

Full wwPDB X-ray Structure Validation Report (i)

Oct 22, 2024 – 06:25 AM JST

:	8YM6
:	Structure of Caspase-8/cFLIP death effector domain assembly
:	Lin, SC.; Yang, CY.
:	2024-03-08
:	3.30 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 (i) 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 (1)) were used in the production of this report:

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure: $X\text{-}RAY \, DIFFRACTION$

The reported resolution of this entry is 3.30 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	$egin{array}{c} { m Whole \ archive} \ (\#{ m Entries}) \end{array}$	${f Similar\ resolution}\ (\#{ m Entries,\ resolution\ range}({ m \AA}))$
R_{free}	164625	1085 (3.32 - 3.28)
Clashscore	180529	1128 (3.32-3.28)
Ramachandran outliers	177936	1125 (3.32-3.28)
Sidechain outliers	177891	1124 (3.32-3.28)
RSRZ outliers	164620	1085 (3.32-3.28)

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 <=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	А	185	85%	12% •	
1	В	185	83%	15%	•
1	С	185	% 80%	17% •	
1	D	185	88%	10%	•
2	F	184	78%	14% 8%	-
2	G	184	% 83%	12% •	



Mol	Chain	Length	Quality of chain		
2	Н	184	75%	20%	5%
2	Ι	184	82%	11%	7%
2	J	184	85%	9%	6%
2	K	184	78%	14%	8%
2	М	184	71%	21%	8%
2	Ν	184	82%	11%	7%
2	О	184	80%	15%	5%



2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 18608 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.

Mol	Chain	Residues		At	oms		ZeroOcc	AltConf	Trace	
1	C	170	70 Total C N O S		0	0	0			
	U	179	1485	939	252	286	8	0	0	0
1	р	191	Total	С	Ν	0	S	0	0	0
1	I D	101	1502	951	254	289	8	0	0	0
1	Δ	170	Total	С	Ν	0	S	0	0	0
1		179	1485	939	252	286	8	0	0	0
1	П	191	Total	С	Ν	0	S	0	0	0
	I D	101	1502	951	254	289	8			U

• Molecule 1 is a protein called Caspase-8 subunit p10.

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
С	122	GLY	PHE	engineered mutation	UNP Q14790
С	123	GLY	LEU	engineered mutation	UNP Q14790
В	122	GLY	PHE	engineered mutation	UNP Q14790
В	123	GLY	LEU	engineered mutation	UNP Q14790
А	122	GLY	PHE	engineered mutation	UNP Q14790
А	123	GLY	LEU	engineered mutation	UNP Q14790
D	122	GLY	PHE	engineered mutation	UNP Q14790
D	123	GLY	LEU	engineered mutation	UNP Q14790

• Molecule 2 is a protein called CASP8 and FADD-like apoptosis regulator subunit p43.

Mol	Chain	Residues		At	oms		ZeroOcc	AltConf	Trace	
9	и	175	Total	С	Ν	0	\mathbf{S}	0	0	0
2	п	175	1424	906	247	263	8	0	0	0
9	С	176	Total	С	Ν	0	S	0	0	0
2	Z G	170	1434	912	250	264	8	0	0	0
9	Б	160	Total	С	Ν	0	S	0	0	0
2	Г	109	1383	881	239	255	8	0	0	0
9	9 V	160	Total	С	N	0	S	0	0	0
	109	1381	879	237	257	8		0	0	



Mol	Chain	Residues		At	\mathbf{oms}			ZeroOcc	AltConf	Trace
9	Т	179	Total	С	Ν	0	S	0	0	0
2	1	172	1403	893	244	258	8	0	0	0
9	т	172	Total	С	Ν	0	S	0	0	0
2	J	175	1407	894	244	261	8	0	0	0
9	М	160	Total	С	Ν	0	S	0	0	0
2		109	1377	877	236	256	8	0	0	0
9	0	175	Total	С	Ν	0	S	0	0	0
2	0	175	1424	906	247	263	8	0	0	0
9	2 N	179	Total	С	Ν	0	S	0	0	0
2		172	1401	891	243	259	8	0	0	0

There are 27 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Н	-2	GLY	-	expression tag	UNP 015519
Н	-1	SER	-	expression tag	UNP 015519
Н	0	HIS	-	expression tag	UNP 015519
G	-2	GLY	-	expression tag	UNP O15519
G	-1	SER	-	expression tag	UNP O15519
G	0	HIS	-	expression tag	UNP O15519
F	-2	GLY	-	expression tag	UNP O15519
F	-1	SER	-	expression tag	UNP 015519
F	0	HIS	-	expression tag	UNP 015519
K	-2	GLY	-	expression tag	UNP O15519
K	-1	SER	-	expression tag	UNP O15519
K	0	HIS	-	expression tag	UNP O15519
Ι	-2	GLY	-	expression tag	UNP 015519
Ι	-1	SER	-	expression tag	UNP O15519
Ι	0	HIS	-	expression tag	UNP O15519
J	-2	GLY	-	expression tag	UNP O15519
J	-1	SER	-	expression tag	UNP O15519
J	0	HIS	-	expression tag	UNP O15519
М	-2	GLY	-	expression tag	UNP O15519
М	-1	SER	-	expression tag	UNP O15519
М	0	HIS	-	expression tag	UNP O15519
0	-2	GLY	-	expression tag	UNP O15519
0	-1	SER	-	expression tag	UNP O15519
0	0	HIS	-	expression tag	UNP O15519
N	-2	GLY	-	expression tag	UNP O15519
N	-1	SER	-	expression tag	UNP 015519
N	0	HIS	-	expression tag	UNP 015519



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: Caspase-8 subunit p10





• Molecule 2: CASP8 and FADD-like apoptosis regulator subunit p43

Chain O:		80%		15%	5%			
GLY SER HIS HIS E17 E17 L24 L24 L24	R64 V 79 V 90 V 96 R94 R94 R94 R94 R96 R96 R96 R98 R98	L112 1113 F114 F114 K117 X119 M120 M120 K124	F131 L132 V135 V136 E137 E137 L149 L149 L151	1159 D163 1168	v175 GLN GLY ALA GLY THR			
SER								

• Molecule 2: CASP8 and FADD-like apoptosis regulator subunit p43

Chain N: 82%												11	L%		79	%										
GLY SER HIS M1	H7	E11	E17	Y60	ION	R64 F65	L68	R76	N79	L83	06N	Y93 R94	K117	M120	G123	K124 ILE	SER LYS	E128 17100	5130 F131	V135	P146	V175	GLN	GLY ALA	GLY	SER



4 Data and refinement statistics (i)

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants	150.31Å 158.64Å 353.29Å	Depositor
a, b, c, α , β , γ	90.00° 90.00° 90.00°	Depositor
Bosolution(A)	29.64 - 3.30	Depositor
Resolution (A)	29.64 - 3.30	EDS
% Data completeness	96.0 (29.64-3.30)	Depositor
(in resolution range)	96.3 (29.64-3.30)	EDS
R_{merge}	0.09	Depositor
R _{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	$1.94 (at 3.31 \text{\AA})$	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
B B.	0.218 , 0.264	Depositor
II, II, <i>free</i>	0.220 , 0.264	DCC
R_{free} test set	3244 reflections $(5.09%)$	wwPDB-VP
Wilson B-factor $(Å^2)$	95.8	Xtriage
Anisotropy	0.953	Xtriage
Bulk solvent $k_{sol}(e/A^3)$, $B_{sol}(A^2)$	0.28 , 62.2	EDS
L-test for $twinning^2$	$ < L >=0.49, < L^2>=0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	18608	wwPDB-VP
Average B, all atoms $(Å^2)$	137.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 2.97% of the height of the origin peak. No significant pseudotranslation is detected.

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.



¹Intensities estimated from amplitudes.

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).

Mal	Chain	Bond	lengths	Bond	angles
IVIOI			# Z > 5	RMSZ	# Z > 5
1	А	0.24	0/1500	0.49	0/2005
1	В	0.24	0/1518	0.48	0/2029
1	С	0.24	0/1500	0.49	0/2005
1	D	0.24	0/1518	0.49	0/2029
2	F	0.25	0/1397	0.52	0/1873
2	G	0.25	0/1450	0.49	0/1946
2	Н	0.24	0/1439	0.49	0/1931
2	Ι	0.25	0/1417	0.52	0/1899
2	J	0.24	0/1421	0.49	0/1906
2	Κ	0.25	0/1395	0.48	0/1872
2	М	0.24	0/1391	0.48	0/1868
2	Ν	0.24	0/1415	0.50	0/1898
2	0	0.26	0/1439	0.51	0/1931
All	All	0.24	0/18800	0.50	0/25192

There are no bond length outliers.

There are no bond angle outliers.

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	А	1485	0	1525	15	0
1	В	1502	0	1539	18	0
1	С	1485	0	1525	21	0



Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	1502	0	1539	12	0
2	F	1383	0	1456	16	0
2	G	1434	0	1514	14	0
2	Н	1424	0	1507	23	0
2	Ι	1403	0	1486	15	0
2	J	1407	0	1482	12	0
2	Κ	1381	0	1454	20	0
2	М	1377	0	1448	22	0
2	Ν	1401	0	1477	11	0
2	0	1424	0	1507	16	0
All	All	18608	0	19459	195	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

All (195) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom 1	Atom 2	Interatomic	Clash	
Atom-1	Atom-2	distance (Å)	overlap (Å)	
2:H:3:ALA:HB3	2:0:118:ASP:HB2	1.72	0.71	
1:B:109:SER:HA	1:B:139:LEU:HD23	1.73	0.71	
1:D:23:LYS:NZ	1:D:35:GLN:O	2.25	0.69	
2:I:99:GLU:OE2	2:I:167:LYS:NZ	2.25	0.69	
2:J:99:GLU:OE2	2:J:167:LYS:NZ	2.25	0.69	
1:A:114:ARG:HD3	1:A:118:ARG:HH21	1.59	0.66	
2:M:64:ARG:NH2	2:M:66:ASP:OD2	2.28	0.66	
2:H:2:SER:HB2	2:0:118:ASP:OD2	1.96	0.65	
2:M:10:GLU:HG3	2:M:38:ARG:HG3	1.79	0.65	
1:B:151:ILE:HB	1:B:159:ILE:HD12	1.78	0.65	
1:A:109:SER:HA	1:A:139:LEU:HD23	1.78	0.65	
2:N:117:LYS:HA	2:N:120:MET:HG2	1.79	0.65	
2:F:60:TYR:HE1	2:F:76:ARG:HG3	1.63	0.64	
2:N:68:LEU:HD11	2:N:79:VAL:HG21	1.81	0.63	
1:A:22:LEU:HD11	1:A:69:ILE:HD13	1.81	0.62	
2:G:61:ARG:HG3	2:G:90:VAL:HG21	1.82	0.62	
1:C:151:ILE:HB	1:C:159:ILE:HD12	1.82	0.61	
2:H:145:ALA:HB3	2:H:148:GLN:HG2	1.82	0.61	
2:I:120:MET:HG3	2:I:122:ARG:H	1.66	0.61	
1:A:151:ILE:HB	1:A:159:ILE:HD12	1.81	0.60	
2:I:10:GLU:HG3	2:I:38:ARG:HB2	1.82	0.60	
1:B:158:ASP:OD1	1:B:158:ASP:N	2.35	0.60	
1:C:168:ASN:OD1	$1:\overline{\text{C:169:LYS:N}}$	2.35	0.59	



		Interatomic	Clash	
Atom-1	Atom-2	distance (Å)	overlap (Å)	
1:A:121:LYS:NZ	1:A:134:ASP:O	2.27	0.59	
1:D:168:ASN:OD1	1:D:169:LYS:N	2.35	0.59	
2:H:100:ILE:HG23	2:H:164:LEU:HD13	1.84	0.58	
2:F:117:LYS:HA	2:F:120:MET:HG2	1.85	0.58	
2:M:128:GLU:HG2	2:M:129:LYS:HG3	1.85	0.58	
2:G:17:GLU:OE2	2:G:64:ARG:HD3	2.03	0.58	
2:M:75:ASP:OD1	2:M:76:ARG:N	2.37	0.57	
2:0:116:MET:O	2:O:120:MET:HG2	2.04	0.57	
2:N:17:GLU:OE2	2:N:64:ARG:HD3	2.05	0.57	
2:H:118:ASP:HB2	2:K:3:ALA:HB3	1.85	0.56	
1:C:25:LEU:HD12	1:C:98:ILE:HG21	1.88	0.56	
2:F:10:GLU:HG3	2:F:38:ARG:HB2	1.87	0.56	
1:A:8:TYR:HA	1:A:42:LEU:HD21	1.87	0.56	
2:J:112:LEU:HD13	2:J:159:ILE:HD13	1.87	0.56	
1:C:114:ARG:NH2	1:D:136:ASP:OD2	2.39	0.55	
1:A:101:TYR:O	1:A:104:MET:HG3	2.07	0.55	
2:F:100:ILE:HD12	2:F:164:LEU:HB3	1.89	0.54	
1:C:65:LEU:HD23	1:C:98:ILE:HD11	1.89	0.54	
1:D:151:ILE:HB	1:D:159:ILE:HD12	1.90	0.54	
2:H:54:ASP:HB3	2:H:89:LEU:HD22	1.88	0.54	
2:H:132:LEU:HA	2:H:135:VAL:HG22	1.89	0.54	
2:I:112:LEU:HD13	2:I:159:ILE:HD13	1.89	0.54	
1:B:128:ILE:HD12	1:B:145:GLU:HG3	1.90	0.54	
2:I:63:ARG:NH2	2:J:120:MET:O	2.41	0.53	
2:K:99:GLU:OE2	2:K:167:LYS:NZ	2.41	0.53	
2:M:22:LEU:HD12	2:M:40:LEU:HD22	1.90	0.53	
2:J:10:GLU:HG3	2:J:38:ARG:HB2	1.89	0.53	
2:0:114:PHE:O	2:O:117:LYS:HB3	2.09	0.52	
1:B:130:LYS:NZ	1:A:116:GLU:OE2	2.33	0.52	
2:K:31:ASP:OD1	2:K:31:ASP:N	2.42	0.52	
1:A:22:LEU:CD1	1:A:69:ILE:HD13	2.40	0.52	
2:O:24:LEU:HB3	2:O:90:VAL:HG11	1.92	0.52	
2:O:149:LEU:HD13	2:O:168:ILE:HG23	1.91	0.51	
2:M:1:MET:HG3	2:M:52:VAL:HG12	1.92	0.51	
2:O:95:VAL:O	2:O:99:GLU:HG2	2.10	0.51	
2:H:43:ILE:HG23	2:H:47:ARG:NH1	2.26	0.51	
2:I:113:ILE:O	2:I:117:LYS:HB3	2.11	0.50	
2:H:10:GLU:HG3	2:H:38:ARG:HB2	1.92	0.50	
2:G:55:LEU:HD23	2:G:72:LEU:HD21	1.92	0.50	
2:M:100:ILE:HG23	2:M:164:LEU:HD13	1.94	0.49	
2:0:17:GLU:OE2	2:O:64:ARG:HD3	2.11	0.49	



		Interatomic	Clash	
Atom-1	Atom-2	distance (Å)	overlap (Å)	
2:H:24:LEU:HD22	2:H:90:VAL:HG11	1.94	0.49	
2:H:21:LEU:HD21	2:H:58:LEU:HB3	1.94	0.49	
2:G:0:HIS:HE1	2:G:45:ARG:HA	1.78	0.49	
2:0:93:TYR:0	2:O:97:MET:HG2	2.13	0.49	
2:M:95:VAL:O	2:M:99:GLU:HG2	2.13	0.49	
2:K:100:ILE:HG23	2:K:164:LEU:HD13	1.95	0.48	
2:H:124:LYS:HE2	2:H:137:GLU:OE2	2.13	0.48	
2:M:116:MET:SD	2:M:138:LEU:HD11	2.53	0.48	
2:N:61:ARG:NH2	2:N:83:LEU:HD21	2.29	0.48	
2:G:57:GLU:OE2	2:G:90:VAL:HG22	2.14	0.48	
2:H:7:HIS:NE2	2:H:11:GLU:OE2	2.46	0.47	
2:M:149:LEU:HD13	2:M:168:ILE:HG23	1.95	0.47	
1:B:168:ASN:HB3	1:B:171:LEU:HG	1.97	0.47	
2:O:119:TYR:CD2	2:O:151:LEU:HD11	2.49	0.47	
2:M:132:LEU:HA	2:M:135:VAL:HG22	1.97	0.47	
1:D:23:LYS:HZ2	1:D:38:ILE:HB	1.79	0.47	
1:B:164:CYS:HB3	1:B:171:LEU:HB2	1.96	0.47	
2:K:61:ARG:HG3	2:K:90:VAL:HG21	1.97	0.47	
1:D:25:LEU:HD23	1:D:102:ARG:HG3	1.97	0.46	
2:J:104:LEU:HD22	2:J:108:ASP:HB3	1.96	0.46	
1:C:101:TYR:O	1:C:104:MET:HG2	2.14	0.46	
1:D:146:MET:HG2	1:D:151:ILE:HD11	1.96	0.46	
1:C:25:LEU:HD12	1:C:98:ILE:HD13	1.98	0.46	
2:K:60:TYR:HB2	2:K:79:VAL:HG11	1.98	0.46	
2:N:7:HIS:CE1	2:N:11:GLU:OE2	2.69	0.46	
2:H:149:LEU:HD13	2:H:168:ILE:HG23	1.97	0.46	
2:K:24:LEU:HB3	2:K:90:VAL:HG11	1.97	0.46	
2:I:22:LEU:HD23	2:I:40:LEU:HD22	1.97	0.46	
2:M:2:SER:OG	2:M:5:VAL:HG23	2.16	0.46	
2:J:163:ASP:N	2:J:163:ASP:OD1	2.49	0.46	
1:A:114:ARG:O	1:A:118:ARG:HG3	2.15	0.45	
1:D:52:ARG:HG3	2:K:162:ILE:HG22	1.97	0.45	
2:G:149:LEU:HD13	2:G:168:ILE:HG23	1.98	0.45	
2:F:42:ASP:OD2	2:M:114:PHE:HE1	1.97	0.45	
2:M:163:ASP:OD1	2:M:163:ASP:N	2.49	0.45	
2:O:131:PHE:O	2:O:135:VAL:HG13	2.16	0.45	
1:C:67:PHE:HB2	1:C:75:LEU:HD11	1.97	0.45	
2:G:93:TYR:CG	2:G:146:PRO:HG3	2.51	0.45	
2:F:57:GLU:O	2:F:61:ARG:HG2	2.16	0.45	
2:H:112:LEU:HG	2:H:159:ILE:HD13	1.97	0.45	
2:O:56:ALA:HB1	2:O:79:VAL:HG22	1.98	0.45	



		Interatomic	Clash	
Atom-1	Atom-2	distance (Å)	overlap (Å)	
1:B:157:LEU:HD11	1:B:178:TYR:HE2	1.81	0.45	
2:N:123:GLY:O	2:N:129:LYS:NZ	2.30	0.45	
2:H:60:TYR:HB2	2:H:79:VAL:HG11	1.99	0.45	
2:N:60:TYR:HB2	2:N:79:VAL:HG11	1.99	0.45	
1:C:28:ASP:OD1	1:C:102:ARG:NH2	2.47	0.45	
2:I:137:GLU:O	2:I:141:LEU:HD13	2.16	0.44	
2:F:117:LYS:HB3	2:F:117:LYS:HE3	1.83	0.44	
2:H:163:ASP:OD1	2:H:163:ASP:N	2.51	0.44	
1:C:101:TYR:OH	1:C:152:LEU:HG	2.17	0.44	
2:I:163:ASP:OD1	2:I:163:ASP:N	2.50	0.44	
2:J:27:ASP:O	2:J:30:ILE:HG13	2.17	0.44	
2:O:124:LYS:HG2	2:O:137:GLU:OE2	2.17	0.44	
1:C:42:LEU:HD22	2:K:114:PHE:CE2	2.52	0.44	
2:H:140:LYS:NZ	2:G:14:ASP:OD2	2.46	0.44	
2:I:34:PRO:HG2	2:I:40:LEU:HD13	2.00	0.44	
1:C:22:LEU:HD22	1:C:65:LEU:HB3	2.00	0.43	
1:B:159:ILE:HG23	1:B:162:ARG:HH21	1.84	0.43	
2:M:57:GLU:HB2	2:M:83:LEU:HD21	2.00	0.43	
1:D:109:SER:HA	1:D:139:LEU:HD23	1.99	0.43	
1:C:47:ARG:NH1	1:C:50:GLU:OE1	2.51	0.43	
1:C:108:ILE:HD11	1:C:164:CYS:SG	2.58	0.43	
2:G:39:ASP:O	2:G:43:ILE:HG13	2.19	0.43	
2:G:43:ILE:O	2:G:47:ARG:HG3	2.19	0.43	
2:F:163:ASP:OD1	2:F:163:ASP:N	2.50	0.43	
2:K:163:ASP:OD1	2:K:163:ASP:N	2.51	0.43	
2:M:20:MET:HE1	2:M:61:ARG:O	2.18	0.43	
1:B:105:LEU:O	1:B:108:ILE:HG22	2.19	0.43	
1:C:87:GLU:O	1:C:91:GLN:HB2	2.19	0.43	
2:H:1:MET:HG3	2:H:50:LEU:O	2.19	0.43	
2:F:129:LYS:HB3	2:F:133:ASP:HB2	2.01	0.43	
2:K:56:ALA:HA	2:K:68:LEU:HD21	2.00	0.43	
1:C:31:PRO:HB2	1:B:12:GLU:O	2.19	0.43	
2:F:90:VAL:HG12	2:F:94:ARG:HB2	2.00	0.43	
2:J:116:MET:O	2:J:120:MET:HG3	2.19	0.43	
2:0:163:ASP:OD1	2:O:163:ASP:N	2.52	0.42	
2:F:145:ALA:HB3	2:F:148:GLN:HB2	2.01	0.42	
2:K:73:LYS:HB2	2:K:73:LYS:HE3	1.80	0.42	
2:I:50:LEU:HA	2:I:54:ASP:HB2	2.01	0.42	
1:C:105:LEU:O	1:C:108:ILE:HG22	2.18	0.42	
1:A:131:CYS:HB3	2:K:13:LEU:O	2.19	0.42	
2:I:116:MET:O	2:I:120:MET:HG2	2.19	0.42	



		Interatomic	Clash	
Atom-1	Atom-2	distance (Å)	overlap (Å)	
2:M:57:GLU:OE2	2:M:90:VAL:HG22	2.18	0.42	
2:0:112:LEU:HG	2:O:159:ILE:HD13	2.01	0.42	
2:H:124:LYS:HD3	2:H:124:LYS:HA	1.81	0.42	
2:H:57:GLU:O	2:H:61:ARG:HG2	2.20	0.42	
2:G:141:LEU:HD21	2:F:63:ARG:HB3	2.01	0.42	
2:K:132:LEU:H	2:K:132:LEU:HD12	1.84	0.42	
1:B:31:PRO:HB2	1:A:12:GLU:O	2.20	0.42	
2:K:28:VAL:HG13	2:K:49:LYS:HD3	2.01	0.42	
1:B:43:MET:O	1:B:47:ARG:HG2	2.20	0.42	
2:F:114:PHE:CD2	2:I:38:ARG:HD2	2.54	0.42	
2:J:22:LEU:HD23	2:J:40:LEU:HD22	2.01	0.41	
2:0:132:LEU:HA	2:0:135:VAL:HG22	2.02	0.41	
1:B:171:LEU:O	1:B:175:ILE:HG13	2.19	0.41	
1:A:65:LEU:HD23	1:A:98:ILE:HD11	2.01	0.41	
2:K:56:ALA:HB1	2:K:79:VAL:HG22	2.02	0.41	
2:K:68:LEU:HD13	2:K:79:VAL:HG21	2.01	0.41	
2:J:112:LEU:HD12	2:J:112:LEU:HA	1.86	0.41	
1:B:8:TYR:HA	1:B:42:LEU:HD21	2.03	0.41	
1:C:55:GLU:HG2	1:C:58:ASN:HB3	2.01	0.41	
1:C:12:GLU:OE2	1:D:33:ARG:NH1	2.45	0.41	
2:N:131:PHE:O	2:N:135:VAL:HG23	2.21	0.41	
1:B:105:LEU:HD23	1:B:105:LEU:HA	1.94	0.41	
1:D:150:VAL:O	1:D:156:LYS:HD3	2.21	0.41	
2:N:90:VAL:HG12	2:N:94:ARG:HB2	2.03	0.41	
1:C:109:SER:HA	1:C:139:LEU:HD23	2.02	0.41	
1:B:22:LEU:HD22	1:B:65:LEU:HB3	2.03	0.41	
2:M:128:GLU:OE1	2:M:128:GLU:N	2.53	0.41	
2:N:93:TYR:CG	2:N:146:PRO:HG3	2.54	0.41	
1:A:31:PRO:HB2	2:H:102:GLU:O	2.20	0.41	
2:F:93:TYR:CG	2:F:146:PRO:HG3	2.56	0.41	
2:M:29:ALA:HB1	2:M:34:PRO:HD3	2.03	0.41	
2:M:55:LEU:HD23	2:M:72:LEU:HD21	2.02	0.41	
1:B:84:GLU:HA	1:B:87:GLU:HG2	2.03	0.41	
2:H:31:ASP:O	2:G:11:GLU:HG3	2.21	0.41	
2:G:160:HIS:CE1	2:K:31:ASP:OD2	2.75	0.40	
2:I:117:LYS:HG2	2:I:118:ASP:N	2.36	0.40	
2:M:17:GLU:CD	2:M:64:ARG:HD2	2.42	0.40	
1:D:22:LEU:HD22	1:D:65:LEU:HB3	2.03	0.40	
2:F:34:PRO:HG2	2:F:40:LEU:HD13	2.03	0.40	
2:J:34:PRO:HG2	2:J:40:LEU:HD13	2.02	0.40	
1:A:92:THR:HA	1:A:93:PRO:HD3	1.98	0.40	



Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:40:LEU:O	2:G:44:LEU:HG	2.20	0.40
2:K:23:PHE:CG	2:K:132:LEU:HD23	2.56	0.40
2:K:34:PRO:HG2	2:K:40:LEU:HD13	2.04	0.40
2:N:65:PHE:CE2	2:N:76:ARG:HD2	2.57	0.40
1:C:52:ARG:NH1	2:J:166:THR:OG1	2.55	0.40
2:F:4:GLU:H	2:F:4:GLU:HG2	1.70	0.40
2:I:117:LYS:HA	2:I:120:MET:HG2	2.02	0.40
2:M:111:SER:O	2:M:115:LEU:HG	2.21	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	Perce	entiles
1	А	177/185~(96%)	171 (97%)	6 (3%)	0	100	100
1	В	179/185~(97%)	175~(98%)	4 (2%)	0	100	100
1	С	177/185~(96%)	172 (97%)	5 (3%)	0	100	100
1	D	179/185~(97%)	174 (97%)	5 (3%)	0	100	100
2	F	163/184~(89%)	157 (96%)	6 (4%)	0	100	100
2	G	174/184~(95%)	168 (97%)	6 (3%)	0	100	100
2	Н	173/184 (94%)	165 (95%)	8 (5%)	0	100	100
2	Ι	168/184 (91%)	161 (96%)	7 (4%)	0	100	100
2	J	169/184~(92%)	162 (96%)	7 (4%)	0	100	100
2	К	165/184 (90%)	158 (96%)	7 (4%)	0	100	100
2	М	165/184~(90%)	160 (97%)	5 (3%)	0	100	100
2	Ν	168/184 (91%)	163 (97%)	5 (3%)	0	100	100
2	Ο	173/184~(94%)	167 (96%)	6 (4%)	0	100	100
All	All	2230/2396~(93%)	2153 (96%)	77 (4%)	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	Perce	ntiles
1	А	168/174~(97%)	168 (100%)	0	100	100
1	В	170/174~(98%)	170 (100%)	0	100	100
1	С	168/174~(97%)	168 (100%)	0	100	100
1	D	170/174~(98%)	170 (100%)	0	100	100
2	F	159/168~(95%)	159 (100%)	0	100	100
2	G	164/168~(98%)	163 (99%)	1 (1%)	84	90
2	Н	163/168~(97%)	163 (100%)	0	100	100
2	Ι	161/168~(96%)	161 (100%)	0	100	100
2	J	161/168~(96%)	161 (100%)	0	100	100
2	Κ	159/168~(95%)	158 (99%)	1 (1%)	84	90
2	М	158/168~(94%)	158 (100%)	0	100	100
2	Ν	160/168~(95%)	160 (100%)	0	100	100
2	Ο	163/168~(97%)	163 (100%)	0	100	100
All	All	2124/2208~(96%)	2122 (100%)	2(0%)	92	96

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	G	37	VAL
2	Κ	10	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 (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^{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>	#RSRZ>2	$OWAB(Å^2)$	Q<0.9
1	А	179/185~(96%)	-0.59	0 100 100	112, 145, 194, 218	0
1	В	181/185~(97%)	-0.66	0 100 100	118, 138, 171, 182	0
1	С	179/185~(96%)	-0.56	1 (0%) 85 78	119, 146, 185, 204	0
1	D	181/185~(97%)	-0.57	0 100 100	125, 149, 185, 221	0
2	F	169/184~(91%)	-0.62	0 100 100	83, 115, 149, 179	0
2	G	176/184~(95%)	-0.70	1 (0%) 85 78	90, 119, 158, 179	0
2	Н	175/184~(95%)	-0.73	0 100 100	100, 132, 162, 175	0
2	Ι	172/184 (93%)	-0.69	0 100 100	99, 126, 163, 188	0
2	J	173/184~(94%)	-0.64	0 100 100	102, 124, 154, 182	0
2	K	169/184~(91%)	-0.72	1 (0%) 85 78	100, 133, 162, 178	0
2	М	169/184~(91%)	-0.67	2 (1%) 76 64	97, 132, 173, 193	0
2	N	172/184~(93%)	-0.64	0 100 100	102, 136, 177, 204	0
2	Ο	175/184 (95%)	-0.58	0 100 100	113, 149, 184, 212	0
All	All	2270/2396~(94%)	-0.64	5 (0%) 92 88	83, 135, 178, 221	0

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	М	121	GLY	3.0
2	G	25	CYS	2.8
1	С	11	GLY	2.4
2	М	25	CYS	2.4
2	К	55	LEU	2.1

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.

