Full wwPDB X-ray Structure Validation Report (i)

May 8, 2024 – 04:31 PM JST

PDB ID	:	8YD7
Title	:	Structure of FADD/Caspase-8/cFLIP death effector domain assembly
Authors	:	Lin, S.-C.; Yang, C.-Y.
Deposited on	:	2024-02-19
Resolution	:	3.32 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:

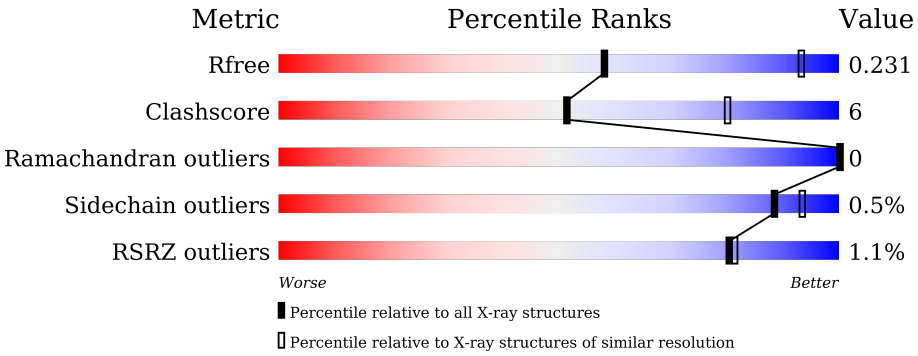
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36.2
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

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 3.32 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	1089 (3.36-3.28)
Clashscore	141614	1137 (3.36-3.28)
Ramachandran outliers	138981	1115 (3.36-3.28)
Sidechain outliers	138945	1114 (3.36-3.28)
RSRZ outliers	127900	1059 (3.36-3.28)

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	G	181	79% 15% • 6%
1	H	181	82% 14% • •
1	I	181	78% 18% • •
1	K	181	83% 11% 6%
2	A	185	76% 23% •
2	B	185	81% 17% •

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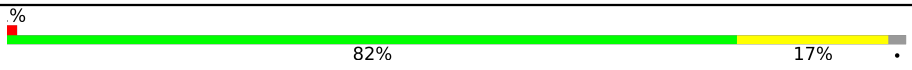
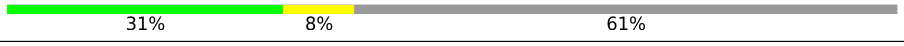
Mol	Chain	Length	Quality of chain
2	C	185	
2	D	185	
2	E	185	
3	L	216	

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 13822 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 CASP8 and FADD-like apoptosis regulator subunit p12.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	G	171	Total	C	N	O	S	Se	0	0	0
			1387	882	238	260	2	5			
1	H	175	Total	C	N	O	S	Se	0	0	0
			1418	902	245	263	2	6			
1	I	175	Total	C	N	O	S	Se	0	0	0
			1418	902	245	263	2	6			
1	K	170	Total	C	N	O	S	Se	0	0	0
			1385	882	237	258	2	6			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	7	GLY	HIS	engineered mutation	UNP O15519
H	7	GLY	HIS	engineered mutation	UNP O15519
I	7	GLY	HIS	engineered mutation	UNP O15519
K	7	GLY	HIS	engineered mutation	UNP O15519

- Molecule 2 is a protein called Caspase-8.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	D	183	Total	C	N	O	S	Se	0	0	0
			1519	962	257	291	2	7			
2	C	182	Total	C	N	O	S	Se	0	0	0
			1510	956	255	290	2	7			
2	B	182	Total	C	N	O	S	Se	0	0	0
			1510	956	255	290	2	7			
2	E	180	Total	C	N	O	S	Se	0	0	0
			1496	948	253	287	2	6			
2	A	182	Total	C	N	O	S	Se	0	0	0
			1510	956	255	290	2	7			

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	122	GLY	PHE	engineered mutation	UNP Q14790
D	123	GLY	LEU	engineered mutation	UNP Q14790
C	122	GLY	PHE	engineered mutation	UNP Q14790
C	123	GLY	LEU	engineered mutation	UNP Q14790
B	122	GLY	PHE	engineered mutation	UNP Q14790
B	123	GLY	LEU	engineered mutation	UNP Q14790
E	122	GLY	PHE	engineered mutation	UNP Q14790
E	123	GLY	LEU	engineered mutation	UNP Q14790
A	122	GLY	PHE	engineered mutation	UNP Q14790
A	123	GLY	LEU	engineered mutation	UNP Q14790

- Molecule 3 is a protein called FAS-associated death domain protein.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
3	L	84	Total	C	N	O	S	Se	0	0	0
			668	420	118	127	1	2			

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
L	9	GLY	HIS	engineered mutation	UNP Q13158
L	209	LEU	-	expression tag	UNP Q13158
L	210	GLU	-	expression tag	UNP Q13158
L	211	HIS	-	expression tag	UNP Q13158
L	212	HIS	-	expression tag	UNP Q13158
L	213	HIS	-	expression tag	UNP Q13158
L	214	HIS	-	expression tag	UNP Q13158
L	215	HIS	-	expression tag	UNP Q13158
L	216	HIS	-	expression tag	UNP Q13158

- Molecule 4 is SELENIUM ATOM (three-letter code: SE) (formula: Se).

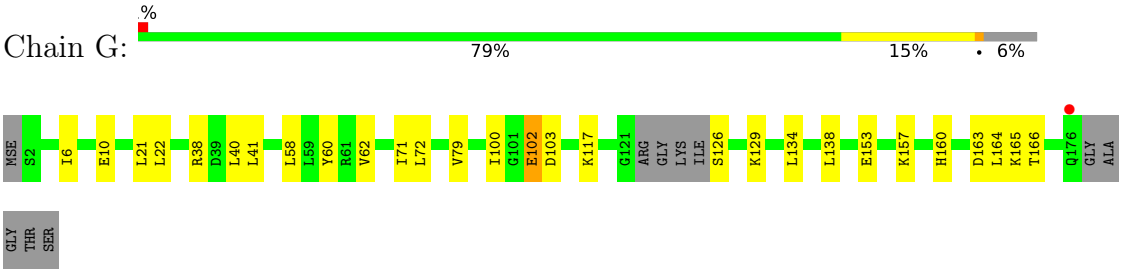
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	G	1	Total	Se	0	0
			1	1		

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.

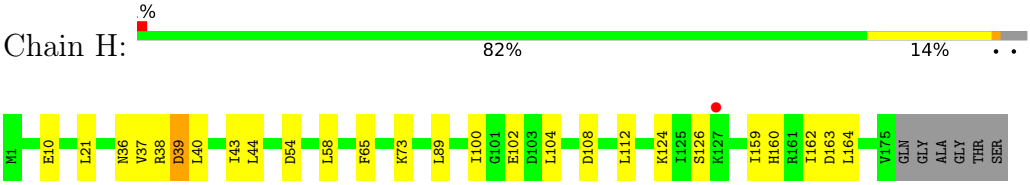
• Molecule 1: CASP8 and FADD-like apoptosis regulator subunit p12

Chain G:



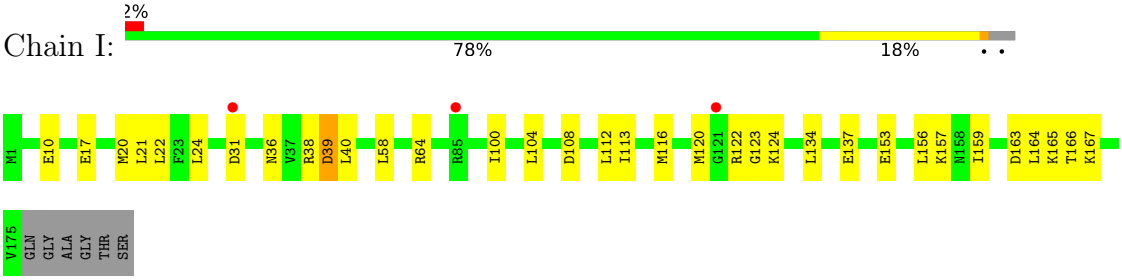
• Molecule 1: CASP8 and FADD-like apoptosis regulator subunit p12

Chain H:



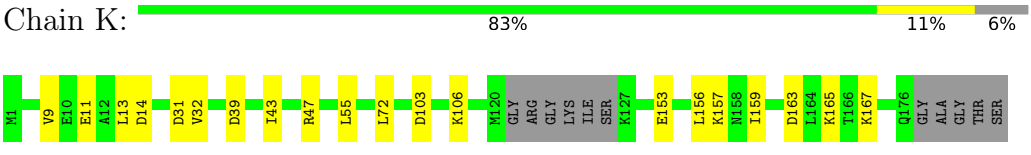
• Molecule 1: CASP8 and FADD-like apoptosis regulator subunit p12

Chain I:



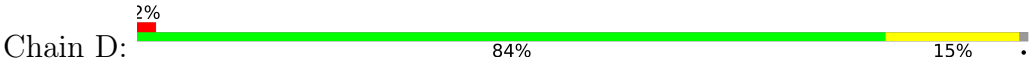
• Molecule 1: CASP8 and FADD-like apoptosis regulator subunit p12

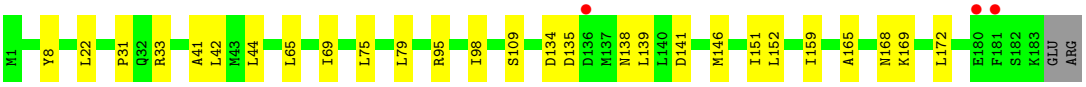
Chain K:



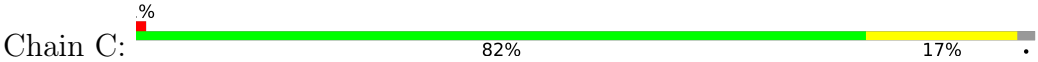
• Molecule 2: Caspase-8

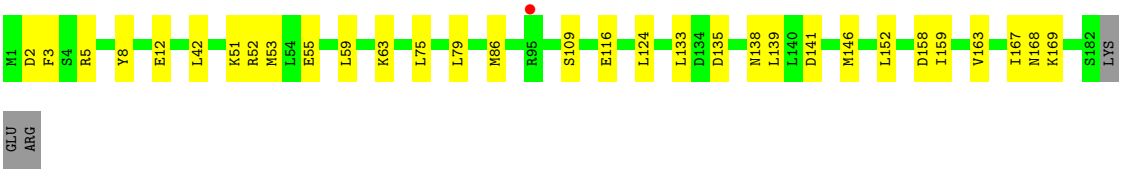
Chain D:



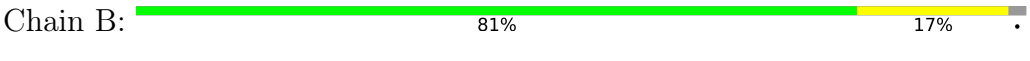


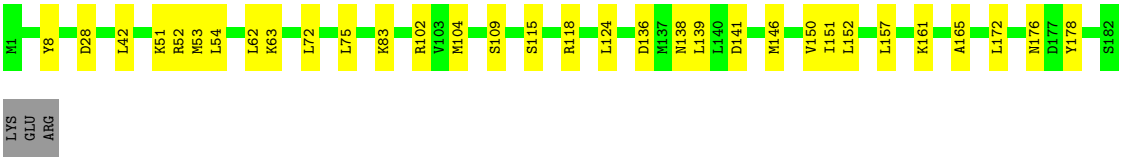
• Molecule 2: Caspase-8



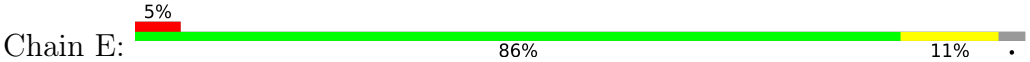


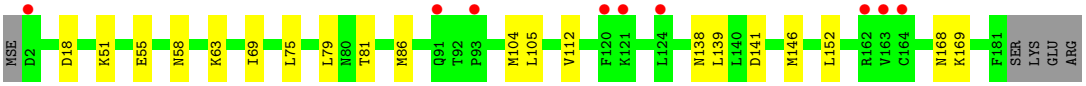
• Molecule 2: Caspase-8



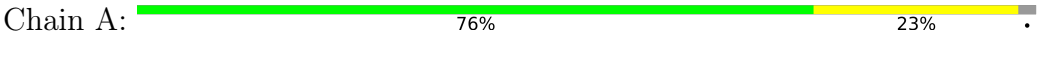


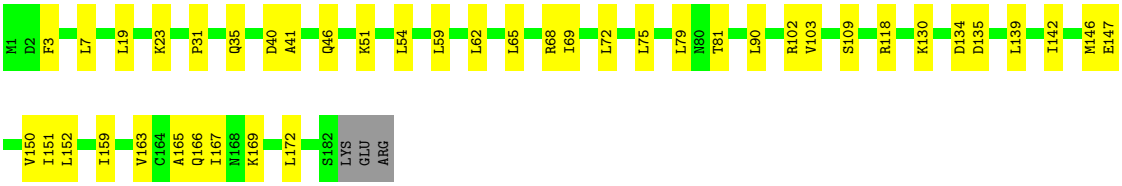
• Molecule 2: Caspase-8



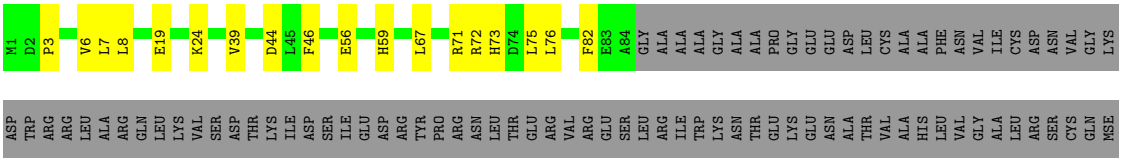


• Molecule 2: Caspase-8





• Molecule 3: FAS-associated death domain protein




ASN LEU VAL ALA ASP LEU VAL GLN GLU VAL GLN GLN ALA ARG ASP LEU GLN ASN ARG SER GLY ALA MSE SER PRO MSE SER TRP ASN SER ASP ALA SER THR SER GLU ALA SER LEU GLU HIS HIS HIS HIS HIS HIS

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	113.94Å 150.06Å 175.70Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.81 – 3.32 29.81 – 3.32	Depositor EDS
% Data completeness (in resolution range)	99.2 (29.81-3.32) 99.0 (29.81-3.32)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	0.12	Depositor
$< I/\sigma(I) >$ [1]	6.19 (at 3.31Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.194 , 0.231 0.195 , 0.231	Depositor DCC
R_{free} test set	2200 reflections (4.91%)	wwPDB-VP
Wilson B-factor (Å^2)	100.8	Xtriage
Anisotropy	0.783	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 59.1	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	13822	wwPDB-VP
Average B, all atoms (Å^2)	112.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.64% 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

Bond lengths and bond angles in the following residue types are not validated in this section: SE

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	G	0.23	0/1395	0.46	0/1864
1	H	0.22	0/1427	0.46	0/1906
1	I	0.22	0/1427	0.45	0/1906
1	K	0.22	0/1393	0.44	0/1861
2	A	0.23	0/1520	0.48	0/2021
2	B	0.23	0/1520	0.45	0/2021
2	C	0.23	0/1520	0.46	0/2021
2	D	0.23	0/1529	0.45	0/2032
2	E	0.23	0/1506	0.46	0/2003
3	L	0.23	0/674	0.52	0/902
All	All	0.23	0/13911	0.46	0/18537

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

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	G	1387	0	1458	18	0
1	H	1418	0	1503	17	0
1	I	1418	0	1503	24	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	K	1385	0	1462	13	0
2	A	1510	0	1551	31	0
2	B	1510	0	1551	19	0
2	C	1510	0	1551	17	0
2	D	1519	0	1564	14	0
2	E	1496	0	1534	11	0
3	L	668	0	691	12	0
4	G	1	0	0	0	0
All	All	13822	0	14368	159	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 (159) 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)
2:A:23:LYS:HE3	2:A:35:GLN:HG2	1.68	0.73
1:G:153:GLU:HG2	1:G:165:LYS:HG3	1.72	0.72
2:E:138:ASN:ND2	2:E:141:ASP:OD2	2.23	0.71
2:C:138:ASN:ND2	2:C:141:ASP:OD2	2.24	0.71
1:H:100:ILE:HG23	1:H:164:LEU:HD13	1.72	0.69
1:K:103:ASP:OD2	1:K:167:LYS:NZ	2.24	0.69
1:H:54:ASP:HB3	1:H:89:LEU:HD22	1.75	0.69
3:L:6:VAL:HG23	2:A:166:GLN:HG2	1.77	0.66
2:D:8:TYR:HA	2:D:42:LEU:HD21	1.77	0.65
2:D:65:LEU:HD12	2:D:98:ILE:HD11	1.78	0.65
1:K:31:ASP:OD2	1:K:47:ARG:NH2	2.31	0.63
1:H:10:GLU:HG3	1:H:38:ARG:HB2	1.80	0.63
1:H:112:LEU:HG	1:H:159:ILE:HD13	1.81	0.62
1:G:117:LYS:NZ	2:A:46:GLN:OE1	2.30	0.61
2:C:146:MSE:HE3	2:C:152:LEU:HD22	1.82	0.60
2:E:146:MSE:HE3	2:E:152:LEU:HD22	1.84	0.60
1:I:31:ASP:OD1	1:I:31:ASP:N	2.35	0.60
1:I:100:ILE:HG23	1:I:164:LEU:HD13	1.85	0.59
1:I:122:ARG:NH1	1:I:137:GLU:OE1	2.35	0.59
2:B:124:LEU:HD21	2:B:146:MSE:SE	2.53	0.58
2:C:109:SER:HA	2:C:139:LEU:HD23	1.86	0.58
2:B:172:LEU:O	2:B:176:ASN:ND2	2.33	0.57
1:K:153:GLU:HG3	1:K:165:LYS:HG3	1.87	0.57
2:A:102:ARG:NH1	2:A:147:GLU:OE2	2.37	0.57
2:C:51:LYS:HD3	2:C:53:MSE:HE2	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:19:GLU:OE2	3:L:72:ARG:HD2	2.05	0.56
2:D:138:ASN:ND2	2:D:141:ASP:OD2	2.39	0.56
1:I:10:GLU:HG3	1:I:38:ARG:HB2	1.87	0.56
1:G:10:GLU:HG3	1:G:38:ARG:HB2	1.88	0.56
1:I:163:ASP:N	1:I:163:ASP:OD1	2.39	0.56
2:E:81:THR:HG21	2:E:86:MSE:HE3	1.86	0.56
2:D:146:MSE:HE2	2:D:152:LEU:HB2	1.88	0.55
2:B:146:MSE:HE3	2:B:152:LEU:HD22	1.87	0.55
1:I:157:LYS:HB2	1:I:165:LYS:HD2	1.89	0.55
2:A:109:SER:HA	2:A:139:LEU:HD23	1.89	0.54
2:B:138:ASN:ND2	2:B:141:ASP:OD2	2.41	0.54
1:I:153:GLU:HG3	1:I:165:LYS:HG3	1.89	0.54
3:L:73:HIS:HA	3:L:76:LEU:HB2	1.90	0.54
2:A:142:ILE:HG22	2:A:146:MSE:HE2	1.90	0.54
1:K:14:ASP:HB3	2:A:130:LYS:HE2	1.90	0.54
2:A:146:MSE:HB3	2:A:152:LEU:HB2	1.88	0.53
2:B:165:ALA:HB2	2:B:172:LEU:HD11	1.90	0.53
1:G:21:LEU:HD11	1:G:58:LEU:HB3	1.91	0.53
2:A:134:ASP:OD1	2:A:135:ASP:N	2.41	0.53
1:G:22:LEU:HD23	1:G:40:LEU:HD22	1.91	0.52
2:C:2:ASP:HB3	2:C:5:ARG:HB3	1.91	0.52
2:B:8:TYR:HA	2:B:42:LEU:HD21	1.91	0.52
2:C:116:GLU:HG2	2:C:167:ILE:HD11	1.92	0.52
2:D:22:LEU:HD21	2:D:69:ILE:HD13	1.92	0.52
3:L:67:LEU:HD21	3:L:75:LEU:HB2	1.92	0.51
2:E:168:ASN:OD1	2:E:169:LYS:N	2.43	0.51
1:I:112:LEU:HD13	1:I:159:ILE:HD13	1.93	0.51
1:I:104:LEU:HD22	1:I:108:ASP:HB3	1.93	0.51
1:I:157:LYS:HD3	1:I:165:LYS:HE3	1.92	0.51
2:D:151:ILE:HG23	2:D:159:ILE:HD12	1.93	0.50
1:K:163:ASP:OD1	1:K:163:ASP:N	2.41	0.50
2:E:63:LYS:HB3	2:E:86:MSE:SE	2.61	0.50
3:L:56:GLU:HG3	3:L:59:HIS:H	1.77	0.50
2:A:68:ARG:HH21	2:A:90:LEU:HD13	1.77	0.50
2:C:52:ARG:HD2	1:I:166:THR:OG1	2.12	0.49
3:L:8:LEU:HD13	3:L:46:PHE:HB3	1.95	0.49
1:H:124:LYS:HG2	1:H:126:SER:H	1.78	0.49
2:B:28:ASP:OD1	2:B:102:ARG:NH2	2.43	0.49
1:H:40:LEU:O	1:H:44:LEU:HG	2.13	0.49
1:K:106:LYS:HD3	1:K:106:LYS:HA	1.63	0.49
1:I:113:ILE:HG12	1:I:134:LEU:HD13	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:24:LYS:HE2	3:L:39:VAL:HB	1.96	0.48
2:C:75:LEU:HD23	2:C:79:LEU:HD12	1.95	0.48
1:I:116:MSE:HB3	1:I:120:MSE:HE2	1.94	0.48
2:A:65:LEU:O	2:A:69:ILE:HG13	2.13	0.48
2:A:75:LEU:HG	2:A:81:THR:HB	1.95	0.48
1:H:65:PHE:HD2	2:A:51:LYS:HA	1.77	0.48
2:E:75:LEU:HD23	2:E:79:LEU:HD12	1.94	0.48
3:L:7:LEU:HD12	3:L:82:PHE:CG	2.49	0.48
2:D:75:LEU:HD23	2:D:79:LEU:HD12	1.96	0.47
1:I:156:LEU:HD23	1:I:159:ILE:HD11	1.96	0.47
2:C:159:ILE:O	2:C:163:VAL:HG22	2.14	0.47
2:A:151:ILE:HG23	2:A:159:ILE:HD13	1.96	0.47
2:C:52:ARG:HG2	2:C:55:GLU:OE2	2.15	0.47
2:C:8:TYR:HA	2:C:42:LEU:HD21	1.96	0.47
1:I:116:MSE:O	1:I:120:MSE:HG2	2.15	0.47
1:H:21:LEU:HD11	1:H:58:LEU:HB3	1.96	0.46
1:K:156:LEU:HD23	1:K:159:ILE:HD11	1.97	0.46
1:I:20:MSE:HE2	1:I:24:LEU:HD11	1.97	0.46
2:E:18:ASP:HA	2:E:69:ILE:HD11	1.96	0.46
1:G:6:ILE:HG23	1:G:41:LEU:HD23	1.98	0.46
2:D:134:ASP:OD1	2:D:135:ASP:N	2.49	0.46
2:B:150:VAL:HG23	2:A:72:LEU:HB2	1.97	0.46
1:H:102:GLU:O	2:A:31:PRO:HB2	2.15	0.46
1:I:163:ASP:O	1:I:167:LYS:HG2	2.15	0.46
2:A:68:ARG:HH11	2:A:103:VAL:HG21	1.80	0.46
2:C:3:PHE:HE1	2:C:59:LEU:HD21	1.81	0.46
1:H:162:ILE:HB	2:A:150:VAL:HG23	1.98	0.46
2:B:115:SER:O	2:B:118:ARG:HG2	2.16	0.46
2:D:165:ALA:HB2	2:D:172:LEU:HD11	1.98	0.46
2:A:163:VAL:O	2:A:167:ILE:HG12	2.16	0.45
2:B:146:MSE:HG2	2:B:151:ILE:HD11	1.98	0.45
1:G:126:SER:HB2	1:G:129:LYS:HE3	1.97	0.45
2:A:68:ARG:HH11	2:A:103:VAL:HG11	1.80	0.45
2:A:7:LEU:HD21	2:A:54:LEU:HD21	1.98	0.45
1:H:160:HIS:NE2	1:K:11:GLU:OE1	2.49	0.45
2:A:169:LYS:HB2	2:A:169:LYS:HE2	1.80	0.45
1:G:157:LYS:HB2	1:G:165:LYS:HD2	1.98	0.45
1:G:166:THR:HG21	2:B:52:ARG:HD2	1.99	0.45
1:H:36:ASN:OD1	1:H:37:VAL:N	2.50	0.45
1:K:55:LEU:HD23	1:K:72:LEU:HD21	1.99	0.44
2:A:62:LEU:HD22	2:A:79:LEU:HD11	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:31:PRO:HB2	2:C:12:GLU:O	2.18	0.44
2:D:33:ARG:HD3	2:C:12:GLU:OE2	2.17	0.44
2:B:72:LEU:HD13	2:B:83:LYS:HB2	2.00	0.44
2:C:168:ASN:OD1	2:C:169:LYS:N	2.50	0.44
1:K:9:VAL:O	1:K:13:LEU:HG	2.19	0.43
3:L:3:PRO:O	3:L:6:VAL:HG12	2.18	0.43
1:K:157:LYS:HB2	1:K:165:LYS:HD2	2.01	0.43
2:A:3:PHE:HE1	2:A:59:LEU:HD21	1.82	0.43
1:G:103:ASP:HA	1:I:124:LYS:H	1.83	0.43
1:H:39:ASP:O	1:H:43:ILE:HG12	2.18	0.43
2:A:19:LEU:HD11	2:A:40:ASP:HA	2.02	0.42
1:G:58:LEU:O	1:G:62:VAL:HG23	2.19	0.42
1:K:31:ASP:OD1	1:K:31:ASP:N	2.43	0.42
1:G:102:GLU:O	1:I:123:GLY:HA3	2.19	0.42
2:B:54:LEU:HD13	2:B:62:LEU:HB2	2.01	0.42
1:K:32:VAL:HG11	1:K:43:ILE:HD13	2.01	0.42
2:D:109:SER:HA	2:D:139:LEU:HD23	2.02	0.42
1:G:160:HIS:HB3	2:B:51:LYS:HE3	2.02	0.42
2:D:41:ALA:O	2:D:44:LEU:HB3	2.19	0.42
2:B:109:SER:HA	2:B:139:LEU:HD23	2.02	0.42
1:H:104:LEU:HD22	1:H:108:ASP:HB3	2.02	0.42
1:I:17:GLU:OE2	1:I:64:ARG:HD3	2.20	0.42
1:G:71:ILE:HG22	1:G:72:LEU:HD23	2.01	0.42
2:B:51:LYS:HB2	2:B:53:MSE:HE2	2.02	0.42
2:E:112:VAL:HG21	2:E:139:LEU:HD22	2.01	0.42
2:A:75:LEU:HD12	2:A:79:LEU:HD12	2.01	0.42
2:E:51:LYS:HE2	3:L:71:ARG:HB2	2.02	0.41
1:I:22:LEU:HD23	1:I:40:LEU:HD22	2.01	0.41
1:I:153:GLU:HG2	1:I:165:LYS:HE2	2.01	0.41
1:G:163:ASP:OD1	1:G:163:ASP:N	2.50	0.41
1:H:163:ASP:OD1	1:H:163:ASP:N	2.52	0.41
2:E:55:GLU:HG2	2:E:58:ASN:HB3	2.03	0.41
1:I:21:LEU:HD11	1:I:58:LEU:HB3	2.03	0.41
3:L:3:PRO:HA	3:L:6:VAL:HG12	2.03	0.41
2:A:19:LEU:HD11	2:A:40:ASP:CA	2.50	0.41
2:A:165:ALA:HA	2:A:172:LEU:HD11	2.01	0.41
2:C:63:LYS:HB3	2:C:86:MSE:SE	2.71	0.41
1:G:134:LEU:O	1:G:138:LEU:HG	2.21	0.41
2:C:124:LEU:O	2:C:133:LEU:HD11	2.21	0.41
2:B:104:MSE:HE2	2:B:178:TYR:CD2	2.56	0.41
1:H:112:LEU:HD23	1:H:112:LEU:HA	1.93	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:40:ASP:OD1	2:A:41:ALA:N	2.52	0.41
1:G:60:TYR:HB2	1:G:79:VAL:HG11	2.03	0.40
2:B:157:LEU:O	2:B:161:LYS:HG3	2.21	0.40
3:L:44:ASP:OD2	2:A:118:ARG:NH2	2.54	0.40
2:D:168:ASN:OD1	2:D:169:LYS:N	2.54	0.40
2:E:104:MSE:SE	2:E:105:LEU:HD12	2.71	0.40
1:H:73:LYS:HA	1:H:73:LYS:HD3	1.85	0.40
1:G:100:ILE:HG23	1:G:164:LEU:HD13	2.03	0.40
2:B:63:LYS:HA	2:B:75:LEU:HD21	2.03	0.40
2:A:68:ARG:NH1	2:A:103:VAL:HG21	2.36	0.40
1:I:36:ASN:ND2	1:I:39:ASP:OD1	2.48	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	G	167/181 (92%)	160 (96%)	7 (4%)	0	100	100
1	H	173/181 (96%)	164 (95%)	9 (5%)	0	100	100
1	I	173/181 (96%)	164 (95%)	9 (5%)	0	100	100
1	K	166/181 (92%)	159 (96%)	7 (4%)	0	100	100
2	A	180/185 (97%)	176 (98%)	4 (2%)	0	100	100
2	B	180/185 (97%)	175 (97%)	5 (3%)	0	100	100
2	C	180/185 (97%)	177 (98%)	3 (2%)	0	100	100
2	D	181/185 (98%)	177 (98%)	4 (2%)	0	100	100
2	E	178/185 (96%)	174 (98%)	4 (2%)	0	100	100
3	L	82/216 (38%)	80 (98%)	2 (2%)	0	100	100
All	All	1660/1865 (89%)	1606 (97%)	54 (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	G	159/159 (100%)	158 (99%)	1 (1%)	86	92
1	H	162/159 (102%)	161 (99%)	1 (1%)	86	92
1	I	162/159 (102%)	161 (99%)	1 (1%)	86	92
1	K	159/159 (100%)	158 (99%)	1 (1%)	86	92
2	A	171/167 (102%)	171 (100%)	0	100	100
2	B	171/167 (102%)	170 (99%)	1 (1%)	86	92
2	C	171/167 (102%)	169 (99%)	2 (1%)	71	84
2	D	172/167 (103%)	171 (99%)	1 (1%)	86	92
2	E	169/167 (101%)	169 (100%)	0	100	100
3	L	77/182 (42%)	77 (100%)	0	100	100
All	All	1573/1653 (95%)	1565 (100%)	8 (0%)	88	93

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	G	102	GLU
2	D	95	ARG
2	C	135	ASP
2	C	158	ASP
2	B	136	ASP
1	H	39	ASP
1	I	39	ASP
1	K	39	ASP

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

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

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

Of 1 ligands modelled in this entry, 1 is monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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	G	166/181 (91%)	-0.08	1 (0%) 89 90	79, 106, 136, 164	0
1	H	169/181 (93%)	-0.11	1 (0%) 89 90	77, 113, 161, 202	0
1	I	169/181 (93%)	-0.20	3 (1%) 68 67	82, 104, 138, 165	0
1	K	164/181 (90%)	-0.21	0 100 100	78, 98, 136, 161	0
2	A	175/185 (94%)	-0.17	0 100 100	76, 99, 136, 143	0
2	B	175/185 (94%)	-0.05	0 100 100	82, 108, 149, 168	0
2	C	175/185 (94%)	-0.17	1 (0%) 89 90	80, 111, 150, 174	0
2	D	176/185 (95%)	-0.14	3 (1%) 70 68	82, 116, 152, 184	0
2	E	174/185 (94%)	0.07	9 (5%) 27 27	91, 122, 160, 181	0
3	L	82/216 (37%)	-0.38	0 100 100	84, 104, 131, 140	0
All	All	1625/1865 (87%)	-0.13	18 (1%) 80 81	76, 108, 150, 202	0

All (18) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	E	120	PHE	3.3
1	I	121	GLY	3.3
2	E	93	PRO	2.5
2	C	95	ARG	2.5
1	G	176	GLN	2.5
2	E	163	VAL	2.4
1	I	85	ARG	2.4
2	E	162	ARG	2.3
2	E	124	LEU	2.3
2	D	181	PHE	2.3
1	I	31	ASP	2.2
2	E	164	CYS	2.2
2	D	180	GLU	2.2

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Mol	Chain	Res	Type	RSRZ
1	H	127	LYS	2.2
2	E	91	GLN	2.1
2	E	121	LYS	2.1
2	D	136	ASP	2.0
2	E	2	ASP	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)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	SE	G	201	1/1	0.91	0.27	175,175,175,175	0

6.5 Other polymers (i)

There are no such residues in this entry.