wwPDB X-ray Structure Validation Summary Report (i)

Jan 2, 2024 – 11:59 am GMT

PDB ID	:	5A5H
Title	:	The crystal structure of the GST-like domains complex of EPRS C92SC105SC123S mutant-AIMP2
Authors	:	Cho, H.Y.; Kang, B.S.
Deposited on	:	2015-06-18
Resolution	:	2.32 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 (i) 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 (i)) were used in the production of this report:

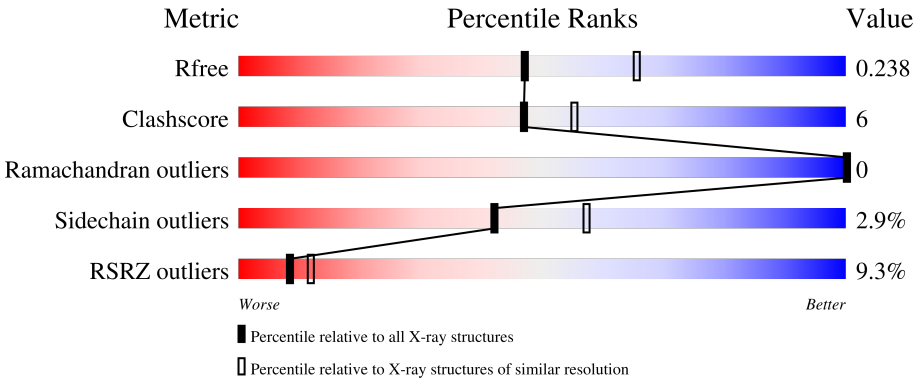
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 2.32 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	5974 (2.34-2.30)
Clashscore	141614	6604 (2.34-2.30)
Ramachandran outliers	138981	6523 (2.34-2.30)
Sidechain outliers	138945	6523 (2.34-2.30)
RSRZ outliers	127900	5855 (2.34-2.30)

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 <=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	175	2% 88% 7% • •
1	C	175	2% 89% 7% •
1	E	175	4% 91% 5% •
1	G	175	7% 86% 10% •
2	B	240	10% 74% 11% • 12%

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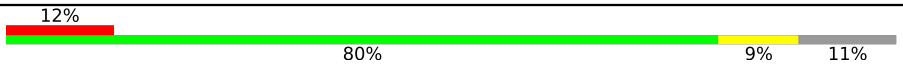
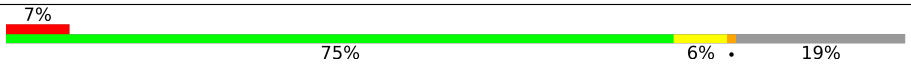
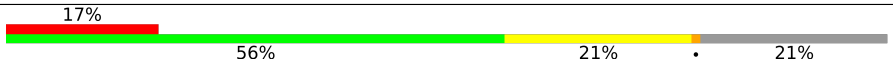
Mol	Chain	Length	Quality of chain
2	D	240	
2	F	240	
2	H	240	

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 11755 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 BIFUNCTIONAL GLUTAMATE/PROLINE--TRNA LIGASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	168	Total	C	N	O	Se	0	0	0
			1293	820	218	254	1			
1	C	168	Total	C	N	O	Se	0	0	0
			1303	827	219	256	1			
1	E	168	Total	C	N	O	Se	0	0	0
			1302	827	219	255	1			
1	G	169	Total	C	N	O	Se	0	0	0
			1308	829	220	258	1			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	92	SER	CYS	engineered mutation	UNP P07814
A	105	SER	CYS	engineered mutation	UNP P07814
A	123	SER	CYS	engineered mutation	UNP P07814
C	92	SER	CYS	engineered mutation	UNP P07814
C	105	SER	CYS	engineered mutation	UNP P07814
C	123	SER	CYS	engineered mutation	UNP P07814
E	92	SER	CYS	engineered mutation	UNP P07814
E	105	SER	CYS	engineered mutation	UNP P07814
E	123	SER	CYS	engineered mutation	UNP P07814
G	92	SER	CYS	engineered mutation	UNP P07814
G	105	SER	CYS	engineered mutation	UNP P07814
G	123	SER	CYS	engineered mutation	UNP P07814

- Molecule 2 is a protein called AMINOACYL TRNA SYNTHASE COMPLEX-INTERACTING MULTIFUNCTIONA L PROTEIN 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	210	Total	C	N	O	S	0	0	0
			1597	1026	276	286	9			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	213	Total	C	N	O	S	0	0	0
			1607	1030	279	290	8			
2	F	195	Total	C	N	O	S	0	0	0
			1492	958	260	266	8			
2	H	189	Total	C	N	O	S	0	0	0
			1444	929	247	259	9			

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	89	MET	-	expression tag	UNP Q13155
B	321	LEU	-	expression tag	UNP Q13155
B	322	GLU	-	expression tag	UNP Q13155
B	323	HIS	-	expression tag	UNP Q13155
B	324	HIS	-	expression tag	UNP Q13155
B	325	HIS	-	expression tag	UNP Q13155
B	326	HIS	-	expression tag	UNP Q13155
B	327	HIS	-	expression tag	UNP Q13155
B	328	HIS	-	expression tag	UNP Q13155
D	89	MET	-	expression tag	UNP Q13155
D	321	LEU	-	expression tag	UNP Q13155
D	322	GLU	-	expression tag	UNP Q13155
D	323	HIS	-	expression tag	UNP Q13155
D	324	HIS	-	expression tag	UNP Q13155
D	325	HIS	-	expression tag	UNP Q13155
D	326	HIS	-	expression tag	UNP Q13155
D	327	HIS	-	expression tag	UNP Q13155
D	328	HIS	-	expression tag	UNP Q13155
F	89	MET	-	expression tag	UNP Q13155
F	321	LEU	-	expression tag	UNP Q13155
F	322	GLU	-	expression tag	UNP Q13155
F	323	HIS	-	expression tag	UNP Q13155
F	324	HIS	-	expression tag	UNP Q13155
F	325	HIS	-	expression tag	UNP Q13155
F	326	HIS	-	expression tag	UNP Q13155
F	327	HIS	-	expression tag	UNP Q13155
F	328	HIS	-	expression tag	UNP Q13155
H	89	MET	-	expression tag	UNP Q13155
H	321	LEU	-	expression tag	UNP Q13155
H	322	GLU	-	expression tag	UNP Q13155
H	323	HIS	-	expression tag	UNP Q13155
H	324	HIS	-	expression tag	UNP Q13155

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Chain	Residue	Modelled	Actual	Comment	Reference
H	325	HIS	-	expression tag	UNP Q13155
H	326	HIS	-	expression tag	UNP Q13155
H	327	HIS	-	expression tag	UNP Q13155
H	328	HIS	-	expression tag	UNP Q13155

- Molecule 3 is water.

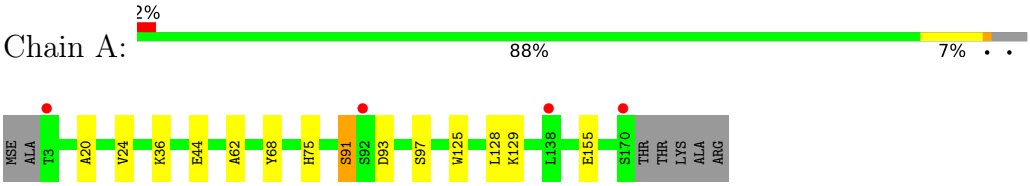
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	54	Total O 54 54	0	0
3	B	42	Total O 42 42	0	0
3	C	100	Total O 100 100	0	0
3	D	44	Total O 44 44	0	0
3	E	72	Total O 72 72	0	0
3	F	66	Total O 66 66	0	0
3	G	26	Total O 26 26	0	0
3	H	5	Total O 5 5	0	0

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.

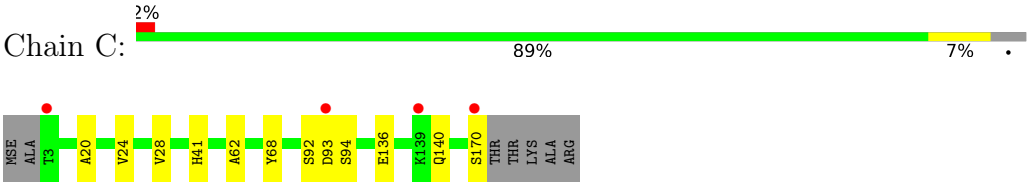
• Molecule 1: BIFUNCTIONAL GLUTAMATE/PROLINE--TRNA LIGASE

Chain A:



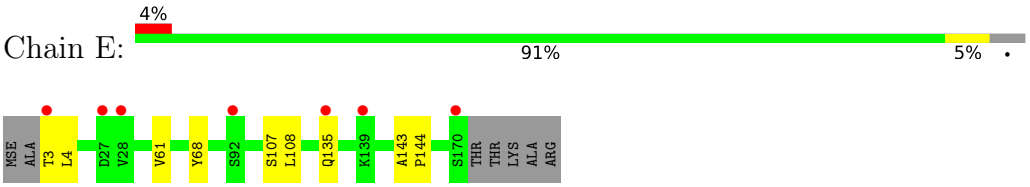
• Molecule 1: BIFUNCTIONAL GLUTAMATE/PROLINE--TRNA LIGASE

Chain C:



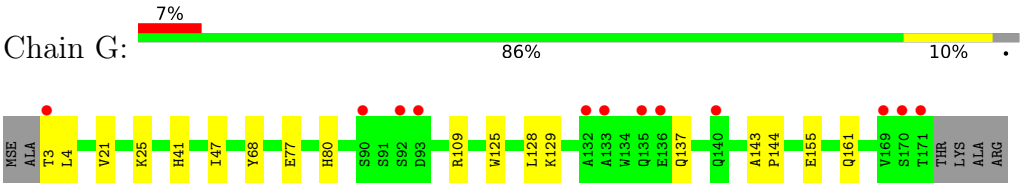
• Molecule 1: BIFUNCTIONAL GLUTAMATE/PROLINE--TRNA LIGASE

Chain E:



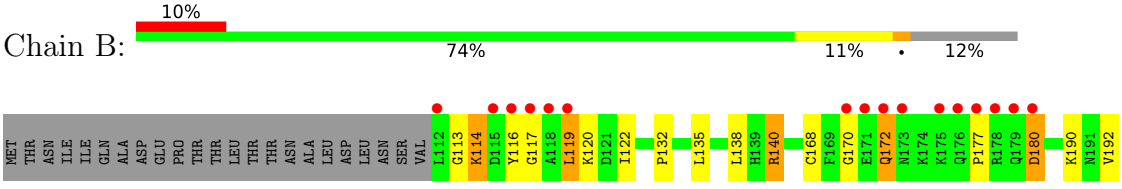
• Molecule 1: BIFUNCTIONAL GLUTAMATE/PROLINE--TRNA LIGASE

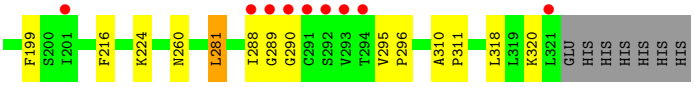
Chain G:



• Molecule 2: AMINOACYL TRNA SYNTHASE COMPLEX-INTERACTING MULTIFUNCTIONA L PROTEIN 2

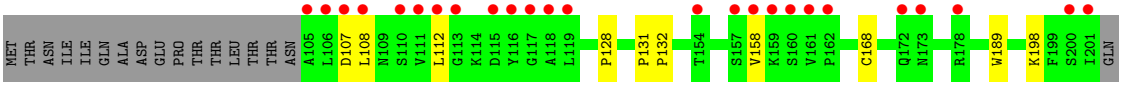
Chain B:

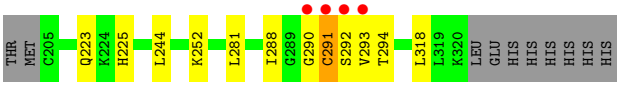




• Molecule 2: AMINOACYL TRNA SYNTHASE COMPLEX-INTERACTING MULTIFUNCTIONA L PROTEIN 2

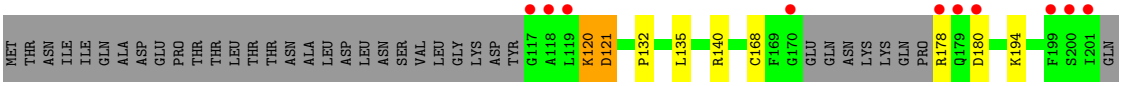
Chain D:

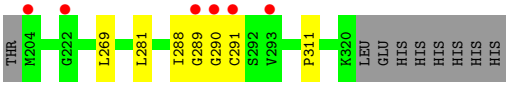




• Molecule 2: AMINOACYL TRNA SYNTHASE COMPLEX-INTERACTING MULTIFUNCTIONA L PROTEIN 2

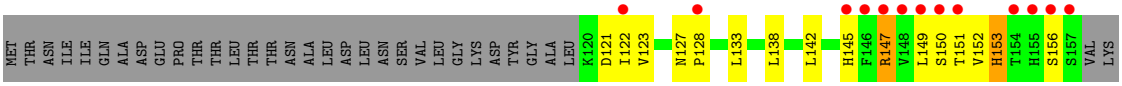
Chain F:

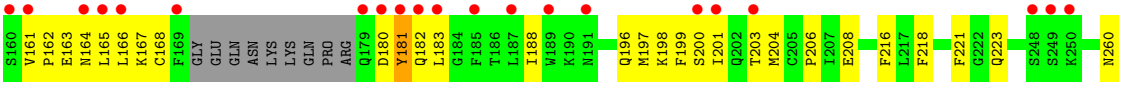


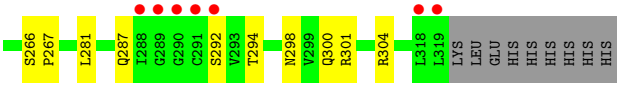


• Molecule 2: AMINOACYL TRNA SYNTHASE COMPLEX-INTERACTING MULTIFUNCTIONA L PROTEIN 2

Chain H:







4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 2 21 21	Depositor
Cell constants a, b, c, α, β, γ	94.69Å 112.79Å 181.25Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	37.80 – 2.32 36.81 – 2.32	Depositor EDS
% Data completeness (in resolution range)	99.0 (37.80-2.32) 95.0 (36.81-2.32)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.16 (at 2.31Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.172 , 0.227 0.189 , 0.238	Depositor DCC
R_{free} test set	1993 reflections (2.38%)	wwPDB-VP
Wilson B-factor (Å^2)	39.5	Xtriage
Anisotropy	0.098	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 50.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	11755	wwPDB-VP
Average B, all atoms (Å^2)	60.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.11% 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

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	0.40	0/1319	0.51	0/1798
1	C	0.49	0/1329	0.56	0/1809
1	E	0.44	0/1328	0.52	0/1807
1	G	0.33	0/1334	0.47	0/1817
2	B	0.53	0/1633	0.73	5/2221 (0.2%)
2	D	0.50	0/1641	0.57	0/2235
2	F	0.54	0/1524	0.61	2/2070 (0.1%)
2	H	0.54	0/1476	0.68	1/2011 (0.0%)
All	All	0.48	0/11584	0.59	8/15768 (0.1%)

There are no bond length outliers.

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	117	GLY	N-CA-C	-11.12	85.31	113.10
2	F	290	GLY	N-CA-C	-10.31	87.33	113.10
2	B	290	GLY	N-CA-C	6.85	130.23	113.10
2	B	281	LEU	CA-CB-CG	-5.72	102.15	115.30
2	B	180	ASP	N-CA-C	5.56	126.00	111.00

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	1293	0	1253	9	0
1	C	1303	0	1272	6	0
1	E	1302	0	1275	3	0
1	G	1308	0	1275	11	0
2	B	1597	0	1587	26	0
2	D	1607	0	1586	12	0
2	F	1492	0	1492	9	0
2	H	1444	0	1430	66	0
3	A	54	0	0	2	0
3	B	42	0	0	0	0
3	C	100	0	0	1	0
3	D	44	0	0	0	0
3	E	72	0	0	1	0
3	F	66	0	0	0	0
3	G	26	0	0	0	0
3	H	5	0	0	0	0
All	All	11755	0	11170	140	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.

The worst 5 of 140 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:D:291:CYS:SG	2:D:292:SER:N	2.19	1.12
2:H:149:LEU:HD22	2:H:181:TYR:CE2	1.85	1.11
2:H:201:ILE:HG13	2:H:203:THR:HG22	1.41	1.03
2:H:149:LEU:HD22	2:H:181:TYR:HE2	1.16	0.96
2:H:151:THR:CG2	2:H:153:HIS:HE1	1.79	0.96

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	166/175 (95%)	160 (96%)	6 (4%)	0	100	100
1	C	166/175 (95%)	163 (98%)	3 (2%)	0	100	100
1	E	166/175 (95%)	163 (98%)	3 (2%)	0	100	100
1	G	167/175 (95%)	163 (98%)	4 (2%)	0	100	100
2	B	208/240 (87%)	198 (95%)	10 (5%)	0	100	100
2	D	209/240 (87%)	205 (98%)	4 (2%)	0	100	100
2	F	189/240 (79%)	183 (97%)	6 (3%)	0	100	100
2	H	183/240 (76%)	174 (95%)	9 (5%)	0	100	100
All	All	1454/1660 (88%)	1409 (97%)	45 (3%)	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	142/149 (95%)	138 (97%)	4 (3%)	43	59
1	C	144/149 (97%)	141 (98%)	3 (2%)	53	70
1	E	144/149 (97%)	141 (98%)	3 (2%)	53	70
1	G	145/149 (97%)	144 (99%)	1 (1%)	84	92
2	B	171/211 (81%)	162 (95%)	9 (5%)	22	31
2	D	171/211 (81%)	168 (98%)	3 (2%)	59	74
2	F	162/211 (77%)	159 (98%)	3 (2%)	57	73
2	H	158/211 (75%)	148 (94%)	10 (6%)	18	24
All	All	1237/1440 (86%)	1201 (97%)	36 (3%)	42	57

5 of 36 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	H	153	HIS
2	H	294	THR

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Mol	Chain	Res	Type
2	H	156	SER
2	H	200	SER
2	B	320	LYS

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

Mol	Chain	Res	Type
2	D	223	GLN
2	D	225	HIS
2	H	196	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)

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)

There are no ligands in this entry.

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, 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	167/175 (95%)	-0.00	4 (2%) 59 66	32, 53, 101, 129	0
1	C	167/175 (95%)	-0.08	4 (2%) 59 66	28, 42, 79, 129	0
1	E	167/175 (95%)	-0.03	7 (4%) 36 43	27, 46, 93, 121	0
1	G	168/175 (96%)	0.20	12 (7%) 16 21	43, 61, 106, 135	0
2	B	210/240 (87%)	0.55	25 (11%) 4 6	25, 52, 119, 158	0
2	D	213/240 (88%)	0.56	29 (13%) 3 4	32, 56, 130, 164	0
2	F	195/240 (81%)	0.36	16 (8%) 11 15	24, 45, 98, 134	0
2	H	189/240 (78%)	0.90	41 (21%) 0 1	30, 81, 138, 160	0
All	All	1476/1660 (88%)	0.33	138 (9%) 8 12	24, 54, 116, 164	0

The worst 5 of 138 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	291	CYS	9.8
2	B	290	GLY	8.5
2	F	290	GLY	8.3
2	D	118	ALA	8.2
2	H	181	TYR	6.8

6.2 Non-standard residues in protein, DNA, RNA chains

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates

There are no monosaccharides in this entry.

6.4 Ligands

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.