



Full wwPDB X-ray Structure Validation Report ⓘ

May 29, 2020 – 07:29 am BST

PDB ID : 5LB8
Title : Crystal structure of human RECQL5 helicase APO form.
Authors : Newman, J.A.; Aitkenhead, H.; Savitsky, P.; Krojer, T.; von Delft, F.; Arrow-smith, C.H.; Edwards, A.M.; Bountra, C.; Gileadi, O.; Structural Genomics Consortium (SGC)
Deposited on : 2016-06-15
Resolution : 3.40 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 ⓘ](#)) 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

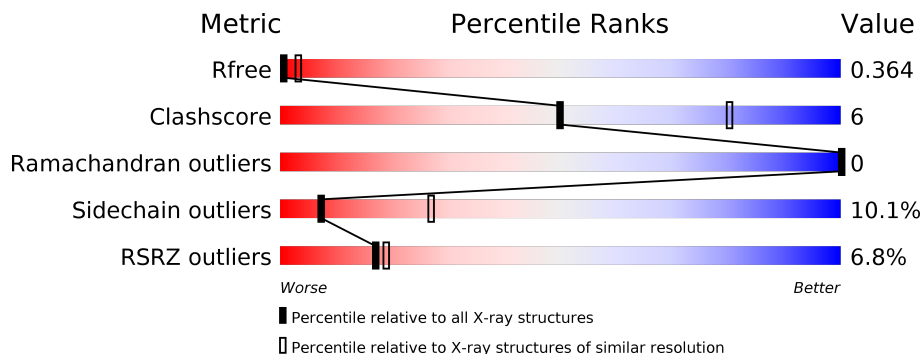
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.40 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	1026 (3.48-3.32)
Clashscore	141614	1055 (3.48-3.32)
Ramachandran outliers	138981	1038 (3.48-3.32)
Sidechain outliers	138945	1038 (3.48-3.32)
RSRZ outliers	127900	2173 (3.50-3.30)

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 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 $\leq 5\%$. 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	518	 6% 63% 18% • 18%
1	D	518	 5% 65% 17% • 18%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 6566 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 ATP-dependent DNA helicase Q5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	427	3266	2070	572	602	22	0	0	0
1	D	426	3298	2087	584	605	22	0	0	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	9	SER	-	expression tag	UNP O94762
A	10	MET	-	expression tag	UNP O94762
D	9	SER	-	expression tag	UNP O94762
D	10	MET	-	expression tag	UNP O94762

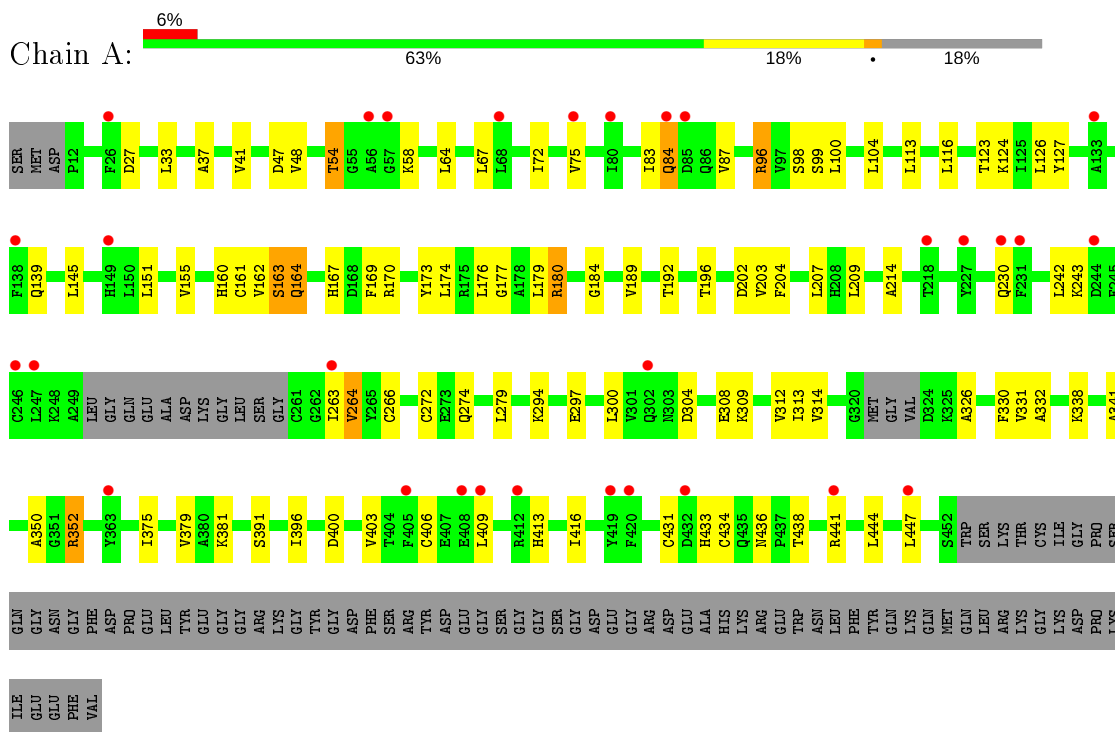
- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Zn	0	0
			1	1		
2	D	1	Total	Zn	0	0
			1	1		

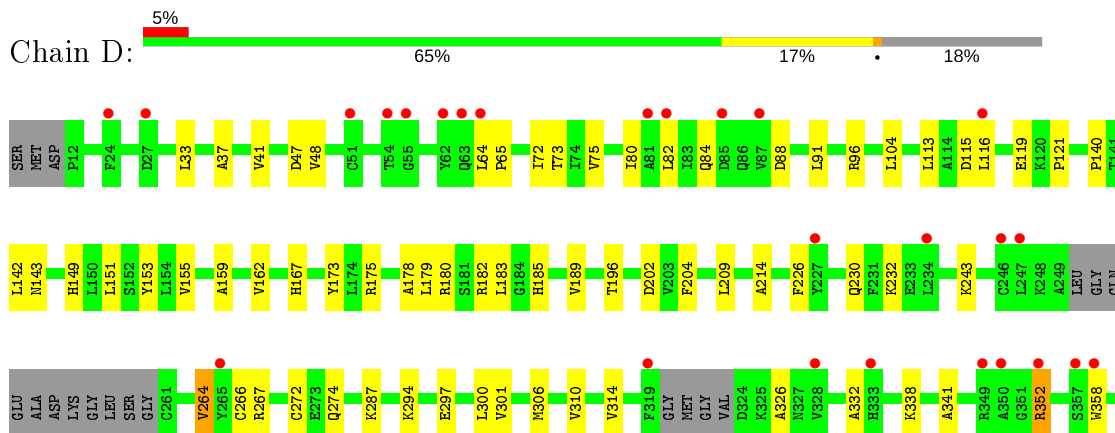
3 Residue-property plots i

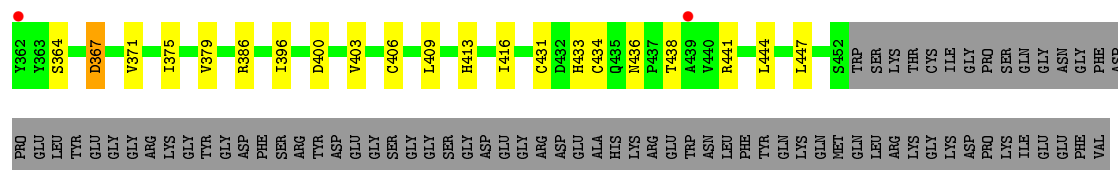
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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: ATP-dependent DNA helicase Q5



• Molecule 1: ATP-dependent DNA helicase Q5





4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α , β , γ	68.74Å 68.74Å 396.31Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.61 – 3.40 48.61 – 3.40	Depositor EDS
% Data completeness (in resolution range)	99.8 (48.61-3.40) 99.8 (48.61-3.40)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.04 (at 3.40Å)	Xtrriage
Refinement program	BUSTER 2.10.2	Depositor
R, R_{free}	0.301 , 0.322 0.317 , 0.364	Depositor DCC
R_{free} test set	684 reflections (4.87%)	wwPDB-VP
Wilson B-factor (Å ²)	139.0	Xtrriage
Anisotropy	0.065	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 118.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	6566	wwPDB-VP
Average B, all atoms (Å ²)	145.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.46% 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	0.45	0/3330	0.63	0/4513
1	D	0.40	0/3362	0.61	0/4550
All	All	0.43	0/6692	0.62	0/9063

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	3266	0	3229	43	0
1	D	3298	0	3290	34	0
2	A	1	0	0	0	0
2	D	1	0	0	0	0
All	All	6566	0	6519	76	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 (76) 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:162:VAL:CG1	1:A:173:TYR:HB3	2.09	0.81
1:A:162:VAL:HG13	1:A:173:TYR:HB3	1.62	0.81
1:A:75:VAL:HA	1:A:155:VAL:HB	1.78	0.66
1:A:54:THR:HA	1:A:58:LYS:HD3	1.80	0.63
1:A:163:SER:O	1:A:169:PHE:HD1	1.80	0.63
1:D:287:LYS:HD2	1:D:301:VAL:HG11	1.82	0.62
1:A:174:LEU:HD22	1:D:175:ARG:HE	1.65	0.62
1:D:48:VAL:HG12	1:D:214:ALA:HB3	1.84	0.59
1:A:48:VAL:HG12	1:A:214:ALA:HB3	1.84	0.59
1:D:149:HIS:HA	1:D:185:HIS:NE2	2.18	0.59
1:D:142:LEU:HD21	1:D:183:LEU:HD11	1.85	0.58
1:A:162:VAL:HG12	1:A:173:TYR:HB3	1.85	0.58
1:A:438:THR:HG22	1:A:441:ARG:HH21	1.71	0.56
1:D:326:ALA:HA	1:D:352:ARG:HB2	1.88	0.56
1:A:326:ALA:HA	1:A:352:ARG:HB2	1.88	0.55
1:A:84:GLN:HA	1:A:87:VAL:HG22	1.89	0.54
1:D:438:THR:HG22	1:D:441:ARG:HH21	1.72	0.54
1:A:116:LEU:HB3	1:A:145:LEU:HD11	1.89	0.53
1:D:75:VAL:HA	1:D:155:VAL:HB	1.90	0.53
1:A:160:HIS:ND1	1:A:192:THR:OG1	2.34	0.53
1:A:180:ARG:HH12	1:A:184:GLY:HA2	1.72	0.53
1:D:364:SER:HB3	1:D:367:ASP:HB2	1.89	0.53
1:A:96:ARG:HB2	1:A:123:THR:HA	1.90	0.53
1:A:163:SER:O	1:A:169:PHE:CD1	2.61	0.52
1:A:48:VAL:HG23	1:A:189:VAL:HG13	1.91	0.51
1:A:400:ASP:HA	1:A:403:VAL:HG22	1.93	0.51
1:D:48:VAL:HG23	1:D:189:VAL:HG13	1.91	0.51
1:A:164:GLN:HG2	1:A:391:SER:HB3	1.93	0.51
1:D:400:ASP:HA	1:D:403:VAL:HG22	1.93	0.51
1:D:264:VAL:HG12	1:D:332:ALA:HB3	1.94	0.50
1:D:226:PHE:HD2	1:D:358:TRP:HD1	1.59	0.50
1:A:431:CYS:HB3	1:A:434:CYS:SG	2.53	0.49
1:D:431:CYS:HB3	1:D:434:CYS:SG	2.53	0.48
1:A:413:HIS:HA	1:A:416:ILE:HD12	1.96	0.48
1:A:204:PHE:HA	1:A:209:LEU:HD12	1.97	0.47
1:D:413:HIS:HA	1:D:416:ILE:HD12	1.97	0.47
1:D:159:ALA:O	1:D:162:VAL:HG22	2.15	0.47
1:D:204:PHE:HA	1:D:209:LEU:HD12	1.96	0.46
1:A:167:HIS:HB3	1:A:341:ALA:HB3	1.98	0.46
1:D:73:THR:HG23	1:D:153:TYR:HB2	1.97	0.46
1:D:267:ARG:HE	1:D:371:VAL:HG22	1.80	0.46
1:D:178:ALA:O	1:D:182:ARG:HB2	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:88:ASP:HA	1:D:91:LEU:HD12	1.97	0.46
1:A:87:VAL:HG11	1:A:99:SER:HB3	1.99	0.45
1:D:115:ASP:O	1:D:121:PRO:HB3	2.17	0.45
1:A:177:GLY:HA2	1:A:207:LEU:HA	1.98	0.45
1:D:64:LEU:HB3	1:D:65:PRO:HD3	1.99	0.45
1:D:167:HIS:HB3	1:D:341:ALA:HB3	1.99	0.44
1:A:96:ARG:HG2	1:A:96:ARG:H	1.59	0.44
1:D:113:LEU:HA	1:D:116:LEU:HD12	2.00	0.44
1:A:161:CYS:HB3	1:A:170:ARG:HG3	1.99	0.43
1:A:331:VAL:HG23	1:A:350:ALA:HB2	1.99	0.43
1:A:338:LYS:HG3	1:A:375:ILE:HD11	1.99	0.43
1:A:173:TYR:HA	1:A:176:LEU:HD12	2.00	0.43
1:A:41:VAL:HG22	1:A:48:VAL:HG21	1.99	0.43
1:D:338:LYS:HG3	1:D:375:ILE:HD12	2.00	0.43
1:A:98:SER:HB3	1:A:123:THR:HG21	2.00	0.43
1:A:312:VAL:HG22	1:A:330:PHE:HZ	1.82	0.43
1:A:37:ALA:O	1:A:41:VAL:HG23	2.19	0.43
1:D:41:VAL:HG22	1:D:48:VAL:HG21	2.01	0.43
1:A:264:VAL:HG12	1:A:332:ALA:HB3	2.00	0.42
1:A:67:LEU:HD23	1:A:124:LYS:HG2	2.01	0.42
1:A:72:ILE:HG22	1:A:124:LYS:HA	2.01	0.42
1:A:242:LEU:HD23	1:A:279:LEU:HD21	2.00	0.42
1:D:266:CYS:SG	1:D:272:CYS:HB3	2.60	0.42
1:D:379:VAL:HG11	1:D:396:ILE:HD11	2.02	0.42
1:D:162:VAL:HG13	1:D:173:TYR:HD2	1.84	0.41
1:A:263:ILE:HG23	1:A:313:ILE:HG23	2.03	0.41
1:A:266:CYS:SG	1:A:272:CYS:HB3	2.61	0.41
1:D:287:LYS:HB2	1:D:310:VAL:HG11	2.03	0.41
1:D:37:ALA:O	1:D:41:VAL:HG23	2.20	0.41
1:A:379:VAL:HG11	1:A:396:ILE:HD11	2.03	0.41
1:A:83:ILE:HG12	1:A:127:TYR:HD1	1.85	0.40
1:D:140:PRO:HA	1:D:143:ASN:HD22	1.86	0.40
1:A:203:VAL:HG13	1:A:207:LEU:HD12	2.03	0.40
1:D:232:LYS:HB2	1:D:364:SER:HB2	2.03	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	421/518 (81%)	394 (94%)	27 (6%)	0	100	100
1	D	420/518 (81%)	390 (93%)	30 (7%)	0	100	100
All	All	841/1036 (81%)	784 (93%)	57 (7%)	0	100	100

There are no Ramachandran outliers to report.

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	344/432 (80%)	306 (89%)	38 (11%)	6	23
1	D	351/432 (81%)	319 (91%)	32 (9%)	9	32
All	All	695/864 (80%)	625 (90%)	70 (10%)	7	27

All (70) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	27	ASP
1	A	33	LEU
1	A	47	ASP
1	A	54	THR
1	A	64	LEU
1	A	84	GLN
1	A	96	ARG
1	A	100	LEU

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Mol	Chain	Res	Type
1	A	104	LEU
1	A	113	LEU
1	A	126	LEU
1	A	139	GLN
1	A	151	LEU
1	A	163	SER
1	A	164	GLN
1	A	179	LEU
1	A	180	ARG
1	A	196	THR
1	A	202	ASP
1	A	230	GLN
1	A	243	LYS
1	A	264	VAL
1	A	274	GLN
1	A	294	LYS
1	A	297	GLU
1	A	300	LEU
1	A	304	ASP
1	A	308	GLU
1	A	309	LYS
1	A	314	VAL
1	A	352	ARG
1	A	381	LYS
1	A	406	CYS
1	A	409	LEU
1	A	433	HIS
1	A	436	ASN
1	A	444	LEU
1	A	447	LEU
1	D	33	LEU
1	D	47	ASP
1	D	72	ILE
1	D	80	ILE
1	D	82	LEU
1	D	84	GLN
1	D	96	ARG
1	D	104	LEU
1	D	119	GLU
1	D	151	LEU
1	D	179	LEU
1	D	180	ARG

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Mol	Chain	Res	Type
1	D	196	THR
1	D	202	ASP
1	D	230	GLN
1	D	243	LYS
1	D	264	VAL
1	D	274	GLN
1	D	294	LYS
1	D	297	GLU
1	D	300	LEU
1	D	306	MET
1	D	314	VAL
1	D	352	ARG
1	D	367	ASP
1	D	386	ARG
1	D	406	CYS
1	D	409	LEU
1	D	433	HIS
1	D	436	ASN
1	D	444	LEU
1	D	447	LEU

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

Mol	Chain	Res	Type
1	A	143	ASN
1	A	164	GLN
1	D	143	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 2 ligands modelled in this entry, 2 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

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, 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	427/518 (82%)	0.45	30 (7%) 16 18	83, 141, 176, 189	0
1	D	426/518 (82%)	0.43	28 (6%) 18 20	115, 149, 179, 199	0
All	All	853/1036 (82%)	0.44	58 (6%) 17 19	83, 146, 178, 199	0

All (58) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	350	ALA	5.7
1	A	246	CYS	5.6
1	D	357	SER	5.2
1	D	85	ASP	5.1
1	D	82	LEU	4.9
1	A	432	ASP	4.8
1	D	55	GLY	4.7
1	A	302	GLN	4.6
1	A	247	LEU	4.5
1	D	358	TRP	4.2
1	A	227	TYR	4.1
1	D	54	THR	4.0
1	D	87	VAL	3.9
1	D	349	ARG	3.9
1	D	352	ARG	3.5
1	A	133	ALA	3.4
1	D	81	ALA	3.4
1	D	246	CYS	3.2
1	A	409	LEU	3.2
1	D	265	TYR	3.2
1	A	56	ALA	3.2
1	A	441	ARG	3.1
1	A	80	ILE	3.1
1	D	227	TYR	3.0

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Mol	Chain	Res	Type	RSRZ
1	D	116	LEU	3.0
1	A	244	ASP	3.0
1	A	84	GLN	3.0
1	D	234	LEU	2.9
1	D	51	CYS	2.8
1	D	64	LEU	2.8
1	A	85	ASP	2.7
1	A	231	PHE	2.7
1	D	319	PHE	2.6
1	D	328	VAL	2.6
1	A	263	ILE	2.6
1	D	27	ASP	2.5
1	A	420	PHE	2.5
1	D	24	PHE	2.5
1	A	75	VAL	2.5
1	D	247	LEU	2.4
1	A	405	PHE	2.4
1	D	63	GLN	2.4
1	A	447	LEU	2.4
1	A	419	TYR	2.3
1	D	333	HIS	2.3
1	A	68	LEU	2.3
1	D	62	TYR	2.3
1	A	26	PHE	2.3
1	A	412	ARG	2.3
1	A	57	GLY	2.2
1	D	362	TYR	2.2
1	A	149	HIS	2.2
1	A	363	TYR	2.1
1	A	218	THR	2.1
1	A	408	GLU	2.1
1	A	230	GLN	2.1
1	A	138	PHE	2.1
1	D	439	ALA	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, 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	A	601	1/1	0.88	0.17	166,166,166,166	0
2	ZN	D	601	1/1	0.90	0.11	132,132,132,132	0

6.5 Other polymers [i](#)

There are no such residues in this entry.