



wwPDB X-ray Structure Validation Summary Report ⓘ

Nov 16, 2021 – 12:05 PM EST

PDB ID : 7LU6
Title : Crystal structure of the mouse Kirrel3 D1 homodimer
Authors : Roman, C.A.; Pak, J.S.; Wang, J.; Ozkan, E.
Deposited on : 2021-02-21
Resolution : 1.95 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 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	:	2.23.2
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)	:	2.23.2

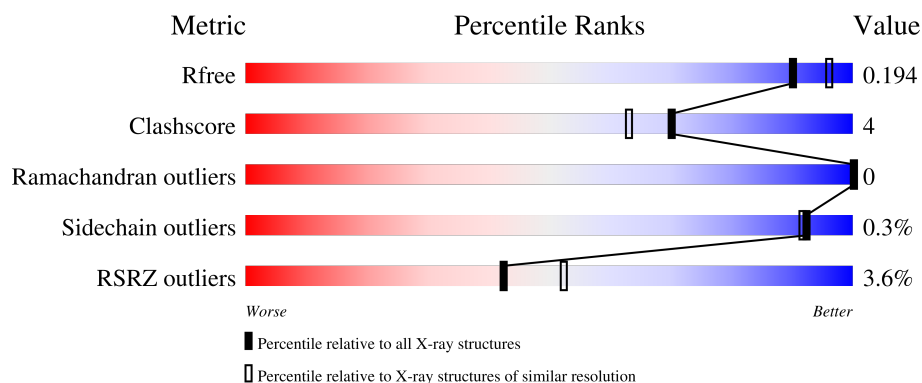
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.95 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	2580 (1.96-1.96)
Clashscore	141614	2705 (1.96-1.96)
Ramachandran outliers	138981	2678 (1.96-1.96)
Sidechain outliers	138945	2678 (1.96-1.96)
RSRZ outliers	127900	2539 (1.96-1.96)

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	109	
1	B	109	
1	C	109	
1	D	109	
1	E	109	

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Mol	Chain	Length	Quality of chain
1	F	109	<div><div></div><div>10%</div><div>78%</div><div>14%</div><div>8%</div></div>
1	G	109	<div><div></div><div>7%</div><div>88%</div><div></div><div>8%</div></div>
1	H	109	<div><div></div><div>5%</div><div>83%</div><div>8%</div><div>9%</div></div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 6752 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 Kin of IRRE-like protein 3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	102	Total	C	N	O	S	0	5	0
			828	529	145	151	3			
1	B	101	Total	C	N	O	S	0	3	0
			802	515	138	146	3			
1	C	102	Total	C	N	O	S	0	4	0
			821	525	143	150	3			
1	D	100	Total	C	N	O	S	0	3	0
			812	517	144	148	3			
1	E	100	Total	C	N	O	S	0	2	0
			792	506	138	145	3			
1	F	100	Total	C	N	O	S	0	3	0
			800	511	138	148	3			
1	G	100	Total	C	N	O	S	0	1	0
			776	496	132	145	3			
1	H	99	Total	C	N	O	S	0	1	0
			777	496	134	144	3			

There are 72 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	44	ALA	-	expression tag	UNP Q8BR86
A	45	ASP	-	expression tag	UNP Q8BR86
A	46	PRO	-	expression tag	UNP Q8BR86
A	147	HIS	-	expression tag	UNP Q8BR86
A	148	HIS	-	expression tag	UNP Q8BR86
A	149	HIS	-	expression tag	UNP Q8BR86
A	150	HIS	-	expression tag	UNP Q8BR86
A	151	HIS	-	expression tag	UNP Q8BR86
A	152	HIS	-	expression tag	UNP Q8BR86
B	44	ALA	-	expression tag	UNP Q8BR86
B	45	ASP	-	expression tag	UNP Q8BR86
B	46	PRO	-	expression tag	UNP Q8BR86
B	147	HIS	-	expression tag	UNP Q8BR86

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Chain	Residue	Modelled	Actual	Comment	Reference
B	148	HIS	-	expression tag	UNP Q8BR86
B	149	HIS	-	expression tag	UNP Q8BR86
B	150	HIS	-	expression tag	UNP Q8BR86
B	151	HIS	-	expression tag	UNP Q8BR86
B	152	HIS	-	expression tag	UNP Q8BR86
C	44	ALA	-	expression tag	UNP Q8BR86
C	45	ASP	-	expression tag	UNP Q8BR86
C	46	PRO	-	expression tag	UNP Q8BR86
C	147	HIS	-	expression tag	UNP Q8BR86
C	148	HIS	-	expression tag	UNP Q8BR86
C	149	HIS	-	expression tag	UNP Q8BR86
C	150	HIS	-	expression tag	UNP Q8BR86
C	151	HIS	-	expression tag	UNP Q8BR86
C	152	HIS	-	expression tag	UNP Q8BR86
D	44	ALA	-	expression tag	UNP Q8BR86
D	45	ASP	-	expression tag	UNP Q8BR86
D	46	PRO	-	expression tag	UNP Q8BR86
D	147	HIS	-	expression tag	UNP Q8BR86
D	148	HIS	-	expression tag	UNP Q8BR86
D	149	HIS	-	expression tag	UNP Q8BR86
D	150	HIS	-	expression tag	UNP Q8BR86
D	151	HIS	-	expression tag	UNP Q8BR86
D	152	HIS	-	expression tag	UNP Q8BR86
E	44	ALA	-	expression tag	UNP Q8BR86
E	45	ASP	-	expression tag	UNP Q8BR86
E	46	PRO	-	expression tag	UNP Q8BR86
E	147	HIS	-	expression tag	UNP Q8BR86
E	148	HIS	-	expression tag	UNP Q8BR86
E	149	HIS	-	expression tag	UNP Q8BR86
E	150	HIS	-	expression tag	UNP Q8BR86
E	151	HIS	-	expression tag	UNP Q8BR86
E	152	HIS	-	expression tag	UNP Q8BR86
F	44	ALA	-	expression tag	UNP Q8BR86
F	45	ASP	-	expression tag	UNP Q8BR86
F	46	PRO	-	expression tag	UNP Q8BR86
F	147	HIS	-	expression tag	UNP Q8BR86
F	148	HIS	-	expression tag	UNP Q8BR86
F	149	HIS	-	expression tag	UNP Q8BR86
F	150	HIS	-	expression tag	UNP Q8BR86
F	151	HIS	-	expression tag	UNP Q8BR86
F	152	HIS	-	expression tag	UNP Q8BR86
G	44	ALA	-	expression tag	UNP Q8BR86

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Chain	Residue	Modelled	Actual	Comment	Reference
G	45	ASP	-	expression tag	UNP Q8BR86
G	46	PRO	-	expression tag	UNP Q8BR86
G	147	HIS	-	expression tag	UNP Q8BR86
G	148	HIS	-	expression tag	UNP Q8BR86
G	149	HIS	-	expression tag	UNP Q8BR86
G	150	HIS	-	expression tag	UNP Q8BR86
G	151	HIS	-	expression tag	UNP Q8BR86
G	152	HIS	-	expression tag	UNP Q8BR86
H	44	ALA	-	expression tag	UNP Q8BR86
H	45	ASP	-	expression tag	UNP Q8BR86
H	46	PRO	-	expression tag	UNP Q8BR86
H	147	HIS	-	expression tag	UNP Q8BR86
H	148	HIS	-	expression tag	UNP Q8BR86
H	149	HIS	-	expression tag	UNP Q8BR86
H	150	HIS	-	expression tag	UNP Q8BR86
H	151	HIS	-	expression tag	UNP Q8BR86
H	152	HIS	-	expression tag	UNP Q8BR86

- Molecule 2 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Na 1 1	0	0
2	B	1	Total Na 1 1	0	0
2	C	1	Total Na 1 1	0	0
2	D	1	Total Na 1 1	0	0
2	E	1	Total Na 1 1	0	0
2	F	1	Total Na 1 1	0	0
2	G	1	Total Na 1 1	0	0
2	H	1	Total Na 1 1	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	80	Total O 80 80	0	0

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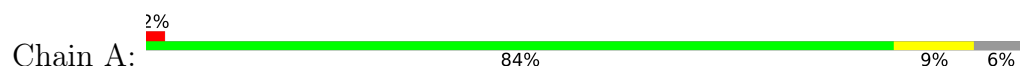
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	61	Total 61	O 61	0	0
3	C	64	Total 64	O 64	0	0
3	D	79	Total 79	O 79	0	0
3	E	19	Total 19	O 19	0	0
3	F	10	Total 10	O 10	0	0
3	G	8	Total 8	O 8	0	0
3	H	15	Total 15	O 15	0	0

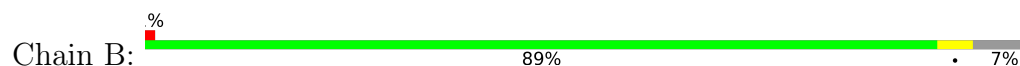
3 Residue-property plots [i](#)

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.

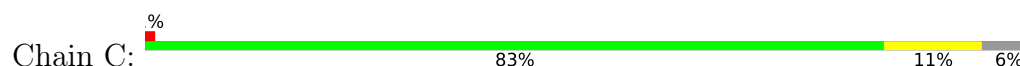
- Molecule 1: Kin of IRRE-like protein 3



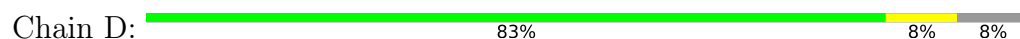
- Molecule 1: Kin of IRRE-like protein 3



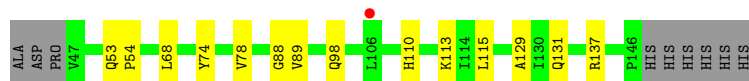
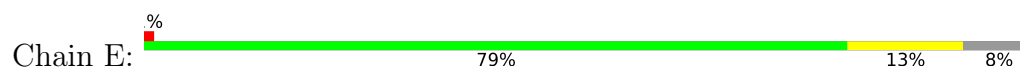
- Molecule 1: Kin of IRRE-like protein 3



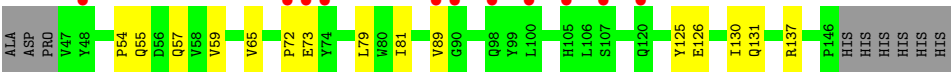
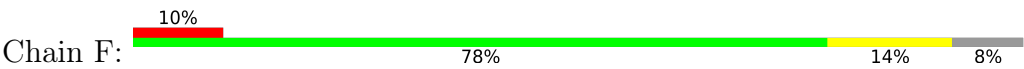
- Molecule 1: Kin of IRRE-like protein 3



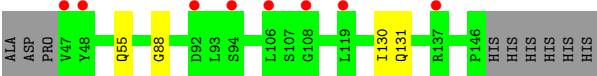
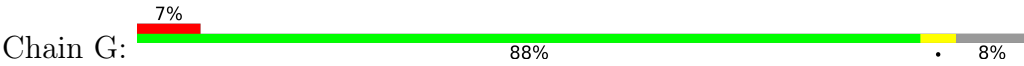
- Molecule 1: Kin of IRRE-like protein 3



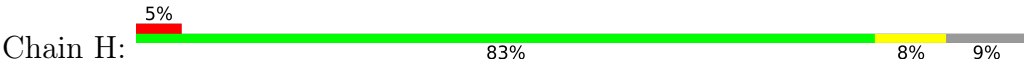
- Molecule 1: Kin of IRRE-like protein 3



● Molecule 1: Kin of IRRE-like protein 3



● Molecule 1: Kin of IRRE-like protein 3



4 Data and refinement statistics

Property	Value	Source
Space group	P 63	Depositor
Cell constants a, b, c, α , β , γ	63.24Å 63.24Å 347.81Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	49.52 – 1.95 49.52 – 1.95	Depositor EDS
% Data completeness (in resolution range)	99.8 (49.52-1.95) 99.8 (49.52-1.95)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	0.11	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.30 (at 1.95Å)	Xtriage
Refinement program	PHENIX 1.19.1_4122	Depositor
R, R_{free}	0.160 , 0.195 0.160 , 0.194	Depositor DCC
R_{free} test set	2846 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	23.2	Xtriage
Anisotropy	0.368	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 33.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	0.328 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	6752	wwPDB-VP
Average B, all atoms (Å ²)	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.34% 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:
NA

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	0.36	0/855	0.59	0/1167
1	B	0.34	0/827	0.57	0/1129
1	C	0.32	0/846	0.55	0/1156
1	D	0.36	0/832	0.58	0/1135
1	E	0.31	0/812	0.54	0/1108
1	F	0.30	0/817	0.54	0/1115
1	G	0.29	0/793	0.51	0/1083
1	H	0.28	0/794	0.52	0/1083
All	All	0.32	0/6576	0.55	0/8976

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	828	0	833	5	0
1	B	802	0	803	3	0
1	C	821	0	819	7	1
1	D	812	0	813	6	0
1	E	792	0	792	10	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	F	800	0	794	12	0
1	G	776	0	761	4	0
1	H	777	0	770	8	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
2	E	1	0	0	0	0
2	F	1	0	0	0	0
2	G	1	0	0	0	0
2	H	1	0	0	0	0
3	A	80	0	0	1	0
3	B	61	0	0	1	0
3	C	64	0	0	2	1
3	D	79	0	0	1	1
3	E	19	0	0	0	0
3	F	10	0	0	0	0
3	G	8	0	0	0	0
3	H	15	0	0	1	1
All	All	6752	0	6385	46	3

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 4.

The worst 5 of 46 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:H:57:GLN:NE2	3:H:1101:HOH:O	2.25	0.70
1:C:105[B]:HIS:ND1	3:C:1102:HOH:O	2.28	0.66
1:H:55:GLN:HA	1:H:137:ARG:NH1	2.16	0.58
1:F:81:ILE:HB	1:F:126:GLU:HG2	1.86	0.57
1:F:59:VAL:HG11	1:F:65[B]:VAL:HG22	1.86	0.57

All (3) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:1157:HOH:O	3:H:1114:HOH:O[5_554]	2.08	0.12
1:C:45:ASP:OD1	1:C:120:GLN:NE2[2_555]	2.18	0.02
3:D:1121:HOH:O	3:D:1122:HOH:O[3_565]	2.19	0.01

5.3 Torsion angles

5.3.1 Protein backbone

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	105/109 (96%)	100 (95%)	5 (5%)	0	100	100
1	B	102/109 (94%)	98 (96%)	4 (4%)	0	100	100
1	C	104/109 (95%)	101 (97%)	3 (3%)	0	100	100
1	D	102/109 (94%)	99 (97%)	3 (3%)	0	100	100
1	E	100/109 (92%)	96 (96%)	4 (4%)	0	100	100
1	F	101/109 (93%)	96 (95%)	5 (5%)	0	100	100
1	G	99/109 (91%)	96 (97%)	3 (3%)	0	100	100
1	H	98/109 (90%)	95 (97%)	3 (3%)	0	100	100
All	All	811/872 (93%)	781 (96%)	30 (4%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains

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	92/93 (99%)	90 (98%)	2 (2%)	52	44
1	B	89/93 (96%)	89 (100%)	0	100	100
1	C	91/93 (98%)	91 (100%)	0	100	100
1	D	89/93 (96%)	88 (99%)	1 (1%)	73	71
1	E	87/93 (94%)	87 (100%)	0	100	100
1	F	88/93 (95%)	88 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	G	84/93 (90%)	84 (100%)	0	100	100
1	H	85/93 (91%)	85 (100%)	0	100	100
All	All	705/744 (95%)	702 (100%)	3 (0%)	92	90

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	91[A]	ARG
1	A	91[B]	ARG
1	D	120	GLN

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

Mol	Chain	Res	Type
1	D	110	HIS
1	E	105	HIS
1	E	110	HIS

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 8 ligands modelled in this entry, 8 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 ⓘ

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 [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	102/109 (93%)	-0.11	2 (1%) 65 73	11, 17, 36, 53	0
1	B	101/109 (92%)	-0.18	1 (0%) 82 87	13, 21, 39, 55	0
1	C	102/109 (93%)	-0.16	1 (0%) 82 87	14, 25, 44, 61	0
1	D	100/109 (91%)	-0.28	0 100 100	12, 20, 33, 44	0
1	E	100/109 (91%)	0.21	1 (1%) 82 87	31, 43, 57, 80	0
1	F	100/109 (91%)	0.67	11 (11%) 5 9	46, 57, 74, 95	0
1	G	100/109 (91%)	0.64	8 (8%) 12 19	43, 57, 78, 84	0
1	H	99/109 (90%)	0.38	5 (5%) 28 37	38, 52, 79, 92	0
All	All	804/872 (92%)	0.14	29 (3%) 42 52	11, 38, 68, 95	0

The worst 5 of 29 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	106	LEU	5.6
1	A	45	ASP	4.3
1	F	90	GLY	4.0
1	G	119	LEU	3.9
1	E	106	LEU	3.7

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(\AA^2)	Q<0.9
2	NA	G	1001	1/1	0.88	0.13	79,79,79,79	0
2	NA	E	1001	1/1	0.92	0.07	53,53,53,53	0
2	NA	F	1001	1/1	0.95	0.12	72,72,72,72	0
2	NA	C	1001	1/1	0.97	0.12	31,31,31,31	0
2	NA	H	1001	1/1	0.97	0.10	60,60,60,60	0
2	NA	A	1001	1/1	0.99	0.09	17,17,17,17	0
2	NA	B	1001	1/1	1.00	0.09	21,21,21,21	0
2	NA	D	1001	1/1	1.00	0.05	21,21,21,21	0

6.5 Other polymers [i](#)

There are no such residues in this entry.