



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 04:47 PM UTC

PDB ID : 6NQ3 / pdb_00006nq3
Title : Crystal Structure of a SUZ12-RBBP4-PHF19-JARID2 Heterotetrameric Complex
Authors : Chen, S.; Jiao, L.; Liu, X.
Deposited on : 2019-01-19
Resolution : 2.89 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:

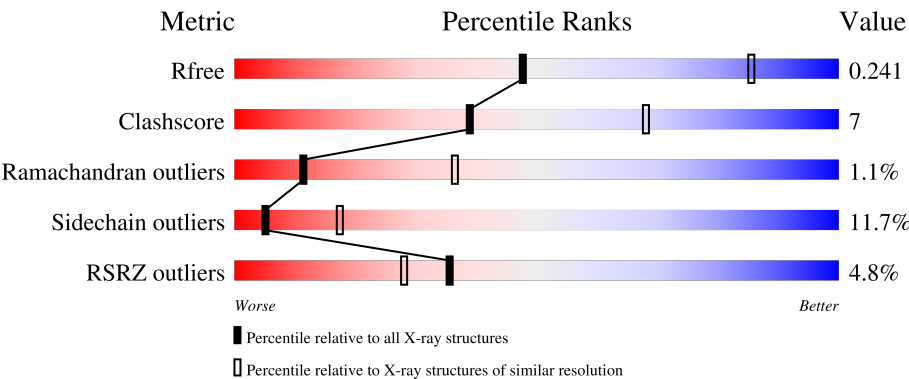
MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

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 2.89 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.



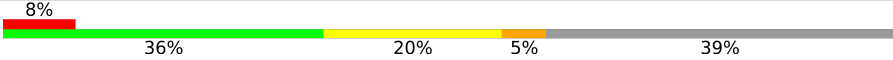
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	2481 (2.90-2.90)
Clashscore	190562	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (2.90-2.90)
RSRZ outliers	180081	2481 (2.90-2.90)

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	439	64%19%13%
1	E	439	2% 64%21%13%
2	B	478	5% 41%16%39%
2	F	478	6% 42%13%42%
3	C	84	42%19%37%

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Mol	Chain	Length	Quality of chain
3	G	84	
4	D	19	
4	H	19	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 11928 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 Histone-binding protein RBBP4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	381	Total	C	N	O	S	0	0	0
			3044	1920	518	596	10			
1	E	382	Total	C	N	O	S	0	0	0
			3045	1920	519	596	10			

There are 28 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-13	MET	-	initiating methionine	UNP Q09028
A	-12	SER	-	expression tag	UNP Q09028
A	-11	HIS	-	expression tag	UNP Q09028
A	-10	HIS	-	expression tag	UNP Q09028
A	-9	HIS	-	expression tag	UNP Q09028
A	-8	HIS	-	expression tag	UNP Q09028
A	-7	HIS	-	expression tag	UNP Q09028
A	-6	HIS	-	expression tag	UNP Q09028
A	-5	LEU	-	expression tag	UNP Q09028
A	-4	VAL	-	expression tag	UNP Q09028
A	-3	PRO	-	expression tag	UNP Q09028
A	-2	ARG	-	expression tag	UNP Q09028
A	-1	GLY	-	expression tag	UNP Q09028
A	0	SER	-	expression tag	UNP Q09028
E	-13	MET	-	initiating methionine	UNP Q09028
E	-12	SER	-	expression tag	UNP Q09028
E	-11	HIS	-	expression tag	UNP Q09028
E	-10	HIS	-	expression tag	UNP Q09028
E	-9	HIS	-	expression tag	UNP Q09028
E	-8	HIS	-	expression tag	UNP Q09028
E	-7	HIS	-	expression tag	UNP Q09028
E	-6	HIS	-	expression tag	UNP Q09028
E	-5	LEU	-	expression tag	UNP Q09028
E	-4	VAL	-	expression tag	UNP Q09028
E	-3	PRO	-	expression tag	UNP Q09028

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Chain	Residue	Modelled	Actual	Comment	Reference
E	-2	ARG	-	expression tag	UNP Q09028
E	-1	GLY	-	expression tag	UNP Q09028
E	0	SER	-	expression tag	UNP Q09028

- Molecule 2 is a protein called Polycomb protein SUZ12.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	291	Total	C	N	O	S	0	0	0
			2418	1551	442	411	14			
2	F	278	Total	C	N	O	S	0	0	0
			2317	1487	422	394	14			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	546	TRP	-	expression tag	UNP Q15022
B	547	SER	-	expression tag	UNP Q15022
B	548	HIS	-	expression tag	UNP Q15022
B	549	PRO	-	expression tag	UNP Q15022
B	550	GLN	-	expression tag	UNP Q15022
B	551	PHE	-	expression tag	UNP Q15022
B	552	GLU	-	expression tag	UNP Q15022
B	553	LYS	-	expression tag	UNP Q15022
F	546	TRP	-	expression tag	UNP Q15022
F	547	SER	-	expression tag	UNP Q15022
F	548	HIS	-	expression tag	UNP Q15022
F	549	PRO	-	expression tag	UNP Q15022
F	550	GLN	-	expression tag	UNP Q15022
F	551	PHE	-	expression tag	UNP Q15022
F	552	GLU	-	expression tag	UNP Q15022
F	553	LYS	-	expression tag	UNP Q15022

- Molecule 3 is a protein called PHD finger protein 19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	53	Total	C	N	O	S	0	0	0
			416	262	71	82	1			
3	G	51	Total	C	N	O	S	0	0	0
			400	254	69	76	1			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	497	SER	-	expression tag	UNP Q5T6S3
C	498	ASN	-	expression tag	UNP Q5T6S3
C	499	ALA	-	expression tag	UNP Q5T6S3
G	497	SER	-	expression tag	UNP Q5T6S3
G	498	ASN	-	expression tag	UNP Q5T6S3
G	499	ALA	-	expression tag	UNP Q5T6S3

- Molecule 4 is a protein called Protein Jumonji.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	17	Total	C	N	O	S	0	0	0
			143	93	26	23	1			
4	H	17	Total	C	N	O	S	0	0	0
			143	93	26	23	1			

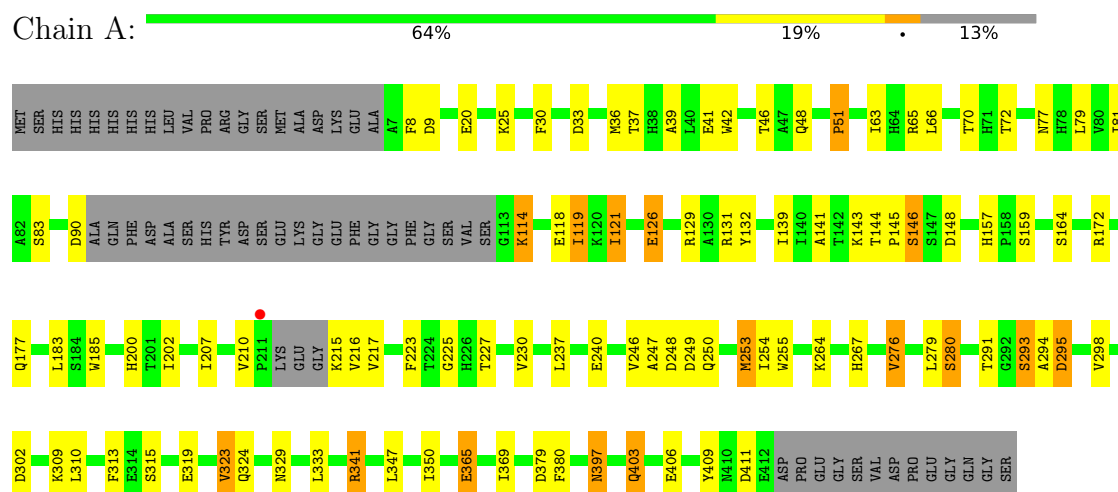
- Molecule 5 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	1	Total	Zn	0	0
			1	1		
5	F	1	Total	Zn	0	0
			1	1		

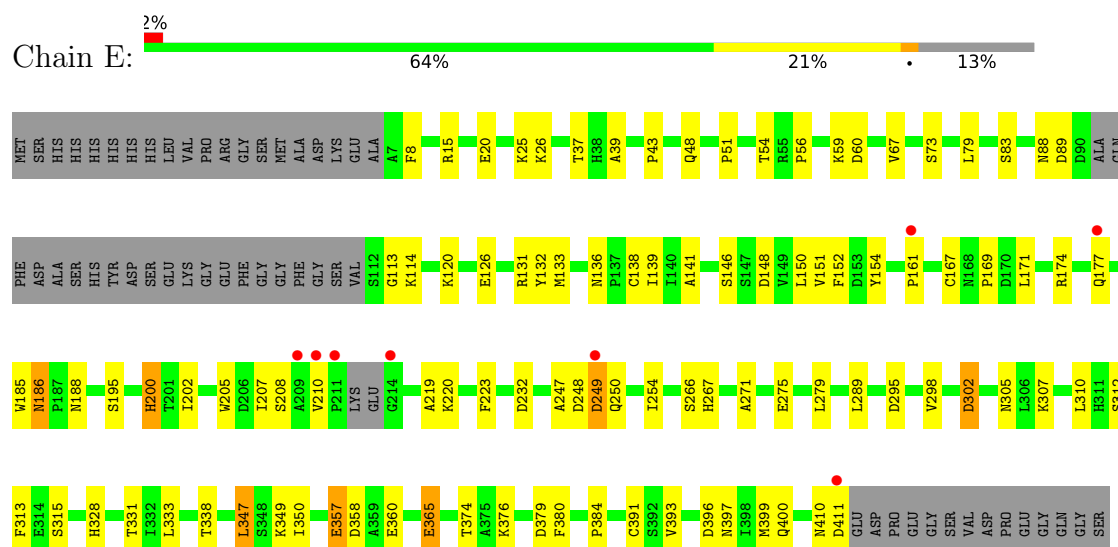
3 Residue-property plots [i](#)

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: Histone-binding protein RBBP4



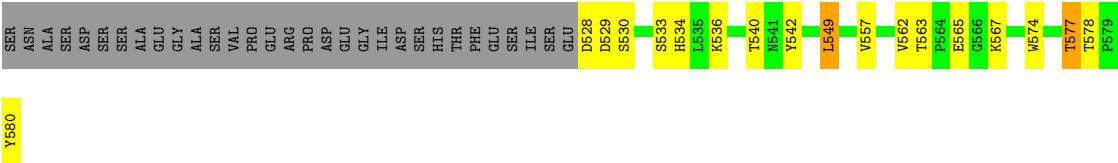
• Molecule 1: Histone-binding protein RBBP4



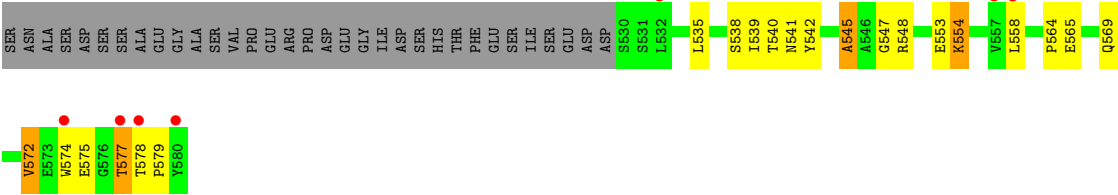
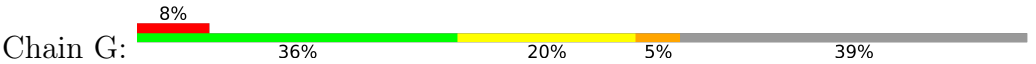
• Molecule 2: Polycomb protein SUZ12



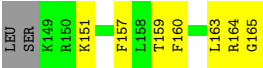




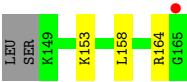
● Molecule 3: PHD finger protein 19



● Molecule 4: Protein Jumonji



● Molecule 4: Protein Jumonji



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	127.71Å 139.60Å 268.08Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.60 – 2.89 46.60 – 2.89	Depositor EDS
% Data completeness (in resolution range)	82.0 (46.60-2.89) 81.9 (46.60-2.89)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.06 (at 2.91Å)	Xtriage
Refinement program	BUSTER 2.10.3	Depositor
R, R_{free}	0.170 , 0.230 0.183 , 0.241	Depositor DCC
R_{free} test set	2180 reflections (4.95%)	wwPDB-VP
Wilson B-factor (Å ²)	50.3	Xtriage
Anisotropy	0.198	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 83.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	11928	wwPDB-VP
Average B, all atoms (Å ²)	67.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.87% 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

5.1 Standard geometry

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

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	0.88	1/3127 (0.0%)	1.31	17/4264 (0.4%)
1	E	0.84	1/3128 (0.0%)	1.32	18/4265 (0.4%)
2	B	0.91	0/2469	1.30	6/3317 (0.2%)
2	F	0.89	0/2365	1.34	14/3172 (0.4%)
3	C	0.82	0/425	1.41	4/574 (0.7%)
3	G	0.83	0/409	1.48	4/552 (0.7%)
4	D	0.82	0/145	1.28	0/191
4	H	0.79	0/145	1.42	0/191
All	All	0.87	2/12213 (0.0%)	1.33	63/16526 (0.4%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	210	VAL	CA-C	7.89	1.61	1.52
1	A	253	MET	SD-CE	-7.19	1.61	1.79

All (63) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	248	ASP	CA-C-N	8.39	132.37	120.28
1	A	248	ASP	C-N-CA	8.39	132.37	120.28
1	E	295	ASP	CA-CB-CG	7.54	120.14	112.60
1	E	396	ASP	CA-CB-CG	7.42	120.02	112.60
1	A	79	LEU	N-CA-C	-6.75	98.25	109.46
1	A	329	ASN	CA-C-N	6.09	128.73	120.38
1	A	329	ASN	C-N-CA	6.09	128.73	120.38
3	G	564	PRO	CA-C-N	6.07	129.03	120.28
3	G	564	PRO	C-N-CA	6.07	129.03	120.28
2	F	234	SER	CA-C-N	5.94	128.84	120.28
2	F	234	SER	C-N-CA	5.94	128.84	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	232	ASP	CA-CB-CG	5.93	118.53	112.60
3	G	572	VAL	CA-C-N	5.79	128.04	120.28
3	G	572	VAL	C-N-CA	5.79	128.04	120.28
1	A	293	SER	N-CA-C	5.74	117.91	109.24
1	A	379	ASP	CA-CB-CG	5.70	118.30	112.60
1	E	248	ASP	CA-C-N	5.67	130.19	120.72
1	E	248	ASP	C-N-CA	5.67	130.19	120.72
1	E	79	LEU	N-CA-C	-5.66	100.06	109.46
1	A	295	ASP	CA-CB-CG	5.65	118.25	112.60
1	E	302	ASP	CA-CB-CG	5.65	118.25	112.60
3	C	562	VAL	CA-C-N	5.58	128.15	120.39
3	C	562	VAL	C-N-CA	5.58	128.15	120.39
1	E	307	LYS	N-CA-C	-5.54	106.19	113.17
1	E	220	LYS	N-CA-C	-5.52	105.17	111.14
2	F	231	ALA	CA-C-N	5.47	127.83	120.50
2	F	231	ALA	C-N-CA	5.47	127.83	120.50
2	B	80	GLN	CA-C-N	5.46	128.15	120.28
2	B	80	GLN	C-N-CA	5.46	128.15	120.28
1	E	250	GLN	N-CA-C	-5.41	106.63	113.23
1	E	146	SER	N-CA-C	-5.40	102.76	110.59
1	A	51	PRO	CA-C-N	5.39	129.13	121.42
1	A	51	PRO	C-N-CA	5.39	129.13	121.42
2	F	146	GLY	CA-C-N	5.38	131.38	121.70
2	F	146	GLY	C-N-CA	5.38	131.38	121.70
3	C	533	SER	CA-C-N	5.37	127.74	120.44
3	C	533	SER	C-N-CA	5.37	127.74	120.44
2	F	303	ASP	CA-CB-CG	5.35	117.95	112.60
1	E	357	GLU	CA-C-N	5.32	127.36	120.44
1	E	357	GLU	C-N-CA	5.32	127.36	120.44
2	B	496	ASP	CA-CB-CG	5.30	117.90	112.60
1	E	379	ASP	CA-CB-CG	5.25	117.85	112.60
1	E	271	ALA	N-CA-C	5.23	116.67	111.07
2	F	244	MET	N-CA-C	-5.21	99.90	108.49
1	A	250	GLN	N-CA-C	-5.18	105.78	113.40
1	A	411	ASP	CA-CB-CG	5.18	117.78	112.60
1	A	37	THR	CB-CA-C	5.17	118.75	110.16
1	A	291	THR	CA-C-N	5.17	126.10	122.33
1	A	291	THR	C-N-CA	5.17	126.10	122.33
2	B	90	PHE	CA-C-N	5.17	127.15	120.44
2	B	90	PHE	C-N-CA	5.17	127.15	120.44
2	B	474	PHE	CA-CB-CG	5.16	118.96	113.80
2	F	143	LYS	CA-C-N	5.16	127.97	120.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	143	LYS	C-N-CA	5.16	127.97	120.79
1	E	200	HIS	CA-CB-CG	5.15	118.95	113.80
1	A	397	ASN	CA-CB-CG	5.11	117.71	112.60
1	E	208	SER	N-CA-C	-5.08	105.38	112.45
1	A	9	ASP	CA-CB-CG	5.07	117.67	112.60
2	F	139	SER	CA-C-N	5.05	127.36	120.54
2	F	139	SER	C-N-CA	5.05	127.36	120.54
2	F	506	ILE	CA-C-N	5.03	128.71	121.71
2	F	506	ILE	C-N-CA	5.03	128.71	121.71
1	E	358	ASP	CA-CB-CG	5.02	117.62	112.60

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	3044	0	2890	45	0
1	E	3045	0	2892	40	0
2	B	2418	0	2461	48	0
2	F	2317	0	2351	31	0
3	C	416	0	402	7	0
3	G	400	0	394	7	0
4	D	143	0	154	4	0
4	H	143	0	154	3	0
5	B	1	0	0	0	0
5	F	1	0	0	0	0
All	All	11928	0	11698	160	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 7.

All (160) 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:B:192:CYS:SG	2:B:244:MET:HE1	1.91	1.10
2:B:308:LEU:HD12	2:B:308:LEU:H	1.42	0.82
1:A:48:GLN:HE22	1:A:131:ARG:HA	1.45	0.81
1:A:121:ILE:HD13	1:A:157:HIS:CD2	2.21	0.76
1:A:48:GLN:NE2	1:A:131:ARG:HA	2.03	0.73
2:B:192:CYS:HG	2:B:244:MET:HE1	1.54	0.73
2:B:241:ASN:OD1	2:B:241:ASN:N	2.22	0.72
1:E:48:GLN:HE22	1:E:131:ARG:HA	1.54	0.72
1:E:48:GLN:NE2	1:E:131:ARG:HA	2.05	0.71
2:B:319:MET:HG2	2:B:353:PRO:HD3	1.73	0.70
2:F:451:PRO:HB2	4:H:158:LEU:HD12	1.75	0.69
2:F:456:ASN:HD22	2:F:458:ARG:H	1.41	0.68
1:A:253:MET:HE3	1:A:255:TRP:CZ2	2.29	0.67
1:A:246:VAL:HB	1:A:276:VAL:HB	1.77	0.66
2:B:437:ASN:HB3	2:B:439:ARG:HD3	1.79	0.64
1:E:48:GLN:HE22	1:E:132:TYR:H	1.45	0.63
1:A:350:ILE:HG12	1:A:365:GLU:HG2	1.81	0.62
2:F:253:ARG:HA	2:F:296:VAL:HG12	1.81	0.62
2:B:182:VAL:HG12	2:B:183:THR:H	1.66	0.61
1:E:298:VAL:HB	1:E:313:PHE:HB2	1.81	0.61
2:B:507:HIS:HB2	3:C:580:TYR:CE2	2.36	0.60
2:F:433:LEU:HD23	2:F:438:THR:HA	1.84	0.59
2:B:192:CYS:HB3	2:B:244:MET:SD	2.43	0.58
1:A:30:PHE:O	2:B:116:THR:HG23	2.03	0.58
1:A:313:PHE:HZ	1:A:347:LEU:HD22	1.68	0.58
1:A:144:THR:HG22	1:A:146:SER:H	1.68	0.57
2:F:434:TYR:O	2:F:435:ASN:HB2	2.05	0.57
2:F:368:LYS:HD2	2:F:369:SER:H	1.70	0.57
2:B:505:ASP:HB3	2:B:508:ARG:HB2	1.86	0.56
2:B:192:CYS:CB	2:B:244:MET:HE1	2.35	0.56
2:F:92:LYS:HB3	2:F:93:PRO:HD3	1.86	0.56
2:B:506:ILE:HG12	3:C:577:THR:HG22	1.85	0.56
2:B:127:ILE:HD12	2:B:128:LYS:H	1.71	0.56
1:E:411:ASP:HB3	2:F:126:ASN:HB2	1.88	0.56
2:F:160:THR:HB	2:F:356:GLN:HB2	1.88	0.56
1:E:138:CYS:HA	1:E:154:TYR:CE2	2.41	0.56
2:F:187:LEU:HB2	2:F:251:LEU:HB3	1.87	0.55
1:E:141:ALA:HB2	1:E:185:TRP:CZ2	2.40	0.55
2:B:161:PHE:HB2	2:B:228:PRO:HB2	1.89	0.55
1:A:39:ALA:O	2:B:524:PRO:HA	2.07	0.55
1:E:350:ILE:HG12	1:E:365:GLU:HG2	1.89	0.55
1:A:202:ILE:HB	1:A:223:PHE:HB2	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:254:ILE:HB	1:A:267:HIS:HB2	1.90	0.53
1:E:374:THR:HB	2:F:513:ALA:HB2	1.91	0.52
1:E:313:PHE:HZ	1:E:347:LEU:HD22	1.75	0.52
1:A:323:VAL:HG22	1:A:333:LEU:HD11	1.90	0.52
1:A:247:ALA:HB3	1:A:249:ASP:HB2	1.91	0.52
1:E:186:ASN:HD22	1:E:188:ASN:H	1.56	0.52
1:E:357:GLU:O	1:E:360:GLU:HB2	2.11	0.51
1:A:302:ASP:HB2	1:A:310:LEU:HD11	1.92	0.51
2:B:244:MET:SD	2:B:244:MET:C	2.93	0.51
3:C:549:LEU:HD13	3:C:574:TRP:HZ3	1.75	0.51
1:E:331:THR:HG21	2:F:129:ARG:CG	2.41	0.51
1:A:293:SER:HB3	1:A:295:ASP:OD1	2.10	0.51
1:A:324:GLN:HB2	1:A:380:PHE:CE2	2.45	0.51
1:A:144:THR:HB	1:A:148:ASP:O	2.11	0.51
3:G:538:SER:O	3:G:541:ASN:HB2	2.10	0.50
1:E:139:ILE:HA	1:E:152:PHE:O	2.12	0.50
1:A:172:ARG:HB3	1:A:216:VAL:HG22	1.92	0.50
1:A:298:VAL:HB	1:A:313:PHE:HB2	1.93	0.50
1:A:309:LYS:HE3	2:B:370:THR:O	2.12	0.50
1:E:393:VAL:HG12	1:E:399:MET:HG3	1.92	0.50
2:B:428:ILE:HD12	2:B:447:ASP:HB2	1.93	0.50
1:E:56:PRO:HB2	1:E:59:LYS:HG3	1.94	0.50
1:E:247:ALA:C	1:E:249:ASP:H	2.19	0.50
1:E:331:THR:HG21	2:F:129:ARG:HG2	1.94	0.49
1:E:338:THR:HG22	1:E:376:LYS:HD3	1.94	0.49
3:G:538:SER:HA	3:G:541:ASN:HD22	1.78	0.49
2:B:190:LYS:HG3	2:B:248:TYR:CE1	2.47	0.49
1:A:141:ALA:HB2	1:A:185:TRP:CZ2	2.48	0.49
1:A:280:SER:HB2	1:A:323:VAL:HG13	1.95	0.49
2:F:506:ILE:HG12	3:G:577:THR:HG22	1.95	0.49
3:C:549:LEU:HD13	3:C:574:TRP:CZ3	2.48	0.49
1:E:150:LEU:HD22	1:E:169:PRO:HG3	1.94	0.48
1:A:144:THR:HG23	1:A:145:PRO:HD2	1.96	0.48
1:E:205:TRP:CD1	1:E:219:ALA:HA	2.49	0.48
2:F:456:ASN:ND2	2:F:458:ARG:H	2.11	0.48
1:A:144:THR:C	1:A:146:SER:H	2.21	0.48
1:A:397:ASN:HB2	2:B:522:ARG:HD3	1.95	0.48
2:F:195:LYS:HG3	2:F:243:HIS:HB3	1.96	0.47
2:B:95:GLN:HE21	3:C:542:TYR:HE2	1.62	0.47
3:C:534:HIS:HE1	4:D:165:GLY:HA3	1.78	0.47
2:B:249:SER:HA	2:B:300:THR:HA	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:505:ASP:C	2:F:507:HIS:H	2.22	0.47
1:A:42:TRP:CG	1:A:72:THR:HG22	2.49	0.47
1:E:37:THR:HG23	2:F:527:HIS:HB3	1.95	0.47
2:B:475:ILE:CD1	2:B:492:ASN:HA	2.45	0.46
1:E:48:GLN:HE22	1:E:132:TYR:N	2.12	0.46
1:A:119:ILE:HG23	1:A:159:SER:HA	1.97	0.46
2:B:449:HIS:NE2	2:B:456:ASN:HB2	2.31	0.46
2:F:97:TYR:CZ	2:F:471:HIS:HA	2.51	0.46
1:A:225:GLY:C	1:A:253:MET:HE1	2.41	0.46
1:E:136:ASN:HD22	1:E:136:ASN:C	2.23	0.46
2:B:164:PHE:HE1	2:B:319:MET:HG3	1.81	0.46
2:B:240:SER:HB3	2:B:245:VAL:HA	1.97	0.46
4:D:159:THR:O	4:D:163:LEU:HG	2.16	0.45
2:B:446:ASP:O	2:B:449:HIS:HB2	2.16	0.45
1:E:202:ILE:HB	1:E:223:PHE:HB2	1.99	0.45
3:C:563:THR:HG22	3:C:565:GLU:H	1.82	0.45
1:E:380:PHE:HA	1:E:391:CYS:O	2.16	0.45
1:A:406:GLU:HA	1:A:409:TYR:CZ	2.51	0.45
2:B:191:VAL:HG22	2:B:193:HIS:CE1	2.51	0.45
1:E:39:ALA:O	2:F:524:PRO:HA	2.17	0.45
1:E:51:PRO:HD3	1:E:132:TYR:CZ	2.52	0.45
3:G:535:LEU:O	3:G:539:ILE:HG12	2.17	0.45
1:E:305:ASN:HB3	2:F:138:LEU:HD11	1.97	0.45
2:B:136:ASP:O	2:B:140:LYS:HG3	2.17	0.44
1:E:120:LYS:HB3	1:E:161:PRO:HG3	1.99	0.44
1:E:328:HIS:HE1	1:E:384:PRO:O	2.00	0.44
1:E:397:ASN:HB2	2:F:522:ARG:HD3	2.00	0.44
2:F:426:LEU:HD22	2:F:484:GLY:HA2	2.00	0.44
1:A:341:ARG:HG3	1:A:369:ILE:HG23	2.00	0.44
2:B:187:LEU:HB2	2:B:251:LEU:HB3	1.99	0.44
1:E:133:MET:HE3	1:E:136:ASN:HB3	2.00	0.44
1:A:253:MET:HE3	1:A:255:TRP:HZ2	1.79	0.44
2:B:93:PRO:HB2	2:B:474:PHE:CZ	2.53	0.43
2:B:158:GLN:HA	2:B:231:ALA:HA	2.00	0.43
2:B:241:ASN:HB2	2:B:242:SER:H	1.49	0.43
2:B:192:CYS:HB3	2:B:244:MET:HE1	2.01	0.43
2:B:91:GLU:OE1	4:D:164:ARG:HD3	2.18	0.43
1:A:139:ILE:HD12	1:A:139:ILE:N	2.34	0.43
2:B:295:PHE:HB3	2:B:319:MET:HB3	2.01	0.42
2:F:301:VAL:HA	2:F:310:LEU:HB2	2.01	0.42
4:D:157:PHE:O	4:D:160:PHE:HB3	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:310:LEU:HA	2:B:310:LEU:HD12	1.88	0.42
2:F:443:GLU:O	4:H:153:LYS:HA	2.19	0.42
1:E:302:ASP:HB2	1:E:310:LEU:HD11	2.00	0.42
2:B:188:LEU:HD11	2:B:237:PHE:CE1	2.54	0.42
2:B:204:ARG:HH12	2:B:207:PRO:HD3	1.85	0.42
1:A:247:ALA:C	1:A:249:ASP:H	2.28	0.42
1:A:294:ALA:HA	1:A:319:GLU:HG2	2.01	0.42
2:B:156:HIS:CD2	2:B:231:ALA:HB1	2.55	0.42
1:E:151:VAL:HB	1:E:171:LEU:HB2	2.01	0.42
2:B:475:ILE:HD11	2:B:492:ASN:HA	2.01	0.41
1:A:310:LEU:O	2:B:376:PRO:HD2	2.20	0.41
2:F:240:SER:HB3	2:F:245:VAL:HA	2.02	0.41
2:F:331:ARG:HA	2:F:331:ARG:HD2	1.87	0.41
2:F:426:LEU:HD23	2:F:426:LEU:HA	1.91	0.41
1:A:20:GLU:OE1	2:B:103:ARG:HD3	2.19	0.41
2:B:110:PHE:CE1	2:B:115:LEU:HD11	2.56	0.41
1:E:195:SER:HB3	1:E:205:TRP:HZ3	1.85	0.41
3:G:545:ALA:HA	3:G:574:TRP:CZ2	2.55	0.41
1:E:254:ILE:HB	1:E:267:HIS:HB2	2.03	0.41
2:F:477:ASN:HB3	2:F:488:ASP:HB2	2.01	0.41
1:A:51:PRO:HD3	1:A:132:TYR:CZ	2.56	0.41
1:E:43:PRO:HA	1:E:397:ASN:HA	2.03	0.41
1:A:77:ASN:ND2	1:A:126:GLU:HA	2.36	0.41
2:B:244:MET:SD	2:B:244:MET:O	2.79	0.41
1:A:33:ASP:HB2	1:A:403:GLN:HG2	2.03	0.41
2:B:532:ARG:HA	2:B:533:PRO:HD3	1.96	0.41
1:A:83:SER:HB3	1:A:118:GLU:HG3	2.02	0.40
3:G:542:TYR:HA	3:G:547:GLY:HA3	2.04	0.40
1:A:46:THR:HB	1:A:129:ARG:HA	2.03	0.40
1:A:225:GLY:HA3	1:A:255:TRP:HH2	1.87	0.40
1:E:20:GLU:HB3	2:F:109:ILE:HG21	2.03	0.40
2:F:451:PRO:HB2	4:H:158:LEU:CD1	2.49	0.40
1:A:210:VAL:HG11	1:A:217:VAL:CG2	2.51	0.40
1:E:15:ARG:HD2	3:G:548:ARG:NH1	2.36	0.40
1:A:36:MET:HE1	1:A:114:LYS:HB3	2.02	0.40
2:B:432:PHE:HB2	2:B:440:GLN:HB3	2.03	0.40

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	375/439 (85%)	354 (94%)	20 (5%)	1 (0%)	36	65
1	E	376/439 (86%)	357 (95%)	15 (4%)	4 (1%)	11	36
2	B	271/478 (57%)	253 (93%)	16 (6%)	2 (1%)	18	48
2	F	258/478 (54%)	225 (87%)	29 (11%)	4 (2%)	7	27
3	C	51/84 (61%)	48 (94%)	2 (4%)	1 (2%)	6	22
3	G	49/84 (58%)	41 (84%)	4 (8%)	4 (8%)	0	2
4	D	15/19 (79%)	14 (93%)	1 (7%)	0	100	100
4	H	15/19 (79%)	15 (100%)	0	0	100	100
All	All	1410/2040 (69%)	1307 (93%)	87 (6%)	16 (1%)	11	36

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	89	ASP
2	F	435	ASN
1	A	315	SER
3	C	529	ASP
1	E	113	GLY
2	F	242	SER
1	E	315	SER
2	F	458	ARG
3	G	545	ALA
3	G	554	LYS
3	G	575	GLU
2	B	458	ARG
2	F	241	ASN
1	E	207	ILE
2	B	352	GLY
3	G	579	PRO

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	343/388 (88%)	310 (90%)	33 (10%)	8	26
1	E	343/388 (88%)	314 (92%)	29 (8%)	10	31
2	B	272/442 (62%)	232 (85%)	40 (15%)	3	10
2	F	259/442 (59%)	225 (87%)	34 (13%)	4	13
3	C	44/70 (63%)	35 (80%)	9 (20%)	1	4
3	G	42/70 (60%)	33 (79%)	9 (21%)	1	4
4	D	16/18 (89%)	15 (94%)	1 (6%)	16	45
4	H	16/18 (89%)	15 (94%)	1 (6%)	16	45
All	All	1335/1836 (73%)	1179 (88%)	156 (12%)	5	17

All (156) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	PHE
1	A	25	LYS
1	A	41	GLU
1	A	63	ILE
1	A	65	ARG
1	A	66	LEU
1	A	70	THR
1	A	81	ILE
1	A	90	ASP
1	A	114	LYS
1	A	119	ILE
1	A	121	ILE
1	A	126	GLU
1	A	143	LYS
1	A	146	SER
1	A	164	SER
1	A	177	GLN
1	A	183	LEU
1	A	200	HIS

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Mol	Chain	Res	Type
1	A	207	ILE
1	A	215	LYS
1	A	227	THR
1	A	230	VAL
1	A	237	LEU
1	A	240	GLU
1	A	264	LYS
1	A	276	VAL
1	A	279	LEU
1	A	280	SER
1	A	323	VAL
1	A	341	ARG
1	A	365	GLU
1	A	403	GLN
2	B	109	ILE
2	B	127	ILE
2	B	128	LYS
2	B	143	LYS
2	B	160	THR
2	B	182	VAL
2	B	183	THR
2	B	188	LEU
2	B	191	VAL
2	B	205	GLN
2	B	234	SER
2	B	238	GLU
2	B	241	ASN
2	B	244	MET
2	B	245	VAL
2	B	249	SER
2	B	254	VAL
2	B	296	VAL
2	B	301	VAL
2	B	308	LEU
2	B	310	LEU
2	B	314	GLU
2	B	316	GLU
2	B	317	VAL
2	B	320	GLN
2	B	337	ILE
2	B	351	GLN
2	B	355	LEU

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Mol	Chain	Res	Type
2	B	356	GLN
2	B	358	THR
2	B	359	LEU
2	B	377	LEU
2	B	433	LEU
2	B	446	ASP
2	B	449	HIS
2	B	472	SER
2	B	490	SER
2	B	506	ILE
2	B	509	GLN
2	B	517	ASN
3	C	528	ASP
3	C	530	SER
3	C	536	LYS
3	C	540	THR
3	C	549	LEU
3	C	557	VAL
3	C	567	LYS
3	C	577	THR
3	C	578	THR
4	D	151	LYS
1	E	8	PHE
1	E	25	LYS
1	E	26	LYS
1	E	54	THR
1	E	60	ASP
1	E	67	VAL
1	E	73	SER
1	E	83	SER
1	E	88	ASN
1	E	114	LYS
1	E	126	GLU
1	E	148	ASP
1	E	167	CYS
1	E	174	ARG
1	E	177	GLN
1	E	186	ASN
1	E	200	HIS
1	E	249	ASP
1	E	266	SER
1	E	275	GLU

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Mol	Chain	Res	Type
1	E	279	LEU
1	E	289	LEU
1	E	312	SER
1	E	333	LEU
1	E	347	LEU
1	E	349	LYS
1	E	365	GLU
1	E	400	GLN
1	E	410	ASN
2	F	101	ARG
2	F	102	THR
2	F	105	LEU
2	F	109	ILE
2	F	123	SER
2	F	124	ARG
2	F	131	THR
2	F	147	GLU
2	F	159	LEU
2	F	194	LYS
2	F	199	VAL
2	F	206	VAL
2	F	230	LEU
2	F	234	SER
2	F	244	MET
2	F	304	LYS
2	F	308	LEU
2	F	310	LEU
2	F	331	ARG
2	F	333	THR
2	F	335	GLU
2	F	354	THR
2	F	355	LEU
2	F	359	LEU
2	F	368	LYS
2	F	447	ASP
2	F	456	ASN
2	F	458	ARG
2	F	459	LYS
2	F	493	GLU
2	F	496	ASP
2	F	506	ILE
2	F	525	ILE

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Mol	Chain	Res	Type
2	F	527	HIS
3	G	540	THR
3	G	553	GLU
3	G	554	LYS
3	G	558	LEU
3	G	565	GLU
3	G	569	GLN
3	G	572	VAL
3	G	577	THR
3	G	578	THR
4	H	164	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (51) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	38	HIS
1	A	48	GLN
1	A	76	GLN
1	A	77	ASN
1	A	85	GLN
1	A	88	ASN
1	A	157	HIS
1	A	186	ASN
1	A	328	HIS
1	A	343	ASN
1	A	354	GLN
1	A	400	GLN
1	A	403	GLN
2	B	83	HIS
2	B	95	GLN
2	B	104	ASN
2	B	120	HIS
2	B	158	GLN
2	B	193	HIS
2	B	298	GLN
2	B	356	GLN
2	B	431	GLN
2	B	435	ASN
2	B	440	GLN
2	B	527	HIS
3	C	534	HIS
1	E	38	HIS

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Mol	Chain	Res	Type
1	E	48	GLN
1	E	85	GLN
1	E	88	ASN
1	E	136	ASN
1	E	168	ASN
1	E	176	HIS
1	E	186	ASN
1	E	250	GLN
1	E	324	GLN
1	E	354	GLN
1	E	400	GLN
1	E	403	GLN
1	E	410	ASN
2	F	205	GLN
2	F	235	ASN
2	F	431	GLN
2	F	435	ASN
2	F	449	HIS
2	F	456	ASN
2	F	492	ASN
2	F	509	GLN
3	G	534	HIS
3	G	541	ASN
3	G	556	GLN

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 oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 2 ligands modelled in this entry, 2 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 [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	381/439 (86%)	-0.52	1 (0%) 90 87	18, 44, 77, 110	0
1	E	382/439 (87%)	-0.27	8 (2%) 63 54	22, 56, 106, 124	0
2	B	291/478 (60%)	0.26	25 (8%) 16 13	24, 63, 110, 131	0
2	F	278/478 (58%)	0.62	28 (10%) 12 10	40, 84, 139, 159	0
3	C	53/84 (63%)	0.21	0 100 100	43, 86, 116, 130	0
3	G	51/84 (60%)	1.20	7 (13%) 6 5	88, 129, 155, 167	0
4	D	17/19 (89%)	-0.44	0 100 100	32, 50, 100, 101	0
4	H	17/19 (89%)	0.54	1 (5%) 28 22	71, 86, 114, 135	0
All	All	1470/2040 (72%)	0.01	70 (4%) 35 28	18, 59, 125, 167	0

All (70) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	337	ILE	5.3
2	F	164	PHE	5.3
2	F	359	LEU	4.9
2	B	359	LEU	4.8
2	F	161	PHE	4.8
2	B	79	VAL	4.5
2	B	164	PHE	4.1
2	F	243	HIS	4.0
2	F	357	PHE	3.8
2	B	254	VAL	3.7
2	F	329	LYS	3.7
2	F	206	VAL	3.6
2	F	254	VAL	3.6
2	F	378	ALA	3.5
1	A	211	PRO	3.4
2	F	353	PRO	3.3

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Mol	Chain	Res	Type	RSRZ
2	F	354	THR	3.3
1	E	211	PRO	3.2
2	B	157	LEU	3.2
3	G	574	TRP	3.2
2	F	298	GLN	3.2
2	B	231	ALA	3.1
2	F	295	PHE	3.1
2	F	230	LEU	3.1
2	F	81	ALA	3.0
2	F	251	LEU	2.9
2	F	332	ALA	2.8
3	G	557	VAL	2.8
1	E	214	GLY	2.8
2	B	161	PHE	2.8
2	B	228	PRO	2.8
2	B	230	LEU	2.8
3	G	558	LEU	2.7
2	B	243	HIS	2.7
2	F	159	LEU	2.7
2	F	252	PHE	2.7
2	B	424	GLN	2.7
2	B	145	LYS	2.6
2	B	329	LYS	2.6
2	F	157	LEU	2.6
3	G	532	LEU	2.6
4	H	165	GLY	2.6
1	E	161	PRO	2.6
2	B	182	VAL	2.6
2	B	183	THR	2.5
2	B	82	ASP	2.5
2	B	162	THR	2.5
2	B	506	ILE	2.4
2	F	203	ILE	2.4
2	B	244	MET	2.4
3	G	577	THR	2.3
2	B	357	PHE	2.3
1	E	177	GLN	2.3
2	B	308	LEU	2.3
1	E	210	VAL	2.3
2	F	321	GLU	2.2
2	B	245	VAL	2.2
2	F	186	VAL	2.1

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Mol	Chain	Res	Type	RSRZ
2	F	434	TYR	2.1
2	B	166	HIS	2.1
2	F	156	HIS	2.1
1	E	411	ASP	2.1
1	E	249	ASP	2.1
1	E	209	ALA	2.1
2	B	425	LYS	2.1
2	F	447	ASP	2.1
3	G	578	THR	2.1
2	F	330	LYS	2.0
2	F	331	ARG	2.0
3	G	580	TYR	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 oligosaccharides 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($\text{\AA}^2$)	Q<0.9
5	ZN	B	1001	1/1	1.00	0.05	40,40,40,40	0
5	ZN	F	1001	1/1	1.00	0.04	61,61,61,61	0

6.5 Other polymers [i](#)

There are no such residues in this entry.