Full wwPDB X-ray Structure Validation Report ⓘ

Aug 30, 2022 – 04:11 pm BST

PDB ID	:	7PK5
Title	:	Phosphodiesterase PdeL (EAL domain of crystals comprising full-length protein)
Authors	:	Fadel, J.; Schirmer, T.
Deposited on	:	2021-08-25
Resolution	:	4.40 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at http://www.wwpdb.org/validation/2017/FAQs#types.

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

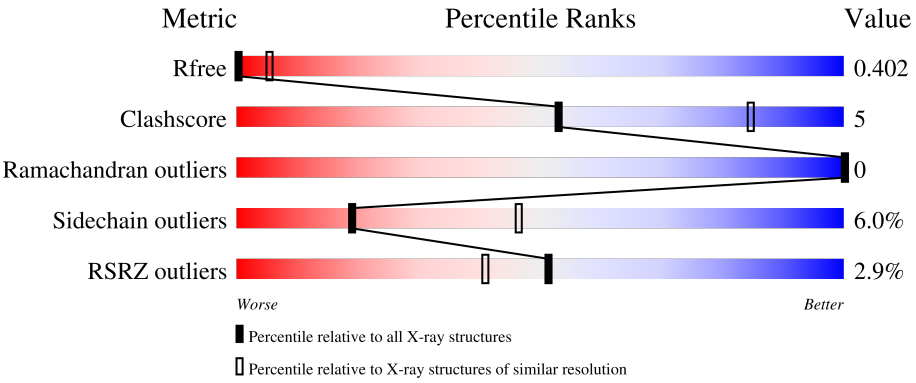
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.30
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0267
CCP4	:	7.1.010 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.30

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 4.40 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	1043 (5.00-3.80)
Clashscore	141614	1111 (5.00-3.80)
Ramachandran outliers	138981	1059 (5.00-3.80)
Sidechain outliers	138945	1041 (5.00-3.80)
RSRZ outliers	127900	1095 (5.08-3.70)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	369	2% 60% 7% 31%
1	B	369	3% 61% 6% 31%
1	C	369	2% 61% 7% 31%
1	D	369	59% 8% 31%

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 7956 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 Cyclic di-GMP phosphodiesterase PdeL.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	253	Total	C	N	O	S	0	2	0
			1989	1288	328	363	10			
1	D	253	Total	C	N	O	S	0	2	0
			1989	1288	328	363	10			
1	B	253	Total	C	N	O	S	0	2	0
			1989	1288	328	363	10			
1	C	253	Total	C	N	O	S	0	2	0
			1989	1288	328	363	10			

There are 32 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	MET	-	initiating methionine	UNP P21514
A	1	ALA	-	expression tag	UNP P21514
A	363	HIS	-	expression tag	UNP P21514
A	364	HIS	-	expression tag	UNP P21514
A	365	HIS	-	expression tag	UNP P21514
A	366	HIS	-	expression tag	UNP P21514
A	367	HIS	-	expression tag	UNP P21514
A	368	HIS	-	expression tag	UNP P21514
D	0	MET	-	initiating methionine	UNP P21514
D	1	ALA	-	expression tag	UNP P21514
D	363	HIS	-	expression tag	UNP P21514
D	364	HIS	-	expression tag	UNP P21514
D	365	HIS	-	expression tag	UNP P21514
D	366	HIS	-	expression tag	UNP P21514
D	367	HIS	-	expression tag	UNP P21514
D	368	HIS	-	expression tag	UNP P21514
B	0	MET	-	initiating methionine	UNP P21514
B	1	ALA	-	expression tag	UNP P21514
B	363	HIS	-	expression tag	UNP P21514
B	364	HIS	-	expression tag	UNP P21514
B	365	HIS	-	expression tag	UNP P21514

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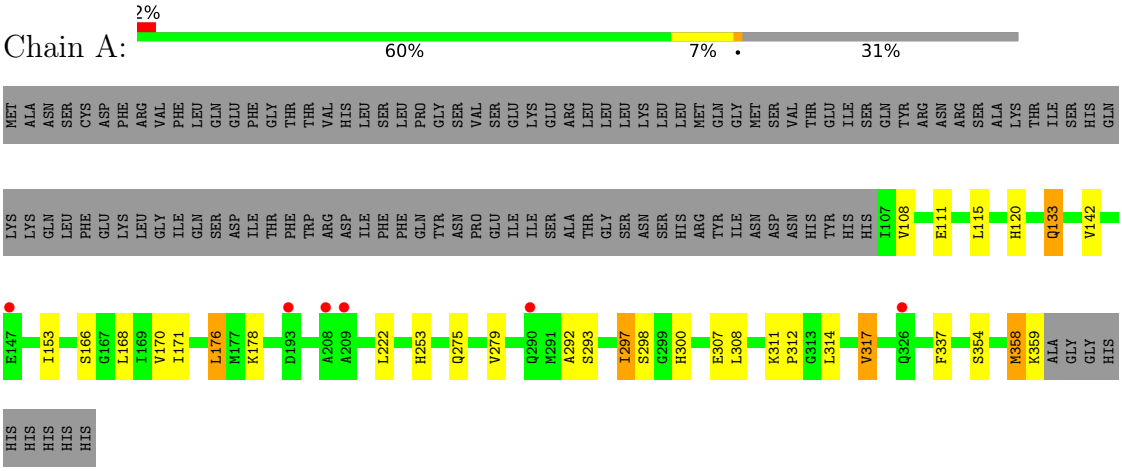
Chain	Residue	Modelled	Actual	Comment	Reference
B	366	HIS	-	expression tag	UNP P21514
B	367	HIS	-	expression tag	UNP P21514
B	368	HIS	-	expression tag	UNP P21514
C	0	MET	-	initiating methionine	UNP P21514
C	1	ALA	-	expression tag	UNP P21514
C	363	HIS	-	expression tag	UNP P21514
C	364	HIS	-	expression tag	UNP P21514
C	365	HIS	-	expression tag	UNP P21514
C	366	HIS	-	expression tag	UNP P21514
C	367	HIS	-	expression tag	UNP P21514
C	368	HIS	-	expression tag	UNP P21514

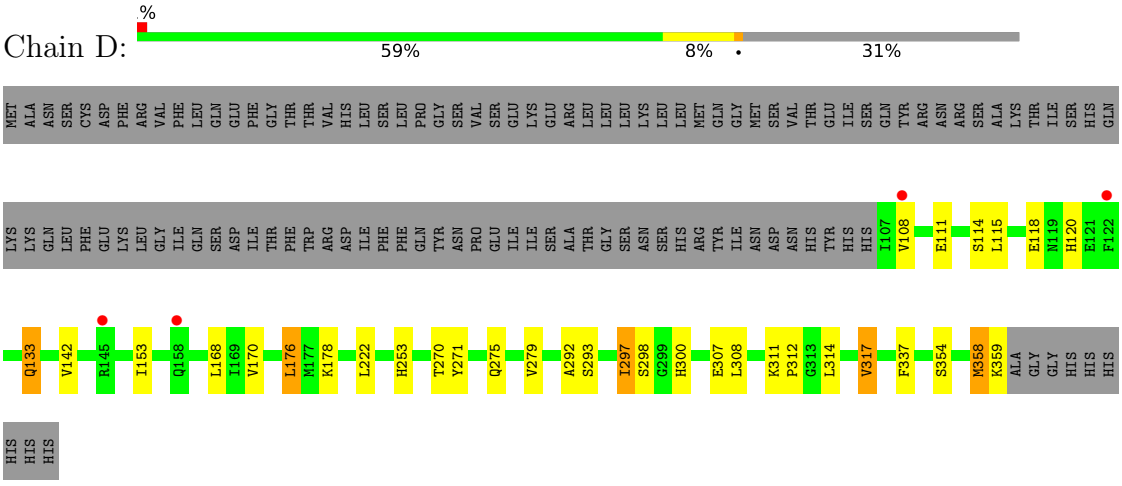
3 Residue-property plots (i)

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.

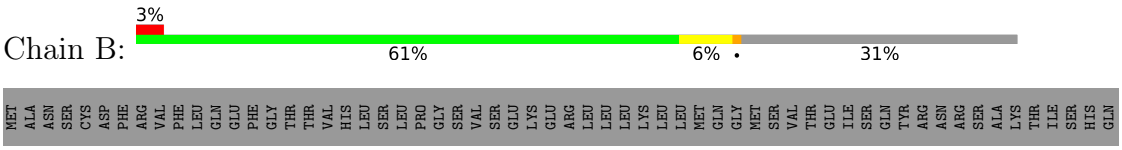
• Molecule 1: Cyclic di-GMP phosphodiesterase PdeL

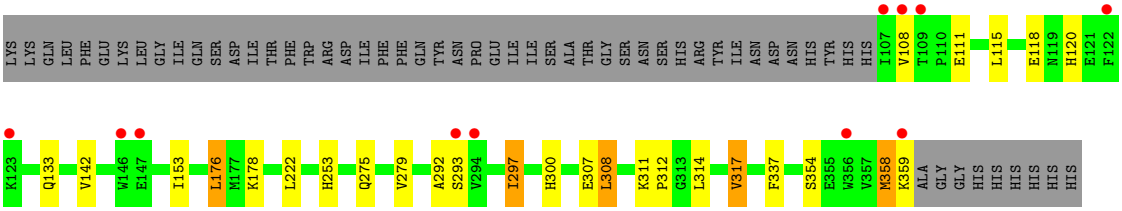


• Molecule 1: Cyclic di-GMP phosphodiesterase PdeL

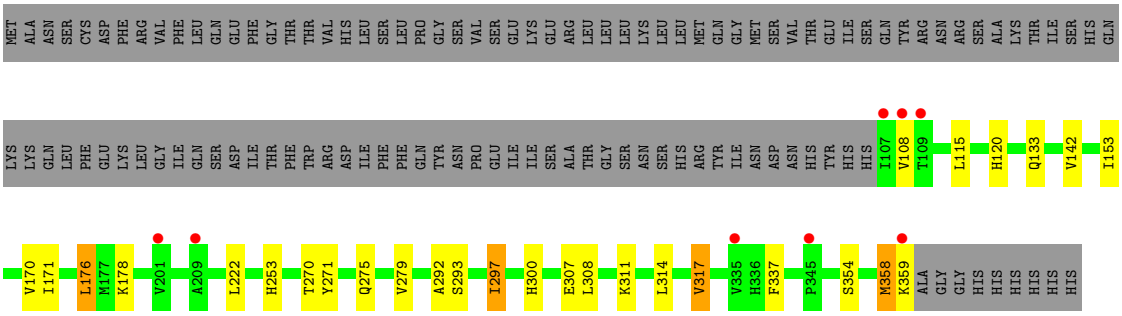


• Molecule 1: Cyclic di-GMP phosphodiesterase PdeL





• Molecule 1: Cyclic di-GMP phosphodiesterase PdeL



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	86.41Å 170.21Å 93.08Å 90.00° 94.37° 90.00°	Depositor
Resolution (Å)	25.00 – 4.40 48.41 – 4.40	Depositor EDS
% Data completeness (in resolution range)	98.4 (25.00-4.40) 80.5 (48.41-4.40)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.35 (at 4.45Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.373 , 0.397 0.379 , 0.402	Depositor DCC
R_{free} test set	791 reflections (4.68%)	wwPDB-VP
Wilson B-factor (Å^2)	173.3	Xtriage
Anisotropy	0.613	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	(Not available) , (Not available)	EDS
L-test for twinning[2]	$< \|L\| > = 0.40$, $< L^2 > = 0.22$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.83	EDS
Total number of atoms	7956	wwPDB-VP
Average B, all atoms (Å^2)	112.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.31% 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

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	0.66	0/2039	0.73	1/2777 (0.0%)
1	B	0.66	0/2039	0.73	1/2777 (0.0%)
1	C	0.66	0/2039	0.73	1/2777 (0.0%)
1	D	0.66	0/2039	0.73	1/2777 (0.0%)
All	All	0.66	0/8156	0.73	4/11108 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	176	LEU	CB-CG-CD1	-6.47	100.00	111.00
1	B	176	LEU	CB-CG-CD1	-6.46	100.02	111.00
1	A	176	LEU	CB-CG-CD1	-6.45	100.03	111.00
1	C	176	LEU	CB-CG-CD1	-6.44	100.05	111.00

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	1989	0	1981	36	16
1	B	1989	0	1981	32	0
1	C	1989	0	1981	33	0
1	D	1989	0	1981	38	16
All	All	7956	0	7924	85	16

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 5.

All (85) 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:118:GLU:OE2	1:C:171:ILE:CG1	1.73	1.34
1:B:118:GLU:OE2	1:C:171:ILE:CD1	1.72	1.33
1:B:118:GLU:OE2	1:C:171:ILE:HG12	1.26	1.26
1:A:171:ILE:CD1	1:D:118:GLU:OE2	1.88	1.20
1:A:171:ILE:HD13	1:D:118:GLU:OE2	1.46	1.10
1:D:297:ILE:HD13	1:C:275:GLN:HG3	1.38	1.04
1:A:171:ILE:CG1	1:D:118:GLU:OE2	2.12	0.97
1:A:297:ILE:CD1	1:B:275:GLN:HA	1.98	0.93
1:B:118:GLU:OE2	1:C:171:ILE:HD13	1.69	0.91
1:D:297:ILE:CD1	1:C:275:GLN:HG3	2.01	0.89
1:A:297:ILE:HD13	1:B:275:GLN:HA	1.53	0.89
1:D:275:GLN:HG3	1:C:297:ILE:HD13	1.54	0.88
1:A:171:ILE:HG12	1:D:118:GLU:OE2	1.75	0.87
1:B:118:GLU:OE2	1:C:171:ILE:HD11	1.76	0.85
1:A:170[A]:VAL:HG21	1:D:111:GLU:HB2	1.59	0.82
1:D:297:ILE:HD13	1:C:275:GLN:CG	2.15	0.77
1:D:275:GLN:HG3	1:C:297:ILE:CD1	2.16	0.75
1:A:297:ILE:CD1	1:B:275:GLN:HG3	2.17	0.75
1:A:297:ILE:HD13	1:B:275:GLN:CA	2.17	0.73
1:A:168:LEU:HD23	1:D:114:SER:OG	1.88	0.73
1:A:298:SER:OG	1:B:275:GLN:OE1	2.10	0.70
1:B:118:GLU:CD	1:C:171:ILE:HG12	2.11	0.69
1:A:297:ILE:HD13	1:B:275:GLN:HG3	1.73	0.69
1:A:297:ILE:HD13	1:B:275:GLN:CB	2.26	0.66
1:A:170[A]:VAL:HG21	1:D:111:GLU:CB	2.27	0.64
1:A:317:VAL:HB	1:A:337:PHE:HB2	1.81	0.63
1:A:297:ILE:HD13	1:B:275:GLN:CG	2.30	0.62
1:D:317:VAL:HB	1:D:337:PHE:HB2	1.81	0.61
1:B:317:VAL:HB	1:B:337:PHE:HB2	1.81	0.61
1:C:317:VAL:HB	1:C:337:PHE:HB2	1.81	0.60
1:D:275:GLN:CG	1:C:297:ILE:HD13	2.28	0.59
1:A:297:ILE:CD1	1:B:275:GLN:CA	2.77	0.58
1:D:311:LYS:HB2	1:C:300:HIS:CE1	2.38	0.58
1:D:311:LYS:CB	1:C:300:HIS:CE1	2.87	0.57
1:A:111:GLU:OE1	1:D:170[B]:VAL:HG11	2.07	0.54
1:A:297:ILE:CG1	1:B:275:GLN:HA	2.37	0.54
1:A:300:HIS:NE2	1:B:308:LEU:O	2.30	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:297:ILE:CD1	1:B:275:GLN:CG	2.85	0.54
1:B:108:VAL:HG13	1:B:108:VAL:O	2.08	0.53
1:C:108:VAL:O	1:C:108:VAL:HG13	2.08	0.53
1:A:108:VAL:HG13	1:A:108:VAL:O	2.08	0.53
1:A:311:LYS:HB2	1:B:300:HIS:CE1	2.43	0.53
1:D:108:VAL:O	1:D:108:VAL:HG13	2.08	0.53
1:D:270:THR:HG22	1:C:270:THR:HG22	1.90	0.52
1:A:170[A]:VAL:CG2	1:D:111:GLU:HB2	2.33	0.52
1:D:292:ALA:O	1:D:293:SER:HB2	2.10	0.51
1:B:292:ALA:O	1:B:293:SER:HB2	2.10	0.51
1:B:111:GLU:HB2	1:C:170[A]:VAL:HG21	1.92	0.51
1:A:166:SER:O	1:D:168:LEU:HD11	2.11	0.51
1:A:292:ALA:O	1:A:293:SER:HB2	2.11	0.51
1:C:292:ALA:O	1:C:293:SER:HB2	2.11	0.51
1:D:300:HIS:CE1	1:C:311:LYS:CB	2.94	0.50
1:D:311:LYS:HB3	1:C:300:HIS:CE1	2.47	0.50
1:D:300:HIS:CE1	1:C:311:LYS:HB2	2.47	0.49
1:A:170[A]:VAL:CG2	1:D:111:GLU:CB	2.91	0.48
1:D:297:ILE:CD1	1:C:275:GLN:CG	2.81	0.48
1:D:358:MET:O	1:D:359:LYS:CB	2.63	0.46
1:C:358:MET:O	1:C:359:LYS:CB	2.63	0.46
1:B:358:MET:O	1:B:359:LYS:CB	2.63	0.46
1:A:358:MET:O	1:A:359:LYS:CB	2.63	0.46
1:D:275:GLN:HA	1:C:297:ILE:HD13	1.98	0.46
1:A:311:LYS:HD3	1:B:300:HIS:HB2	1.99	0.45
1:D:300:HIS:CE1	1:C:311:LYS:HB3	2.52	0.45
1:A:275:GLN:HG3	1:B:297:ILE:CD1	2.47	0.44
1:D:271:TYR:HE1	1:C:271:TYR:HH	1.65	0.43
1:D:275:GLN:HA	1:C:297:ILE:CD1	2.49	0.43
1:D:292:ALA:O	1:D:293:SER:CB	2.67	0.43
1:C:142:VAL:HG12	1:C:176:LEU:HD21	2.00	0.43
1:C:292:ALA:O	1:C:293:SER:CB	2.67	0.43
1:B:142:VAL:HG12	1:B:176:LEU:HD21	2.00	0.43
1:D:142:VAL:HG12	1:D:176:LEU:HD21	2.01	0.43
1:D:298:SER:OG	1:C:275:GLN:OE1	2.35	0.43
1:A:275:GLN:HG3	1:B:297:ILE:HD13	2.00	0.43
1:A:297:ILE:HG12	1:B:275:GLN:HA	1.99	0.43
1:A:292:ALA:O	1:A:293:SER:CB	2.67	0.42
1:B:292:ALA:O	1:B:293:SER:CB	2.66	0.42
1:A:142:VAL:HG12	1:A:176:LEU:HD21	2.01	0.42
1:B:311:LYS:HB3	1:B:312:PRO:HD3	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:297:ILE:HD13	1:C:275:GLN:CB	2.49	0.42
1:A:311:LYS:HB3	1:A:312:PRO:HD3	2.02	0.41
1:C:279:VAL:O	1:C:314:LEU:HD22	2.21	0.40
1:D:311:LYS:HB3	1:D:312:PRO:HD3	2.02	0.40
1:D:279:VAL:O	1:D:314:LEU:HD22	2.21	0.40
1:B:279:VAL:O	1:B:314:LEU:HD22	2.21	0.40
1:A:279:VAL:O	1:A:314:LEU:HD22	2.21	0.40

All (16) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:133:GLN:CD	1:D:133:GLN:CG[2_655]	0.61	1.59
1:A:133:GLN:CG	1:D:133:GLN:CD[2_655]	0.80	1.40
1:A:133:GLN:NE2	1:D:133:GLN:CG[2_655]	1.23	0.97
1:A:133:GLN:NE2	1:D:133:GLN:CB[2_655]	1.26	0.94
1:A:133:GLN:CD	1:D:133:GLN:CD[2_655]	1.44	0.76
1:A:133:GLN:CB	1:D:133:GLN:NE2[2_655]	1.47	0.73
1:A:133:GLN:CG	1:D:133:GLN:OE1[2_655]	1.47	0.73
1:A:133:GLN:OE1	1:D:133:GLN:CG[2_655]	1.50	0.70
1:A:133:GLN:CG	1:D:133:GLN:NE2[2_655]	1.54	0.66
1:A:133:GLN:CA	1:D:133:GLN:NE2[2_655]	1.60	0.60
1:A:133:GLN:NE2	1:D:133:GLN:CA[2_655]	1.68	0.52
1:A:133:GLN:CG	1:D:133:GLN:CG[2_655]	1.76	0.44
1:A:133:GLN:NE2	1:D:133:GLN:CD[2_655]	1.89	0.31
1:A:133:GLN:CB	1:D:133:GLN:CD[2_655]	2.02	0.18
1:A:133:GLN:CD	1:D:133:GLN:CB[2_655]	2.02	0.18
1:A:133:GLN:CD	1:D:133:GLN:NE2[2_655]	2.05	0.15

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	253/369 (69%)	244 (96%)	9 (4%)	0	100	100
1	B	253/369 (69%)	244 (96%)	9 (4%)	0	100	100
1	C	253/369 (69%)	244 (96%)	9 (4%)	0	100	100
1	D	253/369 (69%)	244 (96%)	9 (4%)	0	100	100
All	All	1012/1476 (69%)	976 (96%)	36 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	218/324 (67%)	204 (94%)	14 (6%)	17	44
1	B	218/324 (67%)	204 (94%)	14 (6%)	17	44
1	C	218/324 (67%)	204 (94%)	14 (6%)	17	44
1	D	218/324 (67%)	204 (94%)	14 (6%)	17	44
All	All	872/1296 (67%)	816 (94%)	56 (6%)	19	44

All (56) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	115	LEU
1	A	120[A]	HIS
1	A	120[B]	HIS
1	A	133	GLN
1	A	153	ILE
1	A	178	LYS
1	A	222	LEU
1	A	253	HIS
1	A	297	ILE
1	A	307	GLU
1	A	308	LEU
1	A	317	VAL
1	A	354	SER

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Mol	Chain	Res	Type
1	A	358	MET
1	D	115	LEU
1	D	120[A]	HIS
1	D	120[B]	HIS
1	D	133	GLN
1	D	153	ILE
1	D	178	LYS
1	D	222	LEU
1	D	253	HIS
1	D	297	ILE
1	D	307	GLU
1	D	308	LEU
1	D	317	VAL
1	D	354	SER
1	D	358	MET
1	B	115	LEU
1	B	120[A]	HIS
1	B	120[B]	HIS
1	B	133	GLN
1	B	153	ILE
1	B	178	LYS
1	B	222	LEU
1	B	253	HIS
1	B	297	ILE
1	B	307	GLU
1	B	308	LEU
1	B	317	VAL
1	B	354	SER
1	B	358	MET
1	C	115	LEU
1	C	120[A]	HIS
1	C	120[B]	HIS
1	C	133	GLN
1	C	153	ILE
1	C	178	LYS
1	C	222	LEU
1	C	253	HIS
1	C	297	ILE
1	C	307	GLU
1	C	308	LEU
1	C	317	VAL
1	C	354	SER

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Mol	Chain	Res	Type
1	C	358	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	196	HIS
1	A	275	GLN
1	A	304	ASN
1	D	196	HIS
1	D	275	GLN
1	B	196	HIS
1	B	275	GLN
1	B	304	ASN
1	C	196	HIS
1	C	275	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

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	253/369 (68%)	-0.04	6 (2%) 59 49	74, 95, 120, 146	0
1	B	253/369 (68%)	0.05	11 (4%) 35 29	97, 118, 142, 169	0
1	C	253/369 (68%)	-0.00	8 (3%) 47 37	107, 128, 153, 179	0
1	D	253/369 (68%)	-0.01	4 (1%) 72 62	78, 100, 124, 150	0
All	All	1012/1476 (68%)	0.00	29 (2%) 51 41	74, 111, 144, 179	0

All (29) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	108	VAL	7.9
1	C	107	ILE	7.5
1	B	108	VAL	5.1
1	B	123	LYS	4.6
1	B	294	VAL	3.8
1	A	209	ALA	3.5
1	B	107	ILE	3.4
1	C	209	ALA	3.4
1	C	359	LYS	3.0
1	B	293	SER	2.8
1	A	326	GLN	2.6
1	B	122	PHE	2.6
1	C	109	THR	2.5
1	D	158	GLN	2.5
1	D	108	VAL	2.4
1	C	335	VAL	2.3
1	A	147	GLU	2.3
1	A	208	ALA	2.3
1	B	356	TRP	2.2
1	C	201	VAL	2.2
1	A	193	ASP	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	146	TRP	2.1
1	B	109	THR	2.1
1	D	145	ARG	2.1
1	A	290	GLN	2.1
1	B	359	LYS	2.1
1	B	147	GLU	2.0
1	C	345	PRO	2.0
1	D	122	PHE	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)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.