Full wwPDB X-ray Structure Validation Report ⓘ

May 25, 2020 – 02:59 pm BST

PDB ID	:	6EYS
Title	:	Crystal structure of the periplasmic pyoverdine maturation protein PvdP
Authors	:	Poppe, J.; Blankenfeldt, W.
Deposited on	:	2017-11-13
Resolution	:	2.09 Å(reported)

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

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

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

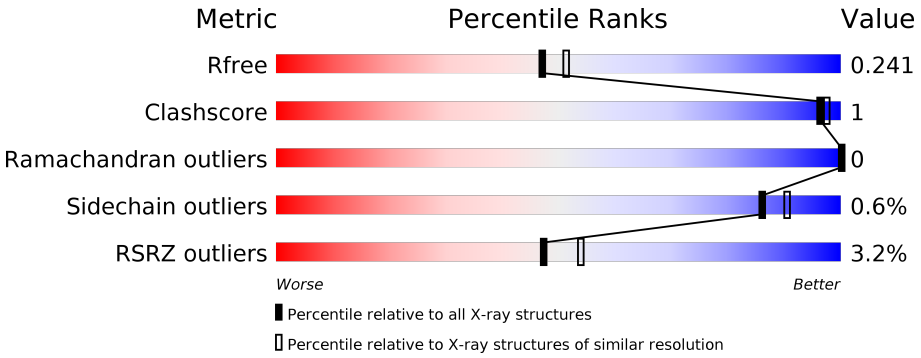
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation 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 2.09 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	5197 (2.10-2.10)
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (2.10-2.10)

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	536	3% 85% • 13%
1	B	536	2% 87% • 11%
1	C	536	3% 86% • 12%
1	D	536	3% 85% • 12%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 30248 atoms, of which 14481 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 PvdP.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	B	478	Total	C	H	N	O	S	0	4	0
			7548	2472	3679	708	682	7			
1	A	469	Total	C	H	N	O	S	0	2	0
			7379	2426	3590	686	670	7			
1	C	470	Total	C	H	N	O	S	0	2	0
			7404	2427	3613	692	664	8			
1	D	472	Total	C	H	N	O	S	0	4	0
			7404	2432	3599	695	671	7			

There are 68 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	9	HIS	-	expression tag	UNP A0A0H2ZBG1
B	10	HIS	-	expression tag	UNP A0A0H2ZBG1
B	11	HIS	-	expression tag	UNP A0A0H2ZBG1
B	12	HIS	-	expression tag	UNP A0A0H2ZBG1
B	13	HIS	-	expression tag	UNP A0A0H2ZBG1
B	14	HIS	-	expression tag	UNP A0A0H2ZBG1
B	15	SER	-	expression tag	UNP A0A0H2ZBG1
B	16	SER	-	expression tag	UNP A0A0H2ZBG1
B	17	GLY	-	expression tag	UNP A0A0H2ZBG1
B	18	LEU	-	expression tag	UNP A0A0H2ZBG1
B	19	GLU	-	expression tag	UNP A0A0H2ZBG1
B	20	VAL	-	expression tag	UNP A0A0H2ZBG1
B	21	LEU	-	expression tag	UNP A0A0H2ZBG1
B	22	PHE	-	expression tag	UNP A0A0H2ZBG1
B	23	GLN	-	expression tag	UNP A0A0H2ZBG1
B	24	GLY	-	expression tag	UNP A0A0H2ZBG1
B	25	THR	-	expression tag	UNP A0A0H2ZBG1
A	9	HIS	-	expression tag	UNP A0A0H2ZBG1
A	10	HIS	-	expression tag	UNP A0A0H2ZBG1
A	11	HIS	-	expression tag	UNP A0A0H2ZBG1
A	12	HIS	-	expression tag	UNP A0A0H2ZBG1

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Chain	Residue	Modelled	Actual	Comment	Reference
A	13	HIS	-	expression tag	UNP A0A0H2ZBG1
A	14	HIS	-	expression tag	UNP A0A0H2ZBG1
A	15	SER	-	expression tag	UNP A0A0H2ZBG1
A	16	SER	-	expression tag	UNP A0A0H2ZBG1
A	17	GLY	-	expression tag	UNP A0A0H2ZBG1
A	18	LEU	-	expression tag	UNP A0A0H2ZBG1
A	19	GLU	-	expression tag	UNP A0A0H2ZBG1
A	20	VAL	-	expression tag	UNP A0A0H2ZBG1
A	21	LEU	-	expression tag	UNP A0A0H2ZBG1
A	22	PHE	-	expression tag	UNP A0A0H2ZBG1
A	23	GLN	-	expression tag	UNP A0A0H2ZBG1
A	24	GLY	-	expression tag	UNP A0A0H2ZBG1
A	25	THR	-	expression tag	UNP A0A0H2ZBG1
C	9	HIS	-	expression tag	UNP A0A0H2ZBG1
C	10	HIS	-	expression tag	UNP A0A0H2ZBG1
C	11	HIS	-	expression tag	UNP A0A0H2ZBG1
C	12	HIS	-	expression tag	UNP A0A0H2ZBG1
C	13	HIS	-	expression tag	UNP A0A0H2ZBG1
C	14	HIS	-	expression tag	UNP A0A0H2ZBG1
C	15	SER	-	expression tag	UNP A0A0H2ZBG1
C	16	SER	-	expression tag	UNP A0A0H2ZBG1
C	17	GLY	-	expression tag	UNP A0A0H2ZBG1
C	18	LEU	-	expression tag	UNP A0A0H2ZBG1
C	19	GLU	-	expression tag	UNP A0A0H2ZBG1
C	20	VAL	-	expression tag	UNP A0A0H2ZBG1
C	21	LEU	-	expression tag	UNP A0A0H2ZBG1
C	22	PHE	-	expression tag	UNP A0A0H2ZBG1
C	23	GLN	-	expression tag	UNP A0A0H2ZBG1
C	24	GLY	-	expression tag	UNP A0A0H2ZBG1
C	25	THR	-	expression tag	UNP A0A0H2ZBG1
D	9	HIS	-	expression tag	UNP A0A0H2ZBG1
D	10	HIS	-	expression tag	UNP A0A0H2ZBG1
D	11	HIS	-	expression tag	UNP A0A0H2ZBG1
D	12	HIS	-	expression tag	UNP A0A0H2ZBG1
D	13	HIS	-	expression tag	UNP A0A0H2ZBG1
D	14	HIS	-	expression tag	UNP A0A0H2ZBG1
D	15	SER	-	expression tag	UNP A0A0H2ZBG1
D	16	SER	-	expression tag	UNP A0A0H2ZBG1
D	17	GLY	-	expression tag	UNP A0A0H2ZBG1
D	18	LEU	-	expression tag	UNP A0A0H2ZBG1
D	19	GLU	-	expression tag	UNP A0A0H2ZBG1
D	20	VAL	-	expression tag	UNP A0A0H2ZBG1

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Chain	Residue	Modelled	Actual	Comment	Reference
D	21	LEU	-	expression tag	UNP A0A0H2ZBG1
D	22	PHE	-	expression tag	UNP A0A0H2ZBG1
D	23	GLN	-	expression tag	UNP A0A0H2ZBG1
D	24	GLY	-	expression tag	UNP A0A0H2ZBG1
D	25	THR	-	expression tag	UNP A0A0H2ZBG1

- Molecule 2 is water.

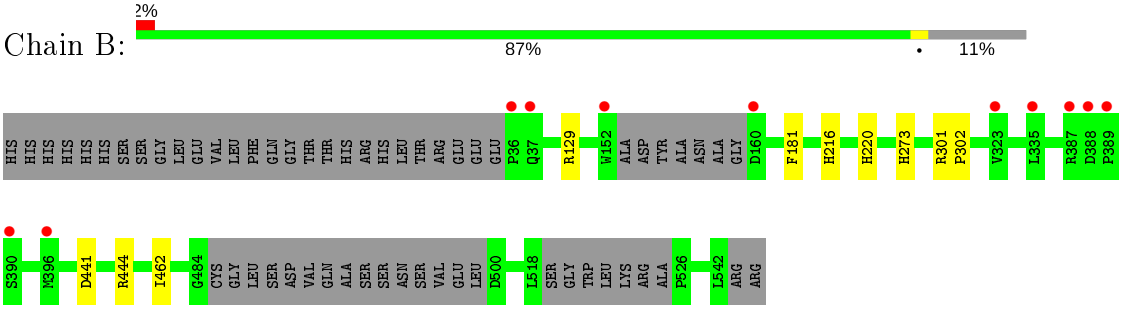
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	B	157	Total O 157 157	0	0
2	A	124	Total O 124 124	0	0
2	C	131	Total O 131 131	0	0
2	D	101	Total O 101 101	0	0

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.

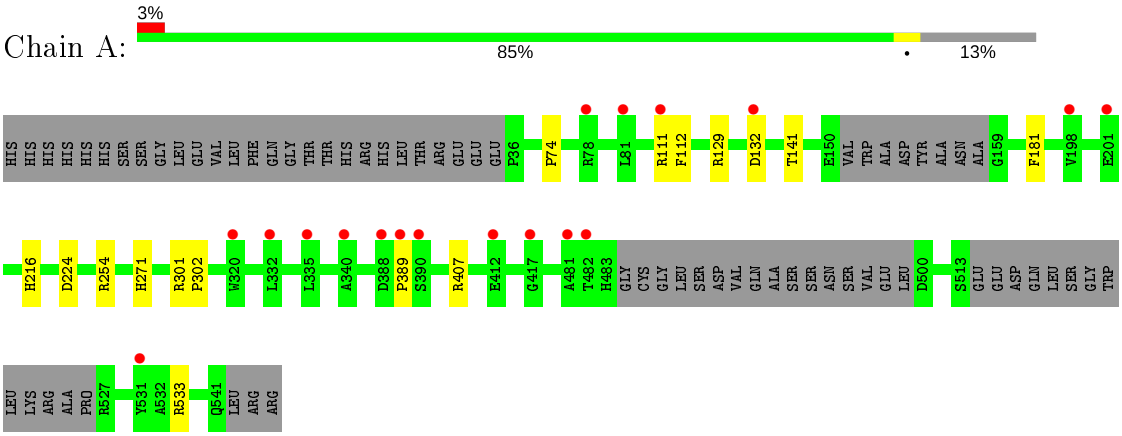
- Molecule 1: PvdP

Chain B:



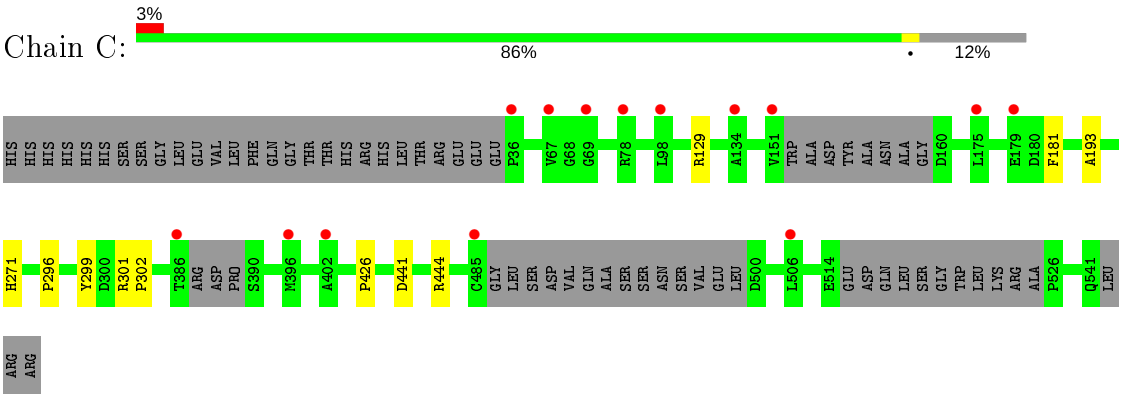
- Molecule 1: PvdP

Chain A:



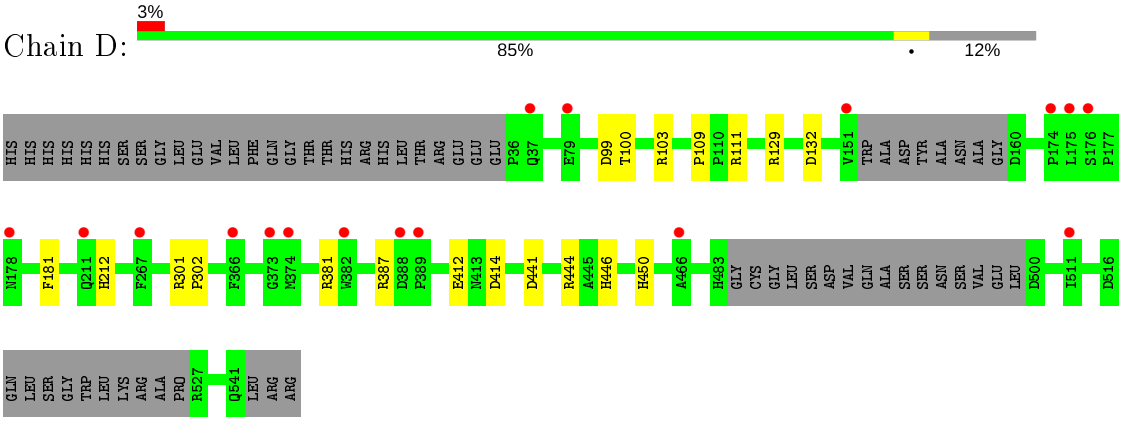
- Molecule 1: PvdP

Chain C:



• Molecule 1: PvdP

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	97.35Å 107.79Å 107.94Å 90.00° 99.97° 90.00°	Depositor
Resolution (Å)	45.61 – 2.09 45.61 – 2.09	Depositor EDS
% Data completeness (in resolution range)	93.2 (45.61-2.09) 66.2 (45.61-2.09)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.18 (at 2.08Å)	Xtriage
Refinement program	PHENIX (dev_2875)	Depositor
R, R_{free}	0.214 , 0.241 0.214 , 0.241	Depositor DCC
R_{free} test set	1999 reflections (2.33%)	wwPDB-VP
Wilson B-factor (Å^2)	35.1	Xtriage
Anisotropy	0.031	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 33.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	30248	wwPDB-VP
Average B, all atoms (Å^2)	52.0	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

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	0.25	0/3921	0.41	0/5336
1	B	0.25	0/4015	0.41	0/5462
1	C	0.25	0/3925	0.41	0/5339
1	D	0.25	0/3945	0.41	0/5372
All	All	0.25	0/15806	0.41	0/21509

There are no bond length outliers.

There are no bond angle outliers.

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	3789	3590	3577	11	0
1	B	3869	3679	3651	5	0
1	C	3791	3613	3602	5	0
1	D	3805	3599	3575	9	0
2	A	124	0	0	3	0
2	B	157	0	0	2	0
2	C	131	0	0	1	0
2	D	101	0	0	1	0
All	All	15767	14481	14405	30	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 1.

All (30) 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:220:HIS:NE2	2:B:601:HOH:O	2.24	0.70
1:C:271:HIS:NE2	2:C:603:HOH:O	2.30	0.64
1:A:111:ARG:NH1	1:A:132:ASP:OD1	2.32	0.63
1:A:111:ARG:HH12	1:A:132:ASP:CG	2.02	0.61
1:A:111:ARG:HG3	1:A:112:PHE:CD2	2.39	0.58
1:D:441:ASP:OD1	1:D:444:ARG:NH2	2.36	0.58
1:A:74:PRO:HB2	1:A:111:ARG:HH21	1.70	0.57
1:B:216:HIS:NE2	2:B:601:HOH:O	2.33	0.56
1:A:224:ASP:OD2	1:A:533:ARG:NH2	2.41	0.53
1:D:381:ARG:NH2	2:D:606:HOH:O	2.41	0.51
1:B:441:ASP:OD1	1:B:444:ARG:NH2	2.44	0.51
1:D:387:ARG:NH1	1:D:412:GLU:OE2	2.44	0.50
1:C:441:ASP:OD1	1:C:444:ARG:NH2	2.46	0.48
1:D:446:HIS:O	1:D:450:HIS:N	2.42	0.48
1:D:387:ARG:NH2	1:D:414:ASP:OD1	2.48	0.47
1:D:111:ARG:NH1	1:D:132:ASP:OD1	2.48	0.46
1:A:132:ASP:HB2	1:A:141:THR:HG21	1.96	0.46
1:D:103:ARG:NH2	1:D:109:PRO:O	2.50	0.45
1:A:216:HIS:NE2	2:A:603:HOH:O	2.36	0.44
1:A:389:PRO:HB2	1:A:407:ARG:O	2.17	0.44
1:C:301:ARG:HB3	1:C:302:PRO:HD3	1.99	0.44
1:B:301:ARG:HB3	1:B:302:PRO:HD3	1.99	0.43
1:D:301:ARG:HB3	1:D:302:PRO:HD3	2.00	0.43
1:C:296:PRO:HG2	1:C:299:TYR:CD2	2.55	0.42
1:C:193:ALA:HB1	1:C:426:PRO:HG2	2.01	0.42
1:D:99:ASP:OD1	1:D:100:THR:N	2.47	0.42
1:A:301:ARG:HB3	1:A:302:PRO:HD3	2.01	0.42
1:A:271:HIS:NE2	2:A:603:HOH:O	2.37	0.41
1:A:254:ARG:NH2	2:A:619:HOH:O	2.52	0.41
1:B:273:HIS:CD2	1:B:462:ILE:HD11	2.57	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	463/536 (86%)	451 (97%)	12 (3%)	0	100	100
1	B	474/536 (88%)	459 (97%)	15 (3%)	0	100	100
1	C	462/536 (86%)	447 (97%)	15 (3%)	0	100	100
1	D	468/536 (87%)	451 (96%)	17 (4%)	0	100	100
All	All	1867/2144 (87%)	1808 (97%)	59 (3%)	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	385/454 (85%)	383 (100%)	2 (0%)	88	92
1	B	395/454 (87%)	393 (100%)	2 (0%)	88	92
1	C	385/454 (85%)	383 (100%)	2 (0%)	88	92
1	D	387/454 (85%)	384 (99%)	3 (1%)	81	86
All	All	1552/1816 (86%)	1543 (99%)	9 (1%)	86	90

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	129	ARG
1	B	181	PHE
1	A	129	ARG
1	A	181	PHE
1	C	129	ARG
1	C	181	PHE
1	D	129	ARG
1	D	181	PHE
1	D	212	HIS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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

There are no ligands in this entry.

5.7 Other polymers

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	A	469/536 (87%)	0.38	18 (3%)	40	46	27, 47, 73, 115	0
1	B	478/536 (89%)	0.19	11 (2%)	60	65	26, 41, 73, 91	1 (0%)
1	C	470/536 (87%)	0.28	14 (2%)	50	56	27, 45, 76, 98	1 (0%)
1	D	472/536 (88%)	0.39	17 (3%)	42	49	27, 48, 77, 108	3 (0%)
All	All	1889/2144 (88%)	0.31	60 (3%)	47	54	26, 45, 76, 115	5 (0%)

All (60) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	390	SER	5.1
1	B	36	PRO	4.8
1	C	36	PRO	4.5
1	B	396	MET	4.1
1	B	387	ARG	3.6
1	D	175	LEU	3.5
1	B	389	PRO	3.5
1	C	386	THR	3.3
1	A	390	SER	3.1
1	A	388	ASP	3.0
1	C	402	ALA	3.0
1	B	37	GLN	3.0
1	A	320	TRP	2.9
1	B	388	ASP	2.8
1	A	482	THR	2.8
1	D	174	PRO	2.7
1	B	323	VAL	2.6
1	C	151	VAL	2.6
1	D	178	ASN	2.5
1	A	81	LEU	2.5
1	C	134	ALA	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	78	ARG	2.4
1	D	388	ASP	2.4
1	D	382	TRP	2.4
1	A	340	ALA	2.3
1	C	69	GLY	2.3
1	C	396	MET	2.3
1	A	412	GLU	2.3
1	C	78	ARG	2.3
1	A	132	ASP	2.3
1	D	511	ILE	2.3
1	C	506	LEU	2.3
1	B	152	TRP	2.3
1	C	67	VAL	2.3
1	D	79	GLU	2.3
1	D	374	MET	2.3
1	B	335	LEU	2.2
1	D	267	PHE	2.2
1	D	366	PHE	2.2
1	A	481	ALA	2.2
1	D	389	PRO	2.2
1	C	179	GLU	2.2
1	A	332	LEU	2.1
1	D	211	GLN	2.1
1	D	151	VAL	2.1
1	D	37	GLN	2.1
1	A	201	GLU	2.1
1	B	160	ASP	2.1
1	C	98	LEU	2.1
1	A	417	GLY	2.1
1	A	531	TYR	2.1
1	D	466	ALA	2.1
1	A	198	VAL	2.1
1	C	485	CYS	2.1
1	D	176	SER	2.1
1	A	389	PRO	2.0
1	C	175	LEU	2.0
1	A	335	LEU	2.0
1	D	373	GLY	2.0
1	A	111	ARG	2.0

6.2 Non-standard residues in protein, DNA, RNA chains

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

6.3 Carbohydrates

There are no carbohydrates in this entry.

6.4 Ligands

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.