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 ⓘ

Jun 19, 2020 – 07:23 pm BST

PDB ID	:	1MF8
Title	:	Crystal Structure of human calcineurin complexed with cyclosporin A and human cyclophilin
Authors	:	Jin, L.; Harrison, S.C.
Deposited on	:	2002-08-09
Resolution	:	3.10 Å(reported)

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

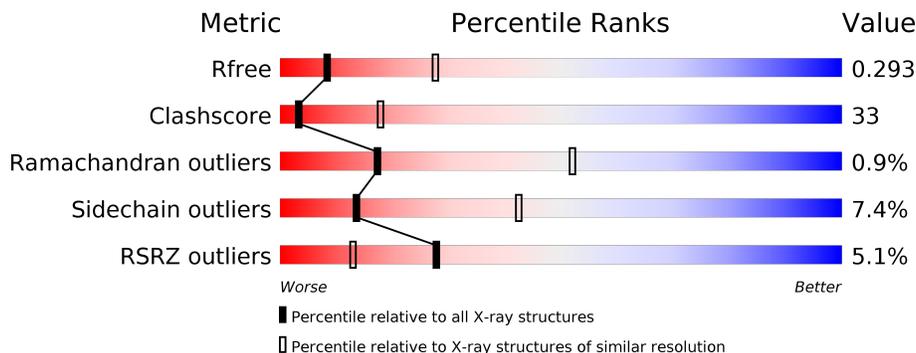|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (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 3.10 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	Percentile Ranks	Value
Rfree		0.293
Clashscore		33
Ramachandran outliers		0.9%
Sidechain outliers		7.4%
RSRZ outliers		5.1%

Worse   Better

■ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1094 (3.10-3.10)
Clashscore	141614	1184 (3.10-3.10)
Ramachandran outliers	138981	1141 (3.10-3.10)
Sidechain outliers	138945	1141 (3.10-3.10)
RSRZ outliers	127900	1067 (3.10-3.10)

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	373	6% / 42% 48% 5% 6%
2	B	170	5% / 52% 40% · ·
3	C	165	2% / 64% 32% · ·
4	D	11	100%

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
4	DAL	D	1	-	-	X	-
4	ABA	D	6	-	-	X	-
5	PO4	A	393	-	-	-	X

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 5522 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 CALMODULIN-DEPENDENT CALCINEURIN A SUBUNIT, ALPHA ISOFORM.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	352	Total 2861	C 1846	N 477	O 518	S 20	31	0	0

- Molecule 2 is a protein called CALCINEURIN B SUBUNIT ISOFORM 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	164	Total 1311	C 828	N 217	O 258	S 8	38	0	0

- Molecule 3 is a protein called PEPTIDYL-PROLYL CIS-TRANS ISOMERASE A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	164	Total 1256	C 797	N 217	O 233	S 9	0	0	0

- Molecule 4 is a protein called CYCLOSPORIN A.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	D	11	Total 85	C 62	N 11	O 12	0	0	0

- Molecule 5 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).
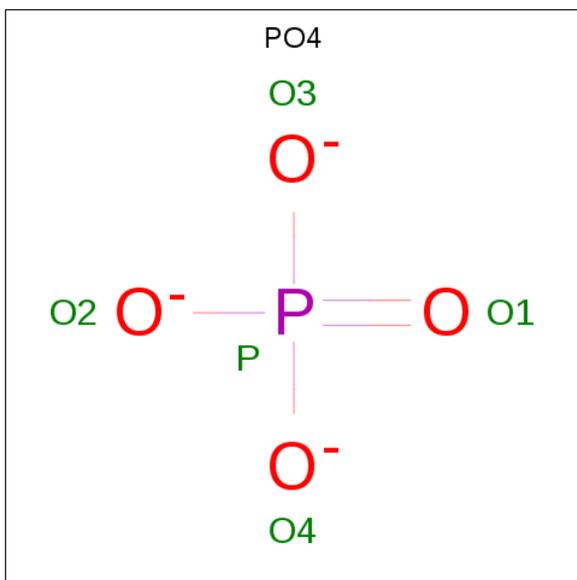
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total 5	O 4	P 1	0	0

- Molecule 6 is CALCIUM ION (three-letter code: CA) (formula: Ca).

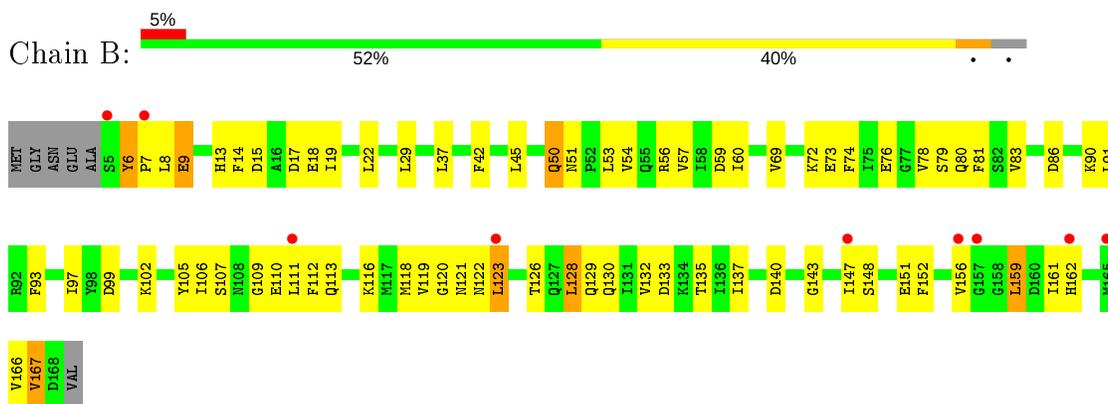| Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	B	4	Total 4	Ca 4	0	0

3 Residue-property plots ⓘ

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: CALMODULIN-DEPENDENT CALCINEURIN A SUBUNIT, ALPHA ISOFORM
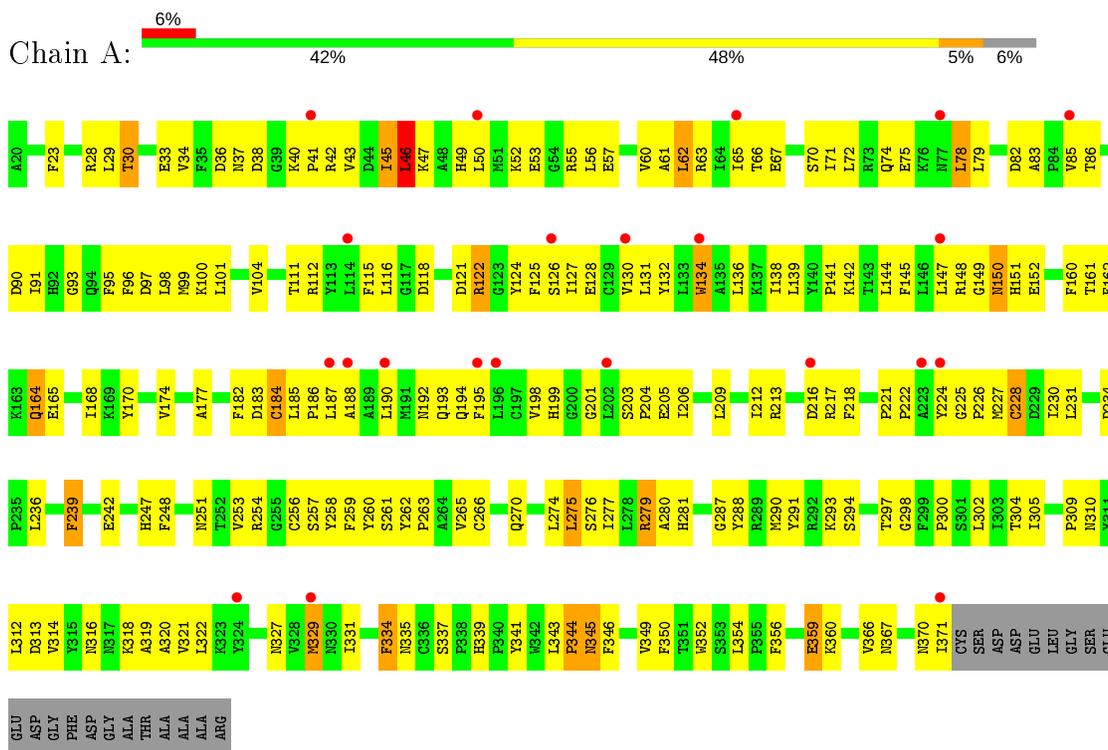
● Molecule 2: CALCINEURIN B SUBUNIT ISOFORM 1

● Molecule 3: PEPTIDYL-PROLYL CIS-TRANS ISOMERASE A

Chain C:

2%

64%

32%

M1 V2 N3 P4 T5 V6 F7 F8 D9 V12 D13 L17 G18 R19 V20 L24 V29 P30 K31 E34 N35 F36 R37 A38 L39 E43 F46 G47 Y48 I57 P58 M61 C62 I78 Y79 K82 F83 E84 D85 E86 N87 F88 I89 H92 T93 I97 L98

A101 M102 T107 Q111 F112 F113 K118 T119 E120 M121 L122 D123 F129 K133 E134 F145 R148 N149 T152 S153 K154 T157 I158 G162 Q163 L164 GLU
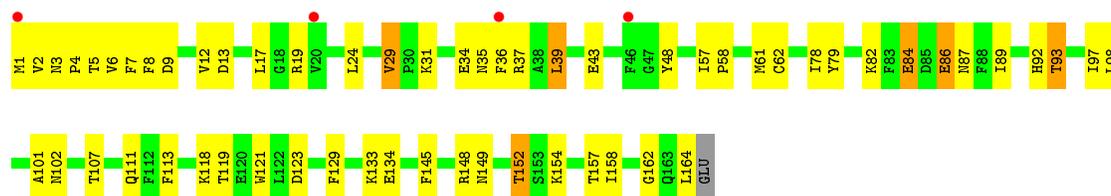
● Molecule 4: CYCLOSPORIN A

Chain D:

100%

A1 L2 L3 V4 T5 A6 G7 L8 V9 L10 A11
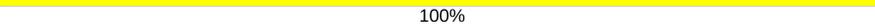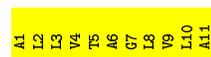
4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	64.95Å 108.33Å 112.84Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	15.00 – 3.10	Depositor
	48.83 – 3.10	EDS
% Data completeness	95.6 (15.00-3.10)	Depositor
(in resolution range)	96.0 (48.83-3.10)	EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
$< I/\sigma(I) >$ [1]	3.50 (at 3.12Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.250 , 0.300	Depositor
	0.257 , 0.293	DCC
R_{free} test set	1065 reflections (7.43%)	wwPDB-VP
Wilson B-factor (Å^2)	100.8	Xtriage
Anisotropy	0.352	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 52.7	EDS
L-test for twinning[2]	$< |L| > = 0.48, < L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.011 for -h,l,k	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	5522	wwPDB-VP
Average B, all atoms (Å^2)	94.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.24% of the height of the origin peak. No significant pseudotranslation is detected.*

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[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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: ABA, MLE, DAL, PO4, MVA, BMT, SAR, CA

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	0.49	0/2940	0.72	0/3990
2	B	0.49	0/1330	0.64	0/1780
3	C	0.45	0/1284	0.67	0/1721
4	D	0.52	0/10	0.64	0/11
All	All	0.48	0/5564	0.69	0/7502

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	2861	0	2794	215	0
2	B	1311	0	1290	78	0
3	C	1256	0	1231	69	0
4	D	85	0	110	24	0
5	A	5	0	0	0	0
6	B	4	0	0	0	0
All	All	5522	0	5425	353	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 33.

The worst 5 of 353 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:322:LEU:HD21	1:A:329:MET:SD	1.80	1.19
3:C:35:ASN:O	3:C:39:LEU:HG	1.46	1.15
2:B:119:VAL:HG21	2:B:123:LEU:HD12	1.24	1.12
1:A:217:ARG:HA	1:A:227:MET:HE1	1.15	1.12
1:A:217:ARG:HA	1:A:227:MET:CE	1.83	1.09

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	350/373 (94%)	316 (90%)	32 (9%)	2 (1%)	25	59
2	B	162/170 (95%)	156 (96%)	5 (3%)	1 (1%)	25	59
3	C	162/165 (98%)	146 (90%)	13 (8%)	3 (2%)	8	33
4	D	1/11 (9%)	1 (100%)	0	0	100	100
All	All	675/719 (94%)	619 (92%)	50 (7%)	6 (1%)	17	52

5 of 6 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	193	GLN
3	C	43	GLU
3	C	86	GLU
1	A	46	LEU
2	B	6	TYR

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	314/328 (96%)	288 (92%)	26 (8%)	11	38
2	B	147/151 (97%)	137 (93%)	10 (7%)	16	45
3	C	132/133 (99%)	124 (94%)	8 (6%)	18	49
4	D	1/1 (100%)	1 (100%)	0	100	100
All	All	594/613 (97%)	550 (93%)	44 (7%)	13	42

5 of 44 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	327	ASN
1	A	345	ASN
3	C	84	GLU
1	A	329	MET
1	A	337	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 12 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	327	ASN
1	A	345	ASN
2	B	121	ASN
1	A	247	HIS
2	B	80	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)

9 non-standard protein/DNA/RNA residues 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	$\#|Z| > 2$
4	SAR	D	7	4	4,4,5	0.77	0	1,3,5	2.09	1 (100%)
4	MVA	D	4	4	6,7,8	0.54	0	7,8,10	1.64	1 (14%)
4	ABA	D	6	4	4,5,6	0.48	0	1,5,7	0.76	0
4	MLE	D	3	4	7,8,9	0.48	0	6,9,11	1.59	2 (33%)
4	MLE	D	10	4	7,8,9	0.72	0	6,9,11	1.78	2 (33%)
4	BMT	D	5	4	11,12,13	1.13	1 (9%)	12,14,16	0.97	0
4	MLE	D	8	4	7,8,9	0.52	0	6,9,11	1.56	1 (16%)
4	MLE	D	2	4	7,8,9	0.42	0	6,9,11	1.78	2 (33%)

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
4	SAR	D	7	4	-	1/1/2/3	-
4	MVA	D	4	4	-	1/6/8/10	-
4	ABA	D	6	4	-	2/3/4/6	-
4	MLE	D	3	4	-	0/5/8/10	-
4	MLE	D	10	4	-	0/5/8/10	-
4	BMT	D	5	4	-	1/13/16/18	-
4	MLE	D	8	4	-	1/5/8/10	-
4	MLE	D	2	4	-	0/5/8/10	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	5	BMT	CD2-CE	-3.17	1.40	1.50

The worst 5 of 9 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	D	4	MVA	CB-CA-C	-3.80	108.28	113.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	2	MLE	CN-N-CA	3.26	123.80	113.64
4	D	8	MLE	CN-N-CA	3.21	123.63	113.64
4	D	10	MLE	CN-N-CA	3.17	123.52	113.64
4	D	3	MLE	CN-N-CA	2.74	122.18	113.64

There are no chirality outliers.

5 of 6 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	D	4	MVA	CB-CA-N-CN
4	D	6	ABA	N-CA-CB-CG
4	D	6	ABA	C-CA-CB-CG
4	D	5	BMT	CB-CA-N-CN
4	D	8	MLE	O-C-CA-CB

There are no ring outliers.

8 monomers are involved in 23 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	7	SAR	2	0
4	D	4	MVA	4	0
4	D	6	ABA	4	0
4	D	3	MLE	5	0
4	D	10	MLE	3	0
4	D	5	BMT	5	0
4	D	8	MLE	5	0
4	D	2	MLE	2	0

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

Of 5 ligands modelled in this entry, 4 are monoatomic - leaving 1 for Mogul analysis.

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	$\#|Z| > 2$
5	PO4	A	393	-	4,4,4	1.01	0	6,6,6	0.43	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 (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	352/373 (94%)	0.27	22 (6%)	20	8	57, 93, 119, 130	12 (3%)
2	B	164/170 (96%)	0.17	9 (5%)	25	11	67, 94, 129, 131	14 (8%)
3	C	164/165 (99%)	0.20	4 (2%)	59	37	70, 100, 116, 128	0
4	D	2/11 (18%)	-0.21	0	100	100	66, 66, 66, 68	0
All	All	682/719 (94%)	0.23	35 (5%)	28	13	57, 96, 122, 131	26 (3%)

The worst 5 of 35 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	202	LEU	4.2
1	A	187	LEU	4.1
2	B	165	MET	4.1
1	A	196	LEU	3.7
2	B	156	VAL	3.7

6.2 Non-standard residues in protein, DNA, RNA chains (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, 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	B-factors(Å^2)	Q<0.9
4	SAR	D	7	5/6	0.94	0.26	59,59,62,67	0
4	MLE	D	8	9/10	0.95	0.58	58,61,78,85	0
4	DAL	D	1	5/6	0.96	0.18	66,67,68,70	0
4	MLE	D	10	9/10	0.96	0.26	52,60,78,81	0
4	BMT	D	5	13/14	0.96	0.33	55,59,91,98	0
4	ABA	D	6	6/7	0.96	0.32	60,62,63,86	0
4	MLE	D	3	9/10	0.97	0.22	60,62,89,89	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å²)	Q<0.9
4	MLE	D	2	9/10	0.97	0.22	62,65,80,82	0
4	MVA	D	4	8/9	0.98	0.26	60,62,80,80	0

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

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, 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	B-factors(Å²)	Q<0.9
5	PO4	A	393	5/5	0.72	0.50	120,130,130,130	0
6	CA	B	401	1/1	0.81	0.10	91,91,91,91	0
6	CA	B	402	1/1	0.95	0.19	77,77,77,77	0
6	CA	B	404	1/1	0.97	0.06	91,91,91,91	0
6	CA	B	403	1/1	0.97	0.04	76,76,76,76	0

6.5 Other polymers ⓘ

There are no such residues in this entry.