



# Full wwPDB X-ray Structure Validation Report i

Dec 20, 2023 – 12:17 pm GMT

PDB ID : 8C0D  
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](mailto: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 i symbol.

The types of validation reports are described at  
<http://www.wwpdb.org/validation/2017/FAQs#types>.

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The following versions of software and data (see [references](#) ①) were used in the production of this report:

MolProbity : 4.02b-467  
Xtriage (Phenix) : 1.13  
EDS : 2.36  
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) : 2.36

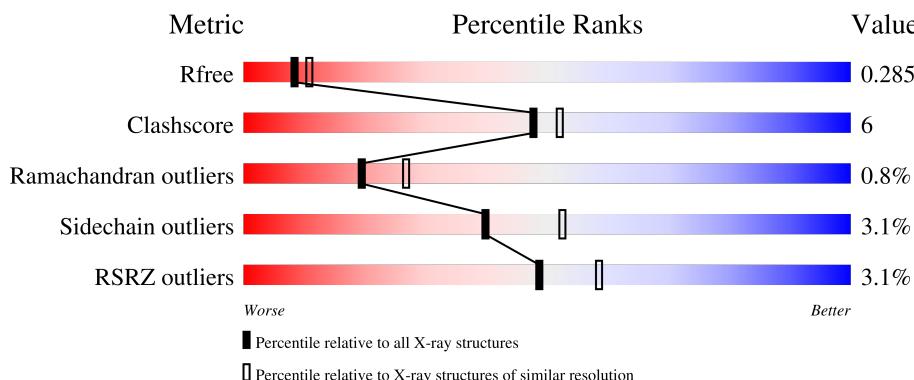
# 1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.56 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))
$R_{free}$	130704	1279 (2.58-2.54)
Clashscore	141614	1327 (2.58-2.54)
Ramachandran outliers	138981	1312 (2.58-2.54)
Sidechain outliers	138945	1312 (2.58-2.54)
RSRZ outliers	127900	1269 (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  $\geq 3$ , 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.



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Mol	Chain	Length	Quality of chain
3	F	168	<div style="width: 2%; background-color: red;">2%</div> <div style="width: 77%; background-color: green;">77%</div> <div style="width: 19%; background-color: yellow;">19%</div> <div style="width: 1%; background-color: gray;">...</div>

## 2 Entry composition (i)

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 1562 491 782 132 156 1	22	0	0
2	E	94	Total C H N O 1449 458 729 124 138	17	0	0

- 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 2532 834 1245 217 232 4	41	0	0
3	F	164	Total C H N O S 2558 839 1260 220 235 4	38	0	0

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 1 1	0	0
4	C	2	Total O 2 2	0	0
4	D	1	Total O 1 1	0	0
4	E	1	Total O 1 1	0	0

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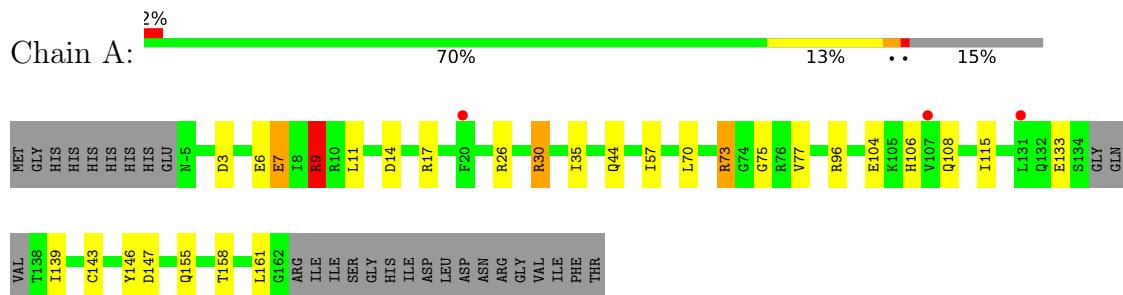
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	F	2	Total 2 2	0	0

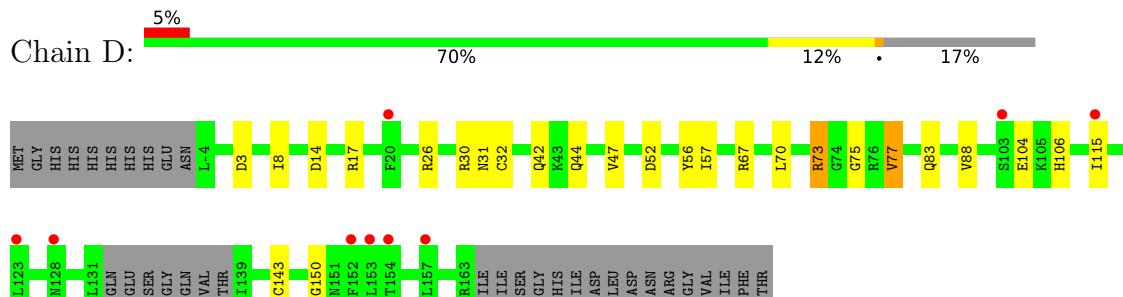
### 3 Residue-property plots [\(i\)](#)

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.

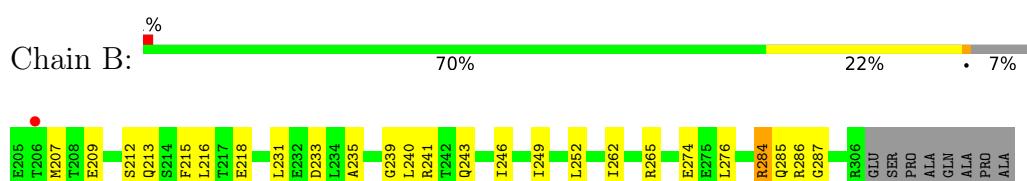
- Molecule 1: E3 UFM1-protein ligase 1



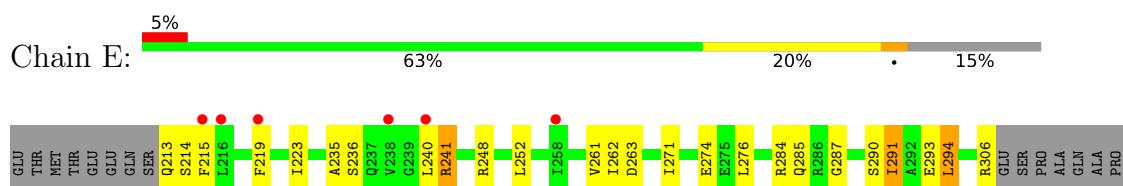
- Molecule 1: E3 UFM1-protein ligase 1



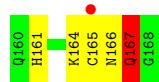
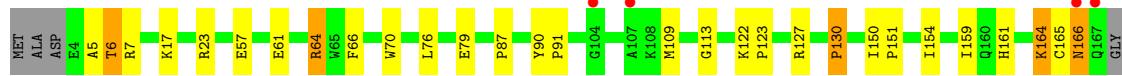
- Molecule 2: DDRGK domain-containing protein 1



- Molecule 2: DDRGK domain-containing protein 1



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



## 4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	79.21 Å   124.56 Å   131.29 Å 90.00°   90.00°   90.00°	Depositor
Resolution (Å)	65.73 – 2.56 65.65 – 2.56	Depositor EDS
% Data completeness (in resolution range)	61.0 (65.73-2.56) 61.0 (65.65-2.56)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$< I/\sigma(I) >$ <sup>1</sup>	2.64 (at 2.58 Å)	Xtriage
Refinement program	REFMAC 5.8.0403	Depositor
$R$ , $R_{free}$	0.232 , 0.286 0.233 , 0.285	Depositor DCC
$R_{free}$ test set	1222 reflections (4.73%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	46.6	Xtriage
Anisotropy	0.215	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.40 , 46.0	EDS
L-test for twinning <sup>2</sup>	$<  L  > = 0.49$ , $< L^2 > = 0.32$	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 <sup>2</sup> )	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.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>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 [\(i\)](#)

### 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	0.53	0/1228	0.94	3/1669 (0.2%)
1	D	0.52	0/1223	0.90	1/1660 (0.1%)
2	B	0.68	3/788 (0.4%)	1.00	1/1068 (0.1%)
2	E	0.66	1/728 (0.1%)	1.08	3/988 (0.3%)
3	C	0.58	0/1324	1.02	7/1806 (0.4%)
3	F	0.62	1/1335 (0.1%)	0.99	5/1818 (0.3%)
All	All	0.59	5/6626 (0.1%)	0.98	20/9009 (0.2%)

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 (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	274	GLU	CD-OE2	-6.54	1.18	1.25
3	F	11	SER	CA-CB	-5.95	1.44	1.52
2	E	274	GLU	CD-OE1	-5.92	1.19	1.25
2	B	274	GLU	CD-OE1	-5.53	1.19	1.25
2	B	218	GLU	CD-OE2	5.36	1.31	1.25

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	9	ARG	NE-CZ-NH2	-9.36	115.62	120.30
1	A	9	ARG	NE-CZ-NH1	8.55	124.57	120.30
3	C	64	ARG	CG-CD-NE	7.44	127.42	111.80
3	C	127	ARG	NE-CZ-NH1	-6.49	117.06	120.30
3	F	64	ARG	CG-CD-NE	6.39	125.21	111.80
3	F	165	CYS	CA-CB-SG	-6.26	102.73	114.00
3	C	23	ARG	NE-CZ-NH1	6.16	123.38	120.30
3	C	127	ARG	NE-CZ-NH2	6.16	123.38	120.30
3	F	23	ARG	NE-CZ-NH1	6.10	123.35	120.30
3	F	23	ARG	NE-CZ-NH2	-5.97	117.31	120.30
2	B	286	ARG	NE-CZ-NH1	5.41	123.01	120.30
3	C	166	ASN	N-CA-CB	-5.39	100.90	110.60
3	F	165	CYS	N-CA-CB	-5.26	101.13	110.60
1	D	73	ARG	NE-CZ-NH2	-5.24	117.68	120.30
1	A	73	ARG	NE-CZ-NH2	-5.19	117.70	120.30
3	C	130	PRO	N-CA-CB	-5.13	96.95	102.60
2	E	241	ARG	NE-CZ-NH1	5.11	122.86	120.30
2	E	284	ARG	NE-CZ-NH1	-5.05	117.77	120.30
2	E	306	ARG	N-CA-CB	5.03	119.65	110.60
3	C	164	LYS	CA-C-O	-5.02	109.57	120.10

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 [\(i\)](#)

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	1216	1189	1123	16	0
1	D	1210	1184	1135	15	0
2	B	780	782	769	14	0
2	E	720	729	719	12	0
3	C	1287	1245	1208	13	0
3	F	1298	1260	1233	22	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	78	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 6.

All (78) 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
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:C:5:ALA:O	3:C:6:THR:C	2.42	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
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:104:GLU:C	1:D:106:HIS:H	2.19	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
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
1:A:104:GLU:C	1:A:106:HIS:H	2.20	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
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:9:ARG:HE	1:A:9:ARG:HB3	1.63	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:213:GLN:C	2:E:215:PHE:H	2.23	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
1:A:146:TYR:O	1:A:147:ASP:C	2.59	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
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
3:F:49:ALA:O	3:F:50:ASP:C	2.58	0.41
3:F:103:ASP:HA	3:F:109:MET:SD	2.61	0.41
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

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	161/194 (83%)	146 (91%)	13 (8%)	2 (1%)	13 17
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%)	14 19
3	C	162/168 (96%)	151 (93%)	8 (5%)	3 (2%)	8 9
3	F	162/168 (96%)	155 (96%)	6 (4%)	1 (1%)	25 33
All	All	834/944 (88%)	785 (94%)	42 (5%)	7 (1%)	19 27

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 [\(i\)](#)

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	112/171 (66%)	108 (96%)	4 (4%)	35 47
1	D	117/171 (68%)	114 (97%)	3 (3%)	46 59
2	B	82/92 (89%)	80 (98%)	2 (2%)	49 63
2	E	74/92 (80%)	69 (93%)	5 (7%)	16 20
3	C	126/146 (86%)	122 (97%)	4 (3%)	39 51
3	F	130/146 (89%)	128 (98%)	2 (2%)	65 77
All	All	641/818 (78%)	621 (97%)	20 (3%)	40 52

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	ASP
1	A	7	GLU
1	A	30	ARG
1	A	108	GLN
2	B	207	MET
2	B	285	GLN
3	C	17	LYS
3	C	61	GLU
3	C	130	PRO
3	C	165	CYS

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Mol	Chain	Res	Type
1	D	3	ASP
1	D	8	ILE
1	D	77	VAL
2	E	252	LEU
2	E	276	LEU
2	E	285	GLN
2	E	291	ILE
2	E	294	LEU
3	F	17	LYS
3	F	167	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
3	C	161	HIS
1	D	44	GLN

### 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 monosaccharides 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

There are no chain breaks in this entry.

## 6 Fit of model and data (i)

### 6.1 Protein, DNA and RNA chains (i)

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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	165/194 (85%)	0.26	3 (1%) 68 75	31, 55, 111, 143	0
1	D	161/194 (82%)	0.39	9 (5%) 24 31	33, 52, 118, 139	0
2	B	102/110 (92%)	0.27	1 (0%) 82 87	32, 45, 68, 75	0
2	E	94/110 (85%)	0.48	6 (6%) 19 24	31, 51, 73, 92	0
3	C	164/168 (97%)	0.32	4 (2%) 59 67	25, 44, 87, 106	0
3	F	164/168 (97%)	0.25	3 (1%) 68 75	28, 43, 77, 96	0
All	All	850/944 (90%)	0.32	26 (3%) 49 58	25, 48, 99, 143	0

All (26) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	E	240	LEU	3.5
3	C	107	ALA	3.0
1	D	103	SER	2.9
3	C	166	ASN	2.9
1	A	131	LEU	2.9
3	F	66	PHE	2.8
2	E	219	PHE	2.8
2	E	215	PHE	2.8
2	E	216	LEU	2.7
1	D	123	LEU	2.7
3	C	104	GLY	2.7
2	B	206	THR	2.5
1	D	153	LEU	2.4
1	D	128	ASN	2.3
1	D	157	LEU	2.3
1	D	20	PHE	2.2
3	F	6	THR	2.2
2	E	238	VAL	2.2
2	E	258	ILE	2.2

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Mol	Chain	Res	Type	RSRZ
3	F	165	CYS	2.2
1	A	107	VAL	2.1
1	A	20	PHE	2.1
1	D	115	ILE	2.1
3	C	167	GLN	2.1
1	D	154	THR	2.0
1	D	152	PHE	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.