



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 17, 2021 – 02:06 AM BST

PDB ID : 6ERF
Title : Complex of APLF factor and Ku heterodimer bound to DNA
Authors : Nemoz, C.; Legrand, P.; Ropars, V.; Charbonnier, J.B.
Deposited on : 2017-10-18
Resolution : 3.01 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 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	:	2.20
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)	:	2.20

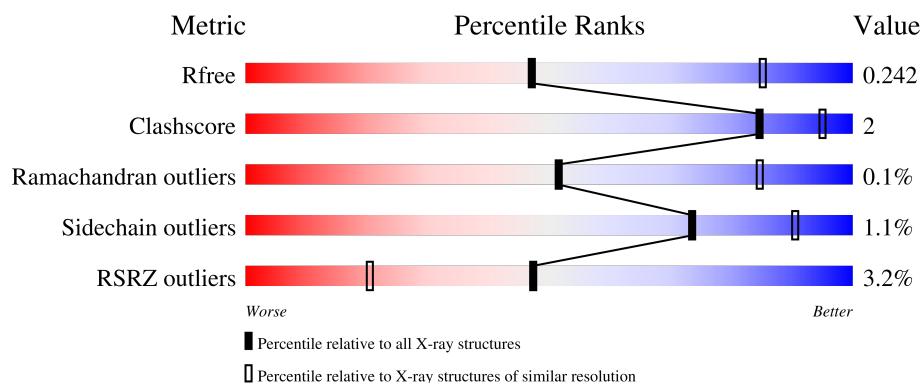
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.01 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	2399 (3.04-3.00)
Clashscore	141614	2734 (3.04-3.00)
Ramachandran outliers	138981	2640 (3.04-3.00)
Sidechain outliers	138945	2643 (3.04-3.00)
RSRZ outliers	127900	2287 (3.04-3.00)

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 $\leq 5\%$. 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	544	<div> <div>4%</div> <div>83%</div> <div>8%</div> <div>9%</div> </div>
1	C	544	<div> <div>4%</div> <div>85%</div> <div>6%</div> <div>8%</div> </div>
1	E	544	<div> <div>%</div> <div>85%</div> <div>7%</div> <div>9%</div> </div>
1	G	544	<div> <div>4%</div> <div>84%</div> <div>7%</div> <div>9%</div> </div>
2	B	572	<div> <div>2%</div> <div>85%</div> <div>6%</div> <div>9%</div> </div>

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Mol	Chain	Length	Quality of chain
2	D	572	
2	F	572	
2	H	572	
3	I	21	
3	K	21	
3	M	21	
3	O	21	
4	J	34	
4	L	34	
4	N	34	
4	P	34	
5	Q	18	
5	R	18	
5	S	18	
5	T	18	

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 35411 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 X-ray repair cross-complementing protein 6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	493	Total	C	N	O	S	0	0	0
			3988	2547	677	747	17			
1	C	500	Total	C	N	O	S	0	0	0
			4035	2578	684	756	17			
1	E	497	Total	C	N	O	S	0	0	0
			4016	2565	682	752	17			
1	G	495	Total	C	N	O	S	0	0	0
			4000	2557	678	748	17			

- Molecule 2 is a protein called X-ray repair cross-complementing protein 5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	521	Total	C	N	O	S	0	0	0
			4168	2666	701	778	23			
2	D	520	Total	C	N	O	S	0	0	0
			4168	2667	701	777	23			
2	F	526	Total	C	N	O	S	0	0	0
			4211	2697	707	784	23			
2	H	526	Total	C	N	O	S	0	0	0
			4211	2697	707	784	23			

There are 72 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-16	MET	-	initiating methionine	UNP P13010
B	-15	HIS	-	expression tag	UNP P13010
B	-14	HIS	-	expression tag	UNP P13010
B	-13	HIS	-	expression tag	UNP P13010
B	-12	HIS	-	expression tag	UNP P13010
B	-11	HIS	-	expression tag	UNP P13010
B	-10	HIS	-	expression tag	UNP P13010
B	-9	HIS	-	expression tag	UNP P13010

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-8	HIS	-	expression tag	UNP P13010
B	-7	HIS	-	expression tag	UNP P13010
B	-6	HIS	-	expression tag	UNP P13010
B	-5	GLU	-	expression tag	UNP P13010
B	-4	ASN	-	expression tag	UNP P13010
B	-3	LEU	-	expression tag	UNP P13010
B	-2	TYR	-	expression tag	UNP P13010
B	-1	PHE	-	expression tag	UNP P13010
B	0	GLN	-	expression tag	UNP P13010
B	1	GLY	-	expression tag	UNP P13010
D	-16	MET	-	initiating methionine	UNP P13010
D	-15	HIS	-	expression tag	UNP P13010
D	-14	HIS	-	expression tag	UNP P13010
D	-13	HIS	-	expression tag	UNP P13010
D	-12	HIS	-	expression tag	UNP P13010
D	-11	HIS	-	expression tag	UNP P13010
D	-10	HIS	-	expression tag	UNP P13010
D	-9	HIS	-	expression tag	UNP P13010
D	-8	HIS	-	expression tag	UNP P13010
D	-7	HIS	-	expression tag	UNP P13010
D	-6	HIS	-	expression tag	UNP P13010
D	-5	GLU	-	expression tag	UNP P13010
D	-4	ASN	-	expression tag	UNP P13010
D	-3	LEU	-	expression tag	UNP P13010
D	-2	TYR	-	expression tag	UNP P13010
D	-1	PHE	-	expression tag	UNP P13010
D	0	GLN	-	expression tag	UNP P13010
D	1	GLY	-	expression tag	UNP P13010
F	-16	MET	-	initiating methionine	UNP P13010
F	-15	HIS	-	expression tag	UNP P13010
F	-14	HIS	-	expression tag	UNP P13010
F	-13	HIS	-	expression tag	UNP P13010
F	-12	HIS	-	expression tag	UNP P13010
F	-11	HIS	-	expression tag	UNP P13010
F	-10	HIS	-	expression tag	UNP P13010
F	-9	HIS	-	expression tag	UNP P13010
F	-8	HIS	-	expression tag	UNP P13010
F	-7	HIS	-	expression tag	UNP P13010
F	-6	HIS	-	expression tag	UNP P13010
F	-5	GLU	-	expression tag	UNP P13010
F	-4	ASN	-	expression tag	UNP P13010
F	-3	LEU	-	expression tag	UNP P13010

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Chain	Residue	Modelled	Actual	Comment	Reference
F	-2	TYR	-	expression tag	UNP P13010
F	-1	PHE	-	expression tag	UNP P13010
F	0	GLN	-	expression tag	UNP P13010
F	1	GLY	-	expression tag	UNP P13010
H	-16	MET	-	initiating methionine	UNP P13010
H	-15	HIS	-	expression tag	UNP P13010
H	-14	HIS	-	expression tag	UNP P13010
H	-13	HIS	-	expression tag	UNP P13010
H	-12	HIS	-	expression tag	UNP P13010
H	-11	HIS	-	expression tag	UNP P13010
H	-10	HIS	-	expression tag	UNP P13010
H	-9	HIS	-	expression tag	UNP P13010
H	-8	HIS	-	expression tag	UNP P13010
H	-7	HIS	-	expression tag	UNP P13010
H	-6	HIS	-	expression tag	UNP P13010
H	-5	GLU	-	expression tag	UNP P13010
H	-4	ASN	-	expression tag	UNP P13010
H	-3	LEU	-	expression tag	UNP P13010
H	-2	TYR	-	expression tag	UNP P13010
H	-1	PHE	-	expression tag	UNP P13010
H	0	GLN	-	expression tag	UNP P13010
H	1	GLY	-	expression tag	UNP P13010

- Molecule 3 is a DNA chain called DNA (5'-D(*GP*TP*TP*TP*TP*TP*AP*GP*TP*TP*TP*AP*TP*TP*GP*GP*GP*CP*GP*CP*G)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	I	14	Total	C	N	O	P	0	0	0
			286	140	40	92	14			
3	K	13	Total	C	N	O	P	0	0	0
			268	130	41	84	13			
3	M	13	Total	C	N	O	P	0	0	0
			268	130	41	84	13			
3	O	14	Total	C	N	O	P	0	0	0
			286	140	40	92	14			

- Molecule 4 is a DNA chain called DNA (34-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	J	12	Total	C	N	O	P	0	0	0
			248	119	52	65	12			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	L	10	Total	C	N	O	P	0	0	0
			206	99	42	55	10			
4	N	14	Total	C	N	O	P	0	0	0
			289	139	59	77	14			
4	P	16	Total	C	N	O	P	0	0	0
			327	157	65	89	16			

- Molecule 5 is a protein called Aprataxin and PNK-like factor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	Q	12	Total	C	N	O	S	0	0	0
			105	69	20	15	1			
5	R	13	Total	C	N	O	S	0	0	0
			113	75	21	16	1			
5	S	12	Total	C	N	O	S	0	0	0
			105	69	20	15	1			
5	T	12	Total	C	N	O	S	0	0	0
			105	69	20	15	1			

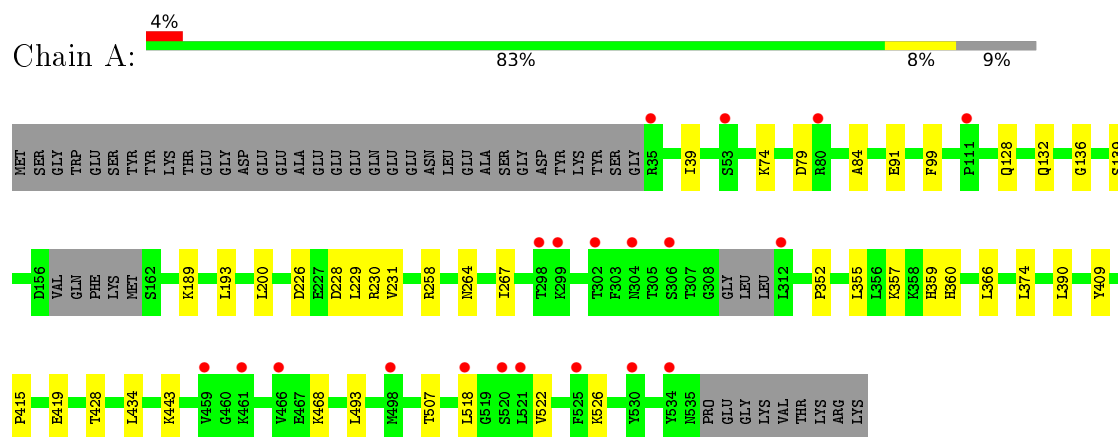
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	B	1	Total	O	0	0
			1	1		
6	E	1	Total	O	1	0
			1	1		
6	F	2	Total	O	0	0
			2	2		
6	G	2	Total	O	0	0
			2	2		
6	H	2	Total	O	0	0
			2	2		

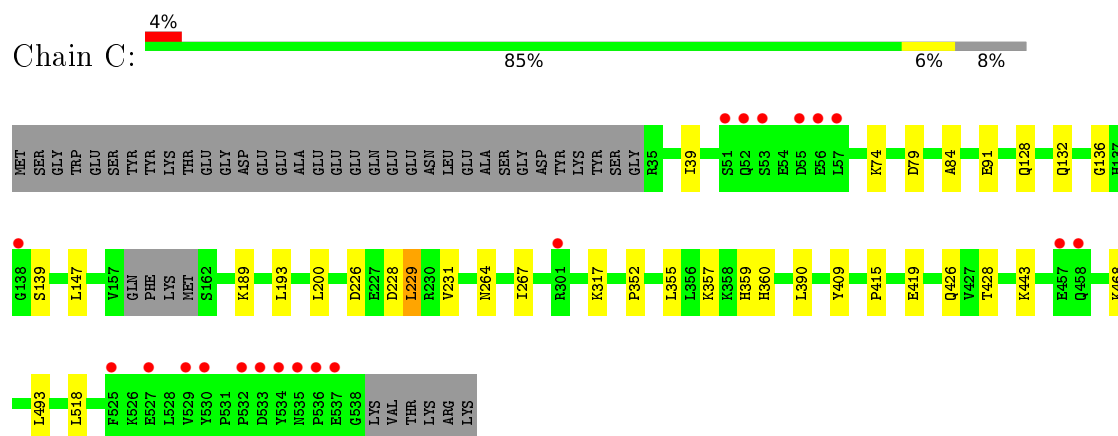
3 Residue-property plots [i](#)

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.

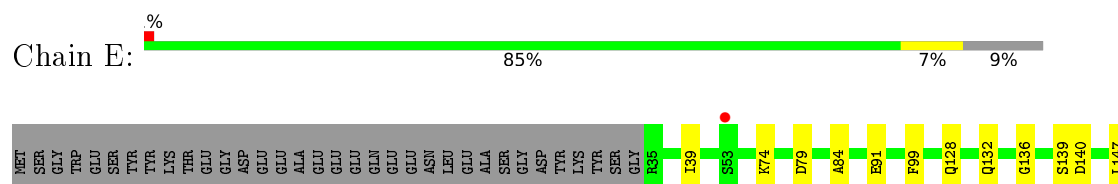
- Molecule 1: X-ray repair cross-complementing protein 6

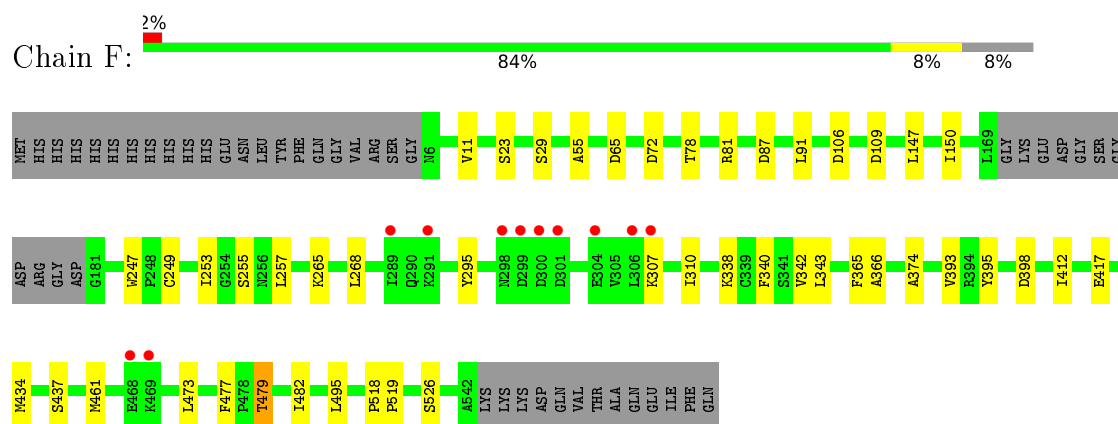


- Molecule 1: X-ray repair cross-complementing protein 6

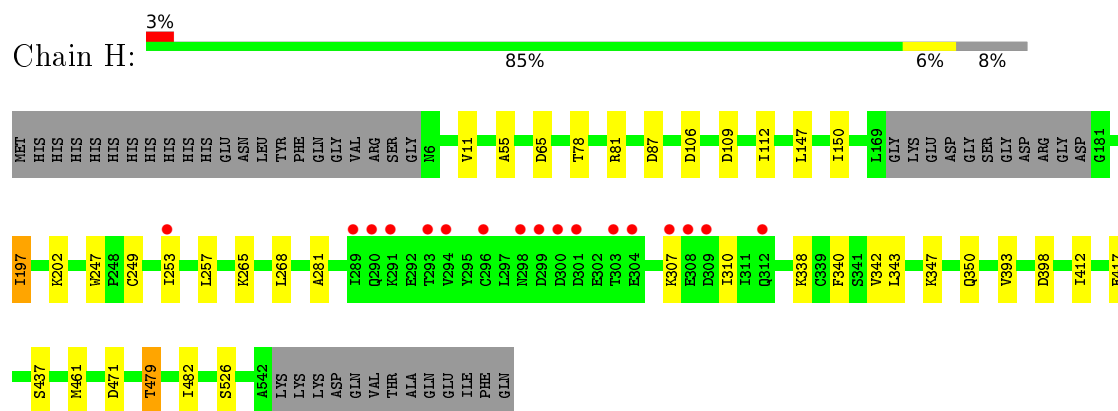


- Molecule 1: X-ray repair cross-complementing protein 6





- Molecule 2: X-ray repair cross-complementing protein 5



- Molecule 3: DNA (5'-D(*GP*TP*TP*TP*TP*TP*AP*GP*TP*TP*TP*AP*TP*TP*GP*GP*GP*CP*GP*CP*G)-3')

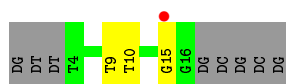


- Molecule 3: DNA (5'-D(*GP*TP*TP*TP*TP*TP*AP*GP*TP*TP*TP*AP*TP*TP*GP*GP*GP*CP*GP*CP*G)-3')

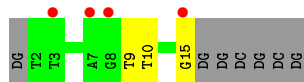


- Molecule 3: DNA (5'-D(*GP*TP*TP*TP*TP*TP*AP*GP*TP*TP*TP*AP*TP*TP*GP*GP*GP*CP*GP*CP*G)-3')

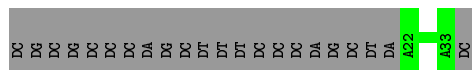




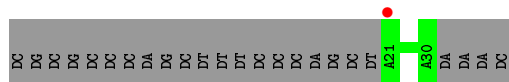
- Molecule 3: DNA (5'-D(*GP*TP*TP*TP*TP*TP*AP*GP*TP*TP*TP*AP*TP*TP*GP*GP*GP*CP*GP*CP*G)-3')



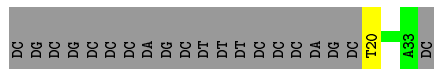
- Molecule 4: DNA (34-MER)



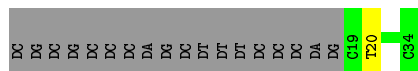
- Molecule 4: DNA (34-MER)



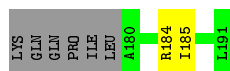
- Molecule 4: DNA (34-MER)



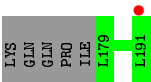
- Molecule 4: DNA (34-MER)



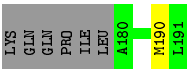
- Molecule 5: Aprataxin and PNK-like factor



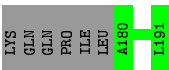
- Molecule 5: Aprataxin and PNK-like factor



● Molecule 5: Aprataxin and PNK-like factor



● Molecule 5: Aprataxin and PNK-like factor



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	98.92Å 140.86Å 150.31Å 68.64° 80.85° 81.23°	Depositor
Resolution (Å)	49.47 – 3.01 49.46 – 3.08	Depositor EDS
% Data completeness (in resolution range)	61.9 (49.47-3.01) 66.1 (49.46-3.08)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.12 (at 3.07Å)	Xtriage
Refinement program	BUSTER 2.10.3	Depositor
R, R_{free}	0.209 , 0.227 0.221 , 0.242	Depositor DCC
R_{free} test set	4537 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	97.5	Xtriage
Anisotropy	0.009	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 65.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	35411	wwPDB-VP
Average B, all atoms (Å ²)	121.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.51% 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	0.37	0/4064	0.58	0/5474
1	C	0.38	0/4113	0.58	0/5543
1	E	0.38	0/4092	0.59	0/5512
1	G	0.37	0/4077	0.59	0/5493
2	B	0.38	0/4251	0.58	0/5734
2	D	0.37	0/4251	0.57	0/5732
2	F	0.37	0/4298	0.58	0/5800
2	H	0.37	0/4298	0.58	0/5800
3	I	1.06	0/317	1.13	0/488
3	K	1.10	0/298	1.15	0/459
3	M	1.11	0/298	1.14	0/459
3	O	1.08	0/317	1.14	0/488
4	J	0.89	0/280	0.98	0/429
4	L	0.94	0/232	1.01	0/355
4	N	0.94	0/326	1.00	0/500
4	P	0.96	0/368	1.02	0/564
5	Q	0.35	0/107	0.55	0/143
5	R	0.40	0/115	0.60	0/154
5	S	0.34	0/107	0.56	0/143
5	T	0.33	0/107	0.55	0/143
All	All	0.45	0/36316	0.63	0/49413

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	3988	0	4053	20	0
1	C	4035	0	4104	21	0
1	E	4016	0	4084	19	0
1	G	4000	0	4073	19	0
2	B	4168	0	4199	21	0
2	D	4168	0	4210	20	0
2	F	4211	0	4252	27	0
2	H	4211	0	4252	20	0
3	I	286	0	165	1	0
3	K	268	0	152	1	0
3	M	268	0	152	2	0
3	O	286	0	165	2	0
4	J	248	0	135	0	0
4	L	206	0	113	0	0
4	N	289	0	158	1	0
4	P	327	0	180	1	0
5	Q	105	0	115	3	0
5	R	113	0	126	0	0
5	S	105	0	115	1	0
5	T	105	0	115	0	0
6	B	1	0	0	0	0
6	E	1	0	0	0	0
6	F	2	0	0	0	0
6	G	2	0	0	0	0
6	H	2	0	0	0	0
All	All	35411	0	34918	159	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 (159) 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)
3:M:15:DG:H1	4:N:20:DT:H3	1.22	0.87
3:O:15:DG:H1	4:P:20:DT:H3	1.22	0.84
1:C:228:ASP:HB3	2:D:437:SER:HB2	1.63	0.81
2:D:467:ASP:HB3	2:D:470:THR:HG22	1.64	0.80
2:H:347:LYS:HG2	2:H:350:GLN:HE21	1.51	0.75
2:B:73:GLN:HG2	5:Q:185:ILE:HG22	1.71	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:106:ASP:HB3	2:B:109:ASP:HB2	1.75	0.69
2:H:106:ASP:HB3	2:H:109:ASP:HB2	1.75	0.69
2:F:106:ASP:HB3	2:F:109:ASP:HB2	1.76	0.68
1:A:390:LEU:HG	1:A:415:PRO:HB2	1.78	0.65
2:D:106:ASP:HB3	2:D:109:ASP:HB2	1.77	0.65
1:G:390:LEU:HG	1:G:415:PRO:HB2	1.79	0.65
2:B:73:GLN:NE2	5:Q:184:ARG:HA	2.13	0.64
1:C:390:LEU:HG	1:C:415:PRO:HB2	1.79	0.64
1:E:390:LEU:HG	1:E:415:PRO:HB2	1.79	0.64
1:A:357:LYS:HB2	1:A:360:HIS:HD2	1.64	0.63
1:E:357:LYS:HB2	1:E:360:HIS:HD2	1.62	0.63
1:C:357:LYS:HB2	1:C:360:HIS:HD2	1.64	0.62
1:A:522:VAL:HG12	1:A:526:LYS:HE2	1.81	0.62
1:G:357:LYS:HB2	1:G:360:HIS:HD2	1.64	0.61
2:F:461:MET:HG3	2:F:526:SER:HB3	1.84	0.60
1:C:426:GLN:HE22	2:D:435:PHE:H	1.49	0.59
2:H:65:ASP:HB3	2:H:78:THR:HG23	1.85	0.58
2:H:461:MET:HG3	2:H:526:SER:HB3	1.85	0.58
2:D:65:ASP:HB3	2:D:78:THR:HG23	1.86	0.57
2:F:65:ASP:HB3	2:F:78:THR:HG23	1.85	0.57
2:B:65:ASP:HB3	2:B:78:THR:HG23	1.87	0.57
2:B:73:GLN:HE21	5:Q:184:ARG:HA	1.70	0.56
2:D:461:MET:HG3	2:D:526:SER:HB3	1.85	0.56
2:B:461:MET:HG3	2:B:526:SER:HB3	1.87	0.56
1:A:39:ILE:HG12	1:A:84:ALA:HB3	1.89	0.55
1:A:357:LYS:HB2	1:A:360:HIS:CD2	2.42	0.54
1:E:39:ILE:HG12	1:E:84:ALA:HB3	1.89	0.54
1:G:39:ILE:HG12	1:G:84:ALA:HB3	1.90	0.54
1:A:507:THR:O	2:B:343:LEU:HD21	2.08	0.53
1:C:39:ILE:HG12	1:C:84:ALA:HB3	1.89	0.53
1:E:352:PRO:HD2	1:E:355:LEU:HD12	1.91	0.53
1:G:228:ASP:HB3	2:H:437:SER:HB2	1.90	0.53
2:H:11:VAL:HG22	2:H:55:ALA:HB3	1.90	0.53
2:B:477:PHE:CE1	2:B:518:PRO:HA	2.44	0.53
2:D:477:PHE:CE1	2:D:518:PRO:HA	2.44	0.52
2:F:11:VAL:HG22	2:F:55:ALA:HB3	1.92	0.52
2:F:477:PHE:CE1	2:F:518:PRO:HA	2.44	0.52
1:C:352:PRO:HD2	1:C:355:LEU:HD12	1.92	0.51
1:C:357:LYS:HB2	1:C:360:HIS:CD2	2.45	0.51
2:D:470:THR:HG23	2:D:472:THR:H	1.75	0.51
2:B:11:VAL:HG22	2:B:55:ALA:HB3	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:197:ILE:HG22	2:H:202:LYS:HG3	1.92	0.50
1:G:352:PRO:HD2	1:G:355:LEU:HD12	1.93	0.50
2:D:11:VAL:HG22	2:D:55:ALA:HB3	1.93	0.50
1:A:226:ASP:HB2	1:A:229:LEU:HB2	1.94	0.50
1:E:360:HIS:HE1	1:E:443:LYS:HE3	1.78	0.49
1:G:507:THR:O	2:H:343:LEU:HD21	2.12	0.49
2:D:265:LYS:HD3	2:D:268:LEU:HD13	1.94	0.49
1:E:357:LYS:HB2	1:E:360:HIS:CD2	2.44	0.48
1:A:264:ASN:HD22	1:A:267:ILE:HD12	1.78	0.48
1:E:228:ASP:HB3	2:F:437:SER:HB3	1.95	0.48
2:D:338:LYS:HB3	2:D:398:ASP:HA	1.96	0.48
2:H:253:ILE:HB	2:H:257:LEU:HD23	1.95	0.48
1:A:352:PRO:HD2	1:A:355:LEU:HD12	1.94	0.47
2:F:479:THR:HA	2:F:482:ILE:HD12	1.96	0.47
1:G:357:LYS:HB2	1:G:360:HIS:CD2	2.46	0.47
2:H:265:LYS:HD3	2:H:268:LEU:HD13	1.96	0.47
2:B:147:LEU:HA	2:B:150:ILE:HD12	1.95	0.47
1:E:91:GLU:HB2	1:E:136:GLY:HA3	1.95	0.47
2:D:253:ILE:HB	2:D:257:LEU:HD23	1.95	0.47
2:D:147:LEU:HA	2:D:150:ILE:HD12	1.96	0.47
1:E:264:ASN:HD22	1:E:267:ILE:HD12	1.80	0.47
2:F:147:LEU:HA	2:F:150:ILE:HD12	1.96	0.47
2:H:147:LEU:HA	2:H:150:ILE:HD12	1.97	0.47
2:F:338:LYS:HB3	2:F:398:ASP:HA	1.96	0.47
1:C:264:ASN:HD22	1:C:267:ILE:HD12	1.80	0.47
1:C:360:HIS:HE1	1:C:443:LYS:HE3	1.79	0.47
1:C:91:GLU:HB2	1:C:136:GLY:HA3	1.97	0.46
1:A:419:GLU:HB3	1:A:428:THR:HB	1.96	0.46
1:E:511:VAL:HG13	2:F:255:SER:HB3	1.96	0.46
2:F:253:ILE:HB	2:F:257:LEU:HD23	1.98	0.46
2:F:265:LYS:HD3	2:F:268:LEU:HD13	1.97	0.46
3:M:9:DT:H2"	3:M:10:DT:C6	2.50	0.46
2:B:253:ILE:HB	2:B:257:LEU:HD23	1.98	0.46
1:E:419:GLU:HB3	1:E:428:THR:HB	1.97	0.46
2:B:265:LYS:HD3	2:B:268:LEU:HD13	1.96	0.46
1:C:317:LYS:HD2	2:D:281:ALA:HA	1.96	0.46
1:C:419:GLU:HB3	1:C:428:THR:HB	1.97	0.45
1:E:352:PRO:HG2	2:F:473:LEU:HD21	1.99	0.45
1:A:228:ASP:HB3	2:B:437:SER:HB2	1.97	0.45
1:G:74:LYS:HD3	1:G:79:ASP:HB2	1.99	0.45
1:A:91:GLU:HB2	1:A:136:GLY:HA3	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:338:LYS:HB3	2:H:398:ASP:HA	1.99	0.45
1:A:193:LEU:HD12	1:A:200:LEU:HD11	1.98	0.45
1:E:128:GLN:O	1:E:132:GLN:HG2	2.17	0.45
2:F:412:ILE:HG23	2:F:417:GLU:HG3	1.99	0.44
1:G:91:GLU:HB2	1:G:136:GLY:HA3	1.99	0.44
1:A:74:LYS:HD3	1:A:79:ASP:HB2	1.99	0.44
1:E:74:LYS:HD3	1:E:79:ASP:HB2	1.98	0.44
3:K:9:DT:H2"	3:K:10:DT:C6	2.53	0.44
1:A:189:LYS:HD2	1:A:189:LYS:HA	1.89	0.44
1:C:147:LEU:HB3	1:C:193:LEU:HD11	1.99	0.44
1:G:264:ASN:HD22	1:G:267:ILE:HD12	1.81	0.44
1:G:360:HIS:HE1	1:G:443:LYS:HE3	1.83	0.44
2:H:479:THR:HA	2:H:482:ILE:HD12	1.98	0.44
1:A:128:GLN:O	1:A:132:GLN:HG2	2.18	0.44
3:I:9:DT:H2"	3:I:10:DT:C6	2.53	0.44
2:B:479:THR:HA	2:B:482:ILE:HD12	2.00	0.43
1:E:193:LEU:HD12	1:E:200:LEU:HD11	2.00	0.43
2:F:477:PHE:HD1	2:F:519:PRO:HD3	1.83	0.43
3:O:9:DT:H2"	3:O:10:DT:C6	2.52	0.43
1:C:128:GLN:O	1:C:132:GLN:HG2	2.18	0.43
1:C:189:LYS:HA	1:C:189:LYS:HD2	1.89	0.43
1:E:189:LYS:HA	1:E:189:LYS:HD2	1.89	0.43
2:D:477:PHE:HD1	2:D:519:PRO:HD3	1.83	0.43
1:G:419:GLU:HB3	1:G:428:THR:HB	2.00	0.43
2:D:247:TRP:HZ3	2:D:249:CYS:HB2	1.83	0.43
2:B:477:PHE:HD1	2:B:519:PRO:HD3	1.82	0.43
1:G:57:LEU:HB3	1:G:61:ASP:HB3	2.01	0.43
1:G:128:GLN:O	1:G:132:GLN:HG2	2.18	0.43
1:C:74:LYS:HD3	1:C:79:ASP:HB2	2.00	0.43
2:F:81:ARG:HH22	2:F:87:ASP:CG	2.22	0.43
1:C:193:LEU:HD12	1:C:200:LEU:HD11	2.01	0.43
1:E:446:MET:SD	2:F:365:PHE:CZ	3.12	0.43
2:H:412:ILE:HG23	2:H:417:GLU:HG3	2.01	0.43
1:G:366:LEU:HD12	1:G:434:LEU:HD22	2.00	0.42
1:C:468:LYS:CB	1:C:518:LEU:HD21	2.50	0.42
1:A:360:HIS:HE1	1:A:443:LYS:HE3	1.84	0.42
2:H:342:VAL:HA	2:H:393:VAL:HG12	2.01	0.42
2:F:247:TRP:HH2	2:F:395:TYR:HE1	1.67	0.42
1:C:352:PRO:HG2	2:D:473:LEU:HD21	2.02	0.42
1:G:189:LYS:HD2	1:G:189:LYS:HA	1.89	0.42
1:G:259:LEU:HD12	1:G:273:ILE:HG13	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:412:ILE:HG23	2:B:417:GLU:HG3	2.02	0.42
2:F:342:VAL:HA	2:F:393:VAL:HG12	2.02	0.42
1:E:147:LEU:HB3	1:E:193:LEU:HD11	2.02	0.42
1:A:468:LYS:CB	1:A:518:LEU:HD21	2.50	0.41
1:G:317:LYS:HD2	2:H:281:ALA:HA	2.02	0.41
2:B:338:LYS:HB3	2:B:398:ASP:HA	2.01	0.41
1:E:507:THR:O	2:F:343:LEU:HD21	2.20	0.41
2:F:23:SER:HB3	2:F:29:SER:HB3	2.01	0.41
2:F:150:ILE:HA	5:S:190:MET:HE3	2.01	0.41
2:F:307:LYS:HA	2:F:310:ILE:HD12	2.03	0.41
2:B:81:ARG:HH22	2:B:87:ASP:CG	2.24	0.41
1:C:360:HIS:CE1	1:C:443:LYS:HE3	2.56	0.41
1:G:147:LEU:HB3	1:G:193:LEU:HD11	2.02	0.41
1:A:258:ARG:HD3	1:A:374:LEU:HD11	2.02	0.41
2:D:412:ILE:HG23	2:D:417:GLU:HG3	2.02	0.41
2:B:307:LYS:HA	2:B:310:ILE:HD12	2.03	0.41
2:B:342:VAL:HA	2:B:393:VAL:HG12	2.02	0.41
2:F:295:TYR:HE2	2:F:307:LYS:HE3	1.86	0.41
2:H:247:TRP:HZ3	2:H:249:CYS:HB2	1.86	0.41
1:A:366:LEU:HD12	1:A:434:LEU:HD22	2.03	0.41
2:D:479:THR:HA	2:D:482:ILE:HD12	2.02	0.41
2:F:247:TRP:HZ3	2:F:249:CYS:HB2	1.85	0.41
2:F:366:ALA:HB1	2:F:374:ALA:HA	2.03	0.41
2:H:112:ILE:HD11	2:H:150:ILE:HD11	2.02	0.41
2:D:407:VAL:HB	2:D:424:LEU:HD11	2.03	0.40
2:H:81:ARG:HH22	2:H:87:ASP:CG	2.24	0.40
2:F:91:LEU:HD13	2:F:495:LEU:HD13	2.04	0.40
2:B:112:ILE:HD11	2:B:150:ILE:HD11	2.04	0.40
2:H:307:LYS:HA	2:H:310:ILE:HD12	2.04	0.40
1:C:226:ASP:HB2	1:C:229:LEU:HB2	2.04	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	487/544 (90%)	474 (97%)	12 (2%)	1 (0%)	47	81
1	C	496/544 (91%)	484 (98%)	11 (2%)	1 (0%)	47	81
1	E	491/544 (90%)	477 (97%)	13 (3%)	1 (0%)	47	81
1	G	491/544 (90%)	479 (98%)	11 (2%)	1 (0%)	47	81
2	B	515/572 (90%)	505 (98%)	10 (2%)	0	100	100
2	D	514/572 (90%)	503 (98%)	11 (2%)	0	100	100
2	F	522/572 (91%)	514 (98%)	8 (2%)	0	100	100
2	H	522/572 (91%)	512 (98%)	10 (2%)	0	100	100
5	Q	10/18 (56%)	10 (100%)	0	0	100	100
5	R	11/18 (61%)	10 (91%)	1 (9%)	0	100	100
5	S	10/18 (56%)	10 (100%)	0	0	100	100
5	T	10/18 (56%)	10 (100%)	0	0	100	100
All	All	4079/4536 (90%)	3988 (98%)	87 (2%)	4 (0%)	51	85

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	359	HIS
1	C	359	HIS
1	E	359	HIS
1	G	359	HIS

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	449/492 (91%)	443 (99%)	6 (1%)	69	88
1	C	454/492 (92%)	449 (99%)	5 (1%)	73	90
1	E	452/492 (92%)	444 (98%)	8 (2%)	59	84

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	G	450/492 (92%)	444 (99%)	6 (1%)	69	88
2	B	468/513 (91%)	463 (99%)	5 (1%)	73	90
2	D	469/513 (91%)	466 (99%)	3 (1%)	86	95
2	F	474/513 (92%)	470 (99%)	4 (1%)	81	93
2	H	474/513 (92%)	470 (99%)	4 (1%)	81	93
5	Q	11/17 (65%)	11 (100%)	0	100	100
5	R	12/17 (71%)	12 (100%)	0	100	100
5	S	11/17 (65%)	11 (100%)	0	100	100
5	T	11/17 (65%)	11 (100%)	0	100	100
All	All	3735/4088 (91%)	3694 (99%)	41 (1%)	73	90

All (41) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	99	PHE
1	A	139	SER
1	A	230	ARG
1	A	231	VAL
1	A	409	TYR
1	A	493	LEU
2	B	72	ASP
2	B	73	GLN
2	B	236	VAL
2	B	340	PHE
2	B	479	THR
1	C	139	SER
1	C	229	LEU
1	C	231	VAL
1	C	409	TYR
1	C	493	LEU
2	D	72	ASP
2	D	340	PHE
2	D	479	THR
1	E	99	PHE
1	E	139	SER
1	E	140	ASP
1	E	229	LEU
1	E	231	VAL
1	E	409	TYR

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Mol	Chain	Res	Type
1	E	493	LEU
1	E	518	LEU
2	F	72	ASP
2	F	340	PHE
2	F	434	MET
2	F	479	THR
1	G	99	PHE
1	G	139	SER
1	G	229	LEU
1	G	409	TYR
1	G	493	LEU
1	G	518	LEU
2	H	197	ILE
2	H	340	PHE
2	H	471	ASP
2	H	479	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	264	ASN
1	A	360	HIS
1	C	101	ASN
1	C	264	ASN
1	C	360	HIS
1	C	423	GLN
1	C	426	GLN
1	E	101	ASN
1	E	264	ASN
1	E	360	HIS
1	G	101	ASN
1	G	264	ASN
1	G	360	HIS
2	H	104	GLN

5.3.3 RNA ⓘ

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, 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	493/544 (90%)	0.05	20 (4%)	37	15	58, 121, 205, 236	0
1	C	500/544 (91%)	0.06	20 (4%)	38	15	66, 121, 189, 202	0
1	E	497/544 (91%)	-0.08	8 (1%)	72	43	60, 112, 171, 233	0
1	G	495/544 (90%)	0.05	22 (4%)	34	13	62, 123, 194, 217	0
2	B	521/572 (91%)	0.04	13 (2%)	57	28	53, 103, 201, 237	0
2	D	520/572 (90%)	-0.04	11 (2%)	63	34	54, 98, 182, 234	0
2	F	526/572 (91%)	-0.09	11 (2%)	63	34	56, 88, 167, 229	0
2	H	526/572 (91%)	0.01	17 (3%)	47	20	47, 106, 181, 225	0
3	I	14/21 (66%)	0.76	2 (14%)	2	1	180, 215, 256, 260	0
3	K	13/21 (61%)	1.45	4 (30%)	0	0	145, 191, 250, 251	0
3	M	13/21 (61%)	0.68	1 (7%)	13	4	150, 183, 234, 239	0
3	O	14/21 (66%)	1.20	4 (28%)	0	0	184, 217, 255, 258	0
4	J	12/34 (35%)	0.24	0	100	100	207, 213, 223, 236	0
4	L	10/34 (29%)	0.66	1 (10%)	7	2	162, 180, 196, 211	0
4	N	14/34 (41%)	-0.02	0	100	100	146, 181, 212, 219	0
4	P	16/34 (47%)	0.61	0	100	100	182, 202, 236, 237	0
5	Q	12/18 (66%)	-0.19	0	100	100	99, 105, 128, 135	0
5	R	13/18 (72%)	-0.12	1 (7%)	13	4	83, 89, 126, 137	0
5	S	12/18 (66%)	-0.21	0	100	100	86, 92, 118, 120	0
5	T	12/18 (66%)	-0.23	0	100	100	94, 96, 117, 119	0
All	All	4233/4756 (89%)	0.02	135 (3%)	47	20	47, 110, 200, 260	0

All (135) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	H	298	ASN	5.9
2	H	301	ASP	5.4
2	D	293	THR	5.4
2	F	304	GLU	5.3
2	H	300	ASP	5.2
2	B	291	LYS	5.1
2	F	300	ASP	4.8
1	C	53	SER	4.5
1	A	53	SER	4.5
2	B	295	TYR	4.5
2	H	291	LYS	4.1
2	F	291	LYS	4.0
1	G	501	GLU	4.0
2	F	298	ASN	4.0
1	A	530	TYR	4.0
2	B	254	GLY	3.9
2	H	304	GLU	3.9
1	A	518	LEU	3.8
2	B	298	ASN	3.8
3	I	15	DG	3.8
1	E	302	THR	3.7
1	G	525	PHE	3.7
2	F	289	ILE	3.7
2	H	307	LYS	3.7
1	C	535	ASN	3.6
2	F	307	LYS	3.6
2	D	189	GLY	3.5
2	F	306	LEU	3.5
2	B	257	LEU	3.5
1	C	55	ASP	3.5
2	D	307	LYS	3.5
4	L	21	DA	3.4
2	D	310	ILE	3.4
2	B	294	VAL	3.2
1	C	527	GLU	3.2
2	D	400	ARG	3.2
2	B	300	ASP	3.2
1	C	525	PHE	3.2
2	H	309	ASP	3.2
1	G	301	ARG	3.2
1	C	534	TYR	3.2
1	G	306	SER	3.1
1	A	299	LYS	3.1

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Mol	Chain	Res	Type	RSRZ
2	D	294	VAL	3.1
1	E	312	LEU	3.1
3	K	15	DG	3.1
1	G	289	TYR	3.1
1	E	501	GLU	3.1
1	A	298	THR	3.0
1	A	302	THR	3.0
1	C	537	GLU	3.0
1	A	466	VAL	3.0
1	E	53	SER	3.0
2	H	289	ILE	2.9
1	C	457	GLU	2.9
2	H	303	THR	2.9
1	C	529	VAL	2.9
1	A	306	SER	2.8
2	H	308	GLU	2.8
1	E	289	TYR	2.8
1	C	536	PRO	2.8
1	C	530	TYR	2.8
2	B	299	ASP	2.8
1	G	365	SER	2.8
1	A	459	VAL	2.8
3	K	14	DT	2.7
2	F	299	ASP	2.7
1	A	525	PHE	2.7
2	B	304	GLU	2.7
1	G	304	ASN	2.7
2	H	299	ASP	2.7
2	B	469	LYS	2.7
3	O	3	DT	2.7
1	C	51	SER	2.6
1	E	306	SER	2.6
1	G	299	LYS	2.6
2	H	294	VAL	2.6
2	B	253	ILE	2.6
1	A	534	TYR	2.6
1	C	301	ARG	2.6
1	G	241	ASP	2.6
1	C	532	PRO	2.6
2	D	296	CYS	2.6
3	K	16	DG	2.5
1	A	520	SER	2.5

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Mol	Chain	Res	Type	RSRZ
2	D	295	TYR	2.5
1	C	52	GLN	2.5
3	O	15	DG	2.5
1	G	292	THR	2.4
1	G	307	THR	2.4
1	A	35	ARG	2.4
1	A	461	LYS	2.4
1	G	466	VAL	2.4
2	D	304	GLU	2.4
3	O	7	DA	2.4
1	G	529	VAL	2.4
1	G	305	THR	2.4
2	H	293	THR	2.4
2	D	309	ASP	2.4
1	C	57	LEU	2.3
1	G	205	LEU	2.3
1	A	304	ASN	2.3
1	G	240	GLU	2.3
2	B	329	GLU	2.3
1	A	312	LEU	2.3
2	F	469	LYS	2.3
1	C	533	ASP	2.2
1	G	295	PRO	2.2
1	G	206	LYS	2.2
1	E	313	PRO	2.2
2	H	312	GLN	2.2
1	G	303	PHE	2.2
1	C	56	GLU	2.2
2	B	323	PHE	2.2
2	F	301	ASP	2.2
2	F	468	GLU	2.2
1	A	80	ARG	2.2
1	A	111	PRO	2.1
3	O	8	DG	2.1
3	I	14	DT	2.1
1	G	527	GLU	2.1
1	G	291	GLU	2.1
3	K	12	DA	2.1
1	A	498	MET	2.1
1	G	452	ILE	2.1
1	C	138	GLY	2.1
2	H	290	GLN	2.1

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Mol	Chain	Res	Type	RSRZ
2	H	296	CYS	2.1
1	E	304	ASN	2.1
3	M	15	DG	2.1
5	R	191	LEU	2.1
1	A	521	LEU	2.1
2	H	253	ILE	2.1
1	C	458	GLN	2.0
2	D	308	GLU	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 [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.