLN:HB3	2.26	0.50
1:B:191:LEU:HG	2:B:1510:GOL:H11	1.93	0.50
1:B:79:LEU:HD23	1:B:83:HIS:CE1	2.46	0.50
1:A:327:GLY:O	1:D:287:GLN:HG2	2.12	0.50
1:B:240:ILE:HD13	1:C:326:GLY:HA3	1.94	0.50
1:B:401:PRO:HD3	1:C:401:PRO:HD3	1.93	0.50
1:B:377:VAL:HG12	1:B:377:VAL:O	2.12	0.49
1:C:58:GLY:HA3	1:C:62:LEU:HB3	1.94	0.49
1:C:1:THR:HG22	1:C:1:THR:O	2.11	0.49
1:A:429:GLU:HG3	4:A:2237:HOH:O	2.11	0.49
1:B:44:GLN:HG2	1:B:50:ARG:HH21	1.78	0.49
1:D:471:GLU:HG3	1:D:491:LEU:HD11	1.94	0.49
1:B:277:GLN:HG3	1:B:283:ARG:NH2	2.27	0.49
1:C:277:GLN:HE21	1:C:283:ARG:CZ	2.26	0.49
1:B:240:ILE:HD11	1:C:324:ILE:HG21	1.94	0.49
1:A:177:VAL:HG23	4:A:2126:HOH:O	2.12	0.49
1:B:45:ILE:HA	1:B:50:ARG:CZ	2.43	0.48
1:D:143:SER:HB2	1:D:414:GLU:OE2	2.13	0.48
1:A:58:GLY:HA3	1:A:67:ILE:HD11	1.94	0.48
1:C:91:LEU:HD22	1:C:95:LEU:HD23	1.96	0.48
1:A:101:VAL:HA	1:A:104:ILE:HD12	1.96	0.48
1:B:277:GLN:HE21	1:B:283:ARG:NE	2.12	0.48
1:B:48:GLU:HB2	1:B:50:ARG:HG3	1.95	0.48
1:C:295:GLN:NE2	1:C:340:ASN:HB3	2.29	0.48
1:D:93:ASP:HB3	1:D:131:TYR:CD2	2.49	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:44:GLN:HG2	1:C:50:ARG:NH2	2.28	0.47
1:B:53:TYR:HA	1:B:57:THR:OG1	2.14	0.47
1:C:475:TYR:OH	1:C:478:ASP:HA	2.15	0.47
1:B:62:LEU:HA	1:B:65:THR:HB	1.97	0.47
1:D:356:ILE:O	1:D:360:MET:HG2	2.14	0.47
1:A:74:ASN:H	1:A:74:ASN:HD22	1.62	0.47
1:C:183:LEU:HG	4:C:2108:HOH:O	2.15	0.47
1:A:159:GLU:O	1:A:171:ALA:HB2	2.15	0.47
1:C:2:GLU:HA	1:C:24:ARG:O	2.15	0.47
1:B:266:VAL:HG22	1:B:455:LEU:HB3	1.96	0.47
1:D:68:ALA:HB1	1:D:70:HIS:CD2	2.50	0.47
1:A:58:GLY:HA3	1:A:62:LEU:HB3	1.97	0.47
1:D:1:THR:HG22	1:D:23:VAL:CG2	2.45	0.47
1:A:117:LYS:CD	1:A:183:LEU:HD21	2.40	0.47
1:A:324:ILE:HD11	1:D:239:ARG:NH2	2.30	0.47
1:A:402:HIS:HB2	1:A:423:ALA:HB2	1.96	0.47
1:C:408:PRO:HB3	1:C:415:ASP:HA	1.96	0.47
1:D:490:GLU:CG	1:D:494:LYS:HE3	2.44	0.47
1:A:114:ILE:HD11	1:A:118:VAL:HG11	1.96	0.46
1:C:187:ALA:O	1:C:188:LYS:HB3	2.15	0.46
1:A:169:LEU:N	1:A:169:LEU:HD23	2.30	0.46
1:A:188:LYS:O	1:A:188:LYS:HG3	2.15	0.46
1:D:58:GLY:HA3	1:D:62:LEU:HB3	1.98	0.46
1:D:24:ARG:HA	1:D:24:ARG:HE	1.80	0.46
1:A:145:ASP:HB3	1:A:148:PRO:HG2	1.97	0.46
1:B:294:THR:O	1:B:298:GLN:HG3	2.15	0.46
1:B:298:GLN:CD	1:C:298:GLN:HB3	2.36	0.46
1:A:190:GLY:O	1:A:194:LEU:HG	2.16	0.46
1:A:48:GLU:HB2	1:A:50:ARG:HG3	1.98	0.46
1:A:18:ILE:HD13	1:A:101:VAL:HG11	1.96	0.46
1:A:377:VAL:O	1:A:377:VAL:HG12	2.16	0.46
1:B:1:THR:O	1:B:1:THR:HG22	2.16	0.46
1:B:411:ALA:O	1:B:412:ASN:HB2	2.15	0.46
1:B:142:ALA:HB3	1:B:417:VAL:HG12	1.97	0.46
1:C:451:LEU:C	1:C:453:LYS:HD3	2.36	0.46
1:C:150:ALA:HA	1:C:194:LEU:HD22	1.97	0.46
1:D:7:PRO:HB2	1:D:109:ARG:HG2	1.98	0.46
1:D:68:ALA:HB1	1:D:70:HIS:NE2	2.31	0.46
1:A:312:ASP:OD1	1:A:313:ASN:N	2.49	0.45
1:B:196:GLY:HA2	1:B:311:SER:O	2.16	0.45
1:B:379:SER:HB3	1:B:382:MET:HE1	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:504:GLY:HA2	4:B:2294:HOH:O	2.17	0.45
1:B:183:LEU:HG	4:B:2105:HOH:O	2.16	0.45
1:B:240:ILE:HD11	1:C:324:ILE:HG22	1.97	0.45
1:D:45:ILE:HA	1:D:50:ARG:CZ	2.46	0.45
1:A:68:ALA:O	1:A:71:ASP:N	2.50	0.45
1:C:76:GLN:NE2	2:C:1510:GOL:H11	2.32	0.45
1:C:46:ILE:HD11	1:C:187:ALA:CB	2.47	0.45
1:D:24:ARG:CA	1:D:24:ARG:HE	2.30	0.45
1:A:396:LYS:NZ	4:A:2217:HOH:O	2.50	0.45
1:A:77:ARG:NH2	1:A:159:GLU:OE2	2.50	0.45
1:B:327:GLY:O	1:C:287:GLN:HG2	2.17	0.45
1:B:361:ASP:OD2	1:B:364:MET:HG2	2.17	0.45
1:D:411:ALA:O	1:D:413:GLN:NE2	2.50	0.45
1:B:145:ASP:HB3	1:B:148:PRO:HG2	1.99	0.45
1:B:79:LEU:HD11	2:B:1510:GOL:H12	1.99	0.45
1:A:377:VAL:CG1	1:C:75:LEU:HD13	2.39	0.45
1:D:77:ARG:NH2	1:D:159:GLU:OE2	2.49	0.45
1:D:109:ARG:NH1	1:D:308:ASN:O	2.50	0.45
1:C:412:ASN:ND2	4:C:2228:HOH:O	2.50	0.45
1:D:62:LEU:O	1:D:65:THR:HB	2.16	0.45
1:A:58:GLY:CA	1:A:67:ILE:HD11	2.47	0.44
1:D:196:GLY:HA2	1:D:311:SER:O	2.16	0.44
1:A:56:ASN:O	1:A:66:ARG:HA	2.17	0.44
1:C:377:VAL:HG12	1:C:377:VAL:O	2.18	0.44
1:D:374:ASN:HB2	1:D:378:ASN:ND2	2.31	0.44
1:B:447:GLN:O	1:B:450:ASP:HB2	2.16	0.44
1:C:283:ARG:NH1	3:C:1511:SO4:O1	2.50	0.44
1:B:76:GLN:NE2	2:B:1510:GOL:H2	2.31	0.44
1:B:77:ARG:NH2	1:B:159:GLU:OE2	2.50	0.44
1:C:79:LEU:HD21	1:C:191:LEU:CD2	2.48	0.44
1:C:145:ASP:HB3	1:C:148:PRO:HG2	2.00	0.44
1:A:313:ASN:ND2	3:A:1511:SO4:O3	2.50	0.44
1:B:24:ARG:HA	1:B:24:ARG:HE	1.82	0.44
1:B:58:GLY:HA3	1:B:62:LEU:HB3	2.00	0.44
1:A:68:ALA:O	1:A:71:ASP:HB2	2.17	0.44
1:C:264:SER:O	1:C:268:LEU:HG	2.18	0.44
1:B:325:SER:OG	1:C:277:GLN:NE2	2.50	0.44
1:B:133:HIS:HB2	1:B:168:TRP:CZ3	2.52	0.43
1:A:74:ASN:N	1:A:74:ASN:HD22	2.16	0.43
1:D:187:ALA:HA	2:D:1510:GOL:HO3	1.82	0.43
1:B:69:SER:O	1:B:72:LEU:HB3	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:411:ALA:O	1:C:413:GLN:NE2	2.50	0.43
1:C:412:ASN:HD21	1:D:412:ASN:HD21	1.67	0.43
1:B:188:LYS:H	2:B:1510:GOL:C3	2.27	0.43
1:B:35:ILE:O	1:B:39:VAL:HG23	2.19	0.43
1:B:239:ARG:HH21	1:C:324:ILE:HD11	1.80	0.43
1:A:58:GLY:CA	1:A:62:LEU:HB3	2.49	0.43
1:C:44:GLN:HG2	1:C:48:GLU:OE2	2.19	0.43
1:A:279:PRO:HG2	1:A:358:LEU:CD1	2.47	0.43
1:A:91:LEU:HD22	1:A:95:LEU:HD23	2.01	0.43
1:B:185:LEU:HD22	1:B:189:GLU:HB3	1.99	0.43
1:D:281:SER:OG	1:D:358:LEU:HD12	2.18	0.43
1:B:111:PHE:HB2	1:B:310:VAL:HG11	2.00	0.42
1:B:439:ALA:HB1	1:B:488:ALA:HB3	2.01	0.42
1:B:83:HIS:HA	1:D:383:ILE:HG13	2.01	0.42
1:C:279:PRO:CG	1:C:358:LEU:HD11	2.41	0.42
1:C:70:HIS:O	1:C:74:ASN:ND2	2.51	0.42
1:C:67:ILE:CG2	1:C:71:ASP:HB2	2.49	0.42
1:A:1:THR:HG21	1:A:22:PRO:O	2.18	0.42
1:B:69:SER:HA	1:B:72:LEU:CB	2.47	0.42
1:D:62:LEU:O	1:D:65:THR:N	2.52	0.42
1:A:163:ARG:HA	1:A:167:GLN:O	2.20	0.42
1:A:360:MET:HE1	1:A:370:PHE:HD1	1.85	0.42
1:B:277:GLN:HB3	1:B:283:ARG:HH21	1.83	0.42
4:A:2217:HOH:O	1:B:396:LYS:NZ	2.51	0.42
1:B:68:ALA:O	1:B:71:ASP:HB2	2.18	0.42
1:C:191:LEU:HG	2:C:1510:GOL:O1	2.19	0.42
1:C:188:LYS:HG3	1:C:188:LYS:O	2.20	0.42
1:C:48:GLU:CD	1:C:50:ARG:HH21	2.22	0.42
1:C:45:ILE:HA	1:C:50:ARG:CZ	2.49	0.42
1:A:222:GLY:HA3	1:A:285:GLN:OE1	2.20	0.42
1:A:266:VAL:HG23	1:A:456:LYS:C	2.39	0.42
1:B:164:TYR:CE2	1:B:165:LYS:HG3	2.54	0.42
1:B:48:GLU:HB2	1:B:50:ARG:NE	2.28	0.42
1:B:266:VAL:HG22	1:B:455:LEU:CB	2.50	0.42
1:B:475:TYR:OH	1:B:478:ASP:HA	2.19	0.42
1:B:58:GLY:N	1:B:67:ILE:HG12	2.35	0.42
1:C:283:ARG:HG3	1:C:283:ARG:O	2.20	0.42
1:C:44:GLN:HG2	1:C:50:ARG:HH21	1.85	0.42
1:A:163:ARG:HD2	4:A:2117:HOH:O	2.19	0.42
1:B:353:GLU:HA	1:B:356:ILE:HD12	2.02	0.42
1:D:222:GLY:O	1:D:226:VAL:HG23	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:190:GLY:O	1:B:194:LEU:HG	2.19	0.41
1:B:374:ASN:HB2	1:B:378:ASN:ND2	2.35	0.41
1:D:59:PHE:HE2	1:D:75:LEU:HD11	1.82	0.41
1:D:66:ARG:O	1:D:67:ILE:HD13	2.19	0.41
1:D:332:GLU:N	1:D:333:PRO:HD2	2.36	0.41
1:A:188:LYS:HE2	1:A:192:ALA:HB2	2.01	0.41
1:A:150:ALA:HA	1:A:194:LEU:HD22	2.03	0.41
1:C:76:GLN:HE22	2:C:1510:GOL:H11	1.86	0.41
1:D:412:ASN:O	1:D:415:ASP:HB3	2.20	0.41
1:C:109:ARG:NH1	1:C:308:ASN:O	2.53	0.41
1:D:259:LEU:CD2	1:D:460:LYS:HD3	2.50	0.41
1:A:325:SER:OG	1:D:277:GLN:NE2	2.53	0.41
1:D:130:VAL:HG11	1:D:174:ALA:HB1	2.03	0.41
1:D:62:LEU:CA	1:D:65:THR:HB	2.51	0.41
1:C:76:GLN:HE22	2:C:1510:GOL:H31	1.85	0.41
1:C:61:LEU:HD23	1:C:61:LEU:N	2.36	0.41
1:A:502:PRO:O	1:A:505:VAL:HG23	2.21	0.40
1:D:1:THR:HG22	1:D:23:VAL:HG23	2.03	0.40
1:D:27:LEU:HD12	1:D:27:LEU:HA	1.94	0.40
1:B:501:LEU:HA	1:B:502:PRO:HD3	1.97	0.40
1:D:194:LEU:HD23	1:D:194:LEU:N	2.34	0.40
1:D:501:LEU:HG	1:D:502:PRO:HD2	2.04	0.40
1:A:75:LEU:HD12	1:A:75:LEU:O	2.21	0.40
1:B:476:ASP:HB2	1:B:477:ARG:H	1.68	0.40
1:C:45:ILE:HG12	1:C:50:ARG:NH1	2.36	0.40
1:D:187:ALA:O	1:D:188:LYS:HB3	2.21	0.40
1:D:51:THR:HG23	1:D:57:THR:HG22	2.04	0.40
1:D:76:GLN:NE2	2:D:1510:GOL:O3	2.50	0.40
1:D:164:TYR:CE2	1:D:165:LYS:HG3	2.56	0.40
1:A:259:LEU:HD22	1:A:460:LYS:HD3	2.03	0.40
1:D:91:LEU:HD22	1:D:95:LEU:HD23	2.03	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	507/509 (100%)	490 (97%)	14 (3%)	3 (1%)	25	15
1	B	507/509 (100%)	491 (97%)	13 (3%)	3 (1%)	25	15
1	C	507/509 (100%)	493 (97%)	12 (2%)	2 (0%)	34	24
1	D	507/509 (100%)	488 (96%)	18 (4%)	1 (0%)	47	38
All	All	2028/2036 (100%)	1962 (97%)	57 (3%)	9 (0%)	34	24

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	275	LYS
1	B	275	LYS
1	A	275	LYS
1	B	374	ASN
1	C	275	LYS
1	B	143	SER
1	A	66	ARG
1	A	143	SER
1	C	143	SER

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	387/387 (100%)	361 (93%)	26 (7%)	16	7
1	B	387/387 (100%)	365 (94%)	22 (6%)	20	11
1	C	387/387 (100%)	362 (94%)	25 (6%)	17	8
1	D	387/387 (100%)	364 (94%)	23 (6%)	19	10
All	All	1548/1548 (100%)	1452 (94%)	96 (6%)	18	9

All (96) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	GLU
1	A	23	VAL
1	A	24	ARG
1	A	26	GLN
1	A	27	LEU
1	A	50	ARG
1	A	64	SER
1	A	79	LEU
1	A	87	ILE
1	A	117	LYS
1	A	169	LEU
1	A	188	LYS
1	A	247	ARG
1	A	259	LEU
1	A	271	LYS
1	A	274	ASP
1	A	312	ASP
1	A	322	ASP
1	A	371	LEU
1	A	373	GLU
1	A	425	LYS
1	A	426	ARG
1	A	429	GLU
1	A	468	LEU
1	A	470	SER
1	A	477	ARG
1	B	2	GLU
1	B	23	VAL
1	B	24	ARG
1	B	26	GLN
1	B	27	LEU
1	B	53	TYR
1	B	61	LEU
1	B	62	LEU
1	B	64	SER
1	B	66	ARG
1	B	79	LEU
1	B	247	ARG
1	B	271	LYS
1	B	274	ASP
1	B	283	ARG
1	B	362	LYS
1	B	371	LEU

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Mol	Chain	Res	Type
1	B	394	GLU
1	B	425	LYS
1	B	426	ARG
1	B	468	LEU
1	B	477	ARG
1	C	2	GLU
1	C	23	VAL
1	C	24	ARG
1	C	26	GLN
1	C	27	LEU
1	C	61	LEU
1	C	62	LEU
1	C	64	SER
1	C	70	HIS
1	C	87	ILE
1	C	116	ARG
1	C	117	LYS
1	C	247	ARG
1	C	259	LEU
1	C	271	LYS
1	C	274	ASP
1	C	322	ASP
1	C	371	LEU
1	C	373	GLU
1	C	425	LYS
1	C	426	ARG
1	C	456	LYS
1	C	468	LEU
1	C	476	ASP
1	C	477	ARG
1	D	2	GLU
1	D	23	VAL
1	D	24	ARG
1	D	26	GLN
1	D	61	LEU
1	D	64	SER
1	D	79	LEU
1	D	87	ILE
1	D	103	LYS
1	D	116	ARG
1	D	117	LYS
1	D	234	SER

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Mol	Chain	Res	Type
1	D	247	ARG
1	D	271	LYS
1	D	274	ASP
1	D	322	ASP
1	D	324	ILE
1	D	371	LEU
1	D	425	LYS
1	D	426	ARG
1	D	468	LEU
1	D	476	ASP
1	D	477	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	74	ASN
1	A	195	ASN
1	A	413	GLN
1	B	167	GLN
1	B	195	ASN
1	B	277	GLN
1	B	363	HIS
1	C	70	HIS
1	C	195	ASN
1	C	270	HIS
1	C	277	GLN
1	C	412	ASN
1	D	26	GLN
1	D	195	ASN
1	D	277	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 (i)

There are no carbohydrates 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	$\#\|Z\| > 2$
3	SO4	C	1511	-	4,4,4	0.64	0	6,6,6	0.07	0
3	SO4	D	1511	-	4,4,4	0.61	0	6,6,6	0.07	0
3	SO4	A	1511	-	4,4,4	0.65	0	6,6,6	0.06	0
2	GOL	B	1510	-	5,5,5	0.64	0	5,5,5	0.59	0
3	SO4	C	1512	-	4,4,4	0.64	0	6,6,6	0.10	0
2	GOL	C	1510	-	5,5,5	0.65	0	5,5,5	0.31	0
2	GOL	A	1510	-	5,5,5	0.61	0	5,5,5	0.40	0
2	GOL	D	1510	-	5,5,5	0.62	0	5,5,5	0.44	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	1510	-	-	2/4/4/4	-
2	GOL	A	1510	-	-	0/4/4/4	-
2	GOL	D	1510	-	-	4/4/4/4	-
2	GOL	B	1510	-	-	4/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	1510	GOL	C1-C2-C3-O3
2	B	1510	GOL	O1-C1-C2-C3
2	C	1510	GOL	O1-C1-C2-C3
2	D	1510	GOL	O1-C1-C2-C3
2	D	1510	GOL	C1-C2-C3-O3
2	B	1510	GOL	O2-C2-C3-O3
2	C	1510	GOL	O1-C1-C2-O2
2	D	1510	GOL	O1-C1-C2-O2
2	D	1510	GOL	O2-C2-C3-O3
2	B	1510	GOL	O1-C1-C2-O2

There are no ring outliers.

5 monomers are involved in 25 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	1511	SO4	1	0
3	A	1511	SO4	1	0
2	B	1510	GOL	9	0
2	C	1510	GOL	7	0
2	D	1510	GOL	7	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	503/509 (98%)	0.04	24 (4%)	30	33	4, 13, 52, 89	0
1	B	504/509 (99%)	0.00	24 (4%)	30	33	4, 13, 51, 89	0
1	C	504/509 (99%)	0.04	23 (4%)	32	35	5, 13, 51, 89	0
1	D	504/509 (99%)	0.08	33 (6%)	18	21	4, 13, 52, 89	0
All	All	2015/2036 (98%)	0.04	104 (5%)	27	30	4, 13, 53, 89	0

All (104) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	276	VAL	9.1
1	C	63	ALA	7.9
1	D	61	LEU	7.8
1	A	61	LEU	7.8
1	D	276	VAL	7.7
1	B	64	SER	7.6
1	B	61	LEU	7.3
1	D	70	HIS	6.2
1	B	276	VAL	6.2
1	D	64	SER	6.1
1	C	1	THR	5.8
1	A	70	HIS	5.7
1	D	65	THR	5.6
1	D	1	THR	5.3
1	D	62	LEU	5.2
1	C	62	LEU	5.2
1	A	69	SER	5.1
1	A	62	LEU	5.1
1	A	68	ALA	5.1
1	C	70	HIS	4.9
1	B	69	SER	4.9

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Mol	Chain	Res	Type	RSRZ
1	B	70	HIS	4.8
1	A	59	PHE	4.6
1	B	1	THR	4.5
1	B	411	ALA	4.5
1	D	412	ASN	4.4
1	C	50	ARG	4.4
1	B	67	ILE	4.3
1	D	410	SER	4.3
1	C	60	GLY	4.2
1	A	1	THR	4.2
1	B	62	LEU	4.1
1	C	64	SER	4.1
1	B	60	GLY	4.0
1	D	50	ARG	4.0
1	D	69	SER	3.9
1	B	50	ARG	3.9
1	D	66	ARG	3.8
1	A	270	HIS	3.8
1	D	59	PHE	3.8
1	C	68	ALA	3.6
1	B	65	THR	3.6
1	A	50	ARG	3.6
1	C	61	LEU	3.5
1	A	64	SER	3.5
1	B	59	PHE	3.4
1	D	67	ILE	3.3
1	C	66	ARG	3.3
1	B	66	ARG	3.3
1	C	270	HIS	3.3
1	D	2	GLU	3.2
1	C	59	PHE	3.2
1	D	47	ALA	3.1
1	A	49	ASP	3.1
1	A	60	GLY	3.0
1	D	63	ALA	3.0
1	C	411	ALA	3.0
1	C	477	ARG	3.0
1	D	51	THR	2.9
1	C	454	GLY	2.9
1	D	477	ARG	2.9
1	B	48	GLU	2.9
1	C	51	THR	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	74	ASN	2.8
1	D	374	ASN	2.8
1	A	377	VAL	2.8
1	B	49	ASP	2.7
1	C	49	ASP	2.7
1	C	375	GLY	2.7
1	B	412	ASN	2.6
1	B	143	SER	2.6
1	B	503	ALA	2.6
1	D	60	GLY	2.6
1	B	51	THR	2.6
1	B	270	HIS	2.6
1	D	53	TYR	2.6
1	A	143	SER	2.6
1	A	51	THR	2.6
1	C	67	ILE	2.5
1	A	477	ARG	2.5
1	C	47	ALA	2.5
1	A	63	ALA	2.5
1	D	58	GLY	2.4
1	D	411	ALA	2.4
1	D	413	GLN	2.4
1	B	374	ASN	2.4
1	D	71	ASP	2.4
1	A	47	ALA	2.3
1	D	376	GLY	2.3
1	D	377	VAL	2.3
1	B	63	ALA	2.3
1	C	65	THR	2.3
1	C	53	TYR	2.2
1	A	412	ASN	2.2
1	A	53	TYR	2.2
1	A	375	GLY	2.2
1	D	46	ILE	2.2
1	D	172	THR	2.1
1	D	48	GLU	2.1
1	D	375	GLY	2.1
1	A	67	ILE	2.1
1	B	477	ARG	2.1
1	D	24	ARG	2.0
1	A	66	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 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, 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	SO4	A	1511	5/5	0.79	0.22	76,86,91,97	0
3	SO4	C	1511	5/5	0.84	0.20	43,89,102,103	0
2	GOL	B	1510	6/6	0.87	0.20	14,32,39,42	0
3	SO4	C	1512	5/5	0.87	0.23	73,103,104,117	0
2	GOL	C	1510	6/6	0.89	0.21	16,46,51,72	0
2	GOL	A	1510	6/6	0.89	0.12	25,34,38,43	0
2	GOL	D	1510	6/6	0.89	0.18	27,36,48,56	0
3	SO4	D	1511	5/5	0.92	0.20	40,81,83,103	0

6.5 Other polymers (i)

There are no such residues in this entry.