Full wwPDB X-ray Structure Validation Report ⓘ

Aug 16, 2020 – 07:56 PM BST

PDB ID	:	6U4Y
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 following versions of software and data (see references ⓘ) were used in the production of this report:

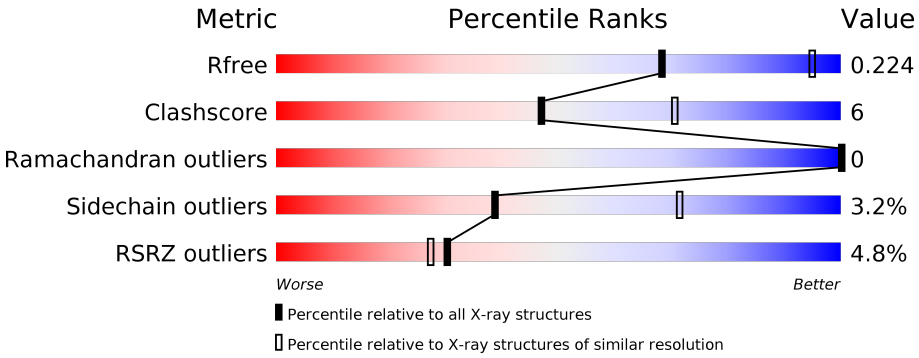
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.13.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.13.1

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 2.91 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}	130704	2307 (2.94-2.90)
Clashscore	141614	2531 (2.94-2.90)
Ramachandran outliers	138981	2462 (2.94-2.90)
Sidechain outliers	138945	2464 (2.94-2.90)
RSRZ outliers	127900	2248 (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 on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	224	15% 52% 18% • 29%
1	B	224	4% 60% 14% 26%
1	C	224	10% 57% 12% • 30%
2	D	366	% 86% 12% •
2	E	366	% 82% 16% •
2	F	366	% 85% 12% •

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:

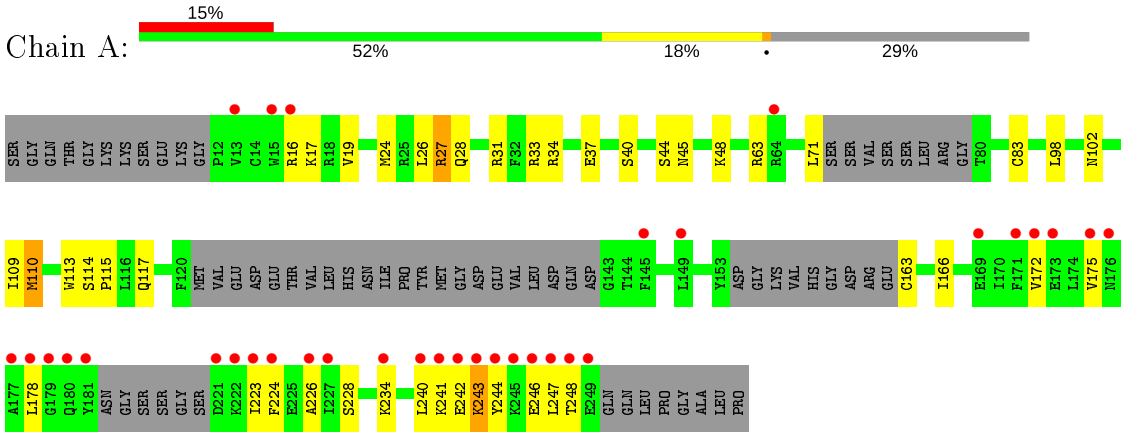
Chain	Residue	Modelled	Actual	Comment	Reference
D	76	GLY	-	expression tag	UNP O75530
D	77	SER	-	expression tag	UNP O75530
E	76	GLY	-	expression tag	UNP O75530
E	77	SER	-	expression tag	UNP O75530
F	76	GLY	-	expression tag	UNP O75530
F	77	SER	-	expression tag	UNP O75530

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.

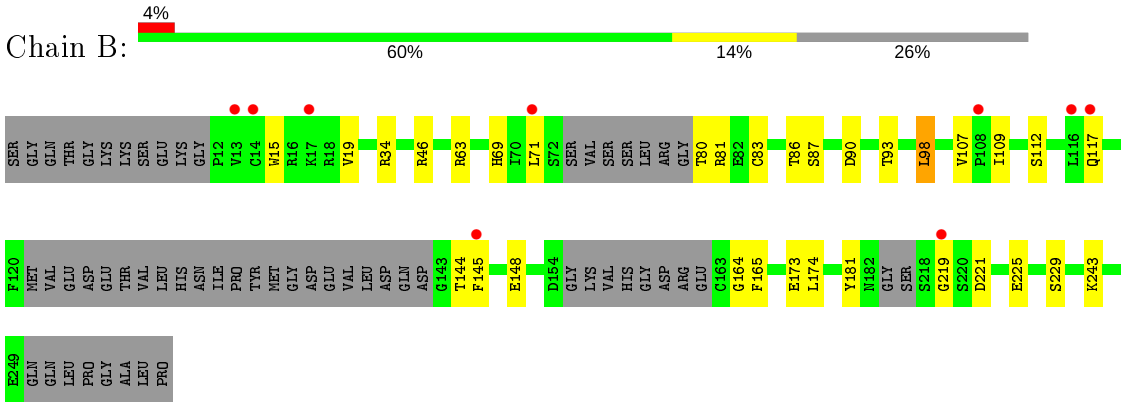
- Molecule 1: Histone-lysine N-methyltransferase EZH2

Chain A:



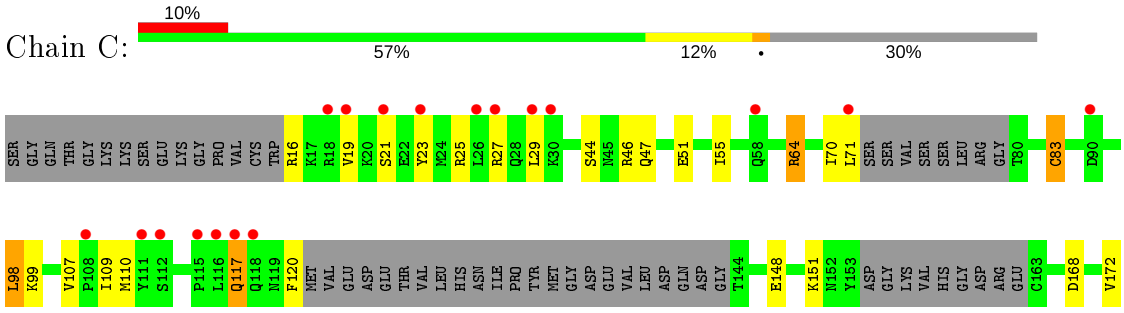
- Molecule 1: Histone-lysine N-methyltransferase EZH2

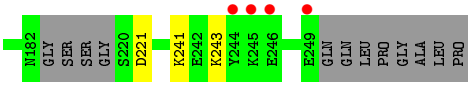
Chain B:



- Molecule 1: Histone-lysine N-methyltransferase EZH2

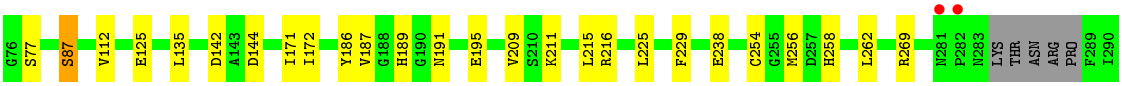
Chain C:

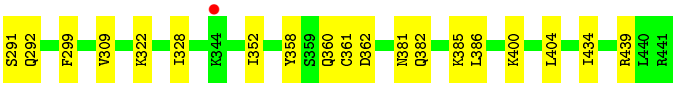




- Molecule 2: Polycomb protein EED

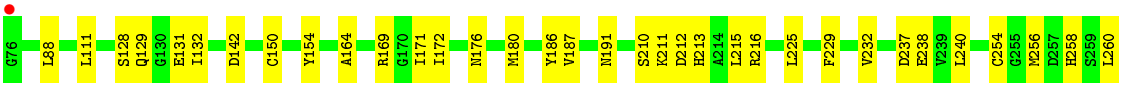
Chain D:

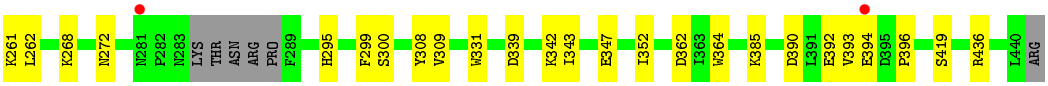




- Molecule 2: Polycomb protein EED

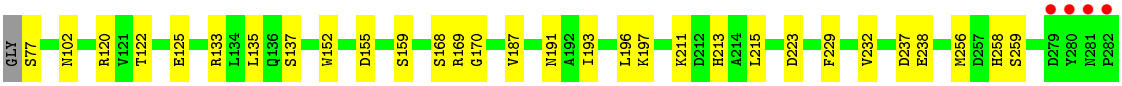
Chain E:

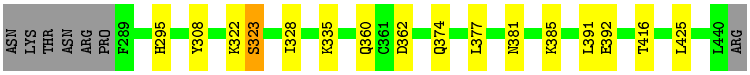




- Molecule 2: Polycomb protein EED

Chain F:





4 Data and refinement statistics (i)

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) 89.1 (48.50-2.91)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [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 (4.73%)	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)	0.34 , 54.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	A	0.34	0/1357	0.56	1/1820 (0.1%)
1	B	0.29	0/1395	0.45	0/1871
1	C	0.28	0/1330	0.45	0/1782
2	D	0.27	0/2991	0.49	0/4048
2	E	0.30	0/2980	0.50	1/4034 (0.0%)
2	F	0.27	0/2968	0.48	0/4018
All	All	0.29	0/13021	0.49	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(^{o})	Ideal(^{o})
1	A	71	LEU	CA-CB-CG	6.81	130.97	115.30
2	E	343	ILE	C-N-CA	-5.09	108.96	121.70

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	1334	0	1347	40	0
1	B	1372	0	1375	26	0
1	C	1310	0	1323	26	1
2	D	2918	0	2829	25	0
2	E	2907	0	2816	34	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	F	2895	0	2807	23	1
All	All	12736	0	12497	157	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 6.

All (157) 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:N	1:A:110:MET:HE3	1.79	0.96
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:A:109:ILE:C	1:A:110:MET:HE3	2.03	0.77
1:C:25:ARG:O	1:C:29:LEU:HD13	1.88	0.72
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:A:109:ILE:C	1:A:110:MET:CE	2.62	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
1:C:16:ARG:HA	1:C:16:ARG:CZ	2.26	0.65
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
1:A:110:MET:N	1:A:110:MET:SD	2.77	0.58
1:B:46:ARG:HD3	2:E:392:GLU:HG3	1.86	0.58
2:E:339:ASP:HB3	2:E:342:LYS:HG3	1.85	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:109:ILE:O	1:A:110:MET:CE	2.52	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
1:A:109:ILE:CA	1:A:110:MET:HE3	2.34	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:262:LEU:HB3	2:D:299:PHE:HB3	1.90	0.53
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: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: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:109:ILE:O	1:A:110:MET:HE3	2.13	0.49
1:A:243:LYS:O	1:A:246:GLU:HG3	2.12	0.49
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
2:F:211:LYS:HG3	2:F:238:GLU:CD	2.34	0.48
2:F:335:LYS:HE3	2:F:335:LYS:HB3	1.69	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:187:VAL:O	2:F:187:VAL:HG12	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
1:A:247:LEU:HA	1:A:247:LEU:HD12	1.51	0.47
2:F:213:HIS:CE1	2:F:237:ASP:HA	2.50	0.47
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:NH1	1:B:46:ARG:HG3	2.31	0.45
1:B:46:ARG:CD	2:E:392:GLU:HG3	2.46	0.45
2:E:347:GLU:HA	2:E:347:GLU:OE2	2.16	0.45
1:A:109:ILE:H	1:A:110:MET:HE3	1.73	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:268:LYS:O	2:E:272:ASN:ND2	2.49	0.44
2:E:260:LEU:HD22	2:E:331:TRP:CZ2	2.52	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:C:168:ASP:O	1:C:172:VAL:HG13	2.18	0.43
1:A:34:ARG:NH2	2:D:352:ILE:O	2.41	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:150:CYS:HA	2:E:164:ALA:O	2.17	0.43
1:A:109:ILE:O	1:A:110:MET:HE2	2.18	0.43
1:C:16:ARG:NE	1:C:16:ARG:HA	2.34	0.43
1:A:17:LYS:HA	1:A:17:LYS:HD3	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:B:219:GLY:C	1:B:221:ASP:H	2.22	0.43
1:C:109:ILE:H	1:C:109:ILE:HD12	1.83	0.43
2:E:260:LEU:HD22	2:E:331:TRP:HZ2	1.83	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
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:386:LEU:HB3	2:D:404:LEU:HB2	2.02	0.41
2:D:87:SER:HA	2:D:434:ILE:O	2.20	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
2:E:232:VAL:HG12	2:E:295:HIS:HB3	2.02	0.41
2:D:381:ASN:ND2	2:D:385:LYS:HB2	2.36	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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 (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	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 (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was

analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	150/203 (74%)	140 (93%)	10 (7%)	16	41
1	B	155/203 (76%)	148 (96%)	7 (4%)	27	59
1	C	148/203 (73%)	138 (93%)	10 (7%)	16	40
2	D	323/328 (98%)	317 (98%)	6 (2%)	57	83
2	E	322/328 (98%)	318 (99%)	4 (1%)	71	90
2	F	321/328 (98%)	312 (97%)	9 (3%)	43	75
All	All	1419/1593 (89%)	1373 (97%)	46 (3%)	39	71

All (46) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	24	MET
1	A	27	ARG
1	A	28	GLN
1	A	40	SER
1	A	44	SER
1	A	63	ARG
1	A	102	ASN
1	A	110	MET
1	A	163	CYS
1	A	243	LYS
1	B	81	ARG
1	B	90	ASP
1	B	98	LEU
1	B	112	SER
1	B	117	GLN
1	B	181	TYR
1	B	243	LYS
1	C	44	SER
1	C	47	GLN
1	C	64	ARG
1	C	71	LEU
1	C	83	CYS
1	C	98	LEU
1	C	99	LYS
1	C	117	GLN
1	C	120	PHE
1	C	243	LYS
2	D	77	SER

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Mol	Chain	Res	Type
2	D	87	SER
2	D	258	HIS
2	D	362	ASP
2	D	382	GLN
2	D	439	ARG
2	E	131	GLU
2	E	258	HIS
2	E	362	ASP
2	E	385	LYS
2	F	77	SER
2	F	120	ARG
2	F	168	SER
2	F	169	ARG
2	F	258	HIS
2	F	259	SER
2	F	323	SER
2	F	362	ASP
2	F	385	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	28	GLN
1	C	102	ASN
1	C	152	ASN
1	C	182	ASN
2	E	129	GLN
2	E	292	GLN
2	F	181	GLN
2	F	185	HIS

5.3.3 RNA (i)

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

There are no monosaccharides in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	160/224 (71%)	0.84	34 (21%) 0 0	40, 82, 136, 161	0
1	B	166/224 (74%)	0.33	9 (5%) 25 22	29, 62, 117, 161	0
1	C	157/224 (70%)	0.58	22 (14%) 2 2	41, 70, 114, 148	0
2	D	361/366 (98%)	-0.42	3 (0%) 86 86	22, 42, 71, 121	0
2	E	360/366 (98%)	-0.33	3 (0%) 86 86	25, 45, 78, 122	0
2	F	358/366 (97%)	-0.39	4 (1%) 80 81	24, 46, 79, 122	0
All	All	1562/1770 (88%)	-0.08	75 (4%) 30 27	22, 51, 107, 161	0

All (75) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	247	LEU	5.3
1	A	241	LYS	5.2
1	A	243	LYS	5.0
1	B	71	LEU	4.6
1	A	145	PHE	4.4
1	A	244	TYR	4.4
1	A	13	VAL	4.1
1	A	171	PHE	4.0
1	B	116	LEU	3.9
1	A	172	VAL	3.7
1	A	249	GLU	3.7
1	A	178	LEU	3.6
1	C	116	LEU	3.6
1	A	221	ASP	3.6
1	C	118	GLN	3.5
1	A	227	ILE	3.4
1	A	173	GLU	3.4
1	A	181	TYR	3.3
2	F	280	TYR	3.3

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Mol	Chain	Res	Type	RSRZ
1	A	240	LEU	3.3
1	B	145	PHE	3.2
1	A	223	ILE	3.1
2	D	281	ASN	3.1
2	D	282	PRO	3.0
2	F	282	PRO	3.0
1	A	226	ALA	3.0
1	C	249	GLU	3.0
1	C	23	TYR	3.0
1	A	176	ASN	2.9
1	C	71	LEU	2.9
1	A	179	GLY	2.9
1	C	244	TYR	2.9
2	F	281	ASN	2.8
1	C	18	ARG	2.7
1	C	29	LEU	2.7
1	A	245	LYS	2.7
1	B	14	CYS	2.7
1	A	15	TRP	2.6
1	B	108	PRO	2.6
1	A	175	VAL	2.5
1	C	112	SER	2.5
1	C	246	GLU	2.5
1	C	27	ARG	2.5
1	B	13	VAL	2.4
2	E	394	GLU	2.4
2	E	76	GLY	2.4
1	B	17	LYS	2.4
1	C	117	GLN	2.4
1	C	58	GLN	2.4
1	C	26	LEU	2.3
1	A	248	THR	2.3
1	B	219	GLY	2.3
1	A	16	ARG	2.3
1	C	30	LYS	2.3
1	A	64	ARG	2.3
1	A	222	LYS	2.2
1	A	242	GLU	2.2
1	B	117	GLN	2.2
2	D	344	LYS	2.2
2	F	279	ASP	2.2
1	C	19	VAL	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	234	LYS	2.1
1	A	149	LEU	2.1
1	A	169	GLU	2.1
1	C	245	LYS	2.1
1	A	180	GLN	2.1
1	C	90	ASP	2.1
1	C	115	PRO	2.0
1	C	21	SER	2.0
1	C	111	TYR	2.0
2	E	281	ASN	2.0
1	A	246	GLU	2.0
1	A	177	ALA	2.0
1	A	224	PHE	2.0
1	C	108	PRO	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.