W O R L D W I D E

wwPDB

P R O T E I N   D A T A   B A N K

wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 08:35 AM GMT

PDB ID	:	3F79
Title	:	Structure of pseudo-centered cell crystal form of the C-terminal phosphatase domain of P. aeruginosa RssB
Authors	:	Levchenko, I.; Grant, R.A.; Sauer, R.T.; Baker, T.A.
Deposited on	:	2008-11-07
Resolution	:	2.80 Å(reported)

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

|		
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

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 2.80 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.
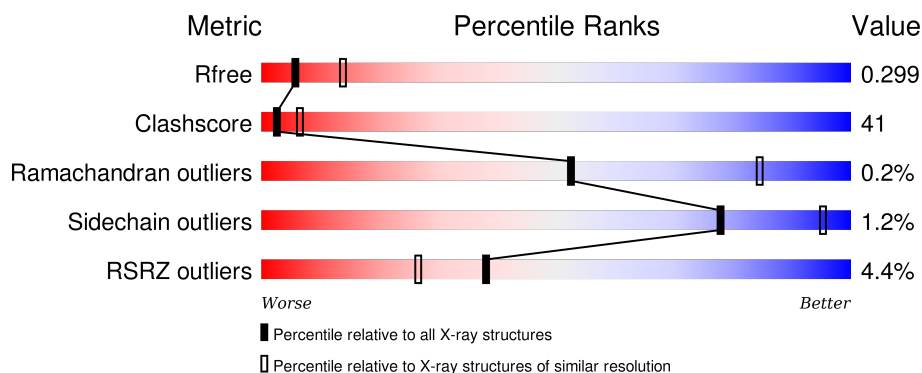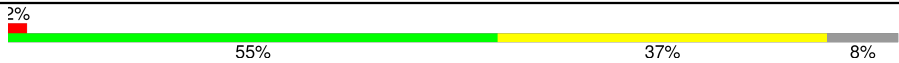

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	2393 (2.80-2.80)
Clashscore	102246	2827 (2.80-2.80)
Ramachandran outliers	100387	2782 (2.80-2.80)
Sidechain outliers	100360	2784 (2.80-2.80)
RSRZ outliers	91569	2404 (2.80-2.80)

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. 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	255	5% / 41% / 46% / 13%
1	B	255	3% / 44% / 45% / · 10%
1	C	255	5% / 38% / 51% / 10%
1	D	255	5% / 39% / 50% / · 10%
1	E	255	4% / 52% / 40% / · 7%

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Mol	Chain	Length	Quality of chain
1	F	255	

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 10386 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 Probable two-component response regulator.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	223	Total 1659	C 1065	N 276	O 312	Se 6	12	0	0
1	B	229	Total 1738	C 1111	N 295	O 326	Se 6	5	0	0
1	C	229	Total 1728	C 1112	N 286	O 325	Se 5	5	0	0
1	D	230	Total 1719	C 1105	N 284	O 324	Se 6	0	0	0
1	E	236	Total 1778	C 1133	N 302	O 337	Se 6	13	0	0
1	F	235	Total 1757	C 1125	N 300	O 327	Se 5	12	0	0

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total 1	Mg 1	0	0
2	D	2	Total 2	Mg 2	0	0
2	C	1	Total 1	Mg 1	0	0
2	F	2	Total 2	Mg 2	0	0
2	E	1	Total 1	Mg 1	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 errors 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: Probable two-component response regulator
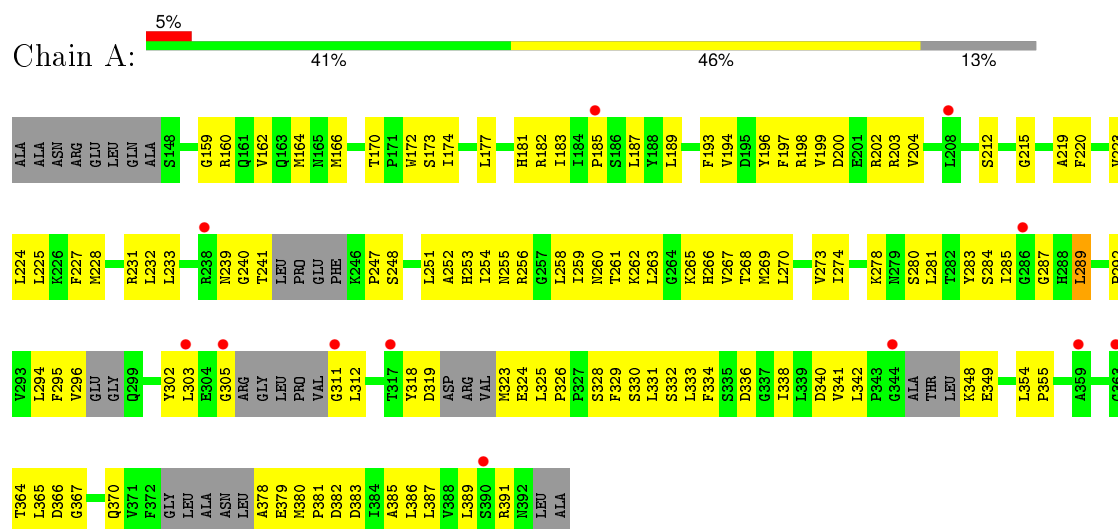
- Molecule 1: Probable two-component response regulator

- Molecule 1: Probable two-component response regulator

● Molecule 1: Probable two-component response regulator

Chain D:

● Molecule 1: Probable two-component response regulator

Chain E:

● Molecule 1: Probable two-component response regulator

Chain F:

L224 L225 K226 F227 M228 R231 L232 L233 R237 R238 N239 G240 THR LEU P243 E244 F245 K246 P247 V250 R256 I259 N260 T261 H266 V267 T268 M269 L270 V273 I274 E277 I285 G286 G287 H288 L289 P290 L291 P292 V293 L294 F295 Q299 A300 R306 GLY LEU P309

V310 G311 L312 L325 S328 F329 S330 L331 S332 L333 F334 S335 D336 G337 I338 L339 D340 V341 L342 K350 L354 P355 T364 L365 D366 R369 Q370 V371 F372 GLY LEU ALA ASN LEU ALA GLU MSE P381 I384 A385 L386 L389 S390 R391 N392 L393 ALA
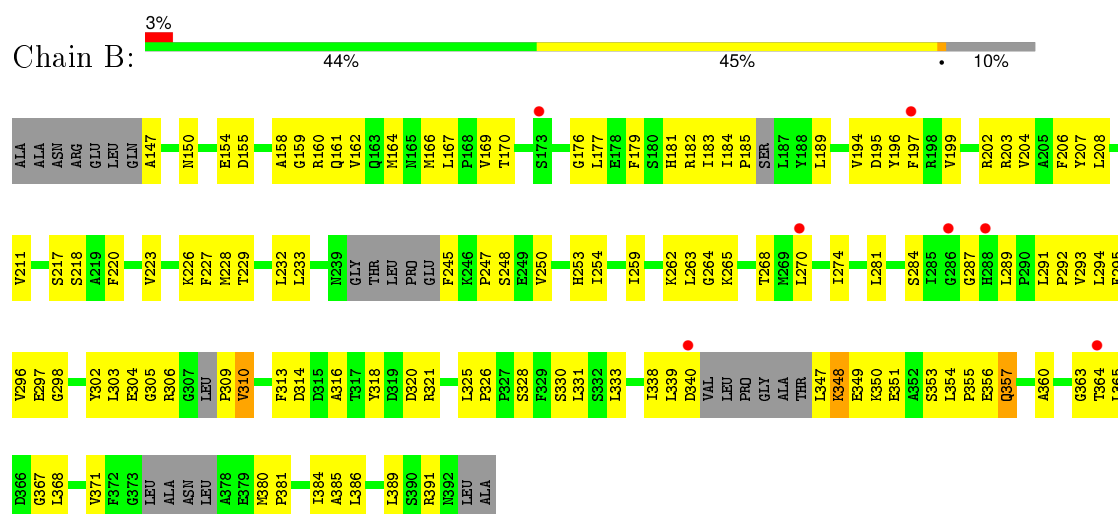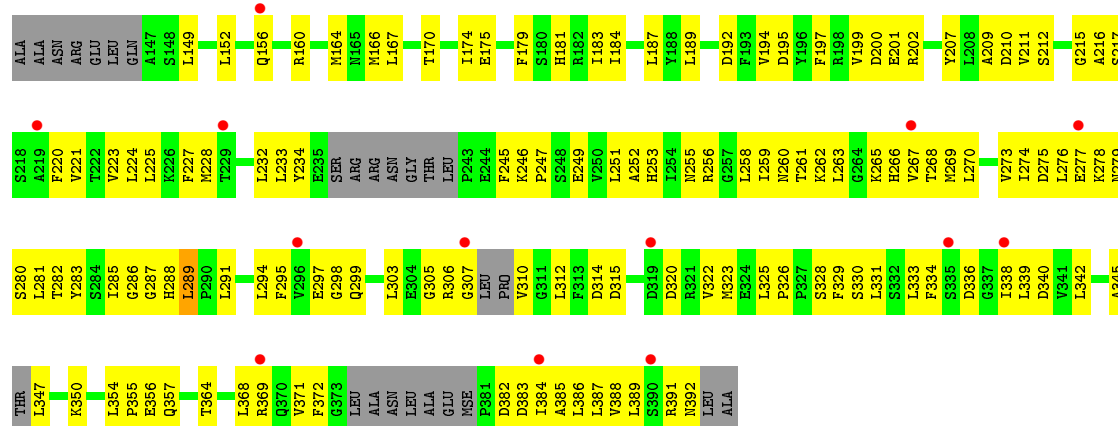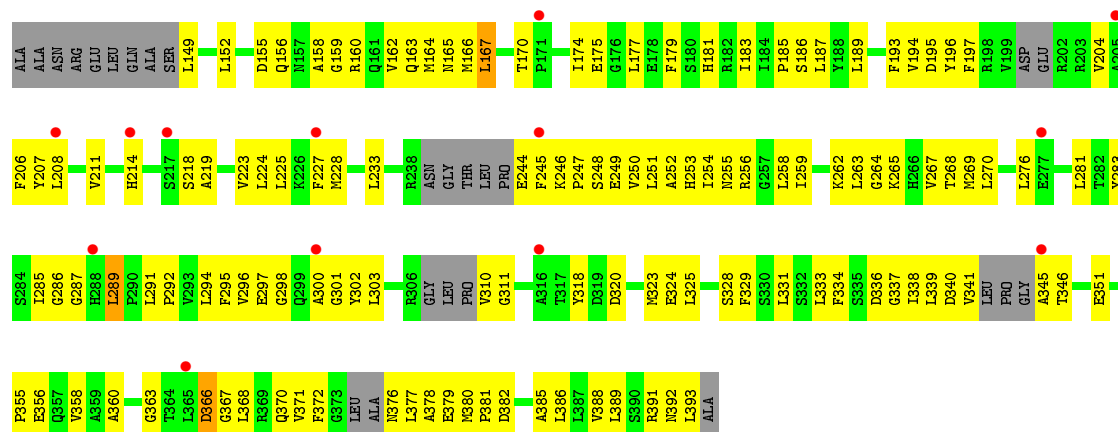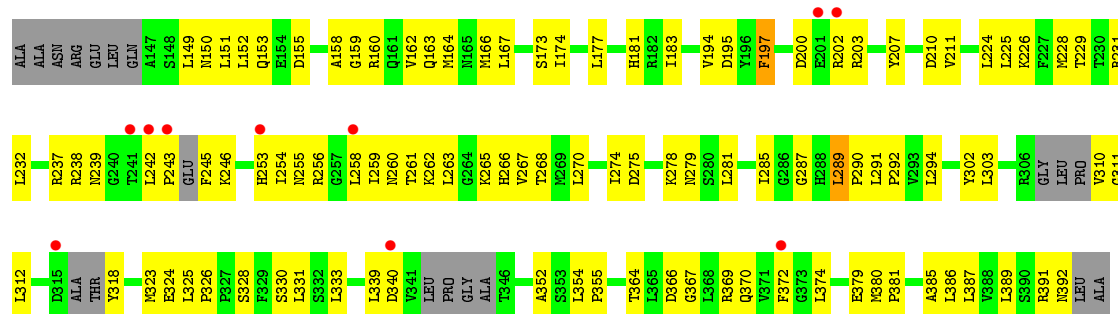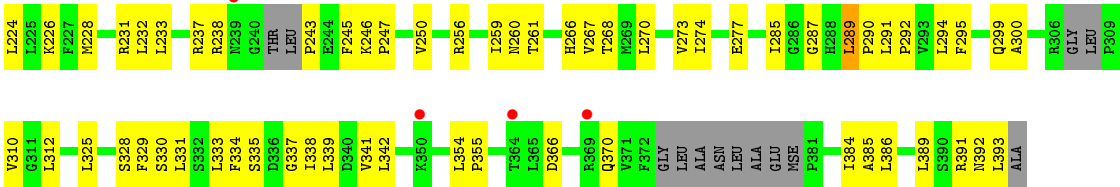
4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 31	Depositor
Cell constants a, b, c, α, β, γ	124.87Å 124.87Å 92.90Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	15.00 – 2.80	Depositor
	37.41 – 2.80	EDS
% Data completeness	98.4 (15.00-2.80)	Depositor
(in resolution range)	99.4 (37.41-2.80)	EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.85 (at 2.81Å)	Xtriage
Refinement program	PHENIX (phenix.refine)	Depositor
R, R_{free}	0.243 , 0.297	Depositor
	0.242 , 0.299	DCC
R_{free} test set	1975 reflections (5.26%)	DCC
Wilson B-factor (Å²)	56.8	Xtriage
Anisotropy	0.597	Xtriage
Bulk solvent k_{sol}(e/Å³), B_{sol}(Å²)	0.27 , 58.9	EDS
Estimated twinning fraction	0.498 for -k,-h,-l 0.047 for -h,-k,l 0.048 for h,-h-k,-l 0.477 for -k,-h,-l	Xtriage
Reported twinning fraction	0.498 for -k,-h,-l	Depositor
L-test for twinning[2]	$< |L| > = 0.46, < L^2 > = 0.28$	Xtriage
Outliers	0 of 39804 reflections	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	10386	wwPDB-VP
Average B, all atoms (Å²)	91.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 48.93 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 8.0149e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: MG

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	0.21	0/1682	0.40	0/2271
1	B	0.24	0/1762	0.41	0/2371
1	C	0.23	0/1756	0.44	0/2374
1	D	0.26	0/1740	0.42	0/2349
1	E	0.22	0/1800	0.42	0/2429
1	F	0.24	0/1785	0.41	0/2413
All	All	0.23	0/10525	0.42	0/14207

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 (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1659	0	1613	128	0
1	B	1738	0	1706	165	0
1	C	1728	0	1687	193	0
1	D	1719	0	1680	190	0
1	E	1778	0	1758	119	0
1	F	1757	0	1713	121	0
2	B	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	1	0	0	0	0
2	D	2	0	0	0	0
2	E	1	0	0	0	0
2	F	2	0	0	0	0
All	All	10386	0	10157	842	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 41.

The worst 5 of 842 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:D:246:LYS:CB	1:D:249:GLU:HB3	1.35	1.51
1:D:246:LYS:HB2	1:D:249:GLU:CB	1.39	1.49
1:D:380:MSE:SE	1:D:381:PRO:HD2	1.85	1.26
1:B:356:GLU:HG3	1:B:357:GLN:NE2	1.56	1.20
1:D:175:GLU:O	1:D:391:ARG:NH2	1.73	1.19

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	209/255 (82%)	193 (92%)	16 (8%)	0	100	100
1	B	217/255 (85%)	202 (93%)	14 (6%)	1 (0%)	34	69
1	C	219/255 (86%)	199 (91%)	20 (9%)	0	100	100
1	D	218/255 (86%)	202 (93%)	15 (7%)	1 (0%)	34	69
1	E	226/255 (89%)	211 (93%)	15 (7%)	0	100	100
1	F	227/255 (89%)	214 (94%)	13 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	1316/1530 (86%)	1221 (93%)	93 (7%)	2 (0%)	52 84

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	310	VAL
1	D	337	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	A	173/206 (84%)	172 (99%)	1 (1%)	90	98
1	B	182/206 (88%)	179 (98%)	3 (2%)	70	93
1	C	181/206 (88%)	179 (99%)	2 (1%)	80	95
1	D	179/206 (87%)	175 (98%)	4 (2%)	60	89
1	E	189/206 (92%)	187 (99%)	2 (1%)	80	95
1	F	181/206 (88%)	180 (99%)	1 (1%)	90	98
All	All	1085/1236 (88%)	1072 (99%)	13 (1%)	78	95

5 of 13 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	289	LEU
1	D	167	LEU
1	E	197	PHE
1	C	187	LEU
1	D	376	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 14 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	253	HIS
1	C	266	HIS
1	E	163	GLN
1	C	163	GLN
1	D	376	ASN

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 carbohydrates in this entry.

5.6   Ligand geometry (i)

Of 7 ligands modelled in this entry, 7 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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 (i)

6.1 Protein, DNA and RNA chains (i)

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, 95th 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	215/255 (84%)	0.19	12 (5%)	28	18	41, 92, 166, 244	0
1	B	222/255 (87%)	-0.11	7 (3%)	51	39	42, 86, 129, 224	0
1	C	223/255 (87%)	0.10	13 (5%)	26	16	43, 91, 141, 234	0
1	D	224/255 (87%)	0.05	13 (5%)	26	16	36, 88, 150, 275	0
1	E	228/255 (89%)	-0.03	10 (4%)	38	26	39, 86, 146, 192	0
1	F	228/255 (89%)	-0.18	4 (1%)	71	61	23, 80, 132, 226	0
All	All	1340/1530 (87%)	0.00	59 (4%)	38	26	23, 88, 146, 275	0

The worst 5 of 59 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	363	GLY	6.2
1	B	288	HIS	5.9
1	A	185	PRO	5.5
1	C	369	ARG	5.5
1	A	238	ARG	5.3

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th 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	LLDF	B-factors(Å^2)	Q<0.9
2	MG	F	4	1/1	0.79	0.19	0.35	94,94,94,94	0
2	MG	B	1	1/1	0.88	0.14	-0.39	61,61,61,61	0
2	MG	D	6	1/1	0.84	0.13	-0.93	78,78,78,78	0
2	MG	D	7	1/1	0.94	0.08	-1.23	40,40,40,40	0
2	MG	E	2	1/1	0.96	0.11	-2.28	39,39,39,39	0
2	MG	F	3	1/1	0.84	0.09	-2.61	47,47,47,47	0
2	MG	C	5	1/1	0.94	0.17	-	50,50,50,50	0

6.5 Other polymers (i)

There are no such residues in this entry.