



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 01:14 PM UTC

PDB ID : 5WAI / pdb_00005wai
Title : Crystal Structure of a Suz12-Rbbp4-Jarid2-Aebp2 Heterotetrameric Complex
Authors : Chen, S.; Jiao, L.; Liu, X.
Deposited on : 2017-06-26
Resolution : 2.90 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:

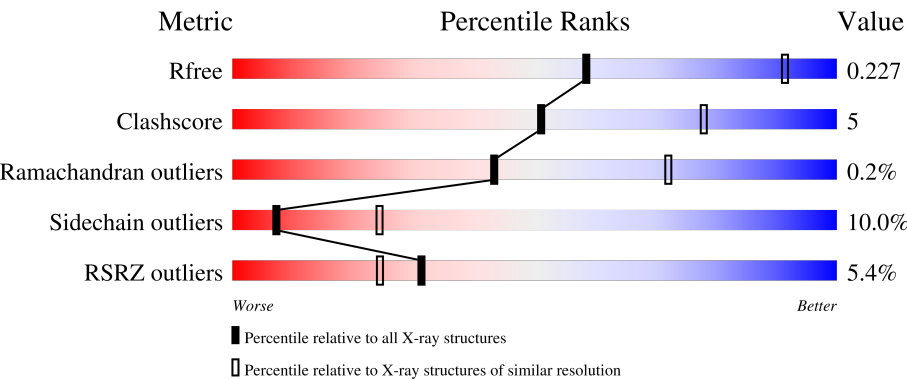
MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
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 2.90 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	3% 71% 17% • 10%
1	E	439	2% 70% 17% • 11%
2	B	478	6% 48% 13% • 37%
2	F	478	5% 45% 13% • 40%
3	C	100	4% 73% 16% • 9%

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Mol	Chain	Length	Quality of chain
3	G	100	 7% 65% 18% 14%
4	D	19	 74% 5% 21%
4	H	19	 47% 32% 21%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 12890 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	397	Total	C	N	O	S	0	0	0
			3157	1992	536	619	10			
1	E	391	Total	C	N	O	S	0	0	0
			3112	1961	530	611	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	300	Total	C	N	O	S	0	1	0
			2504	1599	456	433	16			
2	F	289	Total	C	N	O	S	0	1	0
			2405	1535	440	415	15			

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 Zinc finger protein AEBP2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	91	Total	C	N	O	S	0	0	0
			744	478	136	128	2			
3	G	86	Total	C	N	O	S	0	0	0
			706	453	130	121	2			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	404	SER	-	expression tag	UNP Q6ZN18
C	405	ASN	-	expression tag	UNP Q6ZN18
C	406	ALA	-	expression tag	UNP Q6ZN18
G	404	SER	-	expression tag	UNP Q6ZN18
G	405	ASN	-	expression tag	UNP Q6ZN18
G	406	ALA	-	expression tag	UNP Q6ZN18

- Molecule 4 is a protein called Jumonji, AT-rich interactive domain 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	15	Total	C	N	O	S	0	0	0
			130	85	23	21	1			
4	H	15	Total	C	N	O	S	0	0	0
			130	85	23	21	1			

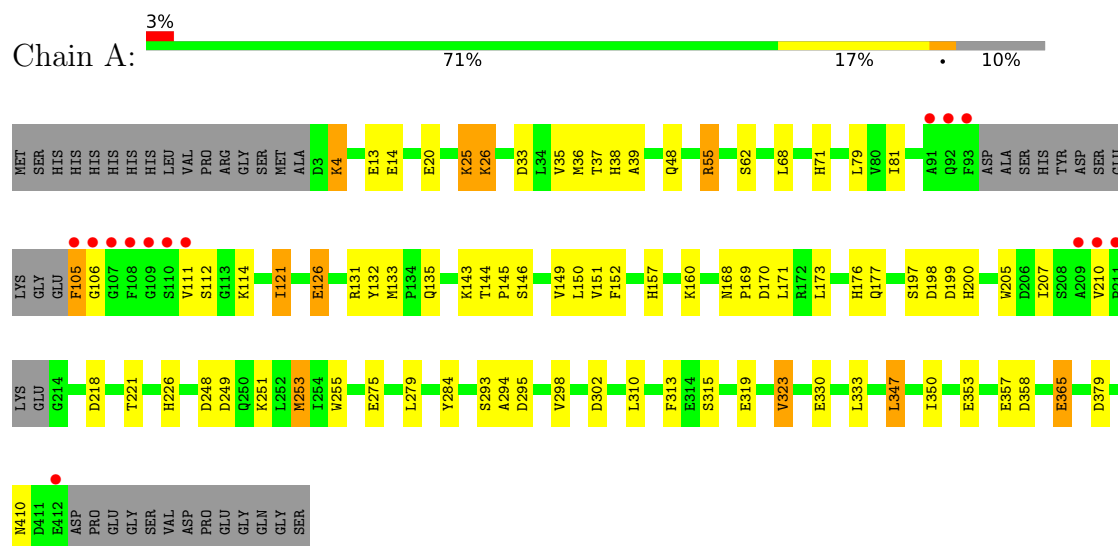
- Molecule 5 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

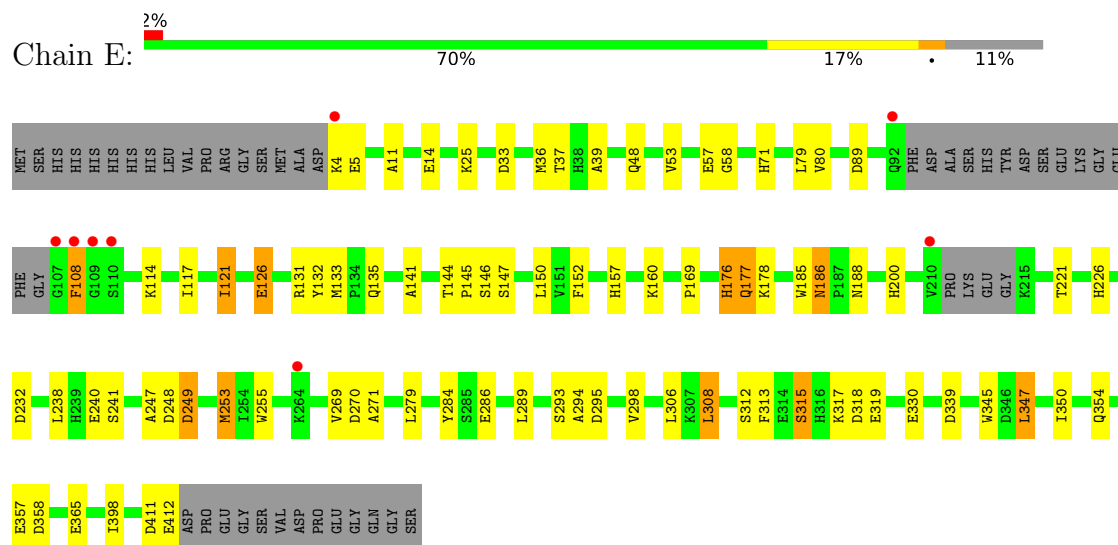
3 Residue-property plots [i](#)

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

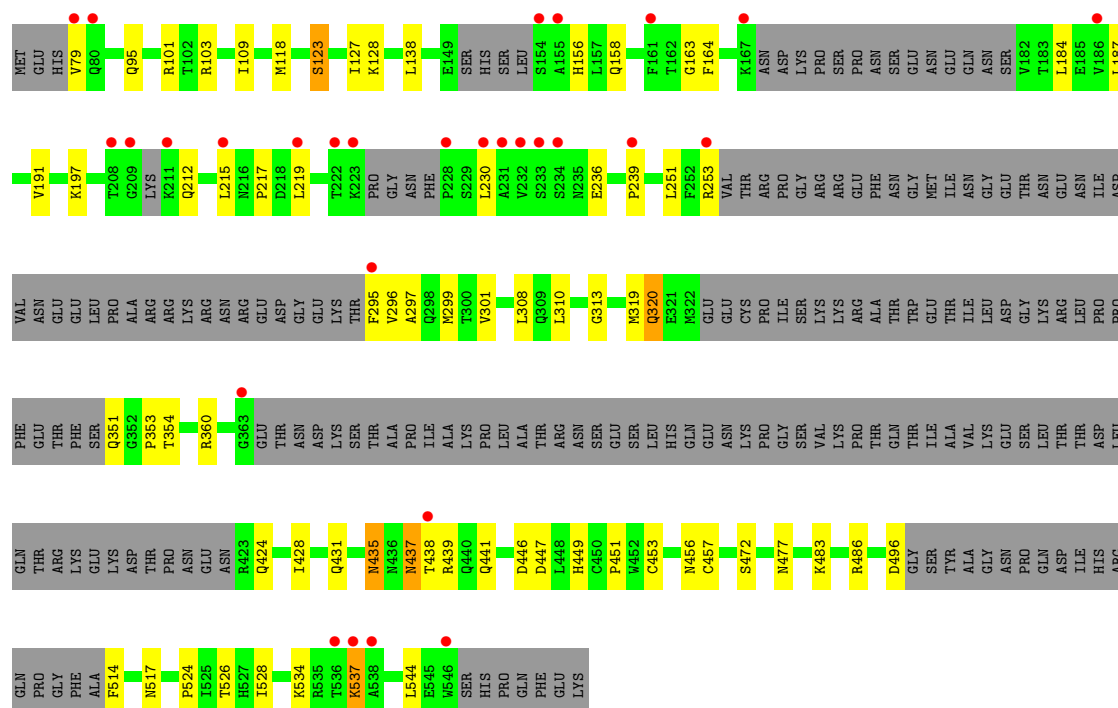


- Molecule 1: Histone-binding protein RBBP4

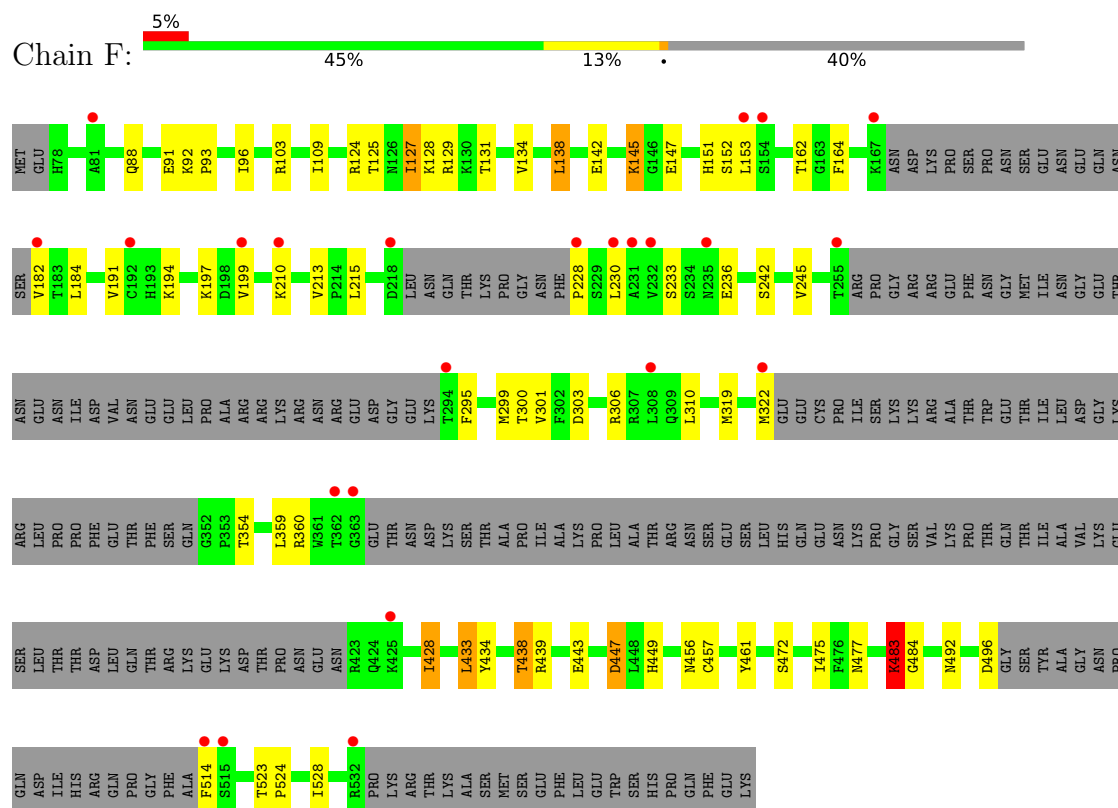


- Molecule 2: Polycomb protein SUZ12



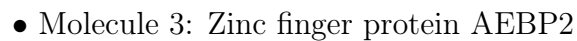


- Molecule 2: Polycomb protein SUZ12



- Molecule 3: Zinc finger protein AEBP2





- Molecule 4: Jumonji, AT-rich interactive domain 2



- Molecule 4: Jumonji, AT-rich interactive domain 2



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	95.30Å 111.43Å 253.25Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.10 – 2.90 48.10 – 2.90	Depositor EDS
% Data completeness (in resolution range)	94.1 (48.10-2.90) 94.3 (48.10-2.90)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.30 (at 2.91Å)	Xtriage
Refinement program	BUSTER 2.10.2	Depositor
R, R_{free}	0.171 , 0.216 0.181 , 0.227	Depositor DCC
R_{free} test set	2867 reflections (4.74%)	wwPDB-VP
Wilson B-factor (Å ²)	52.5	Xtriage
Anisotropy	0.104	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 75.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	12890	wwPDB-VP
Average B, all atoms (Å ²)	66.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.89% 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	0.92	2/3243 (0.1%)	1.30	16/4418 (0.4%)
1	E	0.85	1/3195 (0.0%)	1.31	16/4353 (0.4%)
2	B	0.87	0/2559	1.35	19/3435 (0.6%)
2	F	0.85	1/2460 (0.0%)	1.28	16/3307 (0.5%)
3	C	0.84	0/761	1.32	1/1026 (0.1%)
3	G	0.79	0/722	1.33	5/973 (0.5%)
4	D	0.82	0/132	1.29	0/175
4	H	0.73	0/132	1.26	1/175 (0.6%)
All	All	0.86	4/13204 (0.0%)	1.31	74/17862 (0.4%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	483	LYS	CA-C	7.22	1.60	1.52
1	E	253	MET	SD-CE	-7.11	1.61	1.79
1	A	253	MET	SD-CE	-6.20	1.64	1.79
1	A	210	VAL	CA-C	5.53	1.58	1.53

All (74) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	109	ILE	N-CA-C	-9.10	102.99	111.45
2	B	457	CYS	CA-C-N	-8.87	108.16	122.26
2	B	457	CYS	C-N-CA	-8.87	108.16	122.26
1	E	108	PHE	CA-CB-CG	8.04	121.84	113.80
1	A	295	ASP	CA-CB-CG	7.72	120.32	112.60
2	B	446	ASP	CA-C-N	7.39	131.90	120.82
2	B	446	ASP	C-N-CA	7.39	131.90	120.82
2	B	457	CYS	N-CA-C	-7.34	100.15	110.50
2	B	447	ASP	CA-CB-CG	7.27	119.87	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	295	ASP	CA-CB-CG	7.19	119.79	112.60
2	B	123	SER	CA-C-N	7.04	133.47	120.95
2	B	123	SER	C-N-CA	7.04	133.47	120.95
1	E	176	HIS	N-CA-C	-6.83	99.83	110.42
1	A	248	ASP	CA-C-N	6.76	131.42	120.60
1	A	248	ASP	C-N-CA	6.76	131.42	120.60
2	B	109	ILE	N-CA-C	-6.75	104.42	111.58
2	B	437	ASN	CA-CB-CG	6.72	119.32	112.60
2	F	457	CYS	CA-C-N	-6.25	111.10	121.92
2	F	457	CYS	C-N-CA	-6.25	111.10	121.92
1	E	248	ASP	CA-C-N	6.23	132.05	121.14
1	E	248	ASP	C-N-CA	6.23	132.05	121.14
2	F	514	PHE	CA-CB-CG	6.15	119.95	113.80
2	F	303	ASP	CA-CB-CG	6.07	118.67	112.60
3	C	492	ILE	N-CA-C	-5.92	105.94	111.45
2	F	457	CYS	N-CA-C	-5.90	100.04	109.96
1	A	251	LYS	N-CA-C	5.75	119.10	109.95
1	A	176	HIS	N-CA-C	-5.74	101.70	110.14
1	E	11	ALA	CA-C-N	5.70	127.67	120.72
1	E	11	ALA	C-N-CA	5.70	127.67	120.72
3	G	487	LEU	CA-C-N	5.66	127.86	120.28
3	G	487	LEU	C-N-CA	5.66	127.86	120.28
1	A	358	ASP	CA-CB-CG	5.55	118.15	112.60
3	G	489	ASP	CA-CB-CG	5.54	118.14	112.60
1	E	79	LEU	N-CA-C	-5.52	100.81	109.25
1	E	33	ASP	N-CA-C	-5.47	106.78	113.50
2	F	447	ASP	CA-CB-CG	5.44	118.04	112.60
1	A	275	GLU	CB-CG-CD	5.44	121.84	112.60
2	B	435	ASN	CA-C-N	5.41	129.81	122.07
2	B	435	ASN	C-N-CA	5.41	129.81	122.07
1	A	37	THR	CB-CA-C	5.41	119.49	109.70
2	F	152	SER	CA-C-N	5.40	131.86	121.54
2	F	152	SER	C-N-CA	5.40	131.86	121.54
2	F	129	ARG	N-CA-C	5.38	116.82	111.07
2	F	496	ASP	CA-CB-CG	5.36	117.96	112.60
2	B	127	ILE	N-CA-CB	5.35	116.45	110.62
1	A	293	SER	N-CA-C	5.31	117.06	109.14
2	F	127	ILE	N-CA-CB	5.29	116.18	110.62
2	B	239	PRO	CA-C-N	5.27	129.60	120.58
2	B	239	PRO	C-N-CA	5.27	129.60	120.58
1	E	270	ASP	CA-C-N	5.26	127.33	120.28
1	E	270	ASP	C-N-CA	5.26	127.33	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	G	418	HIS	CA-C-N	5.25	127.94	120.53
3	G	418	HIS	C-N-CA	5.25	127.94	120.53
1	A	33	ASP	CA-CB-CG	5.24	117.84	112.60
4	H	155	GLU	CB-CG-CD	5.24	121.51	112.60
1	A	198	ASP	CA-CB-CG	5.24	117.84	112.60
1	A	379	ASP	CA-CB-CG	5.24	117.84	112.60
1	A	35	VAL	N-CA-CB	5.20	119.10	112.34
1	E	293	SER	N-CA-C	5.16	117.04	109.24
1	E	411	ASP	CA-CB-CG	5.16	117.76	112.60
2	F	461	TYR	CA-C-N	5.14	127.16	120.28
2	F	461	TYR	C-N-CA	5.14	127.16	120.28
1	A	79	LEU	N-CA-C	-5.12	100.83	108.96
2	F	236	GLU	N-CA-C	-5.10	106.90	113.23
2	B	118	MET	CA-C-N	5.09	127.35	120.38
2	B	118	MET	C-N-CA	5.09	127.35	120.38
2	F	523	THR	CB-CA-C	5.06	115.90	110.08
1	E	232	ASP	CA-CB-CG	5.06	117.66	112.60
2	B	313	GLY	N-CA-C	5.05	117.41	110.69
2	B	514	PHE	CA-CB-CG	5.04	118.84	113.80
1	E	271	ALA	N-CA-C	5.02	116.75	111.28
1	A	4	LYS	CA-C-N	5.02	127.01	120.28
1	A	4	LYS	C-N-CA	5.02	127.01	120.28
1	E	318	ASP	CA-CB-CG	5.01	117.61	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	3157	0	2989	40	0
1	E	3112	0	2954	37	0
2	B	2504	0	2533	29	0
2	F	2405	0	2434	20	0
3	C	744	0	781	8	0
3	G	706	0	745	10	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	D	130	0	138	1	0
4	H	130	0	138	1	0
5	B	1	0	0	0	0
5	F	1	0	0	0	0
All	All	12890	0	12712	132	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 5.

All (132) 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:295:PHE:HE2	2:B:353:PRO:CG	1.52	1.23
2:B:295:PHE:CE2	2:B:353:PRO:HG2	1.79	1.16
2:B:295:PHE:HE2	2:B:353:PRO:HG2	1.14	1.02
2:B:295:PHE:CE2	2:B:353:PRO:CG	2.40	0.99
2:B:295:PHE:HA	2:B:320:GLN:O	1.68	0.92
1:E:150:LEU:HD22	1:E:169:PRO:HG3	1.67	0.77
1:A:26:LYS:HG2	1:A:105:PHE:HD1	1.52	0.74
1:A:350:ILE:HG12	1:A:365:GLU:HG2	1.70	0.74
1:A:26:LYS:HG2	1:A:105:PHE:CD1	2.24	0.72
3:C:481:PRO:HB2	3:C:484:THR:HG22	1.72	0.72
1:E:144:THR:HG22	1:E:146:SER:H	1.56	0.71
1:A:150:LEU:HD22	1:A:169:PRO:HG3	1.72	0.69
1:A:144:THR:HG22	1:A:146:SER:H	1.57	0.69
2:F:483:LYS:H	2:F:484:GLY:HA2	1.57	0.69
1:A:133:MET:HE3	1:A:135:GLN:HB2	1.76	0.67
1:A:350:ILE:HG12	1:A:365:GLU:CG	2.26	0.66
1:A:121:ILE:HD11	1:A:152:PHE:CD1	2.32	0.65
2:B:295:PHE:HE2	2:B:353:PRO:CB	2.11	0.64
1:A:294:ALA:HA	1:A:319:GLU:HG2	1.82	0.62
2:B:253:ARG:HB3	2:B:296:VAL:HG22	1.80	0.62
2:B:295:PHE:HE2	2:B:353:PRO:HG3	1.60	0.62
1:A:48:GLN:NE2	1:A:131:ARG:HA	2.14	0.62
1:A:38:HIS:HD2	2:B:526:THR:OG1	1.83	0.61
3:C:440:GLU:HG3	3:C:442:SER:H	1.66	0.60
2:B:296:VAL:CG1	2:B:297:ALA:N	2.63	0.60
2:B:431[A]:GLN:HE22	2:B:441:GLN:HE21	1.49	0.60
1:A:39:ALA:O	2:B:524:PRO:HA	2.02	0.60
2:B:295:PHE:CE2	2:B:353:PRO:CB	2.83	0.60
2:B:187:LEU:HD13	2:B:251:LEU:HD23	1.84	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:435:ASN:HD22	2:B:439:ARG:HH21	1.48	0.60
1:A:55:ARG:HB2	2:B:544:LEU:HD11	1.84	0.59
1:E:186:ASN:HD22	1:E:188:ASN:H	1.50	0.59
2:B:296:VAL:HG12	2:B:297:ALA:N	2.18	0.58
2:F:182:VAL:HG23	2:F:213:VAL:HG13	1.86	0.57
3:C:456:ILE:O	3:C:484:THR:HG21	2.06	0.55
1:E:48:GLN:HE22	1:E:132:TYR:H	1.54	0.55
1:E:48:GLN:HE22	1:E:131:ARG:HA	1.72	0.54
1:A:313:PHE:HZ	1:A:347:LEU:HD22	1.72	0.54
1:A:48:GLN:HE22	1:A:131:ARG:HA	1.72	0.53
1:E:114:LYS:HG2	2:F:528:ILE:HD11	1.90	0.52
3:G:476:HIS:HD2	3:G:478:SER:H	1.56	0.52
1:A:25:LYS:HD2	1:A:105:PHE:CE2	2.45	0.52
2:F:164:PHE:HE1	2:F:319:MET:HG3	1.75	0.52
1:A:323:VAL:HG13	1:A:333:LEU:HD11	1.92	0.52
1:A:226:HIS:CE1	1:A:253:MET:HG3	2.44	0.51
1:E:253:MET:HE3	1:E:255:TRP:CZ2	2.44	0.51
1:E:350:ILE:HG12	1:E:365:GLU:HG2	1.92	0.51
3:G:418:HIS:CE1	3:G:429:VAL:H	2.29	0.51
1:A:48:GLN:HE22	1:A:132:TYR:H	1.59	0.50
2:F:428:ILE:HD12	2:F:447:ASP:HB2	1.93	0.50
1:E:298:VAL:HB	1:E:313:PHE:HB2	1.94	0.50
1:E:269:VAL:HG21	1:E:306:LEU:HD22	1.93	0.49
1:E:354:GLN:HB3	1:E:358:ASP:HB3	1.95	0.49
1:E:247:ALA:C	1:E:249:ASP:H	2.21	0.49
3:C:476:HIS:HD2	3:C:478:SER:OG	1.96	0.49
1:E:36:MET:HG2	2:F:528:ILE:HG12	1.93	0.49
3:G:462:VAL:HG13	3:G:466:GLU:HB3	1.95	0.49
1:E:350:ILE:HG12	1:E:365:GLU:CG	2.43	0.48
1:A:48:GLN:NE2	1:A:132:TYR:H	2.11	0.48
2:B:163:GLY:HA3	2:B:217:PRO:HG3	1.95	0.48
3:C:489:ASP:HB3	3:C:492:ILE:HG13	1.95	0.48
1:E:133:MET:HE3	1:E:135:GLN:HB2	1.96	0.48
3:C:438:ARG:HH11	3:C:446:LYS:HD2	1.78	0.48
1:E:347:LEU:HD12	2:F:134:VAL:HG12	1.96	0.48
2:F:483:LYS:N	2:F:484:GLY:HA2	2.28	0.48
1:E:121:ILE:HD13	1:E:157:HIS:CD2	2.49	0.47
1:E:226:HIS:CE1	1:E:253:MET:HE2	2.49	0.47
1:A:144:THR:HG23	1:A:145:PRO:HD2	1.96	0.47
2:F:138:LEU:HD22	2:F:142:GLU:HG3	1.96	0.47
2:B:431[A]:GLN:NE2	2:B:441:GLN:HE21	2.13	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:253:MET:HE3	1:A:255:TRP:CZ2	2.49	0.47
1:A:71:HIS:ND1	1:A:126:GLU:HG2	2.30	0.46
2:B:537:LYS:H	2:B:537:LYS:HE2	1.80	0.46
1:E:39:ALA:O	2:F:524:PRO:HA	2.16	0.46
1:A:13:GLU:CD	2:B:103:ARG:HH12	2.23	0.46
3:G:462:VAL:HG11	3:G:470:LEU:HD12	1.97	0.45
1:E:141:ALA:HB2	1:E:185:TRP:CZ2	2.51	0.45
1:A:151:VAL:HB	1:A:171:LEU:HB2	1.97	0.45
1:A:253:MET:HE3	1:A:255:TRP:HZ2	1.82	0.45
1:A:302:ASP:HB2	1:A:310:LEU:HD11	1.99	0.45
1:A:55:ARG:HD3	1:A:62:SER:HB3	1.99	0.45
2:B:299:MET:HG2	2:B:310:LEU:HD21	1.99	0.45
1:A:143:LYS:HE3	1:A:149:VAL:HG22	1.98	0.44
1:E:71:HIS:ND1	1:E:126:GLU:HG2	2.32	0.44
1:E:147:SER:HB2	1:E:176:HIS:O	2.17	0.44
2:F:299:MET:HG2	2:F:310:LEU:HD21	2.00	0.44
1:A:197:SER:HB3	1:A:199:ASP:OD1	2.17	0.44
1:E:144:THR:HG23	1:E:145:PRO:HD2	1.98	0.44
1:E:188:ASN:HB2	1:E:240:GLU:HB3	1.99	0.44
2:F:162:THR:HA	2:F:228:PRO:HD2	1.99	0.44
1:A:36:MET:HG2	2:B:528:ILE:HG12	1.99	0.44
1:E:315:SER:HB2	1:E:345:TRP:HH2	1.83	0.44
2:F:93:PRO:HA	2:F:96:ILE:HD12	2.00	0.44
2:F:433:LEU:HD22	2:F:438:THR:HB	2.00	0.43
1:A:284:TYR:CB	1:A:330:GLU:HB3	2.49	0.43
2:B:101:ARG:HG3	2:B:453:CYS:HA	2.00	0.43
2:F:434:TYR:HB3	2:F:439:ARG:HG3	2.00	0.43
2:F:449:HIS:NE2	2:F:456:ASN:HB2	2.33	0.43
2:B:431[A]:GLN:HG3	2:B:486:ARG:HD3	2.00	0.43
1:A:173:LEU:HB3	1:A:205:TRP:CE2	2.53	0.43
1:A:313:PHE:CZ	1:A:347:LEU:HD22	2.53	0.43
1:A:20:GLU:OE1	2:B:103:ARG:HD3	2.19	0.43
1:E:294:ALA:HA	1:E:319:GLU:HG2	2.01	0.43
1:E:48:GLN:NE2	1:E:131:ARG:HA	2.34	0.42
1:E:80:VAL:HG13	1:E:117:ILE:HG23	2.01	0.42
1:E:121:ILE:HD11	1:E:152:PHE:CE2	2.53	0.42
2:F:443:GLU:O	4:H:153:LYS:HA	2.18	0.42
1:A:157:HIS:HE1	1:A:170:ASP:OD2	2.03	0.42
1:E:284:TYR:CB	1:E:330:GLU:HB3	2.50	0.42
1:E:308:LEU:HD21	2:F:145:LYS:HG2	2.00	0.42
1:A:350:ILE:HA	1:A:365:GLU:HG3	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:105:PHE:HB3	1:A:106:GLY:H	1.48	0.42
2:B:451:PRO:HB2	4:D:158:LEU:HD12	2.02	0.42
2:B:164:PHE:HE1	2:B:319:MET:HG3	1.84	0.41
1:E:57:GLU:HA	1:E:58:GLY:HA2	1.77	0.41
1:E:177:GLN:HE21	1:E:177:GLN:HB2	1.73	0.41
1:E:253:MET:HE3	1:E:255:TRP:HZ2	1.84	0.41
2:F:295:PHE:HB3	2:F:319:MET:HB3	2.03	0.41
3:G:434:VAL:HG11	3:G:447:LEU:HD22	2.03	0.41
3:G:456:ILE:HA	3:G:484:THR:OG1	2.20	0.41
1:E:226:HIS:CE1	1:E:253:MET:HG3	2.55	0.41
1:E:339:ASP:HA	3:G:493:TYR:OH	2.20	0.41
3:G:432:SER:HB3	3:G:451:TRP:CZ3	2.56	0.41
1:A:298:VAL:HB	1:A:313:PHE:HB2	2.02	0.41
3:C:476:HIS:CD2	3:C:478:SER:H	2.39	0.41
3:C:476:HIS:CD2	3:C:478:SER:OG	2.73	0.41
1:E:315:SER:HB2	1:E:345:TRP:CH2	2.56	0.41
2:F:475:ILE:HD12	2:F:492:ASN:HA	2.03	0.41
1:A:121:ILE:HD13	1:A:121:ILE:HG21	1.87	0.41
3:G:481:PRO:HB2	3:G:484:THR:HG22	2.04	0.40
2:B:449:HIS:NE2	2:B:456:ASN:HB2	2.37	0.40
3:G:484:THR:HA	3:G:487:LEU:HD23	2.03	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	391/439 (89%)	372 (95%)	18 (5%)	1 (0%)	36	65
1	E	385/439 (88%)	372 (97%)	12 (3%)	1 (0%)	36	65
2	B	283/478 (59%)	263 (93%)	20 (7%)	0	100	100
2	F	276/478 (58%)	259 (94%)	16 (6%)	1 (0%)	30	59

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	C	89/100 (89%)	85 (96%)	4 (4%)	0	100	100
3	G	84/100 (84%)	78 (93%)	6 (7%)	0	100	100
4	D	13/19 (68%)	11 (85%)	2 (15%)	0	100	100
4	H	13/19 (68%)	13 (100%)	0	0	100	100
All	All	1534/2072 (74%)	1453 (95%)	78 (5%)	3 (0%)	43	72

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	315	SER
2	F	153	LEU
1	A	315	SER

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	353/388 (91%)	325 (92%)	28 (8%)	11	34
1	E	349/388 (90%)	320 (92%)	29 (8%)	10	32
2	B	283/442 (64%)	251 (89%)	32 (11%)	5	19
2	F	273/442 (62%)	236 (86%)	37 (14%)	3	12
3	C	85/92 (92%)	77 (91%)	8 (9%)	8	26
3	G	81/92 (88%)	74 (91%)	7 (9%)	10	30
4	D	15/18 (83%)	15 (100%)	0	100	100
4	H	15/18 (83%)	11 (73%)	4 (27%)	0	1
All	All	1454/1880 (77%)	1309 (90%)	145 (10%)	7	24

All (145) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	LYS

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Mol	Chain	Res	Type
1	A	14	GLU
1	A	25	LYS
1	A	26	LYS
1	A	55	ARG
1	A	68	LEU
1	A	81	ILE
1	A	105	PHE
1	A	111	VAL
1	A	112	SER
1	A	114	LYS
1	A	121	ILE
1	A	126	GLU
1	A	160	LYS
1	A	168	ASN
1	A	177	GLN
1	A	200	HIS
1	A	207	ILE
1	A	218	ASP
1	A	221	THR
1	A	249	ASP
1	A	279	LEU
1	A	323	VAL
1	A	347	LEU
1	A	353	GLU
1	A	357	GLU
1	A	365	GLU
1	A	410	ASN
2	B	79	VAL
2	B	95	GLN
2	B	123	SER
2	B	128	LYS
2	B	138	LEU
2	B	156	HIS
2	B	158	GLN
2	B	184	LEU
2	B	191	VAL
2	B	197	LYS
2	B	212	GLN
2	B	215	LEU
2	B	219	LEU
2	B	230	LEU
2	B	236	GLU

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Mol	Chain	Res	Type
2	B	301	VAL
2	B	308	LEU
2	B	320	GLN
2	B	351	GLN
2	B	354	THR
2	B	360	ARG
2	B	424	GLN
2	B	428	ILE
2	B	437	ASN
2	B	438	THR
2	B	472	SER
2	B	477	ASN
2	B	483	LYS
2	B	496	ASP
2	B	517	ASN
2	B	534	LYS
2	B	537	LYS
3	C	416	SER
3	C	420	GLU
3	C	437	LYS
3	C	442	SER
3	C	457	LEU
3	C	462	VAL
3	C	468	HIS
3	C	499	LYS
1	E	4	LYS
1	E	5	GLU
1	E	14	GLU
1	E	25	LYS
1	E	37	THR
1	E	53	VAL
1	E	89	ASP
1	E	108	PHE
1	E	121	ILE
1	E	126	GLU
1	E	160	LYS
1	E	177	GLN
1	E	178	LYS
1	E	186	ASN
1	E	200	HIS
1	E	221	THR
1	E	238	LEU

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Mol	Chain	Res	Type
1	E	241	SER
1	E	249	ASP
1	E	279	LEU
1	E	286	GLU
1	E	289	LEU
1	E	308	LEU
1	E	312	SER
1	E	317	LYS
1	E	347	LEU
1	E	357	GLU
1	E	398	ILE
1	E	412	GLU
2	F	88	GLN
2	F	91	GLU
2	F	92	LYS
2	F	103	ARG
2	F	124	ARG
2	F	125	THR
2	F	127	ILE
2	F	128	LYS
2	F	131	THR
2	F	138	LEU
2	F	145	LYS
2	F	147	GLU
2	F	151	HIS
2	F	184	LEU
2	F	191	VAL
2	F	194	LYS
2	F	197	LYS
2	F	199	VAL
2	F	210	LYS
2	F	215	LEU
2	F	230	LEU
2	F	233	SER
2	F	242	SER
2	F	245	VAL
2	F	300	THR
2	F	301	VAL
2	F	306	ARG
2	F	322	MET
2	F	354	THR
2	F	359	LEU

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Mol	Chain	Res	Type
2	F	360	ARG
2	F	428	ILE
2	F	433	LEU
2	F	438	THR
2	F	472	SER
2	F	477	ASN
2	F	483	LYS
3	G	418	HIS
3	G	424	LYS
3	G	444	LYS
3	G	452	MET
3	G	462	VAL
3	G	487	LEU
3	G	501	LEU
4	H	150	ARG
4	H	151	LYS
4	H	161	LEU
4	H	164	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (57) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	38	HIS
1	A	48	GLN
1	A	76	GLN
1	A	78	HIS
1	A	88	ASN
1	A	157	HIS
1	A	177	GLN
1	A	186	ASN
1	A	311	HIS
1	A	324	GLN
1	A	328	HIS
1	A	354	GLN
1	A	400	GLN
1	A	403	GLN
1	A	410	ASN
2	B	80	GLN
2	B	88	GLN
2	B	104	ASN
2	B	148	GLN
2	B	158	GLN

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Mol	Chain	Res	Type
2	B	216	ASN
2	B	435	ASN
2	B	456	ASN
2	B	492	ASN
3	C	414	ASN
3	C	463	ASN
3	C	468	HIS
3	C	476	HIS
3	C	498	GLN
1	E	38	HIS
1	E	48	GLN
1	E	76	GLN
1	E	78	HIS
1	E	122	ASN
1	E	136	ASN
1	E	177	GLN
1	E	186	ASN
1	E	250	GLN
1	E	260	ASN
1	E	261	ASN
1	E	322	GLN
1	E	324	GLN
1	E	400	GLN
1	E	407	ASN
1	E	410	ASN
2	F	80	GLN
2	F	83	HIS
2	F	104	ASN
2	F	122	ASN
2	F	212	GLN
2	F	298	GLN
2	F	309	GLN
2	F	356	GLN
2	F	437	ASN
2	F	517	ASN
3	G	468	HIS
3	G	476	HIS

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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	397/439 (90%)	-0.31	14 (3%) 47 38	16, 44, 104, 135	0
1	E	391/439 (89%)	-0.18	8 (2%) 65 56	22, 56, 112, 146	0
2	B	300/478 (62%)	0.46	29 (9%) 13 11	18, 77, 135, 160	1 (0%)
2	F	289/478 (60%)	0.41	24 (8%) 17 14	27, 73, 142, 162	1 (0%)
3	C	91/100 (91%)	0.50	4 (4%) 39 30	37, 84, 137, 145	0
3	G	86/100 (86%)	0.82	7 (8%) 18 15	41, 88, 139, 147	0
4	D	15/19 (78%)	-0.47	0 100 100	33, 41, 78, 90	0
4	H	15/19 (78%)	-0.10	0 100 100	37, 48, 77, 109	0
All	All	1584/2072 (76%)	0.11	86 (5%) 31 24	16, 60, 127, 162	2 (0%)

All (86) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	79	VAL	6.2
2	B	209	GLY	6.0
1	A	93	PHE	5.9
1	A	211	PRO	5.5
1	A	105	PHE	5.4
1	A	108	PHE	5.4
2	B	230	LEU	5.2
2	F	230	LEU	4.9
1	A	110	SER	4.9
1	E	210	VAL	4.9
2	B	167	LYS	4.8
2	B	233	SER	4.5
2	F	153	LEU	4.5
2	B	228	PRO	4.3
2	F	363	GLY	4.3
2	B	223	LYS	4.3

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Mol	Chain	Res	Type	RSRZ
2	F	228	PRO	4.2
1	E	108	PHE	4.1
2	B	538	ALA	3.9
2	B	208	THR	3.8
2	B	546	TRP	3.7
2	F	255	THR	3.7
2	B	219	LEU	3.7
1	A	109	GLY	3.7
3	C	413	PHE	3.6
2	F	167	LYS	3.5
2	F	515	SER	3.4
2	F	514	PHE	3.4
3	G	423	GLY	3.3
3	G	482	LYS	3.3
2	B	536	THR	3.1
2	B	222	THR	3.0
3	G	501	LEU	3.0
3	G	439	LYS	3.0
2	F	218	ASP	3.0
3	G	455	ASP	3.0
1	E	110	SER	2.9
2	B	80	GLN	2.9
1	A	92	GLN	2.8
3	C	446	LYS	2.8
1	A	107	GLY	2.8
2	F	182	VAL	2.8
2	B	295	PHE	2.8
1	A	106	GLY	2.8
2	F	294	THR	2.8
1	E	92	GLN	2.7
2	B	232	VAL	2.7
1	A	91	ALA	2.7
3	G	446	LYS	2.7
2	B	363	GLY	2.7
2	B	234	SER	2.6
2	F	532	ARG	2.6
3	C	471	LYS	2.6
1	E	4	LYS	2.5
1	E	107	GLY	2.5
2	B	161	PHE	2.5
2	B	154	SER	2.5
2	F	81	ALA	2.5

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Mol	Chain	Res	Type	RSRZ
3	G	444	LYS	2.5
1	A	210	VAL	2.5
2	B	155	ALA	2.5
2	F	231	ALA	2.5
2	F	210	LYS	2.4
2	F	308	LEU	2.4
2	F	362	THR	2.4
2	B	239	PRO	2.4
2	F	232	VAL	2.3
2	F	322	MET	2.3
1	A	209	ALA	2.3
2	B	438	THR	2.3
1	E	109	GLY	2.3
1	A	412	GLU	2.3
2	F	235	ASN	2.2
2	B	253	ARG	2.2
2	F	192	CYS	2.2
1	A	111	VAL	2.2
2	B	537	LYS	2.2
2	B	215	LEU	2.2
2	B	211	LYS	2.2
2	F	154	SER	2.2
2	B	231	ALA	2.1
2	B	186	VAL	2.1
2	F	199	VAL	2.1
2	F	425	LYS	2.1
1	E	264	LYS	2.1
3	C	445	ILE	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	0.03	30,30,30,30	0
5	ZN	F	1001	1/1	1.00	0.03	39,39,39,39	0

6.5 Other polymers [i](#)

There are no such residues in this entry.