WORLDWIDE wwPDB PROTEIN DATA BANK

wwPDB X-ray Structure Validation Summary Report (i)

Sep 2, 2023 – 10:54 PM EDT

PDB ID	:	3QRF
Title	:	Structure of a domain-swapped FOXP3 dimer
Authors	:	Bandukwala, H.S.; Wu, Y.; Feurer, M.; Chen, Y.; Barbosa, B.; Ghosh, S.; Stroud, J.C.; Benoist, C.; Mathis, D.; Rao, A.; Chen, L.
Deposited on	:	2011-02-17
Resolution	:	2.80 Å(reported)

The following versions of software and data (see references (i)) were used in the production of this report:

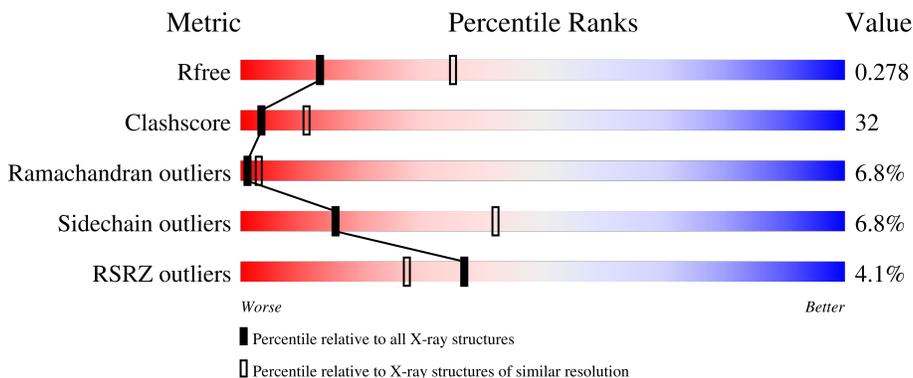|		
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.35
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

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 2.80 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.
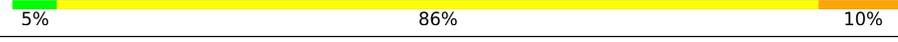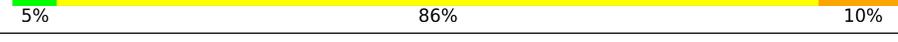
Metric	Percentile Ranks	Value
Rfree		0.278
Clashscore		32
Ramachandran outliers		6.8%
Sidechain outliers		6.8%
RSRZ outliers		4.1%

Worse   *Better*

▌ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R$_{free}$	130704	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)

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	M	286	6% · 41% · 49% · 9%
1	N	286	5% · 43% · 47% · 9%
2	F	82	% · 39% · 54% · 7%
2	G	82	5% · 57% · 39% · •
2	H	82	2% · 44% · 49% · 7%

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Mol	Chain	Length	Quality of chain
2	I	82	2% 57% 39%
3	A	21	24% 71% 5%
3	C	21	19% 76% 5%
4	B	21	5% 86% 10%
4	D	21	5% 86% 10%

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 9105 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 Nuclear factor of activated T-cells, cytoplasmic 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	N	286	Total	C	N	O	S	0	0	0
			2264	1421	413	421	9			
1	M	286	Total	C	N	O	S	0	0	0
			2264	1421	413	421	9			

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
N	393	SER	-	expression tag	UNP Q13469
N	394	SER	-	expression tag	UNP Q13469
N	395	VAL	-	expression tag	UNP Q13469
N	629	ALA	ASP	conflict	UNP Q13469
N	630	ALA	LYS	conflict	UNP Q13469
N	631	ALA	ASP	conflict	UNP Q13469
N	632	ALA	LYS	conflict	UNP Q13469
N	633	ALA	SER	conflict	UNP Q13469
N	634	ALA	GLN	conflict	UNP Q13469
M	393	SER	-	expression tag	UNP Q13469
M	394	SER	-	expression tag	UNP Q13469
M	395	VAL	-	expression tag	UNP Q13469
M	629	ALA	ASP	conflict	UNP Q13469
M	630	ALA	LYS	conflict	UNP Q13469
M	631	ALA	ASP	conflict	UNP Q13469
M	632	ALA	LYS	conflict	UNP Q13469
M	633	ALA	SER	conflict	UNP Q13469
M	634	ALA	GLN	conflict	UNP Q13469

- Molecule 2 is a protein called Forkhead box protein P3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	F	82	Total	C	N	O	S	0	0	0
			714	465	132	114	3			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	G	82	Total 714	C 465	N 132	O 114	S 3	0	0	0
2	H	82	Total 714	C 465	N 132	O 114	S 3	0	0	0
2	I	82	Total 714	C 465	N 132	O 114	S 3	0	0	0

- Molecule 3 is a DNA chain called human hARRE2 DNA (Plus Strand).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	21	Total 431	C 209	N 76	O 126	P 20	0	0	0
3	A	21	Total 431	C 209	N 76	O 126	P 20	0	0	0

- Molecule 4 is a DNA chain called human hARRE2 DNA (Minus Strand).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	21	Total 424	C 206	N 76	O 122	P 20	0	0	0
4	B	21	Total 424	C 206	N 76	O 122	P 20	0	0	0

- Molecule 5 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	F	1	Total 1	Mg 1	0	0
5	G	1	Total 1	Mg 1	0	0
5	H	1	Total 1	Mg 1	0	0
5	I	1	Total 1	Mg 1	0	0

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	N	1	Total 1	O 1	0	0
6	C	2	Total 2	O 2	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	D	3	Total 3	O 3	0	0
6	B	1	Total 1	O 1	0	0

3 Residue-property plots ⓘ

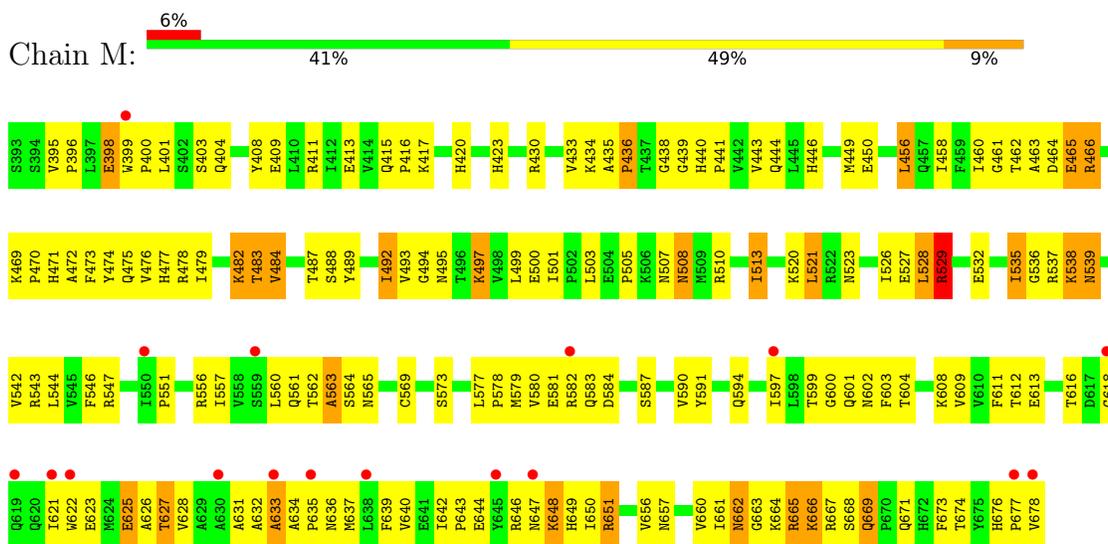These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Nuclear factor of activated T-cells, cytoplasmic 2
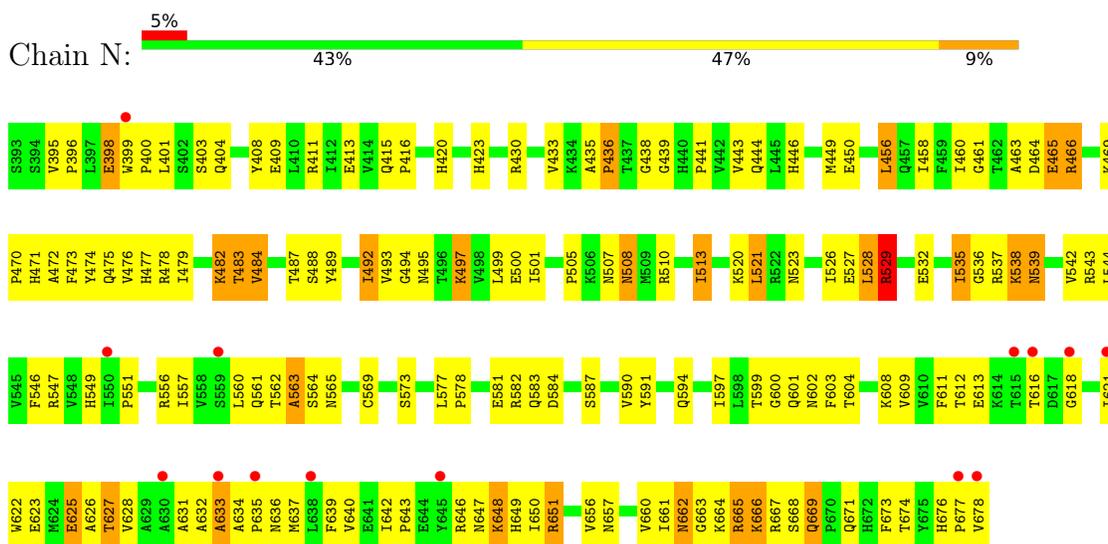
• Molecule 1: Nuclear factor of activated T-cells, cytoplasmic 2

• Molecule 2: Forkhead box protein P3

M336 R337 P338 Y342 I346 R347 W348 A349 I350 L351 E352 A353 P354 E355 K356 Q357 R358 T359 L360 N361 E362 I363 Y364 H365 W366 R369 M370 F371 A372 F373 F374 R375 N376 H377 P378 A379 T380 W381 K382 N383 A384 L389 S390 V396 S400 E401 K402 G403 A404 V405 W406 T407 V408 D409

E410 L411 E412 F413 R414 K415 K416 R417

• Molecule 2: Forkhead box protein P3

Chain G:

M336 R337 P338 P339 F340 T341 R347 L351 E352 A353 R358 T359 L360 N361 E362 I363 Y364 H365 R369 M370 F371 F374 R375 P378 A379 T380 W381 K382 L391 H392 K393 S400 E401 K402 G403 T407 V408 D409 L411 E412 F413 R414 K415 K416 R417

• Molecule 2: Forkhead box protein P3

Chain H:

M336 R337 Y342 I346 R347 W348 A349 I350 L351 E352 A353 P354 E355 K356 Q357 R358 T359 L360 N361 E362 I363 Y364 H365 W366 R369 M370 F371 A372 F373 F374 R375 N376 H377 P378 A379 T380 W381 K382 N383 A384 L389 V396 S400 E401 K402 G403 A404 V405 W406 T407 V408 D409 E410 L411

E412 F413 R414 K415 K416 R417

• Molecule 2: Forkhead box protein P3

Chain I:

M336 R337 P338 P339 F340 R347 L351 E352 A353 R358 T359 L360 N361 E362 I363 Y364 H365 R369 M370 F371 F374 R375 N376 H377 P378 A379 T380 W381 K382 L391 H392 K393 S400 G403 T407 V408 D409 E410 L411 E412 F413 R414 K415 K416 R417

• Molecule 3: human hARRE2 DNA (Plus Strand)

Chain C:

T4001 T4002 A4003 G4004 G4005 A4006 A4007 A4008 A4009 T4010 T4011 T4012 G4013 T4014 T4015 A4018 T4019 A4020 G4021

• Molecule 3: human hARRE2 DNA (Plus Strand)

Chain A:

T4001 T4002 A4003 G4004 G4005 A4006 A4007 A4008 A4009 T4010 T4011 T4012 G4013 T4014 T4015 A4018 T4019 A4020 G4021
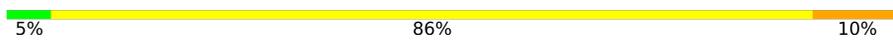
• Molecule 4: human hARRE2 DNA (Minus Strand)

Chain D:

A5001 A5002 C5003 T5004 A5005 T5006 G5007 A5008 A5009 A5010 C5011 A5012 A5013 A5014 T5015 T5016 T5017 T5018 C5019 C5020 T5021

• Molecule 4: human hARRE2 DNA (Minus Strand)

Chain B: 5%   86%   10%

A5001 A5002 C5003 T5004 A5005 T5006 G5007 A5008 A5009 A5010 C5011 A5012 A5013 A5014 T5015 T5016 T5017 T5018 C5019 C5020 T5021

4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	83.67Å 131.23Å 68.67Å 90.00° 89.95° 90.00°	Depositor
Resolution (Å)	50.00 – 2.80 19.93 – 2.80	Depositor EDS
% Data completeness (in resolution range)	(Not available) (50.00-2.80) 96.3 (19.93-2.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.68 (at 2.79Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.248 , 0.283 0.244 , 0.278	Depositor DCC
R_{free} test set	3538 reflections (9.74%)	wwPDB-VP
Wilson B-factor (Å^2)	63.7	Xtriage
Anisotropy	0.645	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.27 , 23.4	EDS
L-test for twinning[2]	$< |L| > = 0.50, < L^2 > = 0.34$	Xtriage
Estimated twinning fraction	0.480 for -h,-k,l	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	9105	wwPDB-VP
Average B, all atoms (Å^2)	65.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.89% of the height of the origin peak. No significant pseudotranslation is detected.*

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[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 ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: MG

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	M	0.38	0/2314	0.65	0/3134
1	N	0.39	0/2314	0.65	0/3134
2	F	0.49	0/738	0.63	0/996
2	G	0.48	0/738	0.62	0/996
2	H	0.50	0/738	0.63	0/996
2	I	0.47	0/738	0.62	0/996
3	A	0.58	0/483	0.89	1/745 (0.1%)
3	C	0.53	0/483	0.88	1/745 (0.1%)
4	B	0.57	0/475	0.82	0/730
4	D	0.55	0/475	0.81	0/730
All	All	0.46	0/9496	0.69	2/13202 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
3	A	0	1
3	C	0	1
4	B	0	2
4	D	0	2
All	All	0	6

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	4006	DA	N9-C1'-C2'	5.36	122.78	112.60
3	C	4006	DA	N9-C1'-C2'	5.25	122.56	112.60

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There are no chirality outliers.

5 of 6 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	A	4018	DA	Sidechain
4	B	5004	DT	Sidechain
3	C	4018	DA	Sidechain
4	D	5004	DT	Sidechain
4	D	5005	DA	Sidechain

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	M	2264	0	2271	168	0
1	N	2264	0	2271	161	0
2	F	714	0	708	51	0
2	G	714	0	708	38	0
2	H	714	0	708	48	0
2	I	714	0	708	38	0
3	A	431	0	242	24	0
3	C	431	0	242	25	0
4	B	424	0	240	24	0
4	D	424	0	240	25	0
5	F	1	0	0	0	0
5	G	1	0	0	0	0
5	H	1	0	0	0	0
5	I	1	0	0	0	0
6	B	1	0	0	0	0
6	C	2	0	0	0	0
6	D	3	0	0	0	0
6	N	1	0	0	0	0
All	All	9105	0	8338	563	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 32.

The worst 5 of 563 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:N:669:GLN:HE21	1:N:671:GLN:HE22	1.07	0.98
1:M:634:ALA:HB3	1:M:637:MET:HB2	1.44	0.98
3:A:4002:DT:H2"	3:A:4003:DA:H5"	1.44	0.98
1:N:475:GLN:HE22	1:N:497:LYS:H	1.04	0.98
3:C:4002:DT:H2"	3:C:4003:DA:H5"	1.45	0.97

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	M	284/286 (99%)	216 (76%)	42 (15%)	26 (9%)	1	1
1	N	284/286 (99%)	217 (76%)	41 (14%)	26 (9%)	1	1
2	F	80/82 (98%)	66 (82%)	10 (12%)	4 (5%)	2	6
2	G	80/82 (98%)	69 (86%)	11 (14%)	0	100	100
2	H	80/82 (98%)	66 (82%)	10 (12%)	4 (5%)	2	6
2	I	80/82 (98%)	69 (86%)	11 (14%)	0	100	100
All	All	888/900 (99%)	703 (79%)	125 (14%)	60 (7%)	1	3

5 of 60 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	N	465	GLU
1	N	563	ALA
1	N	583	GLN
1	N	604	THR
1	N	627	THR

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	M	250/250 (100%)	230 (92%)	20 (8%)	12	34
1	N	250/250 (100%)	230 (92%)	20 (8%)	12	34
2	F	74/74 (100%)	72 (97%)	2 (3%)	44	78
2	G	74/74 (100%)	69 (93%)	5 (7%)	16	42
2	H	74/74 (100%)	72 (97%)	2 (3%)	44	78
2	I	74/74 (100%)	69 (93%)	5 (7%)	16	42
All	All	796/796 (100%)	742 (93%)	54 (7%)	16	42

5 of 54 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	M	398	GLU
1	M	528	LEU
2	I	337	ARG
1	M	403	SER
1	M	492	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 33 such sidechains are listed below:

Mol	Chain	Res	Type
2	H	376	ASN
2	H	377	HIS
2	I	377	HIS
2	F	377	HIS
2	F	376	ASN

5.3.3 RNA (i)

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 monosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 4 ligands modelled in this entry, 4 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 ⓘ

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(Å²)	Q<0.9
1	M	286/286 (100%)	0.20	17 (5%)	22	14	36, 78, 110, 117	0
1	N	286/286 (100%)	0.19	14 (4%)	29	20	36, 78, 110, 117	0
2	F	82/82 (100%)	-0.01	1 (1%)	79	73	31, 50, 82, 98	0
2	G	82/82 (100%)	0.10	4 (4%)	29	20	28, 52, 95, 100	0
2	H	82/82 (100%)	0.06	2 (2%)	59	49	31, 50, 81, 98	0
2	I	82/82 (100%)	0.10	2 (2%)	59	49	29, 52, 95, 100	0
3	A	21/21 (100%)	-0.56	0	100	100	32, 42, 65, 71	0
3	C	21/21 (100%)	-0.50	0	100	100	31, 42, 65, 71	0
4	B	21/21 (100%)	-0.35	0	100	100	32, 43, 68, 81	0
4	D	21/21 (100%)	-0.40	0	100	100	32, 43, 68, 81	0
All	All	984/984 (100%)	0.10	40 (4%)	37	27	28, 66, 105, 117	0

The worst 5 of 40 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	F	336	MET	5.0
2	H	336	MET	4.2
1	N	618	GLY	4.1
2	I	336	MET	3.7
2	I	415	LYS	3.4

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 (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($Å^2$)	Q<0.9
5	MG	I	1	1/1	0.81	0.22	61,61,61,61	0
5	MG	F	1	1/1	0.82	0.09	43,43,43,43	0
5	MG	G	1	1/1	0.85	0.19	62,62,62,62	0
5	MG	H	1	1/1	0.86	0.09	43,43,43,43	0

6.5 Other polymers (i)

There are no such residues in this entry.