Full wwPDB X-ray Structure Validation Report ⓘ

Feb 6, 2024 – 08:30 AM EST

PDB ID	:	2GWF
Title	:	Structure of a USP8-NRDP1 complex
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Deposited on	:	2006-05-04
Resolution	:	2.30 Å(reported)

This is a Full wwPDB X-ray Structure Validation 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 types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

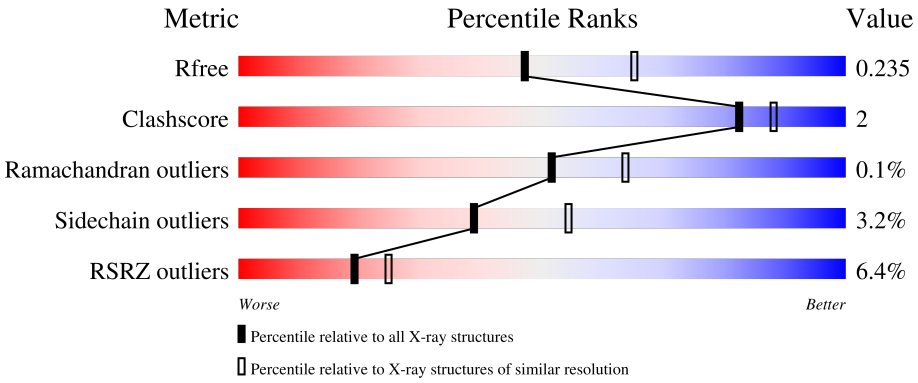
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation 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 2.30 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	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

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	157	4% 79% 6% • 13%
1	C	157	8% 76% 8% • 15%
1	E	157	6% 81% 5% • 13%
2	B	134	3% 83% 7% • 10%
2	D	134	7% 91% • 6%

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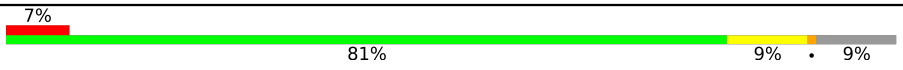
Mol	Chain	Length	Quality of chain
2	F	134	

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 6388 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 Ubiquitin carboxyl-terminal hydrolase 8.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	136	Total	C	N	O	S	0	0	0
			1088	693	178	211	6			
1	C	134	Total	C	N	O	S	0	0	0
			1075	686	175	208	6			
1	E	137	Total	C	N	O	S	0	0	0
			1097	699	180	212	6			

There are 57 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	162	MET	-	initiating methionine	UNP P40818
A	163	GLY	-	cloning artifact	UNP P40818
A	164	SER	-	cloning artifact	UNP P40818
A	165	SER	-	cloning artifact	UNP P40818
A	166	HIS	-	expression tag	UNP P40818
A	167	HIS	-	expression tag	UNP P40818
A	168	HIS	-	expression tag	UNP P40818
A	169	HIS	-	expression tag	UNP P40818
A	170	HIS	-	expression tag	UNP P40818
A	171	HIS	-	expression tag	UNP P40818
A	172	SER	-	cloning artifact	UNP P40818
A	173	SER	-	cloning artifact	UNP P40818
A	174	GLY	-	cloning artifact	UNP P40818
A	175	LEU	-	cloning artifact	UNP P40818
A	176	VAL	-	cloning artifact	UNP P40818
A	177	PRO	-	cloning artifact	UNP P40818
A	178	ARG	-	cloning artifact	UNP P40818
A	179	GLY	-	cloning artifact	UNP P40818
A	180	SER	-	cloning artifact	UNP P40818
C	162	MET	-	initiating methionine	UNP P40818
C	163	GLY	-	cloning artifact	UNP P40818
C	164	SER	-	cloning artifact	UNP P40818
C	165	SER	-	cloning artifact	UNP P40818

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Chain	Residue	Modelled	Actual	Comment	Reference
C	166	HIS	-	expression tag	UNP P40818
C	167	HIS	-	expression tag	UNP P40818
C	168	HIS	-	expression tag	UNP P40818
C	169	HIS	-	expression tag	UNP P40818
C	170	HIS	-	expression tag	UNP P40818
C	171	HIS	-	expression tag	UNP P40818
C	172	SER	-	cloning artifact	UNP P40818
C	173	SER	-	cloning artifact	UNP P40818
C	174	GLY	-	cloning artifact	UNP P40818
C	175	LEU	-	cloning artifact	UNP P40818
C	176	VAL	-	cloning artifact	UNP P40818
C	177	PRO	-	cloning artifact	UNP P40818
C	178	ARG	-	cloning artifact	UNP P40818
C	179	GLY	-	cloning artifact	UNP P40818
C	180	SER	-	cloning artifact	UNP P40818
E	162	MET	-	initiating methionine	UNP P40818
E	163	GLY	-	cloning artifact	UNP P40818
E	164	SER	-	cloning artifact	UNP P40818
E	165	SER	-	cloning artifact	UNP P40818
E	166	HIS	-	expression tag	UNP P40818
E	167	HIS	-	expression tag	UNP P40818
E	168	HIS	-	expression tag	UNP P40818
E	169	HIS	-	expression tag	UNP P40818
E	170	HIS	-	expression tag	UNP P40818
E	171	HIS	-	expression tag	UNP P40818
E	172	SER	-	cloning artifact	UNP P40818
E	173	SER	-	cloning artifact	UNP P40818
E	174	GLY	-	cloning artifact	UNP P40818
E	175	LEU	-	cloning artifact	UNP P40818
E	176	VAL	-	cloning artifact	UNP P40818
E	177	PRO	-	cloning artifact	UNP P40818
E	178	ARG	-	cloning artifact	UNP P40818
E	179	GLY	-	cloning artifact	UNP P40818
E	180	SER	-	cloning artifact	UNP P40818

- Molecule 2 is a protein called RING finger protein 41.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	121	Total	C	N	O	S	0	0	0
			952	595	171	178	8			
2	D	126	Total	C	N	O	S	0	0	0
			994	622	176	188	8			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	F	122	Total	C	N	O	S	0	0	0
			964	604	172	180	8			

There are 27 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	184	SER	-	cloning artifact	UNP Q9H4P4
B	185	SER	-	cloning artifact	UNP Q9H4P4
B	186	GLY	-	cloning artifact	UNP Q9H4P4
B	187	LEU	-	cloning artifact	UNP Q9H4P4
B	188	VAL	-	cloning artifact	UNP Q9H4P4
B	189	PRO	-	cloning artifact	UNP Q9H4P4
B	190	ARG	-	cloning artifact	UNP Q9H4P4
B	191	GLY	-	cloning artifact	UNP Q9H4P4
B	192	SER	-	cloning artifact	UNP Q9H4P4
D	184	SER	-	cloning artifact	UNP Q9H4P4
D	185	SER	-	cloning artifact	UNP Q9H4P4
D	186	GLY	-	cloning artifact	UNP Q9H4P4
D	187	LEU	-	cloning artifact	UNP Q9H4P4
D	188	VAL	-	cloning artifact	UNP Q9H4P4
D	189	PRO	-	cloning artifact	UNP Q9H4P4
D	190	ARG	-	cloning artifact	UNP Q9H4P4
D	191	GLY	-	cloning artifact	UNP Q9H4P4
D	192	SER	-	cloning artifact	UNP Q9H4P4
F	184	SER	-	cloning artifact	UNP Q9H4P4
F	185	SER	-	cloning artifact	UNP Q9H4P4
F	186	GLY	-	cloning artifact	UNP Q9H4P4
F	187	LEU	-	cloning artifact	UNP Q9H4P4
F	188	VAL	-	cloning artifact	UNP Q9H4P4
F	189	PRO	-	cloning artifact	UNP Q9H4P4
F	190	ARG	-	cloning artifact	UNP Q9H4P4
F	191	GLY	-	cloning artifact	UNP Q9H4P4
F	192	SER	-	cloning artifact	UNP Q9H4P4

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	45	Total	O	0	0
			45	45		
3	B	29	Total	O	0	0
			29	29		

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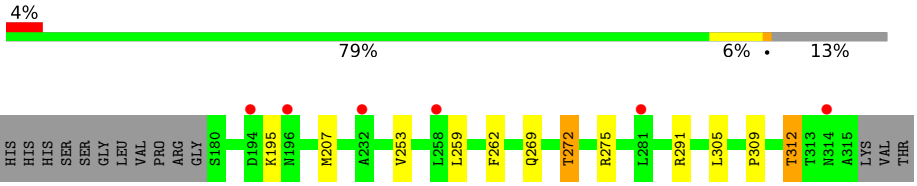
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	C	45	Total O 45 45	0	0
3	D	30	Total O 30 30	0	0
3	E	37	Total O 37 37	0	0
3	F	32	Total O 32 32	0	0

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.

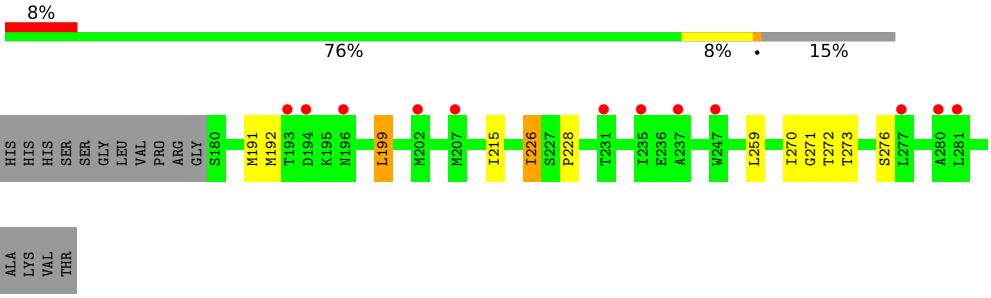
• Molecule 1: Ubiquitin carboxyl-terminal hydrolase 8

Chain A:



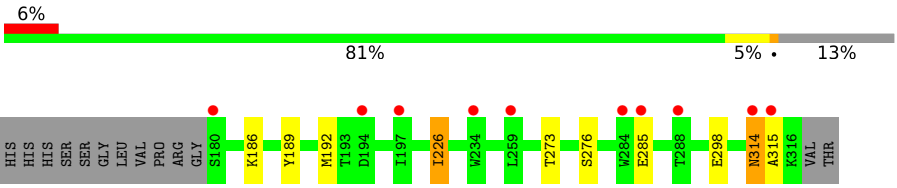
• Molecule 1: Ubiquitin carboxyl-terminal hydrolase 8

Chain C:



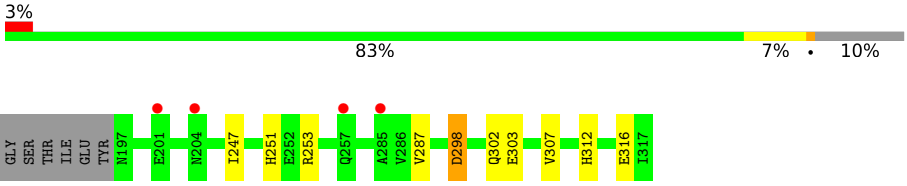
• Molecule 1: Ubiquitin carboxyl-terminal hydrolase 8

Chain E:



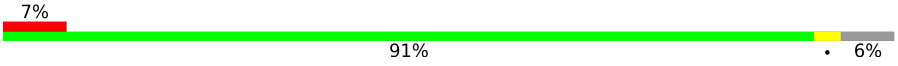
• Molecule 2: RING finger protein 41

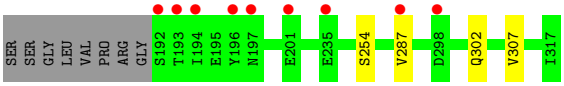
Chain B:



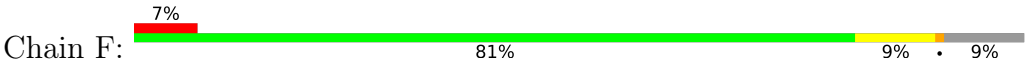
• Molecule 2: RING finger protein 41

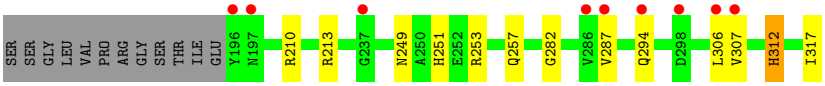
Chain D:





• Molecule 2: RING finger protein 41





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	76.11Å 67.09Å 99.28Å 90.00° 91.12° 90.00°	Depositor
Resolution (Å)	30.00 – 2.30 29.91 – 2.30	Depositor EDS
% Data completeness (in resolution range)	93.2 (30.00-2.30) 93.2 (29.91-2.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$< I/\sigma(I) >$ [1]	3.45 (at 2.31Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.206 , 0.237 0.201 , 0.235	Depositor DCC
R_{free} test set	2093 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å^2)	38.9	Xtriage
Anisotropy	0.131	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 47.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	0.019 for h,-k,-l	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	6388	wwPDB-VP
Average B, all atoms (Å^2)	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.51% 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	0.33	0/1112	0.59	0/1511
1	C	0.34	0/1099	0.58	0/1493
1	E	0.33	0/1121	0.60	0/1522
2	B	0.34	0/970	0.60	0/1316
2	D	0.33	0/1013	0.56	0/1375
2	F	0.34	0/983	0.60	0/1334
All	All	0.33	0/6298	0.59	0/8551

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	1088	0	1074	5	0
1	C	1075	0	1063	10	0
1	E	1097	0	1087	5	0
2	B	952	0	942	4	0
2	D	994	0	980	2	0
2	F	964	0	951	6	0
3	A	45	0	0	0	0
3	B	29	0	0	0	0
3	C	45	0	0	1	0
3	D	30	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	E	37	0	0	0	0
3	F	32	0	0	1	0
All	All	6388	0	6097	30	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.

All (30) 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:F:249:ASN:HB3	2:F:306:LEU:HD12	1.67	0.76
1:E:226:ILE:HD11	1:E:273:THR:HA	1.68	0.75
2:F:251:HIS:HD2	2:F:253:ARG:H	1.35	0.73
1:C:226:ILE:HD12	1:C:276:SER:HB2	1.74	0.70
2:B:251:HIS:HD2	2:B:253:ARG:H	1.40	0.69
1:C:226:ILE:CD1	1:C:276:SER:HB2	2.25	0.67
1:C:192:MET:HE1	1:C:215:ILE:HG21	1.79	0.65
1:E:226:ILE:HD13	1:E:276:SER:HB2	1.79	0.63
2:B:287:VAL:HG12	2:B:307:VAL:HG22	1.82	0.62
1:A:272:THR:HG22	1:A:275:ARG:H	1.68	0.58
1:C:284:TRP:HZ3	3:C:324:HOH:O	1.87	0.57
2:D:287:VAL:HG12	2:D:307:VAL:HG22	1.86	0.57
1:E:314:ASN:CG	1:E:315:ALA:HB2	2.27	0.55
1:C:226:ILE:HD11	1:C:273:THR:O	2.09	0.53
1:A:269:GLN:O	1:A:272:THR:HB	2.09	0.53
2:F:287:VAL:HG12	2:F:307:VAL:HG22	1.92	0.51
1:C:228:PRO:HG3	1:C:271:GLY:HA2	1.95	0.48
1:A:253:VAL:O	1:A:291:ARG:HD3	2.14	0.48
1:A:309:PRO:O	1:A:312:THR:HB	2.16	0.46
2:B:298:ASP:OD2	2:B:298:ASP:N	2.42	0.45
2:F:210:ARG:HB2	2:F:317:ILE:HD13	2.00	0.44
1:E:226:ILE:HG12	1:E:273:THR:HG23	2.00	0.43
1:C:191:MET:HE1	1:C:199:LEU:HB2	2.02	0.42
2:F:213:ARG:HD3	2:F:312:HIS:CD2	2.56	0.41
2:B:316:GLU:CD	2:F:282:GLY:HA2	2.41	0.41
2:D:254:SER:O	2:D:302:GLN:NE2	2.54	0.41
1:E:189:TYR:HA	1:E:192:MET:HE2	2.03	0.40
1:C:270:ILE:HG12	3:F:343:HOH:O	2.20	0.40
1:A:262:PHE:HZ	1:C:285:GLU:HB2	1.86	0.40
1:C:192:MET:HE3	1:C:304:TRP:CH2	2.57	0.40

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	134/157 (85%)	130 (97%)	3 (2%)	1 (1%)	22 26
1	C	132/157 (84%)	128 (97%)	4 (3%)	0	100 100
1	E	135/157 (86%)	128 (95%)	7 (5%)	0	100 100
2	B	119/134 (89%)	117 (98%)	2 (2%)	0	100 100
2	D	124/134 (92%)	122 (98%)	2 (2%)	0	100 100
2	F	120/134 (90%)	118 (98%)	2 (2%)	0	100 100
All	All	764/873 (88%)	743 (97%)	20 (3%)	1 (0%)	51 64

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	195	LYS

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	121/139 (87%)	116 (96%)	5 (4%)	30 43
1	C	120/139 (86%)	116 (97%)	4 (3%)	38 53
1	E	122/139 (88%)	117 (96%)	5 (4%)	30 43

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
2	B	103/114 (90%)	98 (95%)	5 (5%)	25 35
2	D	108/114 (95%)	108 (100%)	0	100 100
2	F	104/114 (91%)	101 (97%)	3 (3%)	42 58
All	All	678/759 (89%)	656 (97%)	22 (3%)	39 54

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	207	MET
1	A	259	LEU
1	A	272	THR
1	A	305	LEU
1	A	312	THR
2	B	247	ILE
2	B	298	ASP
2	B	302	GLN
2	B	303	GLU
2	B	312	HIS
1	C	199	LEU
1	C	226	ILE
1	C	259	LEU
1	C	272	THR
1	E	186	LYS
1	E	226	ILE
1	E	285	GLU
1	E	298	GLU
1	E	314	ASN
2	F	257	GLN
2	F	294	GLN
2	F	312	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	196	ASN
1	A	208	GLN
1	A	269	GLN
2	B	251	HIS
2	B	257	GLN
2	D	244	ASN

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Mol	Chain	Res	Type
1	E	314	ASN
2	F	244	ASN
2	F	251	HIS
2	F	266	GLN
2	F	312	HIS

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 monosaccharides in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

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, 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	136/157 (86%)	0.42	6 (4%)	34	41	18, 26, 39, 44	0
1	C	134/157 (85%)	0.50	12 (8%)	9	12	20, 26, 41, 53	0
1	E	137/157 (87%)	0.63	10 (7%)	15	20	20, 33, 49, 53	0
2	B	121/134 (90%)	0.30	4 (3%)	46	53	17, 29, 39, 43	0
2	D	126/134 (94%)	0.62	9 (7%)	16	21	20, 28, 50, 74	0
2	F	122/134 (91%)	0.40	9 (7%)	14	19	16, 26, 35, 43	0
All	All	776/873 (88%)	0.48	50 (6%)	19	25	16, 28, 44, 74	0

All (50) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	194	ILE	6.5
1	E	285	GLU	6.2
2	D	192	SER	6.0
1	C	194	ASP	5.3
2	F	196	TYR	5.2
2	D	298	ASP	4.6
1	C	196	ASN	4.4
2	D	193	THR	3.8
2	D	196	TYR	3.6
1	C	235	ILE	3.4
2	F	286	VAL	3.4
1	E	284	TRP	3.3
1	E	314	ASN	3.2
2	F	197	ASN	3.1
2	F	298	ASP	3.0
1	C	207	MET	2.9
1	A	232	ALA	2.8
1	E	288	THR	2.8
1	E	197	ILE	2.7

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Mol	Chain	Res	Type	RSRZ
2	D	197	ASN	2.7
2	D	201	GLU	2.7
1	E	259	LEU	2.6
1	E	194	ASP	2.6
1	E	180	SER	2.6
2	B	257	GLN	2.6
2	F	287	VAL	2.4
2	F	306	LEU	2.4
2	F	307	VAL	2.4
2	D	287	VAL	2.4
1	C	280	ALA	2.3
1	A	196	ASN	2.3
1	A	314	ASN	2.2
2	B	204	ASN	2.2
1	C	193	THR	2.2
1	C	231	THR	2.2
1	E	234	TRP	2.2
2	B	201	GLU	2.2
1	C	247	TRP	2.2
1	A	258	LEU	2.1
1	A	281	LEU	2.1
2	F	294	GLN	2.1
1	C	277	LEU	2.1
2	F	237	GLY	2.1
2	D	235	GLU	2.1
1	C	281	LEU	2.1
1	C	202	MET	2.1
1	E	315	ALA	2.1
1	C	237	ALA	2.0
2	B	285	ALA	2.0
1	A	194	ASP	2.0

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

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.