Full wwPDB X-ray Structure Validation Report ⓘ

May 29, 2020 – 09:32 am BST

PDB ID	:	6C5W
Title	:	Crystal structure of the mitochondrial calcium uniporter
Authors	:	Fan, C.; Fan, M.; Fastman, N.; Zhang, J.; Feng, L.
Deposited on	:	2018-01-17
Resolution	:	3.10 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 ①) were used in the production of this report:

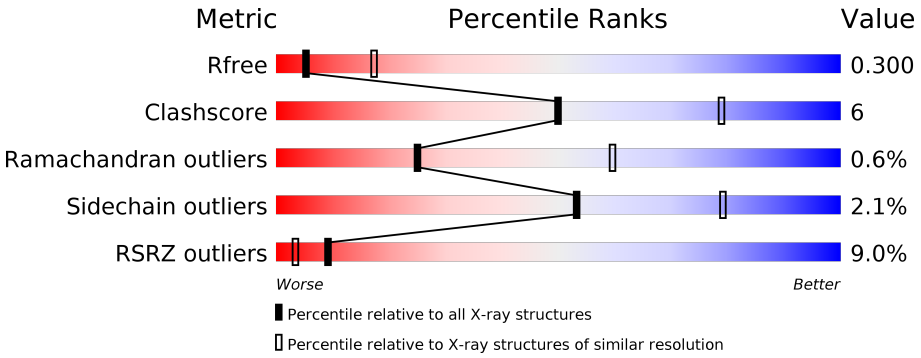
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation 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 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	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	312	10% 78% 12% • 9%
1	B	312	% 56% 13% 30%
2	C	117	2% 91% 9%
2	E	117	24% 80% 20%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 5745 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 calcium uniporter.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	285	Total	C	N	O	S	0	1	0
			2193	1407	384	394	8			
1	B	217	Total	C	N	O	S	0	0	0
			1765	1144	308	306	7			

There are 32 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	GLY	deletion	UNP E9DVV4
A	?	-	GLY	deletion	UNP E9DVV4
A	?	-	ASN	deletion	UNP E9DVV4
A	?	-	LYS	deletion	UNP E9DVV4
A	?	-	SER	deletion	UNP E9DVV4
A	?	-	ASN	deletion	UNP E9DVV4
A	?	-	ASP	deletion	UNP E9DVV4
A	?	-	GLY	deletion	UNP E9DVV4
A	?	-	ARG	deletion	UNP E9DVV4
A	?	-	ARG	deletion	UNP E9DVV4
A	?	-	GLU	deletion	UNP E9DVV4
A	?	-	GLU	deletion	UNP E9DVV4
A	?	-	SER	deletion	UNP E9DVV4
A	?	-	ASN	deletion	UNP E9DVV4
A	?	-	GLY	deletion	UNP E9DVV4
A	?	-	ASN	deletion	UNP E9DVV4
B	?	-	GLY	deletion	UNP E9DVV4
B	?	-	GLY	deletion	UNP E9DVV4
B	?	-	ASN	deletion	UNP E9DVV4
B	?	-	LYS	deletion	UNP E9DVV4
B	?	-	SER	deletion	UNP E9DVV4
B	?	-	ASN	deletion	UNP E9DVV4
B	?	-	ASP	deletion	UNP E9DVV4
B	?	-	GLY	deletion	UNP E9DVV4
B	?	-	ARG	deletion	UNP E9DVV4

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Chain	Residue	Modelled	Actual	Comment	Reference
B	?	-	ARG	deletion	UNP E9DVV4
B	?	-	GLU	deletion	UNP E9DVV4
B	?	-	GLU	deletion	UNP E9DVV4
B	?	-	SER	deletion	UNP E9DVV4
B	?	-	ASN	deletion	UNP E9DVV4
B	?	-	GLY	deletion	UNP E9DVV4
B	?	-	ASN	deletion	UNP E9DVV4

- Molecule 2 is a protein called nanobody.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	117	Total	C	N	O	S	0	0	0
			893	563	157	169	4			
2	E	117	Total	C	N	O	S	0	0	0
			893	563	157	169	4			

- Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca).

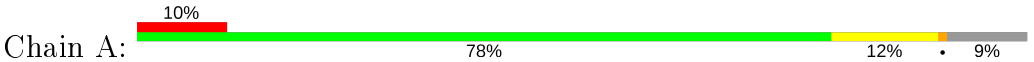
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Ca	0	0
			1	1		

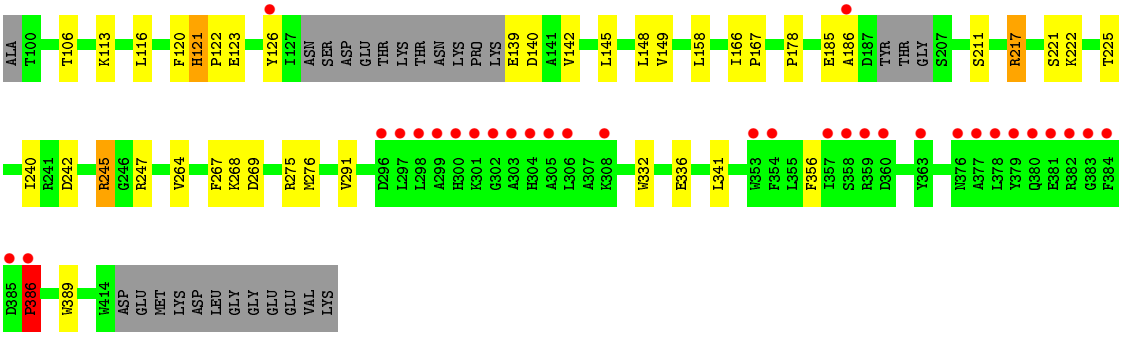
3 Residue-property plots (i)

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: calcium uniporter

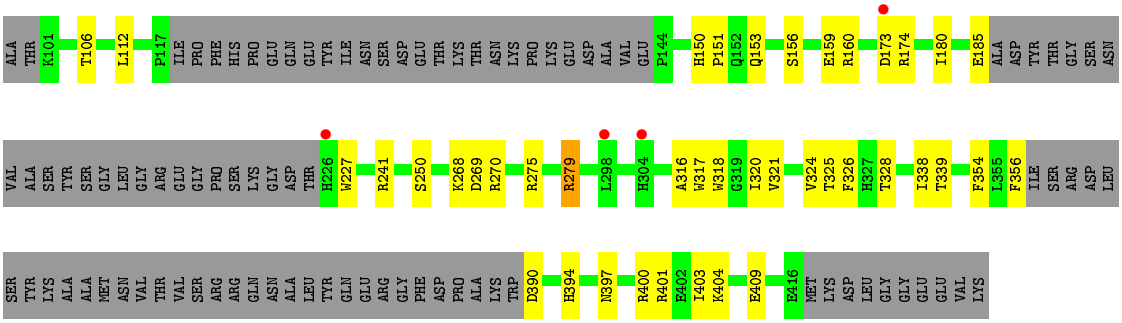
Chain A:





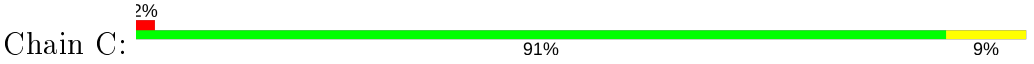
- Molecule 1: calcium uniporter

Chain B:



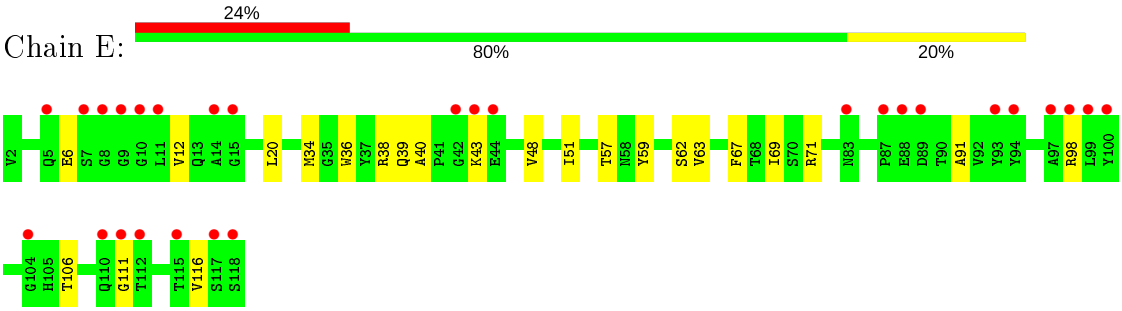
- Molecule 2: nanobody

Chain C:



- Molecule 2: nanobody

Chain E:


24%
80%
20%
V2
Q5
E6
S7
G8
G9
G10
L11
V12
Q13
A14
G15
L20
M34
G35
W36
Y37
R38
Q39
A40
P41
G42
K43
E44
V48
I51
T57
N58
Y59
S62
V63
F67
T68
I69
S70
R71
N83
P87
E88
D89
T90
A91
V92
Y93
Y94
A97
R98
L99
Y100
G104
H105
T106
Q110
G111
T112
T115
V116
S117
S118

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	88.02Å 290.45Å 126.12Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	45.30 – 3.10 42.12 – 3.10	Depositor EDS
% Data completeness (in resolution range)	78.9 (45.30-3.10) 78.9 (42.12-3.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.64 (at 3.12Å)	Xtriage
Refinement program	phenix.refine 1.11.1_2575, PHENIX 1.11.1_2575	Depositor
R, R_{free}	0.256 , 0.299 0.256 , 0.300	Depositor DCC
R_{free} test set	1218 reflections (5.18%)	wwPDB-VP
Wilson B-factor (Å^2)	56.2	Xtriage
Anisotropy	0.099	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.27 , 52.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.82	EDS
Total number of atoms	5745	wwPDB-VP
Average B, all atoms (Å^2)	75.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.59% 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: 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	0.25	0/2248	0.45	1/3053 (0.0%)
1	B	0.23	0/1809	0.41	0/2447
2	C	0.25	0/914	0.44	0/1239
2	E	0.25	0/914	0.46	0/1239
All	All	0.24	0/5885	0.44	1/7978 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	386	PRO	N-CA-CB	6.26	110.81	103.30

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	2193	0	2094	24	0
1	B	1765	0	1770	24	0
2	C	893	0	862	6	0
2	E	893	0	862	14	0
3	A	1	0	0	0	0
All	All	5745	0	5588	66	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 6.

All (66) 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)
2:C:90:THR:HG23	2:C:115:THR:HA	1.70	0.72
1:B:150:HIS:HB3	1:B:153:GLN:HG3	1.70	0.72
1:A:221:SER:HB3	1:A:247:ARG:HD3	1.72	0.72
1:A:123:GLU:HG2	1:A:126:TYR:HA	1.70	0.71
1:A:186:ALA:HA	1:A:245:ARG:HE	1.55	0.71
1:A:139:GLU:OE1	1:A:139:GLU:N	2.30	0.65
1:A:185:GLU:HG3	1:A:225:THR:HB	1.78	0.64
1:A:242:ASP:OD1	1:A:245:ARG:NH1	2.31	0.64
2:E:98:ARG:HG2	2:E:106:THR:HG22	1.78	0.63
1:B:268:LYS:O	1:B:275:ARG:NH1	2.33	0.61
1:A:211:SER:O	1:A:245:ARG:NH2	2.36	0.59
1:B:317:TRP:HH2	1:B:338:ILE:HG22	1.67	0.58
2:C:17:SER:OG	2:C:83:ASN:OD1	2.21	0.58
1:B:241:ARG:HD2	1:B:409:GLU:HB3	1.84	0.58
1:B:275:ARG:HG2	1:B:279:ARG:HH21	1.69	0.58
1:B:275:ARG:HG3	1:B:403:ILE:HD11	1.86	0.58
1:A:341:LEU:HD12	1:B:318:TRP:CE2	2.39	0.58
2:E:63:VAL:HG13	2:E:67:PHE:CD2	2.39	0.58
1:A:122:PRO:HG3	1:A:139:GLU:HB2	1.86	0.57
1:B:156:SER:HA	1:B:159:GLU:HG2	1.85	0.57
2:E:38:ARG:HB2	2:E:91:ALA:HB3	1.89	0.55
2:C:34:MET:HB2	2:C:71:ARG:HD2	1.88	0.55
2:C:12:VAL:HG11	2:C:85:LEU:HD13	1.89	0.54
2:E:34:MET:HB2	2:E:71:ARG:HD2	1.89	0.54
1:A:166:ILE:HG12	1:A:167:PRO:HD2	1.89	0.54
2:E:12:VAL:O	2:E:116:VAL:HA	2.08	0.54
1:A:126:TYR:OH	1:A:178:PRO:HB3	2.07	0.54
2:E:51:ILE:HG12	2:E:57:THR:HB	1.90	0.54
1:B:227:TRP:HZ3	1:B:250:SER:HB2	1.74	0.53
1:A:268:LYS:O	1:A:275:ARG:NH1	2.42	0.52
2:E:39:GLN:H	2:E:91:ALA:HB1	1.74	0.51
1:A:186:ALA:HA	1:A:245:ARG:NE	2.24	0.51
1:A:332:TRP:CE2	1:A:336:GLU:HB2	2.45	0.50
1:B:150:HIS:ND1	1:B:151:PRO:HD2	2.27	0.50
1:B:394:HIS:HA	1:B:397:ASN:HB2	1.93	0.50
1:B:185:GLU:HG2	1:B:227:TRP:CD1	2.47	0.50
2:E:48:VAL:HA	2:E:63:VAL:HG21	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:149:VAL:HG11	1:A:158:LEU:HD13	1.94	0.49
2:E:40:ALA:HB3	2:E:43:LYS:HB2	1.94	0.49
1:B:159:GLU:HB2	1:B:180:ILE:HG12	1.95	0.48
2:E:38:ARG:NH2	2:E:62:SER:OG	2.47	0.47
1:A:291:VAL:HG11	1:A:386:PRO:HA	1.97	0.47
1:B:324:VAL:O	1:B:328:THR:OG1	2.33	0.47
1:A:140:ASP:OD1	1:A:140:ASP:N	2.47	0.46
1:A:116:LEU:HD11	1:A:145:LEU:HD23	1.98	0.46
2:E:59:TYR:CZ	2:E:69:ILE:HG22	2.50	0.46
1:B:159:GLU:HG3	1:B:160:ARG:N	2.32	0.45
2:C:64:LYS:HB2	2:C:64:LYS:HE3	1.82	0.45
1:B:400:ARG:HA	1:B:403:ILE:HG22	1.98	0.45
1:A:106:THR:HG21	1:A:269:ASP:O	2.17	0.44
1:A:113:LYS:HE3	1:A:148:LEU:HD13	2.00	0.44
2:E:6:GLU:OE2	2:E:111:GLY:N	2.45	0.43
1:B:326:PHE:CD2	2:C:54:GLY:HA3	2.53	0.43
1:B:106:THR:HG21	1:B:269:ASP:O	2.18	0.43
1:B:317:TRP:HZ2	1:B:339:THR:HA	1.84	0.43
1:B:159:GLU:HA	1:B:180:ILE:HD11	2.00	0.42
1:B:401:ARG:O	1:B:404:LYS:HG2	2.19	0.42
1:B:316:ALA:O	1:B:320:ILE:HG12	2.19	0.42
1:A:120:PHE:O	1:A:121:HIS:HB2	2.20	0.42
2:E:20:LEU:HB3	2:E:36:TRP:CH2	2.54	0.42
1:A:120:PHE:O	1:A:142:VAL:HG12	2.20	0.41
2:E:57:THR:O	2:E:57:THR:OG1	2.30	0.41
1:A:217:ARG:HG2	1:A:264:VAL:O	2.20	0.41
1:A:240:ILE:HA	1:A:240:ILE:HD13	1.86	0.41
1:B:112:LEU:HD21	1:B:270:ARG:NH1	2.37	0.40
1:B:321:VAL:O	1:B:325:THR:OG1	2.34	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	280/312 (90%)	266 (95%)	11 (4%)	3 (1%)	14 46
1	B	209/312 (67%)	202 (97%)	7 (3%)	0	100 100
2	C	115/117 (98%)	109 (95%)	5 (4%)	1 (1%)	17 52
2	E	115/117 (98%)	108 (94%)	7 (6%)	0	100 100
All	All	719/858 (84%)	685 (95%)	30 (4%)	4 (1%)	25 59

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	121	HIS
1	A	386	PRO
2	C	102	ILE
1	A	389	TRP

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	209/260 (80%)	202 (97%)	7 (3%)	38 69
1	B	181/260 (70%)	175 (97%)	6 (3%)	38 69
2	C	92/92 (100%)	92 (100%)	0	100 100
2	E	92/92 (100%)	92 (100%)	0	100 100
All	All	574/704 (82%)	561 (98%)	13 (2%)	53 77

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	217	ARG
1	A	222	LYS
1	A	245	ARG
1	A	267	PHE
1	A	276[A]	MET
1	A	276[B]	MET
1	A	356	PHE

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Mol	Chain	Res	Type
1	B	173	ASP
1	B	174	ARG
1	B	279	ARG
1	B	354	PHE
1	B	356	PHE
1	B	390	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
2	E	105	HIS

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

Of 1 ligands modelled in this entry, 1 is 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

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	285/312 (91%)	0.41	32 (11%) 5 2	15, 53, 162, 218	0
1	B	217/312 (69%)	0.11	4 (1%) 68 47	22, 60, 123, 164	0
2	C	117/117 (100%)	-0.18	2 (1%) 70 49	28, 49, 81, 111	0
2	E	117/117 (100%)	1.11	28 (23%) 0 0	76, 145, 191, 207	0
All	All	736/858 (85%)	0.34	66 (8%) 9 3	15, 62, 169, 218	0

All (66) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	E	117	SER	7.6
1	A	378	LEU	6.9
1	A	385	ASP	6.2
1	A	300	HIS	6.0
1	A	384	PHE	5.9
2	E	10	GLY	5.7
2	E	118	SER	5.5
1	A	359	ARG	5.4
1	A	358	SER	5.3
1	A	301	LYS	5.3
1	A	297	LEU	5.1
1	A	376	ASN	5.0
1	A	386	PRO	4.6
1	B	226	HIS	4.6
1	A	381	GLU	4.5
1	A	304	HIS	4.5
2	E	11	LEU	4.4
1	A	302	GLY	4.1
1	A	296	ASP	4.0
2	E	7	SER	4.0
1	A	383	GLY	3.9

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Mol	Chain	Res	Type	RSRZ
1	A	303	ALA	3.9
1	A	357	ILE	3.9
1	A	377	ALA	3.9
1	A	379	TYR	3.8
1	A	380	GLN	3.7
2	E	112	THR	3.6
2	E	99	LEU	3.6
1	A	299	ALA	3.5
2	E	83	ASN	3.4
1	B	173	ASP	3.3
1	A	360	ASP	3.3
1	B	304	HIS	3.3
2	E	43	LYS	3.3
1	A	363	TYR	3.2
2	C	103	LEU	3.2
2	E	42	GLY	3.2
1	A	298	LEU	3.1
2	E	111	GLY	3.1
2	E	88	GLU	3.1
2	E	15	GLY	3.1
2	E	115	THR	3.1
1	A	382	ARG	3.0
2	E	8	GLY	2.9
1	A	353	TRP	2.8
2	E	110	GLN	2.8
2	E	100	TYR	2.7
2	E	9	GLY	2.7
2	E	94	TYR	2.5
1	A	186	ALA	2.4
2	E	5	GLN	2.4
1	A	306	LEU	2.4
1	A	126	TYR	2.4
1	B	298	LEU	2.4
2	E	97	ALA	2.3
1	A	305	ALA	2.3
2	E	87	PRO	2.3
1	A	354	PHE	2.3
2	E	104	GLY	2.2
2	E	14	ALA	2.2
2	E	89	ASP	2.1
2	E	44	GLU	2.1
2	C	27	THR	2.1

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Mol	Chain	Res	Type	RSRZ
2	E	93	TYR	2.1
2	E	98	ARG	2.1
1	A	308	LYS	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. 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	B-factors(Å^2)	Q<0.9
3	CA	A	501	1/1	0.98	0.21	32,32,32,32	1

6.5 Other polymers (i)

There are no such residues in this entry.