



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 17, 2026 – 09:27 PM UTC

PDB ID : 8C0D / pdb_00008c0d
Title : UFL1/DDRGK1 bound to UFC1
Authors : Magnussen, H.M.; Kulathu, Y.
Deposited on : 2022-12-16
Resolution : 2.56 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

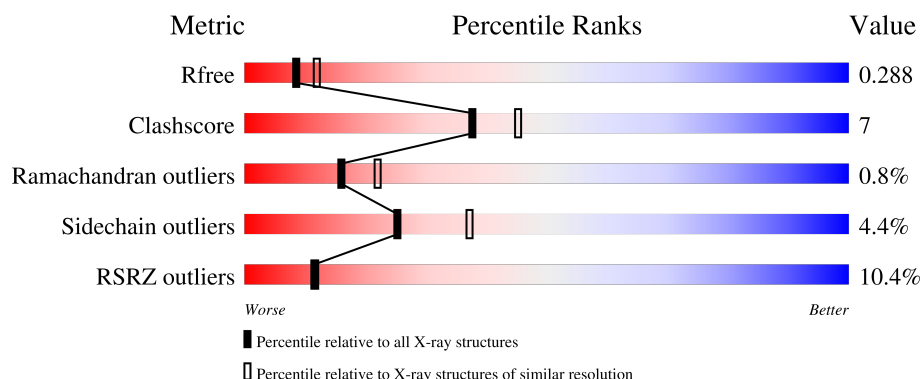
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.56 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	1853 (2.58-2.54)
Clashscore	190562	1897 (2.58-2.54)
Ramachandran outliers	187476	1875 (2.58-2.54)
Sidechain outliers	187428	1875 (2.58-2.54)
RSRZ outliers	180081	1853 (2.58-2.54)

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	194	15% 66% 16% • 15%
1	D	194	14% 67% 15% • 17%
2	B	110	0% 71% 19% • 7%
2	E	110	9% 62% 21% • 15%
3	C	168	7% 78% 15% • •

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Mol	Chain	Length	Quality of chain
3	F	168	5% 74% 21% ...

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 12907 atoms, of which 6389 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 E3 UFM1-protein ligase 1.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	165	Total	C	H	N	O	S	52	0	0
			2405	763	1189	217	232	4			
1	D	161	Total	C	H	N	O	S	45	0	0
			2394	759	1184	214	233	4			

There are 30 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-14	MET	-	initiating methionine	UNP O94874
A	-13	GLY	-	expression tag	UNP O94874
A	-12	HIS	-	expression tag	UNP O94874
A	-11	HIS	-	expression tag	UNP O94874
A	-10	HIS	-	expression tag	UNP O94874
A	-9	HIS	-	expression tag	UNP O94874
A	-8	HIS	-	expression tag	UNP O94874
A	-7	HIS	-	expression tag	UNP O94874
A	-6	GLU	-	expression tag	UNP O94874
A	-5	ASN	-	expression tag	UNP O94874
A	-4	LEU	-	expression tag	UNP O94874
A	-3	TYR	-	expression tag	UNP O94874
A	-2	PHE	-	expression tag	UNP O94874
A	-1	GLN	-	expression tag	UNP O94874
A	0	GLY	-	expression tag	UNP O94874
D	-14	MET	-	initiating methionine	UNP O94874
D	-13	GLY	-	expression tag	UNP O94874
D	-12	HIS	-	expression tag	UNP O94874
D	-11	HIS	-	expression tag	UNP O94874
D	-10	HIS	-	expression tag	UNP O94874
D	-9	HIS	-	expression tag	UNP O94874
D	-8	HIS	-	expression tag	UNP O94874
D	-7	HIS	-	expression tag	UNP O94874
D	-6	GLU	-	expression tag	UNP O94874
D	-5	ASN	-	expression tag	UNP O94874

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-4	LEU	-	expression tag	UNP O94874
D	-3	TYR	-	expression tag	UNP O94874
D	-2	PHE	-	expression tag	UNP O94874
D	-1	GLN	-	expression tag	UNP O94874
D	0	GLY	-	expression tag	UNP O94874

- Molecule 2 is a protein called DDRGK domain-containing protein 1.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	B	102	Total	C	H	N	O	S	22	0	0
			1562	491	782	132	156	1			
2	E	94	Total	C	H	N	O		17	0	0
			1449	458	729	124	138				

- Molecule 3 is a protein called Ubiquitin-fold modifier-conjugating enzyme 1.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
3	C	164	Total	C	H	N	O	S	41	0	0
			2532	834	1245	217	232	4			
3	F	164	Total	C	H	N	O	S	38	0	0
			2558	839	1260	220	235	4			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	116	LYS	CYS	engineered mutation	UNP Q9Y3C8
C	168	GLY	-	expression tag	UNP Q9Y3C8
F	116	LYS	CYS	engineered mutation	UNP Q9Y3C8
F	168	GLY	-	expression tag	UNP Q9Y3C8

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	O	0	0
			1	1		
4	C	2	Total	O	0	0
			2	2		
4	D	1	Total	O	0	0
			1	1		
4	E	1	Total	O	0	0
			1	1		

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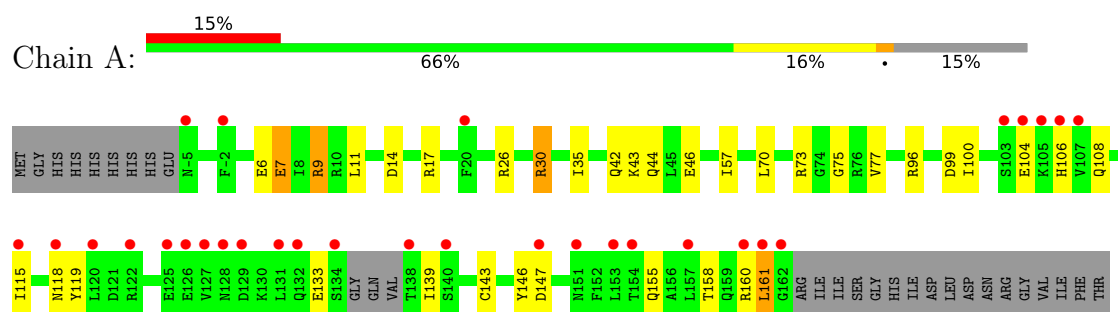
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	F	2	Total	O	0	0
			2	2		

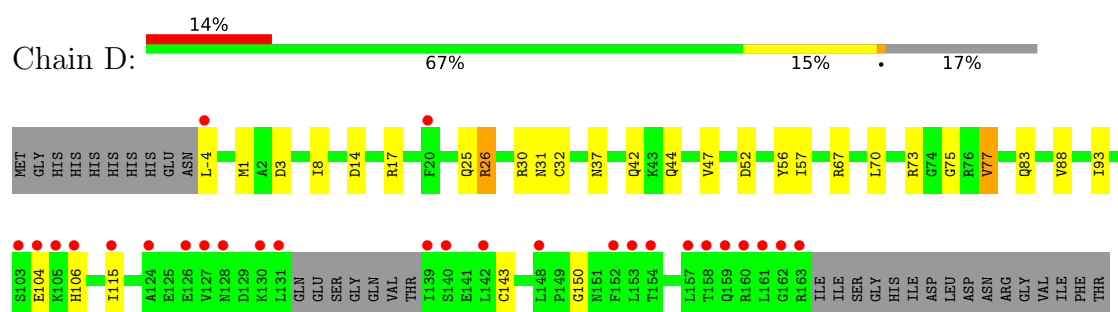
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

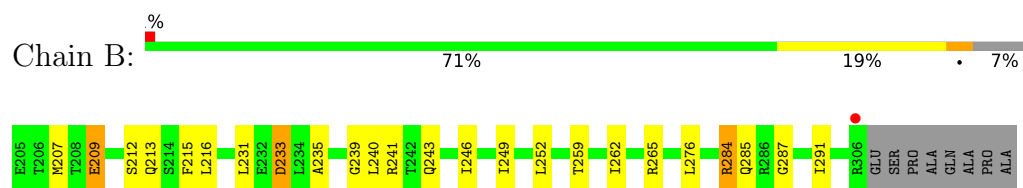
• Molecule 1: E3 UFM1-protein ligase 1



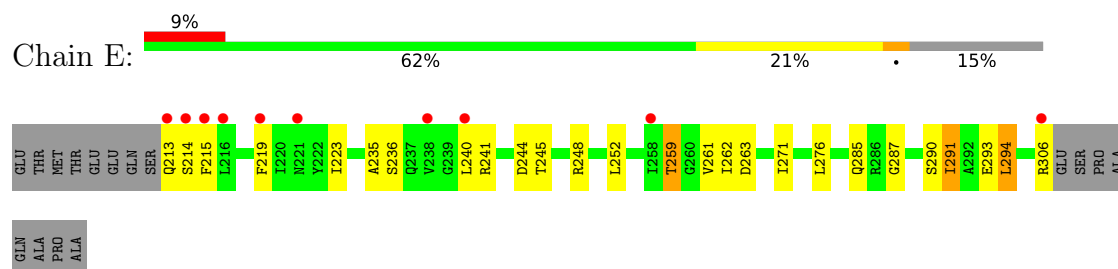
• Molecule 1: E3 UFM1-protein ligase 1



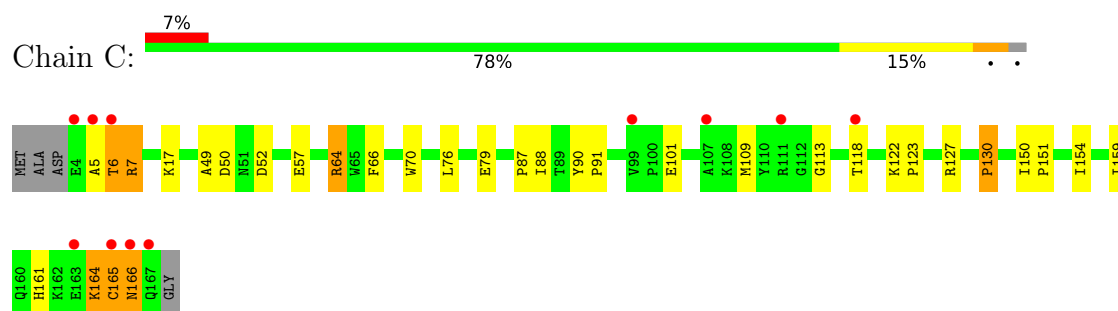
• Molecule 2: DDRGK domain-containing protein 1



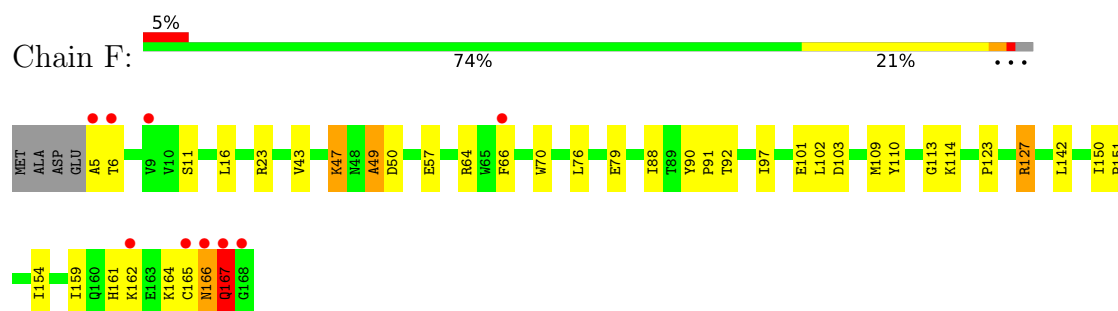
• Molecule 2: DDRGK domain-containing protein 1



- Molecule 3: Ubiquitin-fold modifier-conjugating enzyme 1



- Molecule 3: Ubiquitin-fold modifier-conjugating enzyme 1



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	79.21Å 124.56Å 131.29Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	65.73 – 2.56 65.73 – 2.56	Depositor EDS
% Data completeness (in resolution range)	61.0 (65.73-2.56) 61.0 (65.73-2.56)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.64 (at 2.58Å)	Xtriage
Refinement program	REFMAC 5.8.0403	Depositor
R, R_{free}	0.232 , 0.286 0.230 , 0.288	Depositor DCC
R_{free} test set	1222 reflections (2.88%)	wwPDB-VP
Wilson B-factor (Å ²)	46.6	Xtriage
Anisotropy	0.215	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.40 , 50.8	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	0.91	EDS
Total number of atoms	12907	wwPDB-VP
Average B, all atoms (Å ²)	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 35.38 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 5.8841e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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

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	0.75	0/1228	1.21	1/1669 (0.1%)
1	D	0.75	0/1223	1.21	1/1660 (0.1%)
2	B	0.82	0/788	1.35	1/1068 (0.1%)
2	E	0.84	0/728	1.44	2/988 (0.2%)
3	C	0.82	1/1324 (0.1%)	1.32	11/1806 (0.6%)
3	F	0.83	3/1335 (0.2%)	1.30	8/1818 (0.4%)
All	All	0.80	4/6626 (0.1%)	1.29	24/9009 (0.3%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	4
1	D	0	3
2	B	0	2
2	E	0	1
3	C	0	1
3	F	0	1
All	All	0	12

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	165	CYS	C-O	-6.28	1.18	1.24
3	F	11	SER	CA-CB	-5.92	1.44	1.53
3	F	49	ALA	C-O	-5.09	1.17	1.24
3	F	64	ARG	CD-NE	5.07	1.53	1.46

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	165	CYS	N-CA-C	8.91	119.67	107.73
3	C	164	LYS	CA-C-O	-7.65	109.57	120.51
3	F	166	ASN	O-C-N	7.21	129.50	122.07
3	C	64	ARG	CG-CD-NE	7.01	127.42	112.00
3	F	165	CYS	N-CA-C	6.50	118.45	111.36
3	F	165	CYS	N-CA-CB	-6.10	101.13	110.16
2	B	209	GLU	CB-CG-CD	6.06	122.91	112.60
3	C	50	ASP	CA-CB-CG	6.02	118.62	112.60
3	F	64	ARG	CG-CD-NE	6.01	125.21	112.00
1	D	37	ASN	CA-CB-CG	-5.84	106.76	112.60
3	C	118	THR	N-CA-CB	5.70	118.19	110.38
3	C	166	ASN	N-CA-CB	-5.70	100.90	110.99
1	A	46	GLU	CB-CG-CD	-5.65	102.99	112.60
3	C	50	ASP	CB-CA-C	5.64	118.77	111.50
3	C	52	ASP	CA-CB-CG	5.51	118.11	112.60
3	F	166	ASN	OD1-CG-ND2	-5.42	117.18	122.60
2	E	259	THR	CA-CB-OG1	-5.40	101.49	109.60
2	E	306	ARG	N-CA-CB	5.38	119.65	110.50
3	F	92	THR	OG1-CB-CG2	5.38	120.05	109.30
3	C	49	ALA	N-CA-C	-5.32	103.37	110.55
3	C	49	ALA	O-C-N	-5.27	116.85	122.85
3	F	166	ASN	CA-CB-CG	5.16	117.76	112.60
3	C	130	PRO	N-CA-CB	-5.13	96.95	102.60
3	F	165	CYS	CA-CB-SG	-5.07	102.73	114.40

There are no chirality outliers.

All (12) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	26	ARG	Sidechain
1	A	73	ARG	Sidechain
1	A	9	ARG	Sidechain
1	A	96	ARG	Sidechain
2	B	265	ARG	Sidechain
2	B	284	ARG	Sidechain
3	C	64	ARG	Sidechain
1	D	26	ARG	Sidechain
1	D	67	ARG	Sidechain
1	D	73	ARG	Sidechain
2	E	248	ARG	Sidechain
3	F	127	ARG	Sidechain

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	1216	1189	1123	20	0
1	D	1210	1184	1135	17	0
2	B	780	782	769	15	0
2	E	720	729	719	13	0
3	C	1287	1245	1208	14	0
3	F	1298	1260	1233	24	0
4	A	1	0	0	0	0
4	C	2	0	0	0	0
4	D	1	0	0	0	0
4	E	1	0	0	0	0
4	F	2	0	0	0	0
All	All	6518	6389	6187	89	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 (89) 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:70:LEU:HD13	1:A:77:VAL:HG12	1.50	0.90
3:C:166:ASN:CB	3:F:164:LYS:HA	2.02	0.90
1:D:70:LEU:HD12	1:D:77:VAL:HG13	1.66	0.78
3:C:122:LYS:HB2	3:C:123:PRO:HD3	1.79	0.64
2:B:239:GLY:HA3	3:F:166:ASN:HA	1.80	0.62
3:C:70:TRP:HB3	3:C:79:GLU:HG3	1.81	0.62
1:A:70:LEU:HD13	1:A:77:VAL:CG1	2.28	0.62
3:C:5:ALA:O	3:C:6:THR:C	2.42	0.61
1:A:35:ILE:HG23	2:B:276:LEU:HD23	1.85	0.59
3:C:109:MET:SD	3:C:113:GLY:HA2	2.44	0.58
1:D:75:GLY:O	1:D:115:ILE:HA	2.03	0.58
2:E:235:ALA:HB1	2:E:240:LEU:O	2.04	0.58
3:C:154:ILE:HG13	3:C:159:ILE:HD11	1.87	0.57
3:F:70:TRP:HB3	3:F:79:GLU:HG3	1.87	0.56
1:D:42:GLN:OE1	1:D:44:GLN:NE2	2.40	0.54
2:B:235:ALA:HB1	2:B:240:LEU:O	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:6:GLU:HG3	1:A:9:ARG:HH21	1.73	0.54
1:D:52:ASP:OD1	1:D:52:ASP:N	2.40	0.53
3:F:23:ARG:HG3	3:F:88:ILE:HG23	1.89	0.53
1:A:7:GLU:HG3	1:A:11:LEU:HD12	1.91	0.53
2:E:290:SER:HB3	2:E:293:GLU:HG3	1.89	0.53
1:A:57:ILE:HA	2:B:287:GLY:O	2.09	0.52
1:D:30:ARG:NH1	2:E:262:ILE:O	2.44	0.51
1:D:104:GLU:C	1:D:106:HIS:H	2.19	0.51
3:F:123:PRO:O	3:F:127:ARG:HG3	2.10	0.51
3:F:97:ILE:HD12	3:F:142:LEU:HB2	1.93	0.51
3:C:166:ASN:CB	3:F:164:LYS:CA	2.85	0.51
1:D:47:VAL:HG23	1:D:47:VAL:O	2.12	0.49
2:E:241:ARG:HA	3:F:167:GLN:HB3	1.94	0.49
1:A:104:GLU:C	1:A:106:HIS:H	2.20	0.49
2:E:236:SER:HA	3:F:167:GLN:HE22	1.77	0.49
3:F:109:MET:HG2	3:F:110:TYR:O	2.12	0.49
1:A:139:ILE:HG22	1:A:143:CYS:SG	2.52	0.49
1:D:143:CYS:SG	1:D:150:GLY:HA2	2.52	0.48
3:C:57:GLU:HB3	3:C:66:PHE:CE2	2.48	0.48
2:E:219:PHE:CZ	2:E:223:ILE:HD11	2.48	0.48
3:F:90:TYR:CG	3:F:91:PRO:HA	2.48	0.48
3:C:150:ILE:HB	3:C:151:PRO:HD3	1.94	0.48
1:D:83:GLN:HG3	1:D:88:VAL:O	2.14	0.48
3:F:76:LEU:HB3	3:F:161:HIS:CD2	2.49	0.48
2:B:212:SER:O	2:B:215:PHE:HB3	2.14	0.47
2:B:239:GLY:HA3	3:F:166:ASN:CA	2.44	0.47
1:D:-4:LEU:O	1:D:1:MET:HE1	2.15	0.47
3:C:76:LEU:HB3	3:C:161:HIS:CD2	2.50	0.46
1:D:56:TYR:CE2	2:E:291:ILE:HD13	2.51	0.46
2:B:241:ARG:NH2	2:B:243:GLN:HG2	2.30	0.46
1:A:146:TYR:O	1:A:147:ASP:C	2.59	0.46
3:C:87:PRO:HG2	3:C:90:TYR:HB2	1.98	0.46
3:F:16:LEU:N	3:F:16:LEU:HD12	2.31	0.46
2:E:213:GLN:C	2:E:215:PHE:H	2.23	0.45
1:A:44:GLN:O	2:B:284:ARG:NH2	2.50	0.45
2:B:216:LEU:HD13	2:B:252:LEU:HD23	1.98	0.45
1:A:70:LEU:CD1	1:A:77:VAL:HG12	2.35	0.45
1:D:14:ASP:OD1	1:D:17:ARG:NH1	2.48	0.45
2:B:216:LEU:HD13	2:B:252:LEU:CD2	2.46	0.44
3:F:49:ALA:O	3:F:50:ASP:C	2.58	0.44
1:A:160:ARG:O	1:A:161:LEU:C	2.61	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:209:GLU:H	2:B:209:GLU:CD	2.25	0.44
2:B:209:GLU:O	2:B:213:GLN:HG2	2.18	0.44
3:C:90:TYR:CG	3:C:91:PRO:HA	2.53	0.44
1:A:75:GLY:O	1:A:115:ILE:HA	2.17	0.44
1:D:32:CYS:HB3	2:E:294:LEU:HD23	2.00	0.44
1:D:31:ASN:OD1	2:E:263:ASP:HA	2.17	0.43
1:A:99:ASP:O	1:A:100:ILE:C	2.61	0.43
1:A:42:GLN:O	1:A:43:LYS:C	2.60	0.43
1:A:9:ARG:HE	1:A:9:ARG:HB3	1.63	0.42
3:C:6:THR:O	3:C:7:ARG:C	2.61	0.42
3:F:150:ILE:HB	3:F:151:PRO:HD3	2.01	0.42
3:F:43:VAL:O	3:F:47:LYS:HG2	2.19	0.42
1:A:30:ARG:HE	1:A:30:ARG:HB3	1.63	0.42
3:F:102:LEU:HB2	3:F:109:MET:HE1	2.02	0.42
3:F:109:MET:SD	3:F:113:GLY:HA2	2.58	0.42
3:F:110:TYR:HB2	3:F:114:LYS:HB2	2.02	0.42
1:D:70:LEU:CD1	1:D:77:VAL:HG13	2.44	0.42
2:E:261:VAL:HG22	2:E:271:ILE:HD11	2.01	0.41
3:C:150:ILE:N	3:C:151:PRO:CD	2.83	0.41
2:B:231:LEU:HD12	2:B:246:ILE:HG12	2.03	0.41
2:E:244:ASP:O	2:E:245:THR:C	2.59	0.41
1:A:155:GLN:O	1:A:158:THR:HB	2.21	0.41
2:B:233:ASP:N	2:B:233:ASP:OD1	2.52	0.41
1:D:25:GLN:C	1:D:26:ARG:HG2	2.46	0.41
3:F:103:ASP:HA	3:F:109:MET:SD	2.61	0.41
1:A:118:ASN:O	1:A:119:TYR:C	2.65	0.40
2:B:249:ILE:HG22	2:B:262:ILE:HD11	2.04	0.40
1:D:57:ILE:HA	2:E:287:GLY:O	2.21	0.40
3:F:154:ILE:HG13	3:F:159:ILE:HD11	2.03	0.40
1:A:14:ASP:OD1	1:A:17:ARG:NH1	2.54	0.40
3:F:57:GLU:HB3	3:F:66:PHE:CE2	2.55	0.40
3:F:5:ALA:O	3:F:6:THR:C	2.63	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	161/194 (83%)	146 (91%)	13 (8%)	2 (1%)	10	14
1	D	157/194 (81%)	145 (92%)	12 (8%)	0	100	100
2	B	100/110 (91%)	98 (98%)	2 (2%)	0	100	100
2	E	92/110 (84%)	90 (98%)	1 (1%)	1 (1%)	11	15
3	C	162/168 (96%)	151 (93%)	8 (5%)	3 (2%)	6	7
3	F	162/168 (96%)	155 (96%)	6 (4%)	1 (1%)	21	28
All	All	834/944 (88%)	785 (94%)	42 (5%)	7 (1%)	16	22

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	133	GLU
3	C	164	LYS
1	A	161	LEU
3	C	6	THR
2	E	214	SER
3	F	167	GLN
3	C	7	ARG

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	112/171 (66%)	109 (97%)	3 (3%)	39	55
1	D	117/171 (68%)	113 (97%)	4 (3%)	32	47
2	B	82/92 (89%)	77 (94%)	5 (6%)	17	25
2	E	74/92 (80%)	68 (92%)	6 (8%)	11	16
3	C	126/146 (86%)	120 (95%)	6 (5%)	23	34

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	F	130/146 (89%)	126 (97%)	4 (3%)	35	50
All	All	641/818 (78%)	613 (96%)	28 (4%)	25	37

All (28) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	GLU
1	A	30	ARG
1	A	108	GLN
2	B	207	MET
2	B	233	ASP
2	B	259	THR
2	B	285	GLN
2	B	291	ILE
3	C	17	LYS
3	C	88	ILE
3	C	101	GLU
3	C	127	ARG
3	C	130	PRO
3	C	165	CYS
1	D	3	ASP
1	D	8	ILE
1	D	77	VAL
1	D	93	ILE
2	E	252	LEU
2	E	259	THR
2	E	276	LEU
2	E	285	GLN
2	E	291	ILE
2	E	294	LEU
3	F	47	LYS
3	F	101	GLU
3	F	162	LYS
3	F	167	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	213	GLN
3	C	30	GLN
3	C	161	HIS

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Mol	Chain	Res	Type
1	D	92	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 [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	165/194 (85%)	1.02	30 (18%) 3 3	30, 54, 104, 128	0
1	D	161/194 (82%)	1.00	27 (16%) 4 3	31, 52, 107, 139	0
2	B	102/110 (92%)	0.31	1 (0%) 79 81	31, 44, 68, 75	0
2	E	94/110 (85%)	0.65	10 (10%) 11 11	29, 49, 72, 93	0
3	C	164/168 (97%)	0.47	11 (6%) 24 23	23, 44, 84, 104	0
3	F	164/168 (97%)	0.35	9 (5%) 30 30	27, 43, 75, 97	0
All	All	850/944 (90%)	0.66	88 (10%) 11 12	23, 48, 92, 139	0

All (88) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	131	LEU	9.6
1	D	128	ASN	7.3
1	A	134	SER	6.2
1	D	161	LEU	5.8
1	A	162	GLY	5.4
1	A	132	GLN	5.2
1	A	106	HIS	4.9
2	E	213	GLN	4.7
1	D	163	ARG	4.7
3	C	166	ASN	4.6
3	C	4	GLU	4.6
1	A	-5	ASN	4.5
3	C	167	GLN	4.5
1	A	161	LEU	4.5
1	A	131	LEU	4.4
1	A	127	VAL	4.2
1	A	105	LYS	4.0
1	D	162	GLY	4.0
1	D	158	THR	4.0

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Mol	Chain	Res	Type	RSRZ
1	A	104	GLU	3.9
1	D	139	ILE	3.9
3	F	5	ALA	3.9
1	D	-4	LEU	3.9
3	F	166	ASN	3.8
1	A	140	SER	3.8
1	D	159	GLN	3.7
1	D	130	LYS	3.7
3	C	6	THR	3.6
3	F	165	CYS	3.6
3	F	6	THR	3.6
1	D	103	SER	3.6
1	A	138	THR	3.5
1	D	157	LEU	3.4
1	D	105	LYS	3.4
3	C	5	ALA	3.4
1	D	106	HIS	3.3
1	D	20	PHE	3.3
1	A	122	ARG	3.3
1	A	129	ASP	3.2
3	F	167	GLN	3.1
1	D	104	GLU	3.1
2	E	240	LEU	3.1
2	E	306	ARG	3.1
1	A	151	ASN	3.1
2	B	306	ARG	3.1
1	A	128	ASN	2.9
1	A	126	GLU	2.9
2	E	216	LEU	2.9
3	C	107	ALA	2.9
1	A	120	LEU	2.9
2	E	219	PHE	2.9
1	D	140	SER	2.8
3	F	168	GLY	2.8
1	D	154	THR	2.8
1	D	126	GLU	2.8
1	A	115	ILE	2.7
1	A	153	LEU	2.7
1	A	107	VAL	2.7
2	E	214	SER	2.7
2	E	215	PHE	2.6
1	A	160	ARG	2.6

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Mol	Chain	Res	Type	RSRZ
3	F	9	VAL	2.6
3	C	111	ARG	2.6
1	A	-2	PHE	2.5
1	A	157	LEU	2.5
1	A	125	GLU	2.5
3	C	99	VAL	2.5
1	A	20	PHE	2.5
1	D	152	PHE	2.5
1	D	148	LEU	2.4
3	C	165	CYS	2.4
1	D	142	LEU	2.4
1	D	127	VAL	2.3
2	E	258	ILE	2.3
1	A	147	ASP	2.3
1	D	124	ALA	2.2
3	C	163	GLU	2.2
3	F	66	PHE	2.2
2	E	238	VAL	2.2
1	A	118	ASN	2.2
1	D	160	ARG	2.2
1	A	154	THR	2.1
1	D	153	LEU	2.1
3	F	162	LYS	2.1
3	C	118	THR	2.1
1	A	103	SER	2.1
2	E	221	ASN	2.0
1	D	115	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](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.