



wwPDB X-ray Structure Validation Summary Report ⓘ

May 16, 2020 – 07:25 am BST

PDB ID : 6ATU
Title : Exploring Cystine Dense Peptide Space to Open a Unique Molecular Toolbox
Authors : Gewe, M.M.; Rupert, P.; Strong, R.K.
Deposited on : 2017-08-29
Resolution : 2.40 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	:	2.11
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

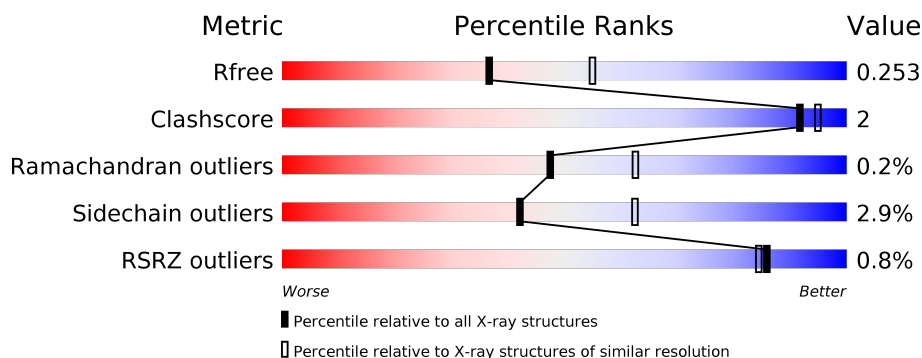
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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.







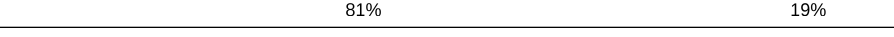
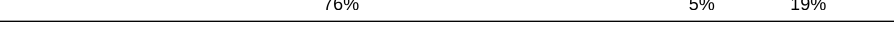
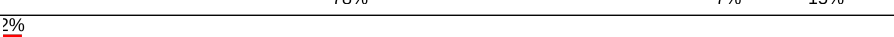
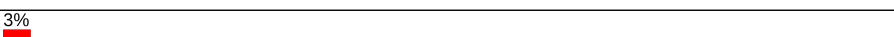




Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (2.40-2.40)

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	59	<div> <div style="width: 83%;"></div> <div style="width: 17%;"></div> </div>
1	B	59	<div> <div style="width: 2%;"></div> <div style="width: 78%;"></div> <div style="width: 5%;"></div> <div style="width: 17%;"></div> </div>
1	C	59	<div> <div style="width: 80%;"></div> <div style="width: 20%;"></div> </div>
1	D	59	<div> <div style="width: 80%;"></div> <div style="width: 20%;"></div> </div>
1	E	59	<div> <div style="width: 76%;"></div> <div style="width: 8%;"></div> <div style="width: 15%;"></div> </div>
1	F	59	<div> <div style="width: 3%;"></div> <div style="width: 78%;"></div> <div style="width: 5%;"></div> <div style="width: 15%;"></div> </div>

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Mol	Chain	Length	Quality of chain
1	G	59	
1	H	59	
1	I	59	
1	J	59	
1	K	59	
1	L	59	
1	M	59	
1	N	59	
1	O	59	
1	P	59	
1	Q	59	
1	R	59	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 6617 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 Elafin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	49	Total	C	N	O	S	0	0	0
			354	218	62	64	10			
1	B	49	Total	C	N	O	S	0	0	0
			354	218	62	64	10			
1	C	47	Total	C	N	O	S	0	0	0
			341	210	60	61	10			
1	D	47	Total	C	N	O	S	0	0	0
			340	210	60	60	10			
1	E	50	Total	C	N	O	S	0	0	0
			361	223	63	65	10			
1	F	50	Total	C	N	O	S	0	0	0
			358	220	63	65	10			
1	G	49	Total	C	N	O	S	0	0	0
			350	215	61	64	10			
1	H	49	Total	C	N	O	S	0	0	0
			351	215	62	64	10			
1	I	50	Total	C	N	O	S	0	0	0
			359	222	62	65	10			
1	J	48	Total	C	N	O	S	0	0	0
			347	213	61	63	10			
1	K	48	Total	C	N	O	S	0	0	0
			347	213	61	63	10			
1	L	48	Total	C	N	O	S	0	0	0
			342	210	60	62	10			
1	M	50	Total	C	N	O	S	0	0	0
			355	220	60	65	10			
1	N	50	Total	C	N	O	S	0	0	0
			358	220	63	65	10			
1	O	50	Total	C	N	O	S	0	0	0
			358	220	63	65	10			
1	P	48	Total	C	N	O	S	0	0	0
			342	211	60	61	10			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	Q	48	Total	C	N	O	S	0	0	0
			346	213	61	62	10			
1	R	49	Total	C	N	O	S	0	0	0
			342	210	60	62	10			

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLY	-	expression tag	UNP P19957
A	0	SER	-	expression tag	UNP P19957
B	-1	GLY	-	expression tag	UNP P19957
B	0	SER	-	expression tag	UNP P19957
C	-1	GLY	-	expression tag	UNP P19957
C	0	SER	-	expression tag	UNP P19957
D	-1	GLY	-	expression tag	UNP P19957
D	0	SER	-	expression tag	UNP P19957
E	-1	GLY	-	expression tag	UNP P19957
E	0	SER	-	expression tag	UNP P19957
F	-1	GLY	-	expression tag	UNP P19957
F	0	SER	-	expression tag	UNP P19957
G	-1	GLY	-	expression tag	UNP P19957
G	0	SER	-	expression tag	UNP P19957
H	-1	GLY	-	expression tag	UNP P19957
H	0	SER	-	expression tag	UNP P19957
I	-1	GLY	-	expression tag	UNP P19957
I	0	SER	-	expression tag	UNP P19957
J	-1	GLY	-	expression tag	UNP P19957
J	0	SER	-	expression tag	UNP P19957
K	-1	GLY	-	expression tag	UNP P19957
K	0	SER	-	expression tag	UNP P19957
L	-1	GLY	-	expression tag	UNP P19957
L	0	SER	-	expression tag	UNP P19957
M	-1	GLY	-	expression tag	UNP P19957
M	0	SER	-	expression tag	UNP P19957
N	-1	GLY	-	expression tag	UNP P19957
N	0	SER	-	expression tag	UNP P19957
O	-1	GLY	-	expression tag	UNP P19957
O	0	SER	-	expression tag	UNP P19957
P	-1	GLY	-	expression tag	UNP P19957
P	0	SER	-	expression tag	UNP P19957
Q	-1	GLY	-	expression tag	UNP P19957
Q	0	SER	-	expression tag	UNP P19957

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Chain	Residue	Modelled	Actual	Comment	Reference
R	-1	GLY	-	expression tag	UNP P19957
R	0	SER	-	expression tag	UNP P19957


- Molecule 2 is water.

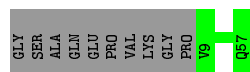
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	26	Total O 26 26	0	0
2	B	32	Total O 32 32	0	0
2	C	11	Total O 11 11	0	0
2	D	8	Total O 8 8	0	0
2	E	27	Total O 27 27	0	0
2	F	20	Total O 20 20	0	0
2	G	9	Total O 9 9	0	0
2	H	13	Total O 13 13	0	0
2	I	32	Total O 32 32	0	0
2	J	19	Total O 19 19	0	0
2	K	26	Total O 26 26	0	0
2	L	8	Total O 8 8	0	0
2	M	5	Total O 5 5	0	0
2	N	18	Total O 18 18	0	0
2	O	12	Total O 12 12	0	0
2	P	26	Total O 26 26	0	0
2	Q	16	Total O 16 16	0	0
2	R	4	Total O 4 4	0	0

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: Elafin

Chain A: 




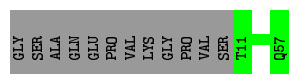
- Molecule 1: Elafin

Chain B: 



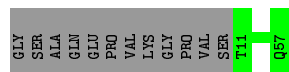
- Molecule 1: Elafin

Chain C: 




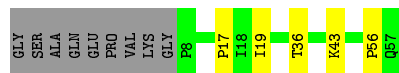
- Molecule 1: Elafin

Chain D: 




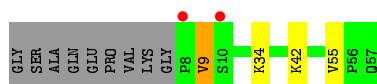
- Molecule 1: Elafin

Chain E: 

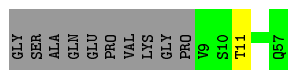
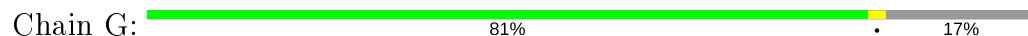


- Molecule 1: Elafin

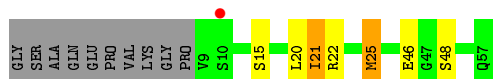
Chain F: 



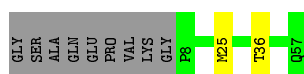
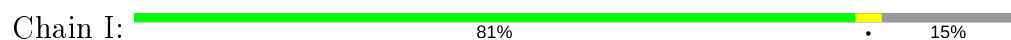
- Molecule 1: Elafin



- Molecule 1: Elafin



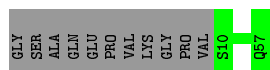
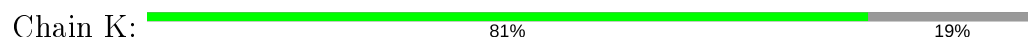
- Molecule 1: Elafin



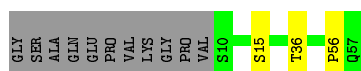
- Molecule 1: Elafin



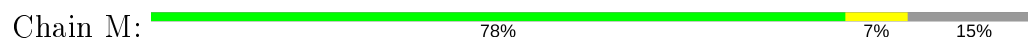
- Molecule 1: Elafin



- Molecule 1: Elafin

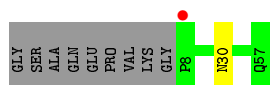
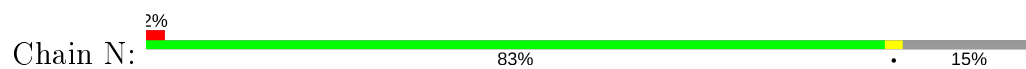


- Molecule 1: Elafin

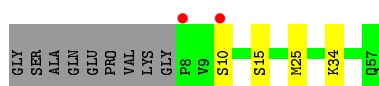
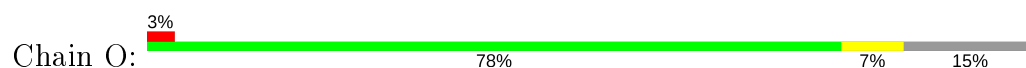




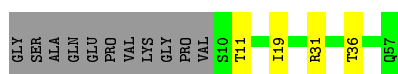
- Molecule 1: Elafin



- Molecule 1: Elafin



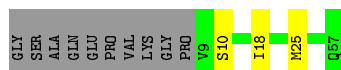
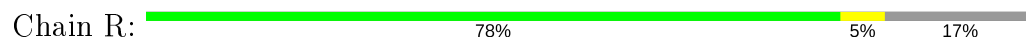
- Molecule 1: Elafin



- Molecule 1: Elafin



- Molecule 1: Elafin



4 Data and refinement statistics

Property	Value	Source
Space group	P 41	Depositor
Cell constants a, b, c, α , β , γ	71.33Å 71.33Å 214.44Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	71.33 – 2.40 49.10 – 2.40	Depositor EDS
% Data completeness (in resolution range)	99.1 (71.33-2.40) 99.1 (49.10-2.40)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.12 (at 2.39Å)	Xtriage
Refinement program	REFMAC 5.8.0158	Depositor
R, R_{free}	0.196 , 0.248 0.201 , 0.253	Depositor DCC
R_{free} test set	2051 reflections (4.94%)	wwPDB-VP
Wilson B-factor (Å ²)	40.0	Xtriage
Anisotropy	0.006	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 11.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.477 for h,-k,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	6617	wwPDB-VP
Average B, all atoms (Å ²)	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.81% 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](#)

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	0.57	0/360	0.59	0/484
1	B	0.59	0/360	0.60	0/484
1	C	0.49	0/347	0.57	0/466
1	D	0.51	0/346	0.53	0/466
1	E	0.54	0/368	0.59	0/495
1	F	0.54	0/365	0.59	0/491
1	G	0.53	0/356	0.56	0/480
1	H	0.57	0/357	0.60	0/480
1	I	0.54	0/366	0.58	0/493
1	J	0.54	0/353	0.60	0/474
1	K	0.57	0/353	0.56	0/474
1	L	0.52	0/348	0.58	0/470
1	M	0.50	0/362	0.53	0/488
1	N	0.55	0/365	0.62	0/491
1	O	0.53	0/365	0.55	0/491
1	P	0.54	0/348	0.60	0/469
1	Q	0.54	0/352	0.60	0/473
1	R	0.50	0/348	0.52	0/471
All	All	0.54	0/6419	0.58	0/8640

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	354	0	358	0	0
1	B	354	0	358	3	0
1	C	341	0	344	0	0
1	D	340	0	344	0	0
1	E	361	0	366	4	0
1	F	358	0	357	2	0
1	G	350	0	347	0	0
1	H	351	0	349	4	0
1	I	359	0	359	2	0
1	J	347	0	349	3	0
1	K	347	0	349	0	0
1	L	342	0	338	1	0
1	M	355	0	355	0	0
1	N	358	0	357	1	0
1	O	358	0	357	1	0
1	P	342	0	343	1	0
1	Q	346	0	346	3	0
1	R	342	0	332	0	0
2	A	26	0	0	0	0
2	B	32	0	0	0	0
2	C	11	0	0	0	0
2	D	8	0	0	0	0
2	E	27	0	0	0	0
2	F	20	0	0	0	0
2	G	9	0	0	0	0
2	H	13	0	0	0	0
2	I	32	0	0	1	0
2	J	19	0	0	0	0
2	K	26	0	0	0	0
2	L	8	0	0	0	0
2	M	5	0	0	0	0
2	N	18	0	0	0	0
2	O	12	0	0	0	0
2	P	26	0	0	1	0
2	Q	16	0	0	1	0
2	R	4	0	0	0	0
All	All	6617	0	6308	20	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 2.

The worst 5 of 20 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:E:36:THR:HB	1:H:25:MET:HE1	1.69	0.74
1:P:19:ILE:HB	2:P:115:HOH:O	1.98	0.62
1:I:36:THR:HB	1:O:25:MET:HE1	1.81	0.62
1:F:9:VAL:HG13	1:F:34:LYS:HB3	1.85	0.57
1:Q:19:ILE:HD12	1:Q:19:ILE:O	2.09	0.53

There are no symmetry-related clashes.

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	47/59 (80%)	45 (96%)	2 (4%)	0	100	100
1	B	47/59 (80%)	45 (96%)	2 (4%)	0	100	100
1	C	45/59 (76%)	42 (93%)	3 (7%)	0	100	100
1	D	45/59 (76%)	42 (93%)	3 (7%)	0	100	100
1	E	48/59 (81%)	47 (98%)	1 (2%)	0	100	100
1	F	48/59 (81%)	47 (98%)	1 (2%)	0	100	100
1	G	47/59 (80%)	45 (96%)	2 (4%)	0	100	100
1	H	47/59 (80%)	43 (92%)	2 (4%)	2 (4%)	2	2
1	I	48/59 (81%)	47 (98%)	1 (2%)	0	100	100
1	J	46/59 (78%)	45 (98%)	1 (2%)	0	100	100
1	K	46/59 (78%)	44 (96%)	2 (4%)	0	100	100
1	L	46/59 (78%)	44 (96%)	2 (4%)	0	100	100
1	M	48/59 (81%)	45 (94%)	3 (6%)	0	100	100
1	N	48/59 (81%)	47 (98%)	1 (2%)	0	100	100
1	O	48/59 (81%)	43 (90%)	5 (10%)	0	100	100
1	P	46/59 (78%)	44 (96%)	2 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	Q	46/59 (78%)	45 (98%)	1 (2%)	0	100	100
1	R	47/59 (80%)	46 (98%)	1 (2%)	0	100	100
All	All	843/1062 (79%)	806 (96%)	35 (4%)	2 (0%)	47	62

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	H	25	MET
1	H	21	ILE

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	43/50 (86%)	43 (100%)	0	100	100
1	B	43/50 (86%)	43 (100%)	0	100	100
1	C	41/50 (82%)	41 (100%)	0	100	100
1	D	41/50 (82%)	41 (100%)	0	100	100
1	E	44/50 (88%)	44 (100%)	0	100	100
1	F	43/50 (86%)	42 (98%)	1 (2%)	50	70
1	G	42/50 (84%)	41 (98%)	1 (2%)	49	68
1	H	42/50 (84%)	40 (95%)	2 (5%)	25	41
1	I	43/50 (86%)	43 (100%)	0	100	100
1	J	42/50 (84%)	40 (95%)	2 (5%)	25	41
1	K	42/50 (84%)	42 (100%)	0	100	100
1	L	41/50 (82%)	39 (95%)	2 (5%)	25	40
1	M	43/50 (86%)	39 (91%)	4 (9%)	9	13
1	N	43/50 (86%)	43 (100%)	0	100	100
1	O	43/50 (86%)	40 (93%)	3 (7%)	15	24
1	P	41/50 (82%)	38 (93%)	3 (7%)	14	22

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	Q	41/50 (82%)	40 (98%)	1 (2%)	49	68
1	R	40/50 (80%)	37 (92%)	3 (8%)	13	21
All	All	758/900 (84%)	736 (97%)	22 (3%)	42	62

5 of 22 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	M	10	SER
1	O	10	SER
1	R	18	ILE
1	M	27	ASN
1	M	34	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	57	GLN
1	I	57	GLN
1	L	57	GLN
1	N	27	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

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, 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	49/59 (83%)	-0.42	0 100 100	26, 35, 50, 68	0
1	B	49/59 (83%)	-0.40	1 (2%) 65 63	26, 36, 50, 70	0
1	C	47/59 (79%)	-0.29	0 100 100	32, 51, 72, 76	0
1	D	47/59 (79%)	-0.30	0 100 100	31, 49, 71, 75	0
1	E	50/59 (84%)	-0.44	0 100 100	26, 37, 62, 93	0
1	F	50/59 (84%)	-0.25	2 (4%) 38 37	29, 39, 69, 87	0
1	G	49/59 (83%)	-0.21	0 100 100	34, 45, 66, 82	0
1	H	49/59 (83%)	-0.33	1 (2%) 65 63	29, 42, 69, 80	0
1	I	50/59 (84%)	-0.33	0 100 100	25, 35, 60, 79	0
1	J	48/59 (81%)	-0.32	0 100 100	27, 40, 62, 94	0
1	K	48/59 (81%)	-0.52	0 100 100	25, 35, 50, 85	0
1	L	48/59 (81%)	-0.30	0 100 100	34, 46, 67, 96	0
1	M	50/59 (84%)	-0.16	0 100 100	35, 51, 72, 96	0
1	N	50/59 (84%)	-0.33	1 (2%) 65 63	28, 37, 67, 93	0
1	O	50/59 (84%)	-0.17	2 (4%) 38 37	32, 42, 79, 99	0
1	P	48/59 (81%)	-0.41	0 100 100	25, 35, 48, 74	0
1	Q	48/59 (81%)	-0.36	0 100 100	29, 40, 61, 86	0
1	R	49/59 (83%)	-0.25	0 100 100	34, 50, 69, 85	0
All	All	879/1062 (82%)	-0.32	7 (0%) 86 84	25, 41, 71, 99	0

The worst 5 of 7 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	N	8	PRO	3.5
1	O	10	SER	3.2
1	B	9	VAL	2.9

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Mol	Chain	Res	Type	RSRZ
1	O	8	PRO	2.8
1	F	8	PRO	2.3

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](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.