



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 06:07 PM UTC

PDB ID : 6U4Y / pdb_00006u4y
Title : Crystal Structure of an EZH2-EED Complex in an Oligomeric State
Authors : Jiao, L.; Liu, X.
Deposited on : 2019-08-26
Resolution : 2.91 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

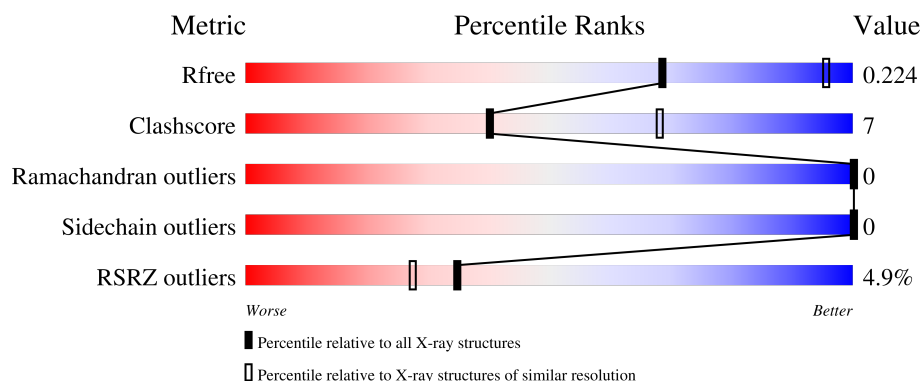
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.91 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	2995 (2.94-2.90)
Clashscore	190562	3213 (2.94-2.90)
Ramachandran outliers	187476	3128 (2.94-2.90)
Sidechain outliers	187428	3130 (2.94-2.90)
RSRZ outliers	180081	2995 (2.94-2.90)

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	224	12% 55% 17% 29%
1	B	224	10% 62% 12% 26%
1	C	224	8% 59% 11% 30%
2	D	366	% 87% 12% .
2	E	366	83% 16% .

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Mol	Chain	Length	Quality of chain
2	F	366	% 86% 11% .

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 12736 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-lysine N-methyltransferase EZH2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	160	Total	C	N	O	S	0	0	0
			1334	853	230	244	7			
1	B	166	Total	C	N	O	S	0	0	0
			1372	872	237	256	7			
1	C	157	Total	C	N	O	S	0	0	0
			1310	834	227	243	6			

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	SER	-	expression tag	UNP Q15910
A	72	SER	THR	conflict	UNP Q15910
A	216	GLY	-	linker	UNP Q15910
A	217	SER	-	linker	UNP Q15910
A	218	SER	-	linker	UNP Q15910
A	219	GLY	-	linker	UNP Q15910
B	1	SER	-	expression tag	UNP Q15910
B	72	SER	THR	conflict	UNP Q15910
B	216	GLY	-	linker	UNP Q15910
B	217	SER	-	linker	UNP Q15910
B	218	SER	-	linker	UNP Q15910
B	219	GLY	-	linker	UNP Q15910
C	1	SER	-	expression tag	UNP Q15910
C	72	SER	THR	conflict	UNP Q15910
C	216	GLY	-	linker	UNP Q15910
C	217	SER	-	linker	UNP Q15910
C	218	SER	-	linker	UNP Q15910
C	219	GLY	-	linker	UNP Q15910

- Molecule 2 is a protein called Polycomb protein EED.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	361	Total	C	N	O	S	0	0	0
			2918	1847	511	538	22			
2	E	360	Total	C	N	O	S	0	0	0
			2907	1841	507	537	22			
2	F	358	Total	C	N	O	S	0	0	0
			2895	1835	504	534	22			

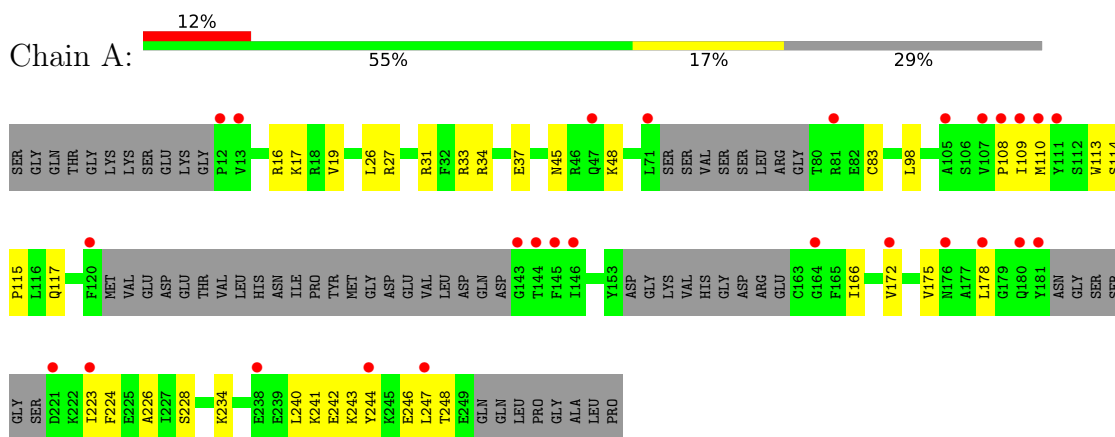
There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	76	GLY	-	expression tag	UNP O75530
D	77	SER	-	expression tag	UNP O75530
E	76	GLY	-	expression tag	UNP O75530
E	77	SER	-	expression tag	UNP O75530
F	76	GLY	-	expression tag	UNP O75530
F	77	SER	-	expression tag	UNP O75530

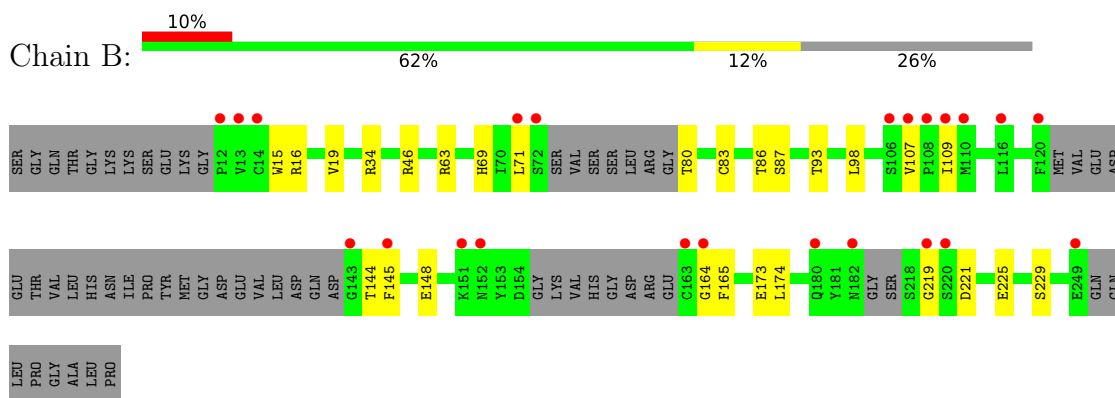
3 Residue-property plots [i](#)

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.

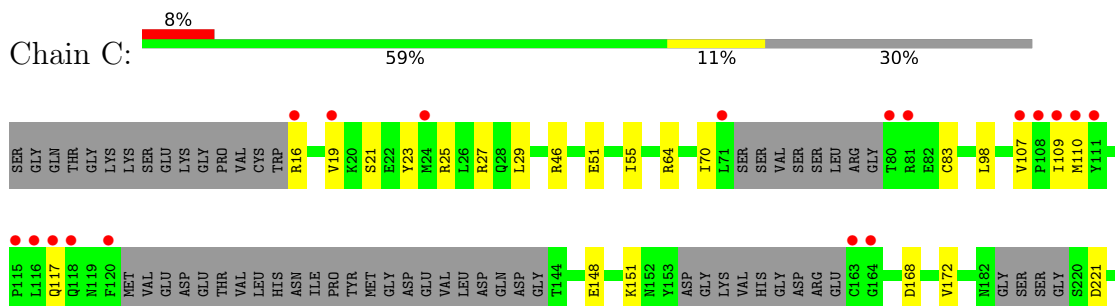
• Molecule 1: Histone-lysine N-methyltransferase EZH2

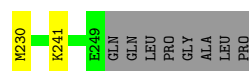


• Molecule 1: Histone-lysine N-methyltransferase EZH2

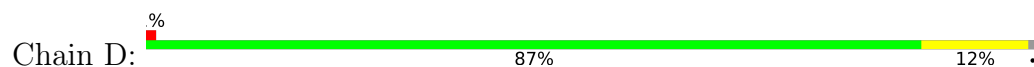


• Molecule 1: Histone-lysine N-methyltransferase EZH2

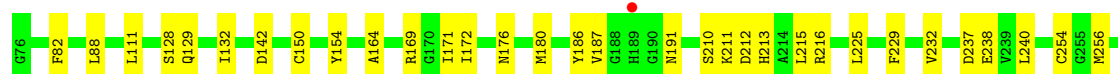
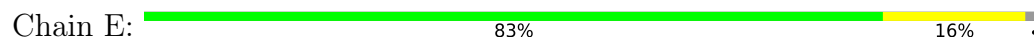




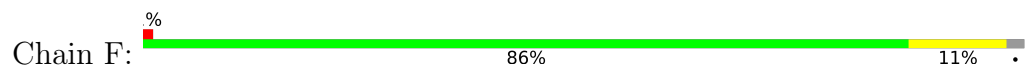
● Molecule 2: Polycomb protein EED



● Molecule 2: Polycomb protein EED



● Molecule 2: Polycomb protein EED



4 Data and refinement statistics

Property	Value	Source
Space group	P 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	181.63Å 114.72Å 131.52Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.50 – 2.91 48.50 – 2.91	Depositor EDS
% Data completeness (in resolution range)	89.1 (48.50-2.91) 89.3 (48.50-2.91)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.57 (at 2.91Å)	Xtriage
Refinement program	BUSTER 2.10.3, PHENIX 1.16_3549	Depositor
R, R_{free}	0.182 , 0.224 0.187 , 0.224	Depositor DCC
R_{free} test set	2577 reflections (4.21%)	wwPDB-VP
Wilson B-factor (Å ²)	53.6	Xtriage
Anisotropy	0.139	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 63.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	12736	wwPDB-VP
Average B, all atoms (Å ²)	57.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.82% 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	0.26	0/1357	0.55	0/1820
1	B	0.20	0/1395	0.42	0/1871
1	C	0.19	0/1330	0.42	0/1782
2	D	0.17	0/2991	0.40	0/4048
2	E	0.21	0/2980	0.44	2/4034 (0.0%)
2	F	0.17	0/2968	0.40	0/4018
All	All	0.19	0/13021	0.43	2/17573 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	343	ILE	CA-C-N	-6.36	108.96	123.15
2	E	343	ILE	C-N-CA	-6.36	108.96	123.15

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	1334	0	1347	38	0
1	B	1372	0	1375	27	0
1	C	1310	0	1323	27	1
2	D	2918	0	2829	28	0
2	E	2907	0	2816	38	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	F	2895	0	2807	26	1
All	All	12736	0	12497	166	1

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 (166) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:109:ILE:O	1:A:110:MET:HE3	1.56	1.04
1:A:109:ILE:C	1:A:110:MET:HE3	1.87	0.99
1:C:221:ASP:OD2	1:C:241:LYS:HE3	1.66	0.93
2:E:191:ASN:HB3	2:E:211:LYS:HB3	1.51	0.92
1:B:107:VAL:HG23	1:B:109:ILE:HD11	1.50	0.91
1:A:166:ILE:O	1:A:234:LYS:NZ	2.06	0.88
1:C:221:ASP:OD2	1:C:241:LYS:CE	2.31	0.78
1:C:25:ARG:O	1:C:29:LEU:HD13	1.88	0.72
1:A:109:ILE:C	1:A:110:MET:CE	2.62	0.71
1:B:107:VAL:O	1:B:109:ILE:HD12	1.91	0.71
2:D:215:LEU:HB2	2:D:229:PHE:HB2	1.73	0.69
1:C:83:CYS:HB3	1:C:98:LEU:HG	1.73	0.69
1:C:25:ARG:O	1:C:29:LEU:CD1	2.41	0.69
2:F:232:VAL:HG12	2:F:295:HIS:HB3	1.74	0.68
1:B:16:ARG:HE	1:C:230:MET:HE3	1.57	0.68
2:F:308:TYR:O	2:F:323:SER:HB2	1.94	0.67
1:B:83:CYS:HB3	1:B:98:LEU:HG	1.77	0.67
2:E:82:PHE:HZ	2:E:376:MET:HE1	1.60	0.66
1:C:16:ARG:CZ	1:C:16:ARG:HA	2.26	0.65
1:A:109:ILE:N	1:A:110:MET:HE1	2.13	0.64
1:C:46:ARG:HD3	2:F:392:GLU:HG2	1.79	0.64
2:F:191:ASN:HB3	2:F:211:LYS:HB3	1.79	0.63
2:E:238:GLU:HB2	2:E:256:MET:HG3	1.81	0.62
1:C:46:ARG:NH2	2:F:374:GLN:O	2.32	0.62
1:A:242:GLU:O	1:A:246:GLU:HG2	1.99	0.61
2:F:238:GLU:HB2	2:F:256:MET:HG3	1.83	0.60
1:A:27:ARG:HE	1:A:31:ARG:HH21	1.50	0.60
1:C:70:ILE:HD11	2:F:133:ARG:NH1	2.17	0.60
1:A:166:ILE:HG23	1:A:234:LYS:HD2	1.85	0.59
1:B:34:ARG:NH2	2:E:352:ILE:O	2.35	0.59
2:D:189:HIS:CE1	2:D:216:ARG:HD2	2.38	0.59
1:B:107:VAL:HG23	1:B:109:ILE:CD1	2.27	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:110:MET:SD	1:A:110:MET:N	2.77	0.58
1:B:46:ARG:HD3	2:E:392:GLU:HG3	1.86	0.58
2:D:82:PHE:HZ	2:D:376:MET:HE1	1.68	0.57
2:E:339:ASP:HB3	2:E:342:LYS:HG3	1.85	0.57
2:F:215:LEU:HB2	2:F:229:PHE:HB2	1.87	0.57
2:D:125:GLU:HB2	2:D:135:LEU:HD11	1.88	0.56
2:E:215:LEU:HB2	2:E:229:PHE:HB2	1.88	0.56
1:B:46:ARG:HH11	1:B:46:ARG:HG3	1.71	0.55
2:E:261:LYS:HG2	2:E:300:SER:HB2	1.87	0.55
2:D:360:GLN:O	2:D:381:ASN:HB2	2.06	0.55
1:A:33:ARG:O	1:A:37:GLU:HG3	2.07	0.54
1:C:107:VAL:O	1:C:109:ILE:HD12	2.07	0.54
1:A:172:VAL:HA	1:A:175:VAL:HG22	1.90	0.54
2:F:196:LEU:O	2:F:197:LYS:HD3	2.08	0.54
2:D:238:GLU:HB2	2:D:256:MET:HG3	1.87	0.54
1:A:240:LEU:HD23	1:A:243:LYS:HD3	1.90	0.54
1:B:87:SER:HB2	2:E:88:LEU:HD23	1.89	0.54
2:D:191:ASN:HB3	2:D:211:LYS:HB3	1.90	0.53
2:F:170:GLY:HA2	2:F:193:ILE:HG13	1.90	0.53
2:D:80:TYR:CG	2:D:376:MET:HE3	2.44	0.53
2:D:262:LEU:HB3	2:D:299:PHE:HB3	1.90	0.53
2:F:211:LYS:HG3	2:F:238:GLU:CD	2.34	0.52
1:A:244:TYR:O	1:A:248:THR:OG1	2.23	0.52
2:F:122:THR:HG23	2:F:137:SER:HB3	1.91	0.52
2:E:172:ILE:HB	2:E:186:TYR:HB2	1.91	0.52
1:A:109:ILE:N	1:A:110:MET:CE	2.73	0.51
1:B:109:ILE:HD12	1:B:109:ILE:H	1.75	0.51
1:A:226:ALA:HB2	1:C:16:ARG:HG3	1.92	0.51
2:E:213:HIS:CE1	2:E:237:ASP:HA	2.46	0.51
2:F:155:ASP:O	2:F:159:SER:N	2.39	0.51
1:A:16:ARG:HA	1:A:19:VAL:HG12	1.92	0.51
1:A:27:ARG:HD2	1:A:31:ARG:HE	1.75	0.51
1:B:107:VAL:O	1:B:109:ILE:CD1	2.59	0.51
1:A:240:LEU:HA	1:A:243:LYS:HB2	1.91	0.51
2:E:254:CYS:HB2	2:E:309:VAL:HB	1.93	0.51
1:C:51:GLU:O	1:C:55:ILE:HG13	2.12	0.50
2:E:82:PHE:CZ	2:E:376:MET:HE1	2.42	0.50
2:E:216:ARG:HB3	2:E:225:LEU:HD11	1.93	0.50
2:F:125:GLU:HB2	2:F:135:LEU:HD11	1.93	0.49
1:C:148:GLU:HA	1:C:151:LYS:HB2	1.94	0.49
1:A:243:LYS:O	1:A:246:GLU:HG3	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:164:GLY:O	1:B:165:PHE:HB2	2.13	0.48
2:E:128:SER:HB3	2:E:129:GLN:NE2	2.27	0.48
1:B:63:ARG:HD3	2:E:154:TYR:CZ	2.48	0.48
1:B:219:GLY:C	1:B:221:ASP:H	2.22	0.47
2:F:335:LYS:HB3	2:F:335:LYS:HE3	1.69	0.47
2:F:187:VAL:HG12	2:F:187:VAL:O	2.14	0.47
2:E:210:SER:OG	2:E:212:ASP:OD1	2.33	0.47
2:D:142:ASP:OD1	2:D:144:ASP:N	2.47	0.47
1:C:25:ARG:O	1:C:29:LEU:HD12	2.15	0.47
2:D:82:PHE:CZ	2:D:376:MET:HE1	2.49	0.47
1:A:247:LEU:HD12	1:A:247:LEU:HA	1.51	0.47
2:F:213:HIS:CE1	2:F:237:ASP:HA	2.50	0.47
1:A:108:PRO:C	1:A:110:MET:HE1	2.40	0.46
2:D:112:VAL:HG12	2:D:125:GLU:HG3	1.97	0.46
1:A:224:PHE:CD2	1:A:241:LYS:HB3	2.51	0.46
2:D:195:GLU:HB3	2:D:209:VAL:HG22	1.97	0.46
2:F:360:GLN:O	2:F:381:ASN:HB2	2.15	0.46
1:A:27:ARG:HE	1:A:31:ARG:NH2	2.14	0.46
2:E:390:ASP:OD2	2:E:393:VAL:HG13	2.15	0.46
2:E:171:ILE:HG23	2:E:187:VAL:HG22	1.97	0.46
1:C:21:SER:O	1:C:25:ARG:HB2	2.15	0.46
2:D:171:ILE:HG12	2:D:187:VAL:HG22	1.97	0.46
2:E:394:GLU:O	2:E:396:PRO:HD3	2.16	0.46
2:E:128:SER:HB3	2:E:129:GLN:HE21	1.81	0.46
1:A:223:ILE:HD12	1:A:223:ILE:H	1.80	0.45
1:B:46:ARG:HG3	1:B:46:ARG:NH1	2.31	0.45
1:B:46:ARG:CD	2:E:392:GLU:HG3	2.46	0.45
2:E:347:GLU:OE2	2:E:347:GLU:HA	2.16	0.45
1:B:107:VAL:CG2	1:B:109:ILE:HD11	2.36	0.45
1:A:178:LEU:HD11	1:C:19:VAL:HG12	1.99	0.44
2:D:328:ILE:HG13	2:D:358:TYR:HE2	1.81	0.44
2:E:111:LEU:HD22	2:E:419:SER:HB2	1.99	0.44
2:E:260:LEU:HD22	2:E:331:TRP:CZ2	2.52	0.44
2:E:268:LYS:O	2:E:272:ASN:ND2	2.49	0.44
1:A:228:SER:HB2	1:A:240:LEU:HD12	2.00	0.44
1:C:109:ILE:HG22	1:C:110:MET:N	2.33	0.44
2:E:132:ILE:HD11	2:E:436:ARG:HB2	2.00	0.44
1:A:83:CYS:HB3	1:A:98:LEU:HG	1.99	0.44
1:C:70:ILE:HD11	2:F:133:ARG:CZ	2.48	0.44
1:A:226:ALA:CB	1:C:16:ARG:HG3	2.48	0.44
1:A:34:ARG:NH2	2:D:352:ILE:O	2.41	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:168:ASP:O	1:C:172:VAL:HG13	2.18	0.43
2:E:215:LEU:C	2:E:216:ARG:HG3	2.44	0.43
2:F:91:ASP:CG	2:F:120:ARG:HH22	2.25	0.43
1:B:69:HIS:HB3	1:B:71:LEU:HG	1.98	0.43
1:C:16:ARG:HA	1:C:16:ARG:NH1	2.33	0.43
2:E:142:ASP:OD2	2:E:169:ARG:NE	2.51	0.43
2:E:262:LEU:HB3	2:E:299:PHE:HB3	2.00	0.43
1:C:107:VAL:O	1:C:109:ILE:CD1	2.66	0.43
2:E:150:CYS:HA	2:E:164:ALA:O	2.17	0.43
1:C:16:ARG:HA	1:C:16:ARG:NE	2.34	0.43
1:A:17:LYS:HD3	1:A:17:LYS:HA	1.75	0.43
1:B:145:PHE:O	1:B:148:GLU:HB2	2.19	0.43
1:C:23:TYR:OH	1:C:27:ARG:NH1	2.52	0.43
2:D:211:LYS:HA	2:D:238:GLU:HG2	2.01	0.43
1:A:16:ARG:HA	1:A:19:VAL:CG1	2.49	0.43
1:A:19:VAL:HG23	1:B:174:LEU:HD21	2.01	0.43
1:C:109:ILE:HD12	1:C:109:ILE:H	1.83	0.43
2:E:260:LEU:HD22	2:E:331:TRP:HZ2	1.83	0.43
2:F:82:PHE:HZ	2:F:376:MET:HE1	1.84	0.43
1:B:15:TRP:O	1:B:19:VAL:HG23	2.18	0.42
2:D:322:LYS:HB3	2:D:328:ILE:HG12	2.00	0.42
1:C:64:ARG:HE	1:C:64:ARG:HB3	1.57	0.42
1:A:224:PHE:N	1:A:224:PHE:CD1	2.87	0.42
2:F:416:THR:HB	2:F:425:LEU:HD11	2.02	0.42
2:F:322:LYS:HB3	2:F:328:ILE:HG12	2.00	0.42
1:B:144:THR:O	1:B:148:GLU:HG3	2.20	0.42
2:F:102:ASN:HB2	2:F:152:TRP:CE2	2.54	0.42
2:D:172:ILE:HB	2:D:186:TYR:HB2	2.02	0.42
2:E:240:LEU:HD11	2:E:256:MET:HG2	2.02	0.42
2:F:82:PHE:CZ	2:F:376:MET:HE1	2.54	0.42
1:B:86:THR:HG22	1:B:93:THR:HG23	2.01	0.42
2:D:225:LEU:O	2:D:291:SER:HB3	2.20	0.42
2:D:254:CYS:HB2	2:D:309:VAL:HB	2.02	0.41
2:D:211:LYS:HG3	2:D:238:GLU:HG2	2.02	0.41
2:D:87:SER:HA	2:D:434:ILE:O	2.20	0.41
2:D:386:LEU:HB3	2:D:404:LEU:HB2	2.02	0.41
2:E:180:MET:HE3	2:E:180:MET:HB2	1.79	0.41
1:B:80:THR:HB	2:D:400:LYS:HG2	2.02	0.41
1:A:45:ASN:HA	1:A:48:LYS:HD2	2.02	0.41
1:B:225:GLU:O	1:B:229:SER:OG	2.26	0.41
2:F:377:LEU:HB2	2:F:391:LEU:HD11	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:381:ASN:ND2	2:D:385:LYS:HB2	2.36	0.41
2:E:232:VAL:HG12	2:E:295:HIS:HB3	2.02	0.41
2:E:308:TYR:HB2	2:E:364:TRP:CH2	2.55	0.41
1:B:87:SER:HB2	2:E:88:LEU:CD2	2.51	0.41
1:A:114:SER:HB3	1:A:117:GLN:H	1.85	0.40
2:D:269:ARG:HH21	2:D:292:GLN:HG3	1.85	0.40
1:A:26:LEU:HD22	1:B:173:GLU:HB3	2.03	0.40
2:D:358:TYR:HE1	2:D:361:CYS:HB3	1.87	0.40
1:A:113:TRP:CH2	1:A:115:PRO:HG3	2.56	0.40
1:A:224:PHE:N	1:A:224:PHE:HD1	2.19	0.40
2:E:176:ASN:O	2:E:180:MET:N	2.51	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:117:GLN:NE2	2:F:223:ASP:OD2[4_559]	1.94	0.26

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	150/224 (67%)	144 (96%)	6 (4%)	0	100	100
1	B	156/224 (70%)	150 (96%)	6 (4%)	0	100	100
1	C	147/224 (66%)	145 (99%)	2 (1%)	0	100	100
2	D	357/366 (98%)	347 (97%)	10 (3%)	0	100	100
2	E	356/366 (97%)	343 (96%)	13 (4%)	0	100	100
2	F	354/366 (97%)	340 (96%)	14 (4%)	0	100	100
All	All	1520/1770 (86%)	1469 (97%)	51 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	150/203 (74%)	150 (100%)	0	100	100
1	B	155/203 (76%)	155 (100%)	0	100	100
1	C	148/203 (73%)	148 (100%)	0	100	100
2	D	323/328 (98%)	323 (100%)	0	100	100
2	E	322/328 (98%)	322 (100%)	0	100	100
2	F	321/328 (98%)	321 (100%)	0	100	100
All	All	1419/1593 (89%)	1419 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	62	GLN
1	B	119	ASN
1	C	28	GLN
1	C	152	ASN
1	C	182	ASN
2	D	204	ASN
2	D	213	HIS
2	E	129	GLN
2	E	146	ASN
2	F	181	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 oligosaccharides 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	160/224 (71%)	0.76	27 (16%)	4 3	40, 82, 136, 161	0
1	B	166/224 (74%)	0.40	23 (13%)	6 5	29, 62, 117, 161	0
1	C	157/224 (70%)	0.49	18 (11%)	9 8	41, 70, 114, 148	0
2	D	361/366 (98%)	-0.50	4 (1%)	78 71	22, 42, 71, 121	0
2	E	360/366 (98%)	-0.43	1 (0%)	90 87	25, 45, 78, 122	0
2	F	358/366 (97%)	-0.40	3 (0%)	82 76	24, 46, 79, 122	0
All	All	1562/1770 (88%)	-0.14	76 (4%)	35 27	22, 51, 107, 161	0

All (76) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	71	LEU	6.1
1	C	71	LEU	5.0
1	A	71	LEU	4.9
1	A	12	PRO	4.5
1	A	108	PRO	4.5
2	F	282	PRO	4.4
1	C	109	ILE	4.2
1	A	13	VAL	4.1
2	D	76	GLY	4.0
1	B	12	PRO	3.9
1	A	110	MET	3.7
1	B	116	LEU	3.7
2	F	290	ILE	3.7
1	A	109	ILE	3.6
1	C	107	VAL	3.5
1	C	108	PRO	3.5
1	B	108	PRO	3.5
1	C	164	GLY	3.3
1	C	110	MET	3.2

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Mol	Chain	Res	Type	RSRZ
1	B	180	GLN	3.2
1	C	16	ARG	3.1
1	A	145	PHE	3.1
1	B	72	SER	3.0
1	C	116	LEU	3.0
1	C	80	THR	3.0
1	B	110	MET	2.9
1	A	181	TYR	2.8
1	A	180	GLN	2.8
1	B	219	GLY	2.8
1	A	146	ILE	2.7
1	B	163	CYS	2.7
1	B	106	SER	2.7
1	B	107	VAL	2.7
1	B	109	ILE	2.6
1	C	163	CYS	2.6
1	B	152	ASN	2.6
1	C	111	TYR	2.6
2	D	441	ARG	2.6
1	C	115	PRO	2.5
1	B	220	SER	2.5
1	B	120	PHE	2.5
2	E	189	HIS	2.5
1	C	120	PHE	2.5
2	D	282	PRO	2.4
1	A	107	VAL	2.4
1	A	143	GLY	2.4
1	A	105	ALA	2.4
1	C	19	VAL	2.4
1	A	144	THR	2.4
1	A	244	TYR	2.4
1	B	151	LYS	2.3
1	B	143	GLY	2.3
1	A	176	ASN	2.3
1	B	145	PHE	2.3
2	D	283	ASN	2.3
1	C	117	GLN	2.3
1	A	223	ILE	2.3
1	A	172	VAL	2.3
1	A	47	GLN	2.2
1	B	14	CYS	2.2
1	A	178	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	120	PHE	2.2
1	C	81	ARG	2.2
1	B	249	GLU	2.2
1	A	81	ARG	2.1
1	B	182	ASN	2.1
2	F	180	MET	2.1
1	A	164	GLY	2.1
1	C	24	MET	2.1
1	A	247	LEU	2.1
1	C	118	GLN	2.1
1	B	164	GLY	2.1
1	A	221	ASP	2.1
1	A	238	GLU	2.0
1	A	111	TYR	2.0
1	B	13	VAL	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](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.