Full wwPDB X-ray Structure Validation Report (i)

Jun 27, 2016 – 03:13 PM EDT

PDB ID	:	5CRF
Title	:	Structure of the penicillin-binding protein PonA1 from Mycobacterium Tuberculosis
Authors	:	Filippova, E.V.; Wawrzak, Z.; Kiryukhina, O.; Kieser, K.; Endres, M.; Rubin, E.; Sacchettini, J.; Joachimiak, A.; Anderson, W.F.; Midwest Center for Structural Genomics (MCSG); Structures of Mtb Proteins Conferring Susceptibility to Known Mtb Inhibitors (MTBI)
Deposited on	:	2015-07-22
Resolution	:	1.80 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
http://wwpdb.org/validation/2016/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:

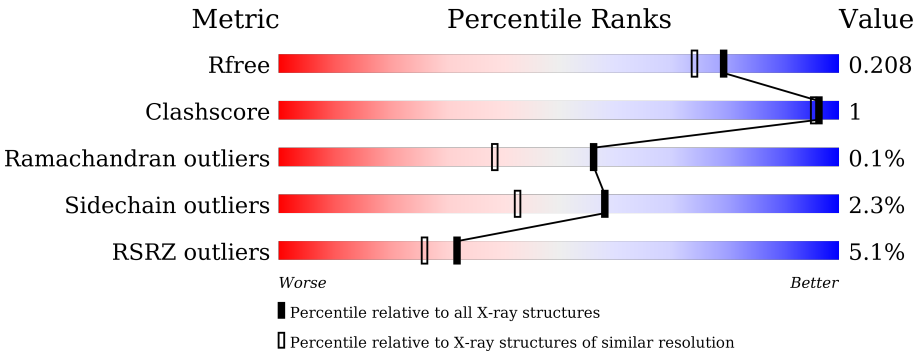
MolProbity	:	4.02b-467
Mogul	:	1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20027790
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20027790

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 1.80 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	4533 (1.80-1.80)
Clashscore	102246	5383 (1.80-1.80)
Ramachandran outliers	100387	5320 (1.80-1.80)
Sidechain outliers	100360	5319 (1.80-1.80)
RSRZ outliers	91569	4547 (1.80-1.80)

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	430	3% 85% • • 10%
1	B	430	4% 85% 5% 10%
1	C	430	7% 85% • 11%
1	D	430	5% 83% 5% 12%

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	PO4	B	702	-	-	-	X
2	PO4	D	702	-	-	-	X

2 Entry composition

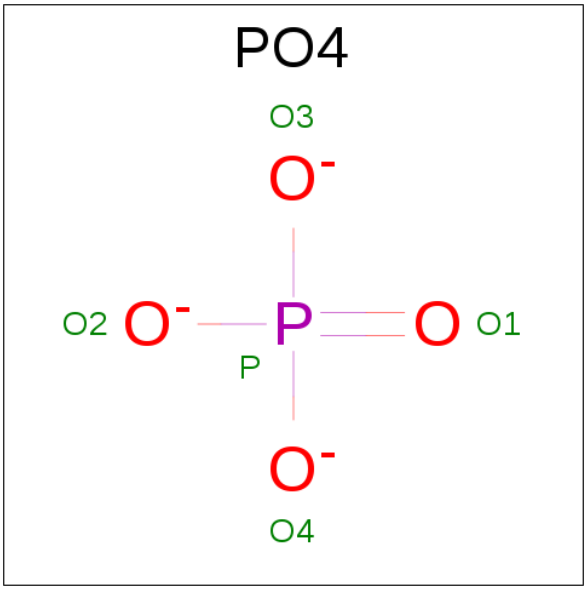
There are 3 unique types of molecules in this entry. The entry contains 12240 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Penicillin-binding protein 1A.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	386	Total	C	N	O	S	Se	0	2	0
			2835	1768	490	568	2	7			
1	B	388	Total	C	N	O	S	Se	0	2	0
			2842	1777	486	570	2	7			
1	C	382	Total	C	N	O	S	Se	0	1	0
			2786	1740	479	558	2	7			
1	D	380	Total	C	N	O	S	Se	0	2	0
			2788	1740	480	559	2	7			

- Molecule 2 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	P	0	0
			5	4	1		
2	B	1	Total	O	P	0	0
			5	4	1		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	B	1	Total O P 5 4 1	0	0
2	D	1	Total O P 5 4 1	0	0
2	D	1	Total O P 5 4 1	0	0

- Molecule 3 is water.

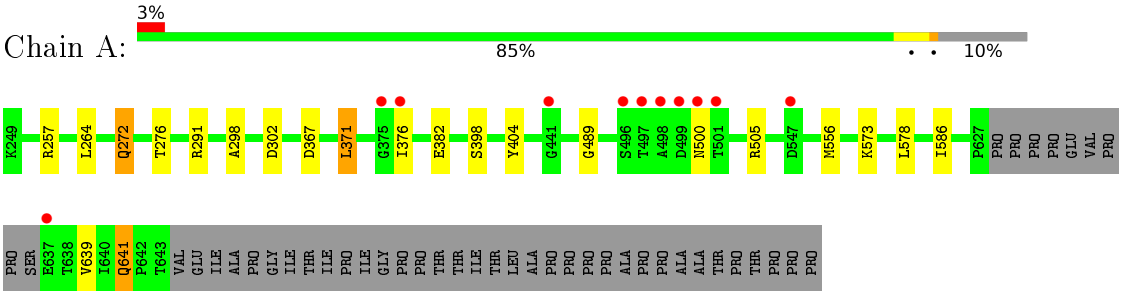
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	280	Total O 280 280	0	0
3	B	291	Total O 293 293	0	2
3	C	191	Total O 191 191	0	0
3	D	200	Total O 200 200	0	0

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.

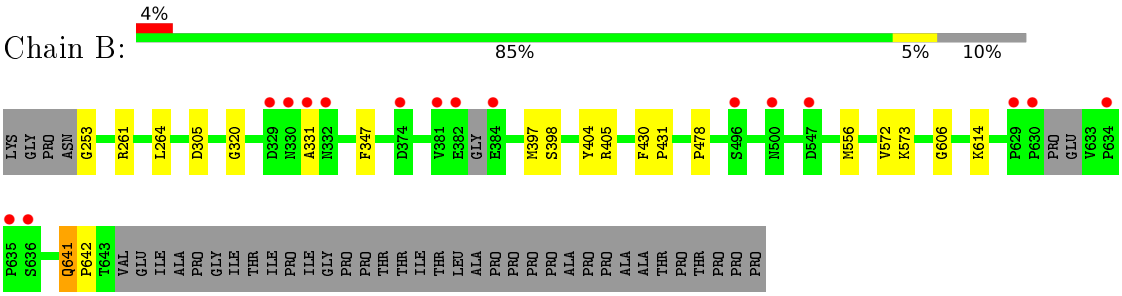
- Molecule 1: Penicillin-binding protein 1A

Chain A:



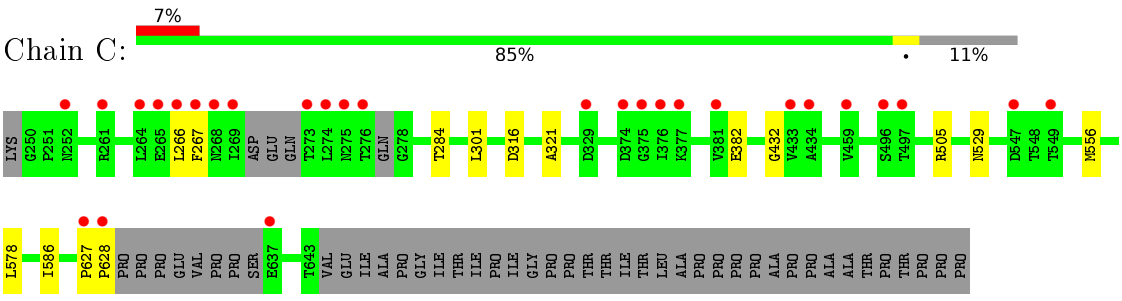
- Molecule 1: Penicillin-binding protein 1A

Chain B:



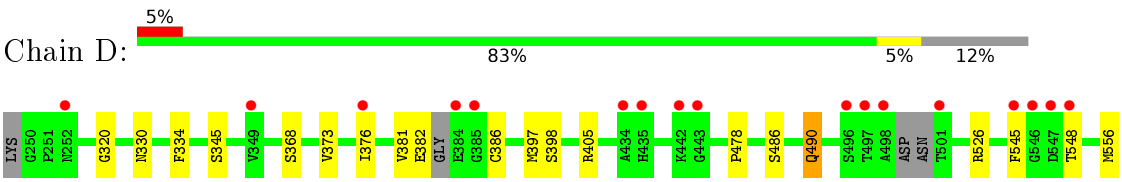
- Molecule 1: Penicillin-binding protein 1A

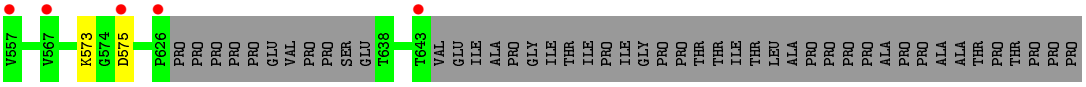
Chain C:



- Molecule 1: Penicillin-binding protein 1A

Chain D:




V557
V567
K573
G574
D575
P626
PRO PRO PRO PRO PRO GLU VAL PRO PRO SER GLU
T638
T643
VAL GLU ILE ALA PRO GLY ILE THR ILE PRO ILE GLY PRO PRO THR THR ILE THR LEU ALA PRO PRO PRO PRO ALA PRO PRO ALA ALA THR PRO THR PRO PRO PRO

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	46.01Å 333.31Å 47.53Å 90.00° 108.37° 90.00°	Depositor
Resolution (Å)	30.00 – 1.80 29.66 – 1.80	Depositor EDS
% Data completeness (in resolution range)	96.6 (30.00-1.80) 96.6 (29.66-1.80)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.64 (at 1.80Å)	Xtriage
Refinement program	REFMAC 5.8.0103	Depositor
R, R_{free}	0.161 , 0.205 0.164 , 0.208	Depositor DCC
R_{free} test set	6019 reflections (5.25%)	DCC
Wilson B-factor (Å^2)	23.5	Xtriage
Anisotropy	0.207	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 49.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.032 for l,-k,h	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	12240	wwPDB-VP
Average B, all atoms (Å^2)	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.75% 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: PO4

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	0.78	0/2883	0.85	5/3915 (0.1%)
1	B	0.73	0/2894	0.83	4/3937 (0.1%)
1	C	0.68	0/2833	0.78	2/3849 (0.1%)
1	D	0.69	0/2833	0.81	2/3846 (0.1%)
All	All	0.72	0/11443	0.82	13/15547 (0.1%)

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	C	0	1

There are no bond length outliers.

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	261	ARG	NE-CZ-NH1	9.50	125.05	120.30
1	A	371	LEU	CA-CB-CG	8.15	134.06	115.30
1	B	261	ARG	NE-CZ-NH2	-7.14	116.73	120.30
1	A	257	ARG	NE-CZ-NH2	-6.90	116.85	120.30
1	A	367	ASP	CB-CG-OD1	6.41	124.07	118.30
1	D	526	ARG	NE-CZ-NH1	6.12	123.36	120.30
1	D	405	ARG	NE-CZ-NH1	5.63	123.11	120.30
1	B	305	ASP	CB-CG-OD1	5.62	123.36	118.30
1	B	405	ARG	NE-CZ-NH1	5.56	123.08	120.30
1	C	316	ASP	CB-CG-OD1	5.33	123.10	118.30
1	C	505	ARG	NE-CZ-NH1	5.32	122.96	120.30
1	A	505	ARG	NE-CZ-NH1	5.19	122.90	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	257	ARG	NE-CZ-NH1	5.07	122.83	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	432	GLY	Peptide

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	2835	0	2759	9	0
1	B	2842	0	2760	10	0
1	C	2786	0	2706	6	0
1	D	2788	0	2708	7	0
2	A	5	0	0	0	0
2	B	10	0	0	0	0
2	D	10	0	0	0	0
3	A	280	0	0	2	0
3	B	293	0	0	2	0
3	C	191	0	0	0	0
3	D	200	0	0	1	0
All	All	12240	0	10933	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:431[A]:PRO:O	3:B:801:HOH:O	2.08	0.72
1:B:397:MSE:SE	1:C:382:GLU:O	2.60	0.69
1:D:386:CYS:HB3	1:D:397:MSE:HE1	1.76	0.67
1:C:266:LEU:HD23	1:C:267:PHE:CZ	2.41	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:373:VAL:O	1:D:376:ILE:HG12	2.07	0.55
1:B:253:GLY:HA3	1:B:331:ALA:HB1	1.89	0.55
1:B:253:GLY:N	3:B:803:HOH:O	2.43	0.51
1:D:545:PHE:CE1	1:D:575:ASP:HA	2.47	0.49
1:D:545:PHE:HE1	1:D:575:ASP:HA	1.78	0.48
1:A:371:LEU:HD21	1:A:404:TYR:CD1	2.49	0.48
1:B:572:VAL:HG13	1:B:573:LYS:HG2	1.97	0.47
1:A:639:VAL:HG21	3:D:813:HOH:O	2.14	0.46
1:C:284:THR:HB	1:C:321:ALA:HB1	1.98	0.46
1:C:578:LEU:HG	1:C:586:ILE:HB	1.98	0.46
1:B:430:PHE:HB2	1:B:431[A]:PRO:CD	2.47	0.45
1:A:500:ASN:HB3	3:A:921:HOH:O	2.17	0.44
1:D:368:SER:OG	1:D:386:CYS:O	2.36	0.44
1:B:320:GLY:O	1:B:478:PRO:HA	2.18	0.43
1:A:376:ILE:HD11	3:A:1033:HOH:O	2.18	0.43
1:A:298:ALA:O	1:A:302:ASP:HB2	2.19	0.42
1:A:639:VAL:HG13	1:A:641:GLN:HE22	1.83	0.42
1:D:320:GLY:O	1:D:478:PRO:HA	2.20	0.42
1:A:489:GLY:HA2	1:B:606:GLY:O	2.20	0.41
1:D:486:SER:OG	1:D:490:GLN:HB2	2.21	0.41
1:A:272:GLN:O	1:A:276:THR:HG23	2.21	0.41
1:C:627:PRO:HA	1:C:628:PRO:HD3	1.97	0.40
1:B:253:GLY:HA3	1:B:331:ALA:CB	2.50	0.40
1:A:578:LEU:HG	1:A:586:ILE:HD12	2.04	0.40
1:B:641:GLN:CB	1:B:642:PRO:HA	2.51	0.40
1:C:266:LEU:HD23	1:C:267:PHE:CE2	2.56	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	384/430 (89%)	381 (99%)	3 (1%)	0	100	100
1	B	384/430 (89%)	378 (98%)	6 (2%)	0	100	100
1	C	375/430 (87%)	367 (98%)	8 (2%)	0	100	100
1	D	374/430 (87%)	369 (99%)	4 (1%)	1 (0%)	46	29
All	All	1517/1720 (88%)	1495 (98%)	21 (1%)	1 (0%)	56	38

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	381	VAL

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	292/321 (91%)	284 (97%)	8 (3%)	52	36
1	B	295/321 (92%)	288 (98%)	7 (2%)	57	41
1	C	287/321 (89%)	284 (99%)	3 (1%)	82	77
1	D	287/321 (89%)	278 (97%)	9 (3%)	47	30
All	All	1161/1284 (90%)	1134 (98%)	27 (2%)	58	42

All (27) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	264	LEU
1	A	272	GLN
1	A	291	ARG
1	A	382	GLU
1	A	398	SER
1	A	556	MSE
1	A	573	LYS
1	A	641	GLN
1	B	264	LEU
1	B	347	PHE

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Mol	Chain	Res	Type
1	B	398	SER
1	B	404	TYR
1	B	556	MSE
1	B	614	LYS
1	B	641	GLN
1	C	301	LEU
1	C	529	ASN
1	C	556	MSE
1	D	330	ASN
1	D	334	PHE
1	D	345	SER
1	D	382	GLU
1	D	398	SER
1	D	490	GLN
1	D	548	THR
1	D	556	MSE
1	D	573	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	456	GLN
1	C	268	ASN
1	C	529	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)

5 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	$\#\|Z\| > 2$
2	PO4	A	701	-	4,4,4	1.13	0	6,6,6	0.26	0
2	PO4	B	701	-	4,4,4	0.90	0	6,6,6	0.27	0
2	PO4	B	702	-	4,4,4	0.64	0	6,6,6	0.28	0
2	PO4	D	701	-	4,4,4	0.77	0	6,6,6	0.23	0
2	PO4	D	702	-	4,4,4	1.57	0	6,6,6	0.23	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	PO4	A	701	-	-	0/0/0/0	0/0/0/0
2	PO4	B	701	-	-	0/0/0/0	0/0/0/0
2	PO4	B	702	-	-	0/0/0/0	0/0/0/0
2	PO4	D	701	-	-	0/0/0/0	0/0/0/0
2	PO4	D	702	-	-	0/0/0/0	0/0/0/0

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

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	379/430 (88%)	-0.11	11 (2%)	55	49	12, 24, 48, 75	0
1	B	381/430 (88%)	-0.14	16 (4%)	40	34	15, 26, 54, 74	0
1	C	375/430 (87%)	0.11	28 (7%)	17	13	25, 33, 59, 93	0
1	D	373/430 (86%)	0.01	22 (5%)	26	21	17, 33, 56, 88	0
All	All	1508/1720 (87%)	-0.03	77 (5%)	32	26	12, 30, 56, 93	0

All (77) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	332	ASN	7.3
1	B	331	ALA	6.8
1	C	266	LEU	6.2
1	B	635	PRO	5.8
1	C	269	ILE	5.8
1	C	376	ILE	5.0
1	D	501	THR	4.6
1	C	267	PHE	4.5
1	D	497	THR	4.2
1	B	629	PRO	4.2
1	D	498	ALA	4.1
1	A	500	ASN	4.0
1	D	547	ASP	4.0
1	C	627	PRO	3.8
1	D	384	GLU	3.7
1	A	547	ASP	3.7
1	C	265	GLU	3.7
1	B	374	ASP	3.7
1	A	637	GLU	3.6
1	B	330	ASN	3.6
1	A	499	ASP	3.6

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Mol	Chain	Res	Type	RSRZ
1	C	252	ASN	3.5
1	C	547	ASP	3.5
1	A	376	ILE	3.4
1	C	268	ASN	3.4
1	B	547	ASP	3.4
1	C	375	GLY	3.3
1	A	497	THR	3.3
1	B	630	PRO	3.2
1	C	274	LEU	3.2
1	D	442	LYS	3.2
1	C	276	THR	3.2
1	C	434	ALA	3.1
1	D	643	THR	3.0
1	B	384	GLU	3.0
1	D	546	GLY	2.9
1	D	385	GLY	2.9
1	C	381	VAL	2.9
1	D	548	THR	2.9
1	D	496	SER	2.8
1	C	377	LYS	2.8
1	D	545	PHE	2.7
1	C	628	PRO	2.6
1	A	501	THR	2.6
1	B	500	ASN	2.6
1	C	264	LEU	2.6
1	C	275	ASN	2.5
1	C	637	GLU	2.5
1	C	549	THR	2.5
1	C	329	ASP	2.5
1	C	497	THR	2.5
1	B	496	SER	2.5
1	A	496	SER	2.5
1	C	433	VAL	2.5
1	A	375	GLY	2.4
1	A	498	ALA	2.4
1	D	575	ASP	2.4
1	D	567	VAL	2.4
1	B	634	PRO	2.4
1	B	382	GLU	2.4
1	B	381	VAL	2.4
1	D	434	ALA	2.4
1	D	443	GLY	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	636	SER	2.4
1	D	252	ASN	2.2
1	C	496	SER	2.2
1	D	376	ILE	2.1
1	C	459	VAL	2.1
1	D	435	HIS	2.1
1	C	273	THR	2.1
1	D	626	PRO	2.1
1	A	441	GLY	2.1
1	B	329	ASP	2.0
1	C	374	ASP	2.0
1	C	261	ARG	2.0
1	D	349	VAL	2.0
1	D	557	VAL	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. 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, 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	LLDF	B-factors(Å^2)	Q<0.9
2	PO4	D	702	5/5	0.92	0.30	5.70	69,71,72,73	0
2	PO4	B	702	5/5	0.97	0.13	5.19	31,31,37,38	0
2	PO4	B	701	5/5	0.98	0.12	1.99	38,41,43,47	0
2	PO4	D	701	5/5	0.97	0.14	-	50,51,53,54	0
2	PO4	A	701	5/5	0.98	0.07	-	45,45,48,51	0

6.5 Other polymers (i)

There are no such residues in this entry.