wwPDB X-ray Structure Validation Summary Report (i)

Oct 24, 2024 – 12:32 AM EDT

PDB ID	:	2AXZ
Title	:	Crystal structure of PrgX/cCF10 complex
Authors	:	Shi, K.; Brown, C.K.; Gu, Z.Y.; Kozlowicz, B.K.; Dunny, G.M.; Ohlendorf, D.H.; Earhart, C.A.
Deposited on	:	2005-09-06
Resolution	:	3.00 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:

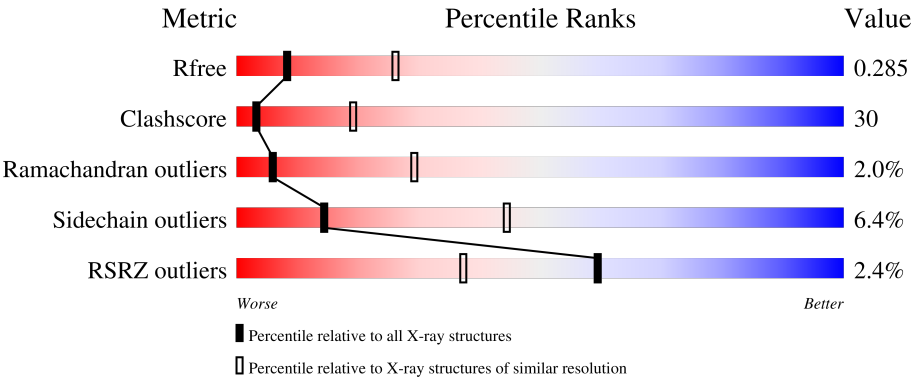
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

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 3.00 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}	164625	2511 (3.00-3.00)
Clashscore	180529	2866 (3.00-3.00)
Ramachandran outliers	177936	2778 (3.00-3.00)
Sidechain outliers	177891	2781 (3.00-3.00)
RSRZ outliers	164620	2523 (3.00-3.00)

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	317	51% 40% 5% ·
1	B	317	56% 36% · ·
1	C	317	6% 38% 43% 7% 12%
1	D	317	2% 46% 45% 5% ·
2	E	7	14% 71% 14%

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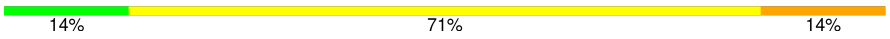
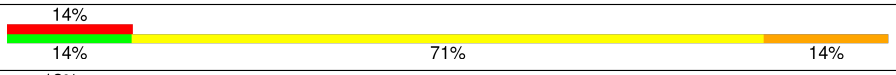
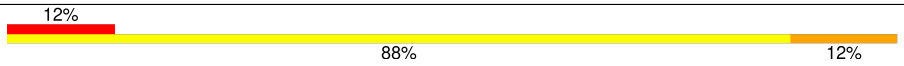
Mol	Chain	Length	Quality of chain
2	F	7	
2	H	7	
3	I	8	

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 10170 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 PrgX.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	306	Total	C	N	O	Se	0	0	0
			2532	1645	406	475	6			
1	B	305	Total	C	N	O	Se	0	0	0
			2523	1640	405	472	6			
1	C	279	Total	C	N	O	Se	0	0	0
			2309	1499	374	432	4			
1	D	305	Total	C	N	O	Se	0	0	0
			2523	1640	405	472	6			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MSE	MET	modified residue	UNP Q04114
A	27	MSE	MET	modified residue	UNP Q04114
A	67	MSE	MET	modified residue	UNP Q04114
A	175	MSE	MET	modified residue	UNP Q04114
A	203	MSE	MET	modified residue	UNP Q04114
A	297	MSE	MET	modified residue	UNP Q04114
B	1	MSE	MET	modified residue	UNP Q04114
B	27	MSE	MET	modified residue	UNP Q04114
B	67	MSE	MET	modified residue	UNP Q04114
B	175	MSE	MET	modified residue	UNP Q04114
B	203	MSE	MET	modified residue	UNP Q04114
B	297	MSE	MET	modified residue	UNP Q04114
C	1	MSE	MET	modified residue	UNP Q04114
C	27	MSE	MET	modified residue	UNP Q04114
C	67	MSE	MET	modified residue	UNP Q04114
C	175	MSE	MET	modified residue	UNP Q04114
C	203	MSE	MET	modified residue	UNP Q04114
C	297	MSE	MET	modified residue	UNP Q04114
D	1	MSE	MET	modified residue	UNP Q04114
D	27	MSE	MET	modified residue	UNP Q04114
D	67	MSE	MET	modified residue	UNP Q04114

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Chain	Residue	Modelled	Actual	Comment	Reference
D	175	MSE	MET	modified residue	UNP Q04114
D	203	MSE	MET	modified residue	UNP Q04114
D	297	MSE	MET	modified residue	UNP Q04114

- Molecule 2 is a protein called LVTLVFV peptide.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	E	7	Total	C	N	O	0	0	0
			56	40	7	9			
2	F	7	Total	C	N	O	0	0	0
			56	40	7	9			
2	H	7	Total	C	N	O	0	0	0
			56	40	7	9			

- Molecule 3 is a protein called TPPKEVT(MSE) peptide.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	I	8	Total	C	N	O	Se	0	0	0
			62	39	9	13	1			

- Molecule 4 is water.

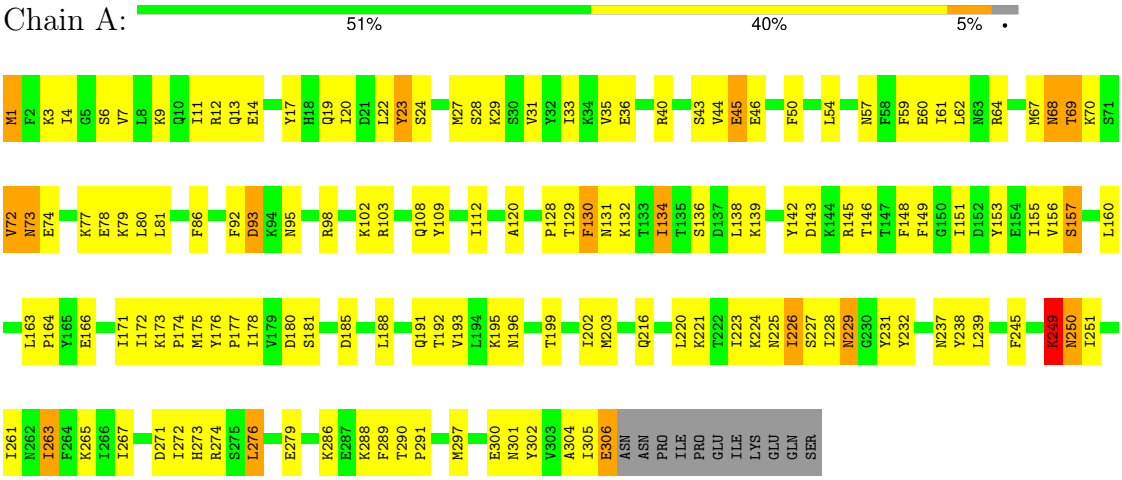
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	23	Total	O	0	0
			23	23		
4	B	18	Total	O	0	0
			18	18		
4	C	5	Total	O	0	0
			5	5		
4	D	7	Total	O	0	0
			7	7		

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.

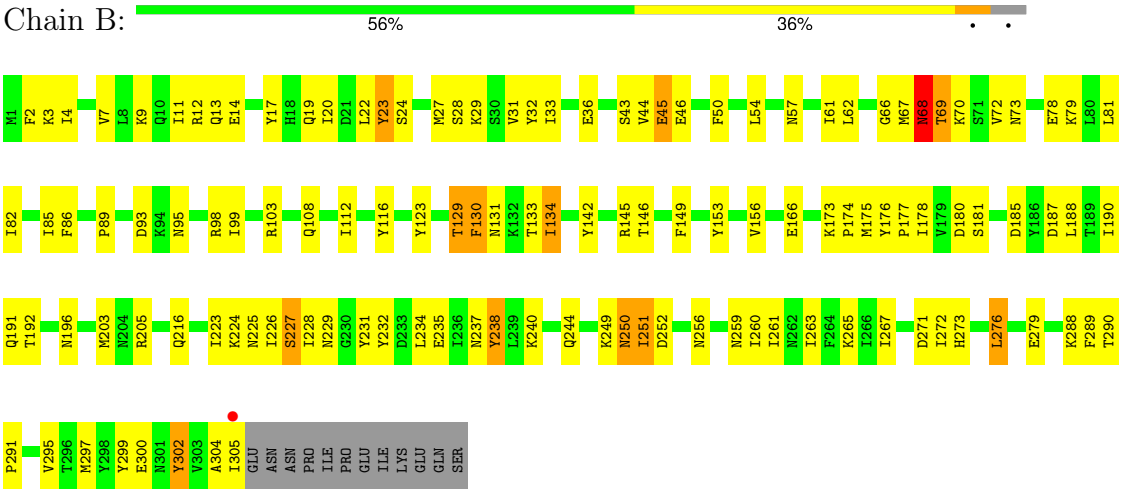
- Molecule 1: PrgX

Chain A:



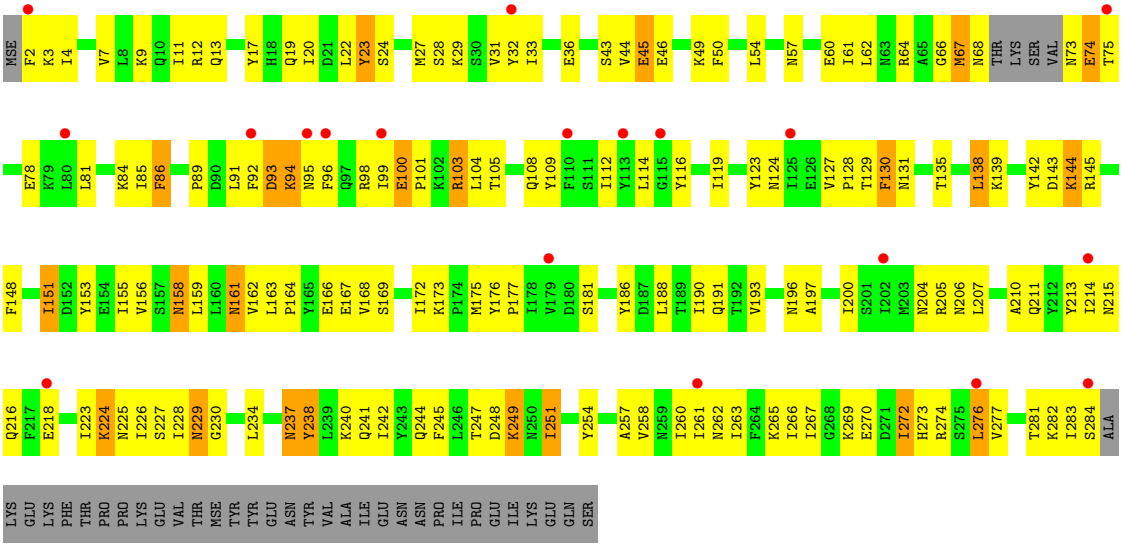
- Molecule 1: PrgX

Chain B:



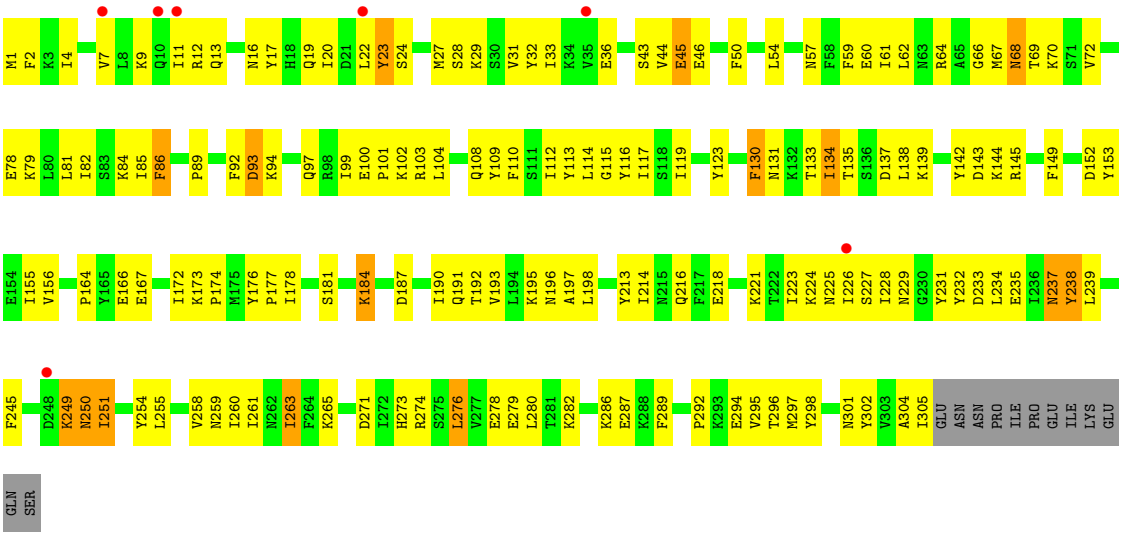
- Molecule 1: PrgX

Chain C:



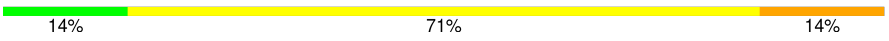
- Molecule 1: PrgX

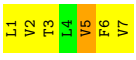
Chain D:



- Molecule 2: LVTLVFV peptide

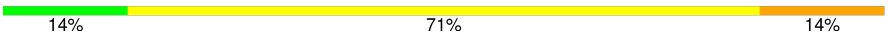
Chain E:





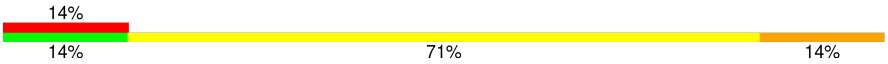
- Molecule 2: LVTLVFV peptide

Chain F:



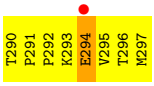
- Molecule 2: LVTLVFV peptide

Chain H:



• Molecule 3: TPPKEVT(MSE) peptide

Chain I:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	71.08Å 83.90Å 286.80Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.00 – 3.00 40.00 – 3.00	Depositor EDS
% Data completeness (in resolution range)	(Not available) (40.00-3.00) 92.6 (40.00-3.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.52 (at 2.77Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.228 , 0.288 0.232 , 0.285	Depositor DCC
R_{free} test set	1626 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å^2)	61.4	Xtriage
Anisotropy	0.209	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 73.3	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	0.92	EDS
Total number of atoms	10170	wwPDB-VP
Average B, all atoms (Å^2)	71.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.41% 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	0.28	0/2579	0.50	0/3475
1	B	0.27	0/2570	0.50	0/3463
1	C	0.28	0/2350	0.50	0/3165
1	D	0.27	0/2570	0.49	0/3463
2	E	0.42	0/56	0.68	0/75
2	F	0.43	0/56	0.67	0/75
2	H	0.43	0/56	0.61	0/75
3	I	0.40	0/62	0.70	0/81
All	All	0.28	0/10299	0.50	0/13872

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

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	2532	0	2570	153	0
1	B	2523	0	2564	144	0
1	C	2309	0	2342	180	0
1	D	2523	0	2564	171	0
2	E	56	0	67	11	0
2	F	56	0	67	11	0
2	H	56	0	67	15	0
3	I	62	0	64	24	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	23	0	0	2	0
4	B	18	0	0	1	0
4	C	5	0	0	1	0
4	D	7	0	0	0	0
All	All	10170	0	10305	614	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 30.

The worst 5 of 614 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:227:SER:HB2	1:B:300:GLU:HG3	1.36	1.04
1:D:81:LEU:HA	1:D:84:LYS:HD3	1.42	1.01
1:C:20:ILE:H	1:C:20:ILE:HD12	1.29	0.97
1:C:163:LEU:HD12	1:C:164:PRO:HD2	1.46	0.97
1:B:20:ILE:HD12	1:B:20:ILE:H	1.29	0.95

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	304/317 (96%)	273 (90%)	24 (8%)	7 (2%)	5 26
1	B	303/317 (96%)	276 (91%)	22 (7%)	5 (2%)	7 33
1	C	275/317 (87%)	252 (92%)	16 (6%)	7 (2%)	4 24
1	D	303/317 (96%)	276 (91%)	22 (7%)	5 (2%)	7 33
2	E	5/7 (71%)	5 (100%)	0	0	100 100
2	F	5/7 (71%)	5 (100%)	0	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	H	5/7 (71%)	5 (100%)	0	0	100	100
3	I	6/8 (75%)	4 (67%)	2 (33%)	0	100	100
All	All	1206/1297 (93%)	1096 (91%)	86 (7%)	24 (2%)	6	29

5 of 24 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	69	THR
1	B	69	THR
1	C	74	GLU
1	D	68	ASN
1	A	68	ASN

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	288/293 (98%)	268 (93%)	20 (7%)	13	42
1	B	287/293 (98%)	272 (95%)	15 (5%)	19	52
1	C	263/293 (90%)	242 (92%)	21 (8%)	10	35
1	D	287/293 (98%)	273 (95%)	14 (5%)	21	54
2	E	7/7 (100%)	6 (86%)	1 (14%)	2	13
2	F	7/7 (100%)	6 (86%)	1 (14%)	2	13
2	H	7/7 (100%)	6 (86%)	1 (14%)	2	13
3	I	8/7 (114%)	7 (88%)	1 (12%)	3	17
All	All	1154/1200 (96%)	1080 (94%)	74 (6%)	14	44

5 of 74 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	45	GLU
2	F	5	VAL

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Mol	Chain	Res	Type
1	D	134	ILE
1	D	259	ASN
1	B	86	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 68 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	124	ASN
1	D	206	ASN
1	D	250	ASN
1	B	216	GLN
1	B	215	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 oligosaccharides 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	300/317 (94%)	-0.39	0 100 100	15, 40, 91, 144	0
1	B	299/317 (94%)	-0.28	1 (0%) 90 81	15, 46, 98, 165	0
1	C	275/317 (86%)	0.59	19 (6%) 24 14	41, 102, 176, 185	0
1	D	299/317 (94%)	0.20	7 (2%) 61 39	30, 80, 145, 174	0
2	E	7/7 (100%)	-0.66	0 100 100	20, 31, 33, 61	0
2	F	7/7 (100%)	-0.29	0 100 100	35, 43, 55, 60	0
2	H	7/7 (100%)	0.14	1 (14%) 7 4	43, 50, 56, 103	0
3	I	7/8 (87%)	0.49	1 (14%) 7 4	68, 112, 161, 177	0
All	All	1201/1297 (92%)	0.02	29 (2%) 59 37	15, 63, 146, 185	0

The worst 5 of 29 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	115	GLY	4.9
1	C	96	PHE	4.3
1	C	80	LEU	3.3
2	H	7	VAL	3.3
3	I	294	GLU	3.3

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.