



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 10, 2024 – 04:43 AM EDT

PDB ID : 4FC5
Title : Crystal Structure of Ton_0340
Authors : Lee, S.G.; Lee, K.H.; An, Y.J.; Cha, S.S.; Oh, B.H.
Deposited on : 2012-05-24
Resolution : 2.30 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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 : 2.36
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) : 2.36

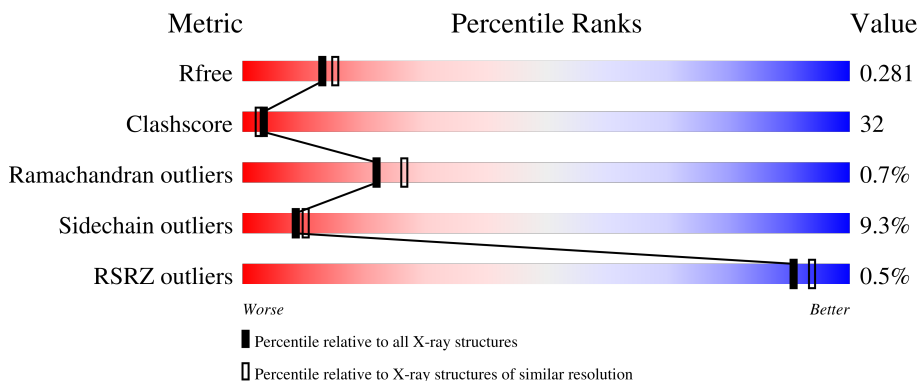
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

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 of 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 $\leq 5\%$. 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	270	
1	B	270	
1	C	270	
1	D	270	
1	E	270	

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Mol	Chain	Length	Quality of chain
1	F	270	 55% 39% 6%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 13532 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 Putative uncharacterized protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	259	Total 1963	C 1250	N 334	O 372	S 7	0	0	0
1	B	268	Total 2022	C 1288	N 343	O 384	S 7	0	0	0
1	C	269	Total 2035	C 1297	N 344	O 386	S 8	0	0	0
1	D	268	Total 2022	C 1288	N 343	O 384	S 7	0	0	0
1	E	258	Total 1959	C 1248	N 333	O 371	S 7	0	0	0
1	F	269	Total 2035	C 1297	N 344	O 386	S 8	0	0	0

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	269	LYS	-	expression tag	UNP B6YTD8
A	270	LEU	-	expression tag	UNP B6YTD8
B	269	LYS	-	expression tag	UNP B6YTD8
B	270	LEU	-	expression tag	UNP B6YTD8
C	269	LYS	-	expression tag	UNP B6YTD8
C	270	LEU	-	expression tag	UNP B6YTD8
D	269	LYS	-	expression tag	UNP B6YTD8
D	270	LEU	-	expression tag	UNP B6YTD8
E	269	LYS	-	expression tag	UNP B6YTD8
E	270	LEU	-	expression tag	UNP B6YTD8
F	269	LYS	-	expression tag	UNP B6YTD8
F	270	LEU	-	expression tag	UNP B6YTD8

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	8	Total 8	Zn 8	0	0
2	B	11	Total 11	Zn 11	0	0
2	C	8	Total 8	Zn 8	0	0
2	D	7	Total 7	Zn 7	0	0
2	E	11	Total 11	Zn 11	0	0
2	F	8	Total 8	Zn 8	0	0

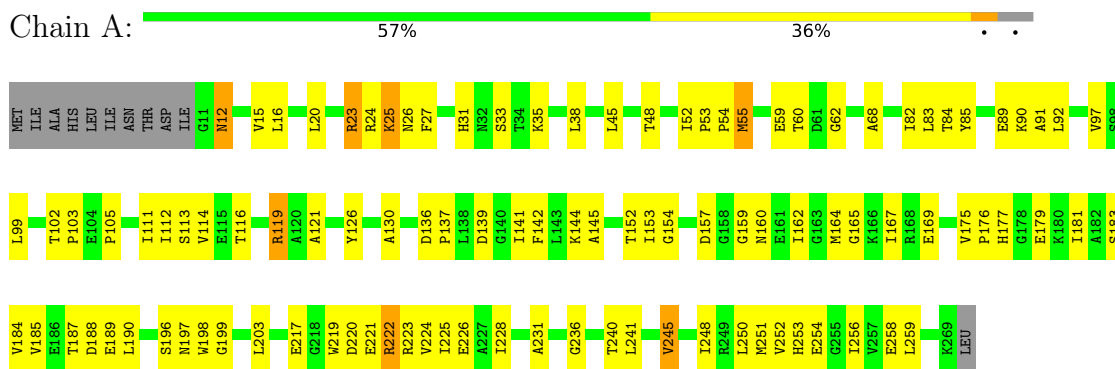
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	260	Total 260	O 260	0	0
3	B	309	Total 309	O 309	0	0
3	C	170	Total 170	O 170	0	0
3	D	191	Total 191	O 191	0	0
3	E	218	Total 218	O 218	0	0
3	F	295	Total 295	O 295	0	0

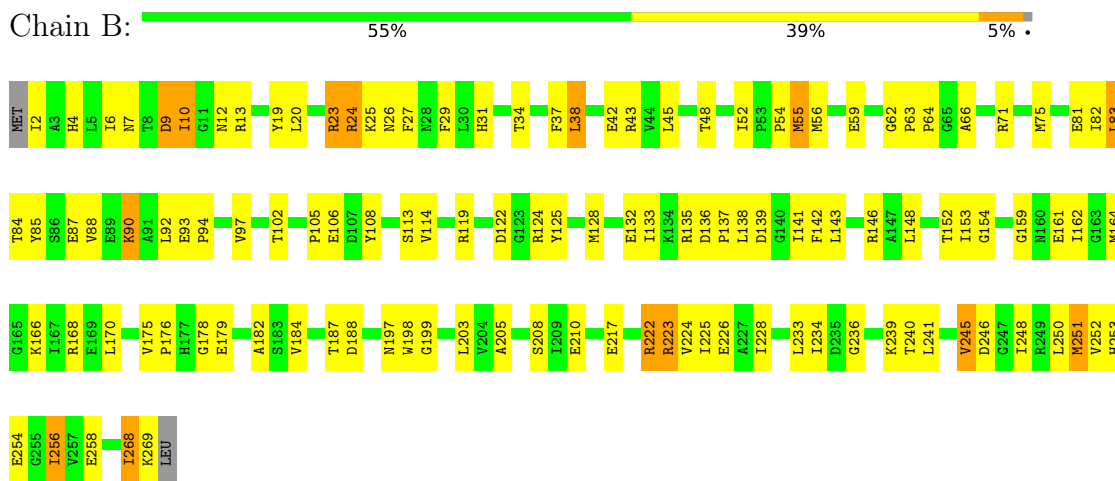
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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.

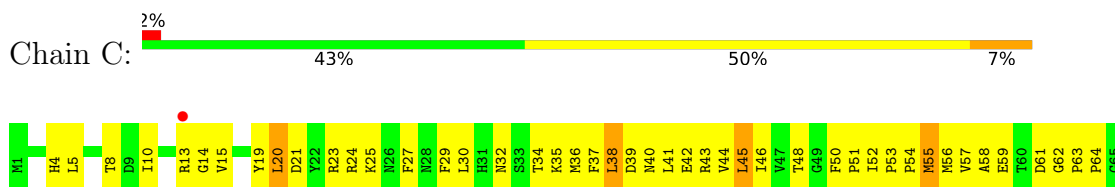
- Molecule 1: Putative uncharacterized protein

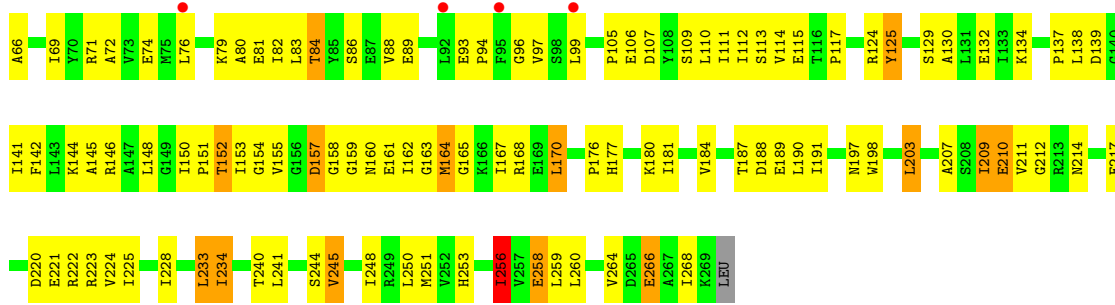


- Molecule 1: Putative uncharacterized protein

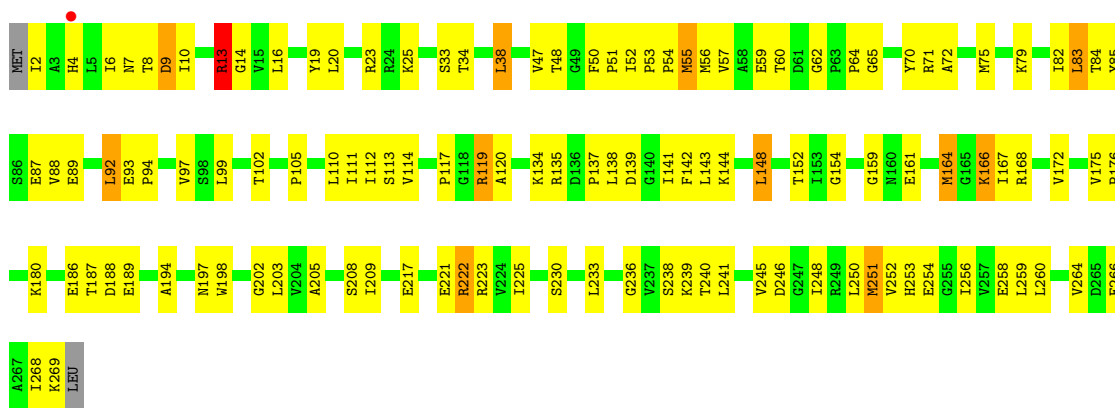


- Molecule 1: Putative uncharacterized protein

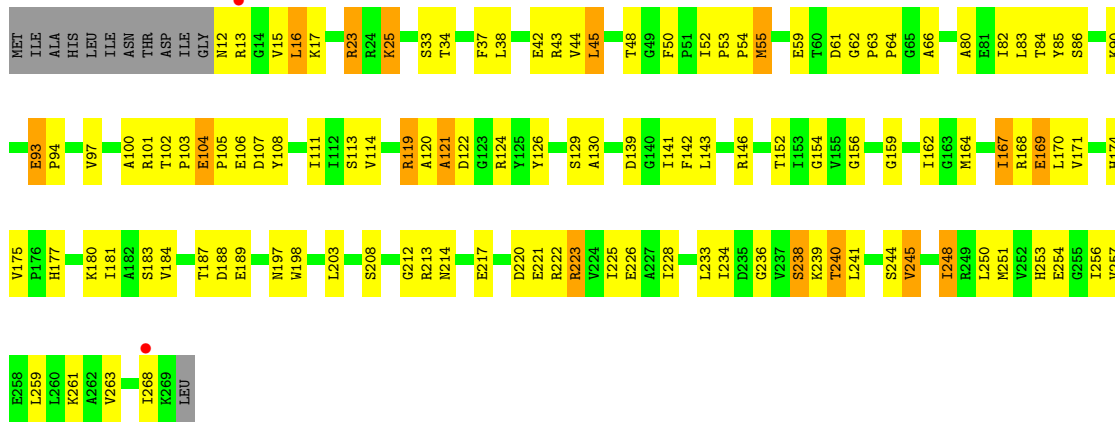




• Molecule 1: Putative uncharacterized protein



• Molecule 1: Putative uncharacterized protein



• Molecule 1: Putative uncharacterized protein



P94	G178	E266
V97	E179	A267
T102	K180	I268
P103	I181	K269
E104	A182	LEU
P106	S183	
E106	V184	
D107	T187	
I111	D188	
I112	M197	
S113	W198	
V114		
E115	L203	
T116	V204	
P117	A205	
G118	S208	
R119	L209	
R124	E210	
Y125	V211	
Y126	G212	
S129	R213	
A130	E221	
L131	R222	
E132	I225	
I133	I228	
K134	L233	
R135	I234	
D139	D235	
G140	G236	
I141	K239	
F142	T240	
L143	L241	
K144	A242	
G149	P243	
T152	S244	
I153	V245	
G154	I248	
D157	R249	
G158	L250	
G159	M251	
M160	V252	
E161	H253	
I162	E254	
G163	G255	
M164	I256	
R168	L259	
E169	L260	
L170	V264	
H177	D265	

4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α , β , γ	107.18Å 107.18Å 356.38Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	44.45 – 2.30 44.45 – 2.22	Depositor EDS
% Data completeness (in resolution range)	94.1 (44.45-2.30) 92.8 (44.45-2.22)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.68 (at 2.22Å)	Xtrriage
Refinement program	CNS	Depositor
R, R_{free}	0.223 , 0.281 0.223 , 0.281	Depositor DCC
R_{free} test set	9588 reflections (9.98%)	wwPDB-VP
Wilson B-factor (Å ²)	19.9	Xtrriage
Anisotropy	0.040	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 54.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.42$, $\langle L^2 \rangle = 0.24$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	13532	wwPDB-VP
Average B, all atoms (Å ²)	34.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.72% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ 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:
ZN

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	0.47	0/1997	0.71	1/2707 (0.0%)
1	B	0.57	0/2057	0.75	0/2791
1	C	0.58	0/2070	0.75	1/2808 (0.0%)
1	D	0.57	0/2057	0.78	2/2791 (0.1%)
1	E	0.62	0/1993	0.78	0/2702
1	F	0.50	0/2070	0.70	0/2808
All	All	0.55	0/12244	0.74	4/16607 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	13	ARG	N-CA-C	6.20	127.73	111.00
1	C	256	ILE	CG1-CB-CG2	-6.19	97.79	111.40
1	D	166	LYS	CD-CE-NZ	-5.31	99.49	111.70
1	A	35	LYS	CB-CG-CD	-5.28	97.86	111.60

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	1963	0	1996	112	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	2022	0	2043	144	0
1	C	2035	0	2070	186	0
1	D	2022	0	2044	130	0
1	E	1959	0	1993	124	0
1	F	2035	0	2070	127	0
2	A	8	0	0	0	0
2	B	11	0	0	0	0
2	C	8	0	0	0	0
2	D	7	0	0	0	0
2	E	11	0	0	0	0
2	F	8	0	0	0	0
3	A	260	0	0	16	0
3	B	309	0	0	19	0
3	C	170	0	0	15	0
3	D	191	0	0	11	0
3	E	218	0	0	14	0
3	F	295	0	0	14	0
All	All	13532	0	12216	780	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 32.

The worst 5 of 780 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:125:TYR:HB2	1:B:133:ILE:CD1	1.65	1.25
1:D:82:ILE:HD12	1:D:97:VAL:HG11	1.20	1.17
1:A:159:GLY:HA2	1:A:164:MET:HG2	1.24	1.14
1:B:159:GLY:HA2	1:B:164:MET:HG2	1.26	1.12
1:E:159:GLY:HA2	1:E:164:MET:HG2	1.26	1.12

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	257/270 (95%)	242 (94%)	15 (6%)	0	100	100
1	B	266/270 (98%)	243 (91%)	22 (8%)	1 (0%)	34	42
1	C	267/270 (99%)	230 (86%)	32 (12%)	5 (2%)	8	7
1	D	266/270 (98%)	239 (90%)	26 (10%)	1 (0%)	34	42
1	E	256/270 (95%)	228 (89%)	25 (10%)	3 (1%)	13	14
1	F	267/270 (99%)	254 (95%)	12 (4%)	1 (0%)	34	42
All	All	1579/1620 (98%)	1436 (91%)	132 (8%)	11 (1%)	22	26

5 of 11 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	210	GLU
1	D	13	ARG
1	E	268	ILE
1	C	164	MET
1	E	121	ALA

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	208/219 (95%)	195 (94%)	13 (6%)	18	24
1	B	213/219 (97%)	193 (91%)	20 (9%)	8	10
1	C	216/219 (99%)	192 (89%)	24 (11%)	6	7
1	D	213/219 (97%)	196 (92%)	17 (8%)	12	15
1	E	208/219 (95%)	185 (89%)	23 (11%)	6	7
1	F	216/219 (99%)	194 (90%)	22 (10%)	7	8
All	All	1274/1314 (97%)	1155 (91%)	119 (9%)	9	10

5 of 119 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	9	ASP
1	F	143	LEU
1	D	233	LEU
1	F	141	ILE
1	F	256	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 17 such sidechains are listed below:

Mol	Chain	Res	Type
1	F	40	ASN
1	F	253	HIS
1	B	253	HIS
1	C	197	ASN
1	D	197	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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 53 ligands modelled in this entry, 53 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	259/270 (95%)	-0.65	0 100 100	5, 23, 43, 65	0
1	B	268/270 (99%)	-0.64	0 100 100	10, 29, 53, 76	0
1	C	269/270 (99%)	-0.08	5 (1%) 66 73	22, 45, 69, 83	0
1	D	268/270 (99%)	-0.61	1 (0%) 92 95	14, 29, 48, 72	0
1	E	258/270 (95%)	-0.46	2 (0%) 86 89	20, 39, 59, 84	0
1	F	269/270 (99%)	-0.66	0 100 100	9, 26, 43, 52	0
All	All	1591/1620 (98%)	-0.52	8 (0%) 91 94	5, 32, 58, 84	0

The worst 5 of 8 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	99	LEU	3.1
1	C	76	LEU	3.1
1	C	92	LEU	3.0
1	E	13	ARG	3.0
1	C	95	PHE	2.7

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 monosaccharides 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, 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
2	ZN	F	308	1/1	0.59	0.24	106,106,106,106	0
2	ZN	E	306	1/1	0.65	0.13	141,141,141,141	0
2	ZN	A	308	1/1	0.73	0.18	164,164,164,164	0
2	ZN	C	301	1/1	0.80	0.08	103,103,103,103	0
2	ZN	F	307	1/1	0.84	0.07	100,100,100,100	0
2	ZN	E	311	1/1	0.85	0.07	128,128,128,128	0
2	ZN	C	307	1/1	0.86	0.12	124,124,124,124	0
2	ZN	B	309	1/1	0.86	0.07	137,137,137,137	0
2	ZN	E	310	1/1	0.86	0.20	109,109,109,109	0
2	ZN	F	301	1/1	0.87	0.05	87,87,87,87	0
2	ZN	B	310	1/1	0.88	0.07	136,136,136,136	0
2	ZN	B	308	1/1	0.89	0.07	133,133,133,133	0
2	ZN	D	306	1/1	0.90	0.07	122,122,122,122	0
2	ZN	F	302	1/1	0.90	0.07	104,104,104,104	0
2	ZN	D	307	1/1	0.90	0.08	124,124,124,124	0
2	ZN	E	304	1/1	0.90	0.07	73,73,73,73	0
2	ZN	B	311	1/1	0.93	0.18	125,125,125,125	0
2	ZN	E	308	1/1	0.93	0.06	110,110,110,110	0
2	ZN	B	307	1/1	0.93	0.08	67,67,67,67	0
2	ZN	B	305	1/1	0.93	0.03	89,89,89,89	0
2	ZN	D	301	1/1	0.94	0.04	83,83,83,83	0
2	ZN	C	306	1/1	0.94	0.11	89,89,89,89	0
2	ZN	A	307	1/1	0.94	0.23	96,96,96,96	0
2	ZN	D	303	1/1	0.95	0.05	69,69,69,69	0
2	ZN	E	307	1/1	0.95	0.06	104,104,104,104	0
2	ZN	C	308	1/1	0.95	0.05	132,132,132,132	0
2	ZN	C	304	1/1	0.96	0.14	72,72,72,72	0
2	ZN	F	306	1/1	0.96	0.07	62,62,62,62	0
2	ZN	B	302	1/1	0.96	0.11	58,58,58,58	0
2	ZN	E	309	1/1	0.96	0.10	75,75,75,75	0
2	ZN	A	306	1/1	0.97	0.05	44,44,44,44	0
2	ZN	C	302	1/1	0.98	0.10	51,51,51,51	0
2	ZN	E	302	1/1	0.98	0.05	47,47,47,47	0
2	ZN	E	303	1/1	0.98	0.06	66,66,66,66	0
2	ZN	D	305	1/1	0.98	0.10	39,39,39,39	0
2	ZN	B	304	1/1	0.98	0.09	67,67,67,67	0
2	ZN	C	305	1/1	0.99	0.07	54,54,54,54	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	ZN	A	302	1/1	0.99	0.11	45,45,45,45	0
2	ZN	E	305	1/1	0.99	0.06	46,46,46,46	0
2	ZN	A	303	1/1	0.99	0.08	30,30,30,30	0
2	ZN	B	301	1/1	0.99	0.07	39,39,39,39	0
2	ZN	A	304	1/1	0.99	0.12	68,68,68,68	0
2	ZN	D	302	1/1	0.99	0.04	35,35,35,35	0
2	ZN	B	303	1/1	0.99	0.08	47,47,47,47	0
2	ZN	D	304	1/1	0.99	0.09	34,34,34,34	0
2	ZN	A	305	1/1	0.99	0.07	52,52,52,52	0
2	ZN	A	301	1/1	0.99	0.06	30,30,30,30	0
2	ZN	F	303	1/1	0.99	0.06	40,40,40,40	0
2	ZN	C	303	1/1	0.99	0.12	49,49,49,49	0
2	ZN	E	301	1/1	0.99	0.11	46,46,46,46	0
2	ZN	B	306	1/1	0.99	0.03	55,55,55,55	0
2	ZN	F	305	1/1	1.00	0.07	32,32,32,32	0
2	ZN	F	304	1/1	1.00	0.08	30,30,30,30	0

6.5 Other polymers [i](#)

There are no such residues in this entry.