WORLDWIDE wwPDB PROTEIN DATA BANK

Full wwPDB X-ray Structure Validation Report (i)

Jul 19, 2022 – 06:22 AM JST

PDB ID	:	7XGE
Title	:	Crystal structure of MCL-1 in complex with computationally designed inhibitor protein
Authors	:	Oh, B.-H.; Kim, S.
Deposited on	:	2022-04-04
Resolution	:	2.38 Å(reported)

The following versions of software and data (see references (i)) were used in the production of this report:

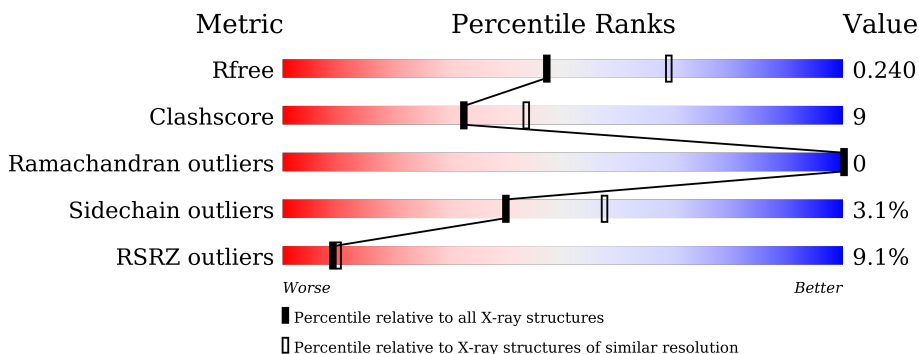|		
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.29
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.29

1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:
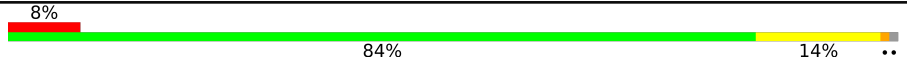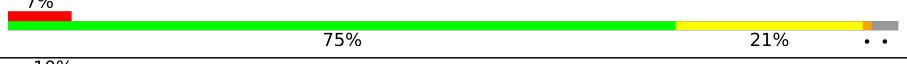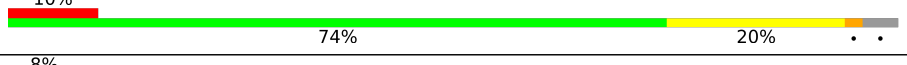*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.38 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.
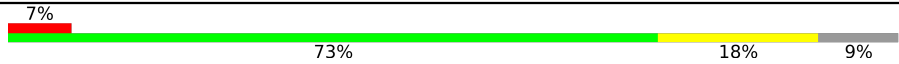
Metric	Percentile Ranks	Value
Rfree		0.240
Clashscore		9
Ramachandran outliers		0
Sidechain outliers		3.1%
RSRZ outliers		9.1%

Worse   *Better*

▮ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	5509 (2.40-2.36)
Clashscore	141614	6082 (2.40-2.36)
Ramachandran outliers	138981	5973 (2.40-2.36)
Sidechain outliers	138945	5975 (2.40-2.36)
RSRZ outliers	127900	5397 (2.40-2.36)

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	A	169	8% / 84% 14% ••
1	C	169	11% / 76% 17% • 5%
1	E	169	10% / 69% 16% •• 11%
1	G	169	7% / 75% 21% ••
2	B	156	10% / 74% 20% ••
2	D	156	8% / 76% 17% 8%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	F	156	7% 73% 18% 9%
2	H	156	7% 70% 18% 11%

2 Entry composition ⓘ

There are 3 unique types of molecules in this entry. The entry contains 9956 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 BCL-xL and MCL-1 dual binder 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	168	Total	C	N	O	S	0	0	0
			1336	844	243	248	1			
1	C	161	Total	C	N	O	S	0	0	0
			1281	809	231	240	1			
1	E	151	Total	C	N	O	S	0	0	0
			1205	766	219	219	1			
1	G	164	Total	C	N	O	S	0	0	0
			1304	824	235	244	1			

- Molecule 2 is a protein called Induced myeloid leukemia cell differentiation protein Mcl-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	150	Total	C	N	O	S	0	0	0
			1208	759	223	222	4			
2	D	144	Total	C	N	O	S	0	0	0
			1162	731	213	215	3			
2	F	142	Total	C	N	O	S	0	0	0
			1145	721	210	211	3			
2	H	139	Total	C	N	O	S	0	0	0
			1128	711	207	207	3			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	3	MET	-	initiating methionine	UNP Q07820
B	154	SER	-	expression tag	UNP Q07820
B	155	ARG	-	expression tag	UNP Q07820
B	156	GLY	-	expression tag	UNP Q07820
B	157	LYS	-	expression tag	UNP Q07820
B	158	LEU	-	expression tag	UNP Q07820
D	3	MET	-	initiating methionine	UNP Q07820
D	154	SER	-	expression tag	UNP Q07820

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
D	155	ARG	-	expression tag	UNP Q07820
D	156	GLY	-	expression tag	UNP Q07820
D	157	LYS	-	expression tag	UNP Q07820
D	158	LEU	-	expression tag	UNP Q07820
F	3	MET	-	initiating methionine	UNP Q07820
F	154	SER	-	expression tag	UNP Q07820
F	155	ARG	-	expression tag	UNP Q07820
F	156	GLY	-	expression tag	UNP Q07820
F	157	LYS	-	expression tag	UNP Q07820
F	158	LEU	-	expression tag	UNP Q07820
H	3	MET	-	initiating methionine	UNP Q07820
H	154	SER	-	expression tag	UNP Q07820
H	155	ARG	-	expression tag	UNP Q07820
H	156	GLY	-	expression tag	UNP Q07820
H	157	LYS	-	expression tag	UNP Q07820
H	158	LEU	-	expression tag	UNP Q07820

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	25	Total 25	O 25	0	0
3	B	23	Total 23	O 23	0	0
3	C	34	Total 34	O 34	0	0
3	D	21	Total 21	O 21	0	0
3	E	22	Total 22	O 22	0	0
3	F	19	Total 19	O 19	0	0
3	G	24	Total 24	O 24	0	0
3	H	19	Total 19	O 19	0	0

3 Residue-property plots ⓘ

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the propo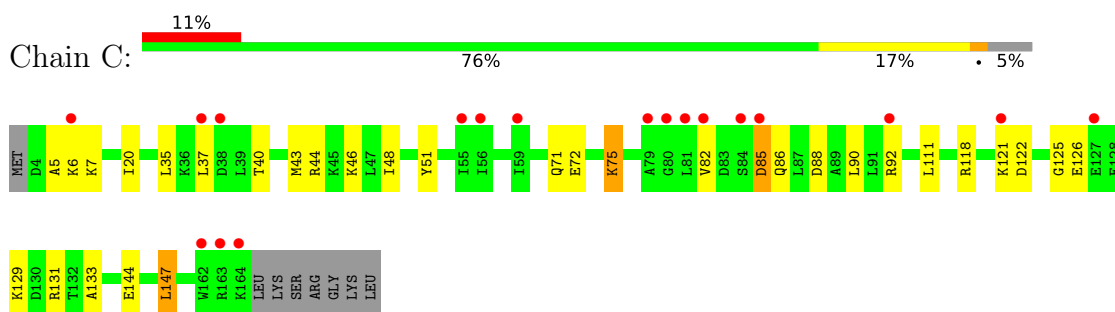rtions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, 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.
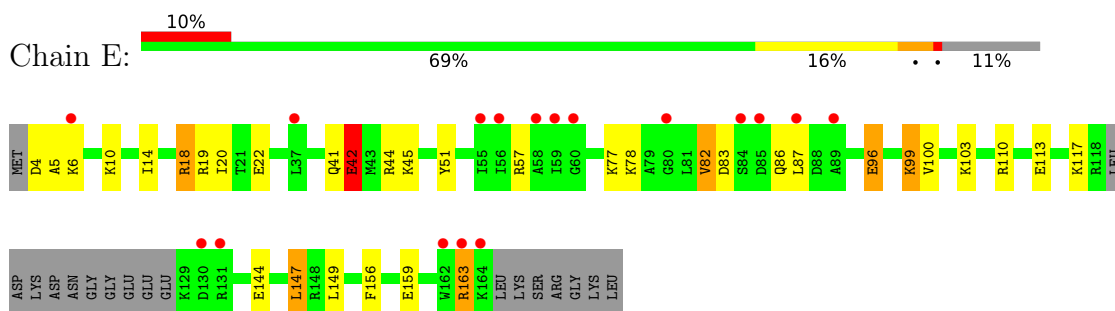
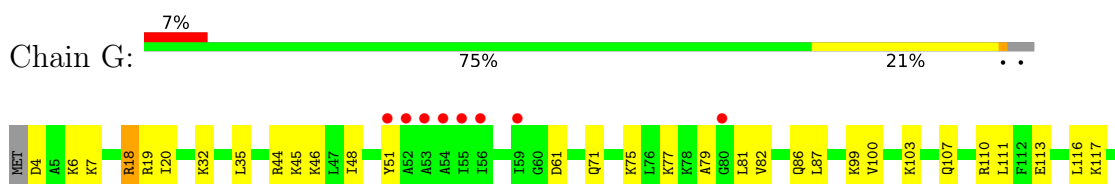- Molecule 1: BCL-xL and MCL-1 dual binder 2

Chain A:

- Molecule 1: BCL-xL and MCL-1 dual binder 2

Chain C:

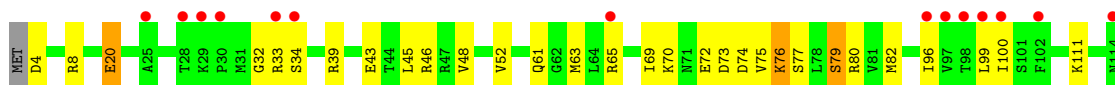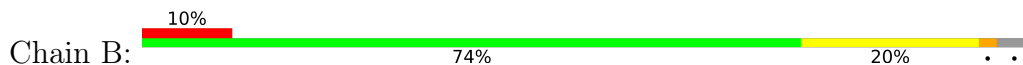- Molecule 1: BCL-xL and MCL-1 dual binder 2

Chain E:

- Molecule 1: BCL-xL and MCL-1 dual binder 2

Chain G:

G124 K129 E139 L147 R148 K160 K164 L165 K166 S167 ARG GLY LYS LEU

• **Molecule 2: Induced myeloid leukemia cell differentiation protein Mcl-1**

Chain B:

10%

74% 20%

MET D4 R8 E20 A25 T28 K29 P30 M31 G32 R33 S34 R39 E43 T44 L45 R46 R47 V48 V52 Q61 G62 M63 L64 R65 I69 K70 N71 E72 D73 D74 V75 K76 S77 L78 S79 R80 V81 M82 I96 V97 T98 L99 I100 S101 F102 K111 N114

Q115 E116 I126 V129 L130 R135 V153 SER ARG GLY LYS LEU

• **Molecule 2: Induced myeloid leukemia cell differentiation protein Mcl-1**

Chain D:

8%

76% 17% 8%

MET D4 E5 R8 Q9 R16 E20 D27 THR LYS PRO MET GLY ARG SER G35 A36 T37 K40 F60 Q61 G62 M63 L64 R65 K66 K70 K76 S77 L78 S79 M82 I96 V97 T98 L99 I100 S101 F102 G103 A104 F105 K111 E116 L122 S125

K140 E149 V153 S154 ARG GLY LYS LEU

• **Molecule 2: Induced myeloid leukemia cell differentiation protein Mcl-1**

Chain F:

7%

73% 18% 9%

MET D4 L11 E12 S15 R16 E20 A25 LYS ASP THR LYS PRO MET GLY ARG SER G35 S38 R39 R46 Q61 L64 R65 K76 S77 L78 S79 R80 V81 M82 S87 I96 V97 T98 L99 I100 S101 F102 V106 A107 K108 H109 T112 I113 L122
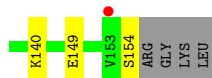

D128 V129 L130 T133 H152 V153 S154 ARG GLY LYS LEU

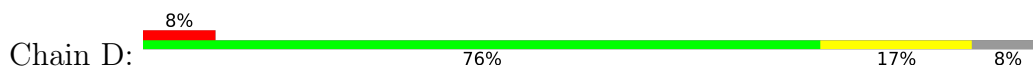• **Molecule 2: Induced myeloid leukemia cell differentiation protein Mcl-1**

Chain H:

7%

70% 18% 11%

MET D4 E12 R16 R19 T23 G24 A25 LYS ASP THR LYS PRO MET GLY ARG SER GLY A36 E57 Q61 K66 L67 D68 I69 K70 N71 E72 D73 L78 S79 R80 V81 M82 F86 S87 V97 T98 L99 I100 S101 F102 T112 I113 N114 Q115 E116 I119

V129 T133 K134 R135 D136 W137 K140 Q141 E149 H152 VAL SER ARG GLY LYS LEU

4 Data and refinement statistics (i)

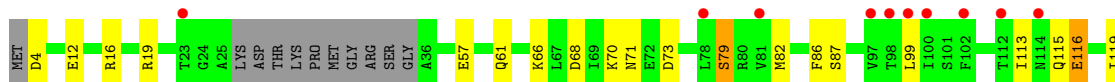| Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	67.99Å 74.77Å 92.16Å 70.83° 89.59° 67.58°	Depositor
Resolution (Å)	29.46 – 2.38 29.46 – 2.38	Depositor EDS
% Data completeness (in resolution range)	97.3 (29.46-2.38) 97.3 (29.46-2.38)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.93 (at 2.39Å)	Xtriage
Refinement program	PHENIX 1.17.1_3660	Depositor
R, R_{free}	0.202 , 0.240 0.202 , 0.240	Depositor DCC
R_{free} test set	3064 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	53.5	Xtriage
Anisotropy	0.264	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 49.4	EDS
L-test for twinning[2]	$< |L| > = 0.50, < L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	9956	wwPDB-VP
Average B, all atoms (Å^2)	70.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.81% of the height of the origin peak. No significant pseudotranslation is detected.*

---

[1]Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$|Z|$ >5	RMSZ	#$|Z|$ >5
1	A	0.30	0/1345	0.53	1/1795 (0.1%)
1	C	0.37	0/1290	0.59	2/1724 (0.1%)
1	E	0.47	2/1213 (0.2%)	0.67	4/1620 (0.2%)
1	G	0.31	0/1313	0.51	0/1754
2	B	0.35	0/1228	0.59	3/1651 (0.2%)
2	D	0.40	1/1180 (0.1%)	0.75	6/1586 (0.4%)
2	F	0.31	0/1163	0.49	0/1564
2	H	0.31	0/1146	0.50	1/1541 (0.1%)
All	All	0.36	3/9878 (0.0%)	0.58	17/13235 (0.1%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	65	ARG	CG-CD	5.77	1.66	1.51
1	E	96	GLU	CB-CG	5.48	1.62	1.52
1	E	42	GLU	CD-OE1	-5.33	1.19	1.25

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(º)	Ideal(º)
2	D	65	ARG	NE-CZ-NH2	10.14	125.37	120.30
2	D	65	ARG	NE-CZ-NH1	-9.53	115.53	120.30
1	C	75	LYS	CB-CG-CD	8.09	132.65	111.60
1	A	75	LYS	CA-CB-CG	7.71	130.37	113.40
2	D	65	ARG	CB-CG-CD	-7.51	92.07	111.60
2	H	140	LYS	CD-CE-NZ	6.81	127.36	111.70
2	D	65	ARG	CG-CD-NE	6.39	125.21	111.80
1	E	96	GLU	CA-CB-CG	6.35	127.36	113.40
2	D	66	LYS	CA-CB-CG	6.17	126.96	113.40
2	B	73	ASP	CB-CG-OD2	-6.09	112.82	118.30
1	E	163	ARG	NE-CZ-NH2	-5.96	117.32	120.30
2	D	65	ARG	CA-CB-CG	5.68	125.90	113.40
2	B	20	GLU	CA-CB-CG	5.58	125.68	113.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	69	ILE	CG1-CB-CG2	-5.57	99.15	111.40
1	E	82	VAL	CG1-CB-CG2	5.37	119.49	110.90
1	C	147	LEU	CA-CB-CG	-5.35	103.00	115.30
1	E	147	LEU	CA-CB-CG	-5.17	103.40	115.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1336	0	1417	16	0
1	C	1281	0	1348	34	1
1	E	1205	0	1285	25	0
1	G	1304	0	1376	28	1
2	B	1208	0	1220	21	0
2	D	1162	0	1167	16	0
2	F	1145	0	1150	20	0
2	H	1128	0	1133	24	0
3	A	25	0	0	0	0
3	B	23	0	0	0	0
3	C	34	0	0	1	0
3	D	21	0	0	0	0
3	E	22	0	0	0	0
3	F	19	0	0	0	0
3	G	24	0	0	2	0
3	H	19	0	0	0	0
All	All	9956	0	10096	175	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 9.

All (175) 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:F:76:LYS:NZ	2:F:79:SER:OG	1.76	1.18
1:C:82:VAL:HG23	1:C:86:GLN:HB2	1.20	1.12
1:C:126:GLU:HA	1:C:129:LYS:HD2	1.45	0.97
2:F:20:GLU:OE1	2:F:46:ARG:NH1	1.99	0.94
1:C:82:VAL:CG2	1:C:86:GLN:HB2	2.00	0.91
1:C:71:GLN:HG2	1:C:75:LYS:HE3	1.51	0.90
2:B:111:LYS:NZ	2:B:116:GLU:OE1	2.07	0.87
1:G:82:VAL:HG23	1:G:86:GLN:HB2	1.55	0.87
1:C:125:GLY:O	1:C:129:LYS:HG2	1.78	0.83
1:C:37:LEU:HD21	1:C:129:LYS:NZ	1.95	0.81
1:A:6:LYS:HD2	1:A:159:GLU:HG2	1.63	0.80
1:E:6:LYS:HE2	1:E:159:GLU:HG2	1.63	0.80
1:C:35:LEU:HD22	1:C:129:LYS:HB2	1.63	0.79
2:B:76:LYS:HE3	2:B:80:ARG:HH12	1.51	0.76
1:E:113:GLU:OE1	2:F:65:ARG:NH1	2.19	0.75
1:G:82:VAL:HG23	1:G:86:GLN:CB	2.16	0.74
2:F:12:GLU:O	2:F:16:ARG:HG3	1.87	0.73
2:F:35:GLY:N	2:F:38:SER:HG	1.85	0.73
1:E:83:ASP:H	1:E:86:GLN:HE21	1.35	0.73
2:B:20:GLU:OE1	2:B:46:ARG:NE	2.23	0.69
1:C:85:ASP:HA	1:C:88:ASP:OD1	1.92	0.69
1:G:35:LEU:HD22	1:G:129:LYS:HG2	1.75	0.69
1:C:37:LEU:HD21	1:C:129:LYS:HZ2	1.55	0.68
1:E:18:ARG:HD2	1:E:19:ARG:HD3	1.77	0.67
1:E:99:LYS:NZ	1:E:100:VAL:HG13	2.10	0.66
2:D:36:ALA:O	2:D:40:LYS:HG3	1.97	0.65
1:C:20:ILE:HG13	1:C:147:LEU:HD22	1.77	0.64
2:H:57:GLU:O	2:H:61:GLN:HB2	1.98	0.64
1:C:85:ASP:O	1:C:88:ASP:OD1	2.16	0.64
2:D:61:GLN:HG2	2:D:105:PHE:CZ	2.33	0.64
1:A:68:GLN:O	1:A:71:GLN:HG2	1.98	0.62
2:F:76:LYS:NZ	2:F:79:SER:HG	1.98	0.61
2:D:82:MET:HG2	2:D:99:LEU:HD22	1.84	0.60
2:D:76:LYS:O	2:D:79:SER:HB2	2.02	0.60
1:G:18:ARG:NH1	1:G:148:ARG:HH22	2.01	0.59
1:C:85:ASP:C	1:C:88:ASP:OD1	2.42	0.58
2:H:149:GLU:O	2:H:152:HIS:ND1	2.36	0.58
1:G:20:ILE:HG13	1:G:147:LEU:HD22	1.86	0.58
1:E:82:VAL:HG22	1:E:86:GLN:HB2	1.85	0.58
1:C:72:GLU:O	1:C:75:LYS:HB2	2.04	0.57
2:B:82:MET:HG2	2:B:99:LEU:HD22	1.87	0.57
1:C:71:GLN:HG2	1:C:75:LYS:CE	2.29	0.57

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:147:LEU:O	1:C:147:LEU:HG	2.05	0.56
2:D:149:GLU:O	2:D:149:GLU:HG3	2.03	0.56
1:E:42:GLU:OE1	1:E:42:GLU:N	2.34	0.56
2:B:61:GLN:O	2:B:65:ARG:HG3	2.05	0.56
1:A:160:LYS:HD3	1:A:163:ARG:HH21	1.71	0.56
2:H:16:ARG:HG2	2:H:19:ARG:NH2	2.22	0.55
1:C:72:GLU:HA	1:C:75:LYS:CG	2.37	0.55
1:G:6:LYS:HG3	1:G:7:LYS:N	2.21	0.55
1:E:41:GLN:O	1:E:45:LYS:HG2	2.06	0.55
2:F:82:MET:HG2	2:F:99:LEU:HD22	1.88	0.55
2:H:86:PHE:CG	2:H:134:LYS:HE2	2.42	0.54
2:D:61:GLN:HG2	2:D:105:PHE:HZ	1.71	0.54
1:E:99:LYS:O	1:E:103:LYS:HG3	2.09	0.53
1:G:111:LEU:HD21	1:G:139:GLU:HB3	1.90	0.53
1:C:37:LEU:HD21	1:C:129:LYS:HZ3	1.75	0.52
1:G:46:LYS:NZ	3:G:204:HOH:O	2.42	0.52
2:F:79:SER:HB2	2:F:129:VAL:HG21	1.91	0.52
2:H:57:GLU:HG2	2:H:61:GLN:HE21	1.75	0.52
2:H:68:ASP:CG	2:H:70:LYS:HE3	2.30	0.52
1:C:85:ASP:CA	1:C:88:ASP:OD1	2.56	0.52
1:E:99:LYS:HD2	1:E:100:VAL:N	2.25	0.51
2:H:82:MET:HG2	2:H:99:LEU:HD22	1.93	0.51
2:D:9:GLN:NE2	2:D:37:THR:OG1	2.43	0.51
2:B:45:LEU:HD21	2:B:100:ILE:HG21	1.93	0.51
1:C:126:GLU:HA	1:C:129:LYS:CD	2.30	0.51
1:E:99:LYS:HZ2	1:E:100:VAL:HG13	1.75	0.51
1:C:37:LEU:CD2	1:C:129:LYS:NZ	2.71	0.50
1:A:160:LYS:HD3	1:A:163:ARG:NH2	2.27	0.50
1:G:44:ARG:O	1:G:48:ILE:HG12	2.10	0.50
1:G:18:ARG:HH12	1:G:148:ARG:HH22	1.59	0.50
1:A:32:LYS:NZ	1:A:137:GLU:OE2	2.36	0.50
2:D:5:GLU:OE2	2:D:8:ARG:NH1	2.39	0.50
2:H:113:ILE:HD12	2:H:115:GLN:HG3	1.93	0.50
1:A:20:ILE:HG13	1:A:147:LEU:HD22	1.93	0.49
1:A:68:GLN:HG2	1:A:71:GLN:NE2	2.27	0.49
2:B:20:GLU:OE1	2:B:46:ARG:NH2	2.44	0.49
2:B:96:ILE:HG12	2:B:130:LEU:HD21	1.94	0.49
2:H:12:GLU:O	2:H:16:ARG:HG3	2.10	0.49
2:D:78:LEU:HD23	2:D:122:LEU:HD11	1.94	0.49
2:F:78:LEU:HD23	2:F:122:LEU:HD11	1.94	0.49
2:F:96:ILE:HG12	2:F:130:LEU:HD11	1.95	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:140:LYS:O	2:D:140:LYS:HD3	2.11	0.49
1:A:49:GLU:OE2	2:B:77:SER:OG	2.25	0.49
1:E:147:LEU:O	1:E:147:LEU:HG	2.10	0.49
2:B:4:ASP:OD2	2:B:135:ARG:NH2	2.39	0.49
1:C:35:LEU:HD11	1:C:133:ALA:HB2	1.95	0.49
1:C:37:LEU:CD2	1:C:129:LYS:HZ3	2.26	0.49
1:C:118:ARG:O	1:C:122:ASP:HB2	2.12	0.49
1:G:82:VAL:CG2	1:G:86:GLN:HB2	2.34	0.49
2:B:39:ARG:O	2:B:43:GLU:HG3	2.14	0.48
1:A:122:ASP:OD1	1:A:128:GLU:HG3	2.13	0.48
2:F:64:LEU:HD13	2:F:106:VAL:HG22	1.96	0.48
2:H:79:SER:HB2	2:H:129:VAL:HG21	1.96	0.48
1:C:72:GLU:HA	1:C:75:LYS:HG2	1.95	0.48
1:G:45:LYS:HE2	1:G:45:LYS:HB2	1.54	0.48
1:G:99:LYS:O	1:G:103:LYS:HG2	2.14	0.48
1:G:77:LYS:HB2	1:G:87:LEU:HD13	1.95	0.48
2:D:79:SER:OG	2:D:125:SER:OG	2.32	0.47
1:E:96:GLU:O	1:E:100:VAL:HG22	2.14	0.47
2:B:111:LYS:CE	2:B:116:GLU:OE1	2.63	0.47
1:G:116:LEU:HD13	2:H:66:LYS:HD2	1.95	0.47
1:A:72:GLU:O	1:A:75:LYS:HB3	2.14	0.47
1:E:110:ARG:NH1	1:E:113:GLU:HB3	2.30	0.47
1:E:96:GLU:CD	1:E:99:LYS:HE3	2.35	0.47
2:F:35:GLY:O	2:F:39:ARG:HG3	2.14	0.47
2:B:72:GLU:O	2:B:75:VAL:HG12	2.15	0.46
1:G:166:LYS:HE3	1:G:166:LYS:HA	1.96	0.46
2:B:70:LYS:HD2	2:B:74:ASP:OD2	2.14	0.46
2:H:4:ASP:OD2	2:H:135:ARG:NH2	2.44	0.46
1:C:40:THR:HG23	1:C:43:MET:H	1.81	0.46
1:E:20:ILE:HG13	1:E:147:LEU:HD22	1.96	0.46
1:E:4:ASP:OD1	1:E:5:ALA:N	2.49	0.46
2:H:71:ASN:OD1	2:H:73:ASP:HB2	2.16	0.45
1:C:88:ASP:O	1:C:92:ARG:HG3	2.16	0.45
2:B:48:VAL:O	2:B:52:VAL:HG23	2.17	0.45
1:E:149:LEU:HD12	1:E:149:LEU:HA	1.79	0.45
2:F:78:LEU:O	2:F:82:MET:HG3	2.16	0.45
1:G:19:ARG:HD2	1:G:61:ASP:HB3	1.99	0.45
1:C:126:GLU:O	1:C:129:LYS:HG3	2.17	0.45
2:H:137:TRP:CH2	2:H:141:GLN:HG3	2.52	0.45
2:D:16:ARG:O	2:D:20:GLU:HB3	2.18	0.44
2:D:5:GLU:OE1	2:D:8:ARG:NH1	2.51	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:7:LYS:HA	1:A:7:LYS:HD3	1.72	0.44
2:H:116:GLU:HA	2:H:119:ILE:HG13	1.98	0.44
1:A:134:LYS:HG3	1:E:156:PHE:HZ	1.82	0.44
1:A:120:ASP:OD2	1:A:121:LYS:HE3	2.18	0.44
1:G:4:ASP:HB2	1:G:6:LYS:HG2	2.00	0.44
1:G:32:LYS:HB3	1:G:32:LYS:HE2	1.84	0.44
1:A:68:GLN:O	1:A:72:GLU:HG2	2.17	0.43
1:C:129:LYS:HG2	1:C:129:LYS:H	1.61	0.43
2:B:8:ARG:NH1	2:B:32:GLY:HA3	2.33	0.43
1:A:44:ARG:O	1:A:48:ILE:HG12	2.17	0.43
2:D:5:GLU:CD	2:D:8:ARG:NH1	2.72	0.43
1:G:99:LYS:HG3	1:G:100:VAL:N	2.32	0.43
1:G:79:ALA:HB3	1:G:81:LEU:HD12	2.00	0.43
2:B:33:ARG:NE	2:B:33:ARG:HA	2.33	0.43
1:C:5:ALA:HB1	1:C:90:LEU:HD22	2.00	0.43
1:E:99:LYS:HZ3	1:E:100:VAL:HG13	1.82	0.43
2:F:11:LEU:O	2:F:15:SER:HB2	2.19	0.43
2:F:108:LYS:O	2:F:112:THR:HG23	2.19	0.43
1:A:34:ALA:HB1	1:A:119:LEU:HD21	2.00	0.42
2:B:76:LYS:H	2:B:76:LYS:HG2	1.65	0.42
1:C:6:LYS:HG3	1:C:7:LYS:N	2.34	0.42
2:F:87:SER:HA	2:H:133:THR:O	2.19	0.42
2:F:16:ARG:O	2:F:20:GLU:HG2	2.20	0.42
2:D:61:GLN:CG	2:D:105:PHE:HZ	2.32	0.42
1:C:111:LEU:HD23	1:C:111:LEU:HA	1.93	0.42
1:G:71:GLN:O	1:G:75:LYS:HG3	2.19	0.42
1:C:72:GLU:HA	1:C:75:LYS:HG3	2.02	0.42
1:E:57:ARG:NH2	2:H:136:ASP:OD2	2.37	0.42
2:H:68:ASP:OD2	2:H:70:LYS:HE3	2.20	0.42
1:C:44:ARG:O	1:C:48:ILE:HG12	2.20	0.41
2:B:79:SER:HB2	2:B:129:VAL:HG21	2.02	0.41
1:E:44:ARG:HH11	1:E:45:LYS:NZ	2.19	0.41
2:H:86:PHE:CD2	2:H:134:LYS:HE2	2.55	0.41
2:F:109:HIS:O	2:F:113:ILE:HG12	2.20	0.41
2:B:63:MET:HB3	2:B:63:MET:HE2	1.93	0.41
1:C:51:TYR:OH	3:C:201:HOH:O	2.17	0.41
1:E:77:LYS:HB2	1:E:87:LEU:HD13	2.03	0.41
2:F:133:THR:O	2:H:87:SER:HA	2.20	0.41
1:G:160:LYS:HG2	1:G:164:LYS:HE2	2.03	0.41
2:F:76:LYS:HE3	2:F:76:LYS:HB3	1.76	0.41
1:G:18:ARG:NH1	3:G:201:HOH:O	2.24	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:70:LYS:HE3	2:D:70:LYS:HB2	1.75	0.41
1:E:14:ILE:HD13	1:E:14:ILE:HA	1.89	0.41
2:H:133:THR:O	2:H:134:LYS:HG3	2.21	0.41
2:B:20:GLU:OE1	2:B:46:ARG:CZ	2.69	0.40
1:G:113:GLU:HG2	2:H:66:LYS:HZ3	1.85	0.40
1:E:18:ARG:HD3	1:E:22:GLU:OE2	2.21	0.40
1:G:103:LYS:O	1:G:107:GLN:HG3	2.21	0.40
1:G:117:LYS:O	1:G:117:LYS:HD2	2.21	0.40
2:H:16:ARG:HG2	2:H:19:ARG:HH22	1.86	0.40
1:G:48:ILE:HD12	2:H:66:LYS:HB3	2.04	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:131:ARG:NH2	1:G:7:LYS:NZ[1_556]	2.13	0.07

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	166/169 (98%)	164 (99%)	2 (1%)	0	100	100
1	C	159/169 (94%)	157 (99%)	2 (1%)	0	100	100
1	E	147/169 (87%)	146 (99%)	1 (1%)	0	100	100
1	G	162/169 (96%)	160 (99%)	2 (1%)	0	100	100
2	B	148/156 (95%)	142 (96%)	6 (4%)	0	100	100
2	D	140/156 (90%)	138 (99%)	2 (1%)	0	100	100
2	F	138/156 (88%)	136 (99%)	2 (1%)	0	100	100
2	H	135/156 (86%)	132 (98%)	3 (2%)	0	100	100

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	1195/1300 (92%)	1175 (98%)	20 (2%)	0	100 100

There are no Ramachandran outliers to report.

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	133/134 (99%)	129 (97%)	4 (3%)	41	59
1	C	127/134 (95%)	123 (97%)	4 (3%)	40	57
1	E	119/134 (89%)	110 (92%)	9 (8%)	13	18
1	G	130/134 (97%)	126 (97%)	4 (3%)	40	57
2	B	131/136 (96%)	128 (98%)	3 (2%)	50	68
2	D	126/136 (93%)	122 (97%)	4 (3%)	39	56
2	F	124/136 (91%)	123 (99%)	1 (1%)	81	91
2	H	122/136 (90%)	120 (98%)	2 (2%)	62	78
All	All	1012/1080 (94%)	981 (97%)	31 (3%)	40	57

All (31) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	45	LYS
1	A	51	TYR
1	A	128	GLU
1	A	141	ARG
2	B	34	SER
2	B	76	LYS
2	B	79	SER
1	C	46	LYS
1	C	85	ASP
1	C	121	LYS
1	C	144	GLU
2	D	27	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	D	111	LYS
2	D	116	GLU
2	D	154	SER
1	E	10	LYS
1	E	18	ARG
1	E	42	GLU
1	E	51	TYR
1	E	78	LYS
1	E	99	LYS
1	E	117	LYS
1	E	144	GLU
1	E	163	ARG
2	F	128	ASP
1	G	18	ARG
1	G	51	TYR
1	G	110	ARG
1	G	139	GLU
2	H	79	SER
2	H	116	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	25	GLN
1	A	71	GLN
2	D	9	GLN
1	E	86	GLN
1	G	107	GLN
2	H	61	GLN

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 ⓘ

There are no ligands in this entry.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	168/169 (99%)	0.26	14 (8%)	11	12	42, 63, 107, 156	0
1	C	161/169 (95%)	0.45	18 (11%)	5	6	42, 67, 130, 157	0
1	E	151/169 (89%)	0.48	17 (11%)	5	5	43, 66, 121, 139	0
1	G	164/169 (97%)	0.31	11 (6%)	17	19	41, 64, 107, 126	0
2	B	150/156 (96%)	0.34	16 (10%)	6	6	40, 64, 114, 148	0
2	D	144/156 (92%)	0.34	13 (9%)	9	10	42, 63, 93, 137	0
2	F	142/156 (91%)	0.35	11 (7%)	13	14	44, 67, 101, 120	0
2	H	139/156 (89%)	0.34	11 (7%)	12	13	42, 69, 102, 116	0
All	All	1219/1300 (93%)	0.36	111 (9%)	9	10	40, 65, 113, 157	0

All (111) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	37	LEU	6.6
1	E	37	LEU	6.3
1	E	162	TRP	5.7
1	G	165	LEU	5.6
1	C	162	TRP	5.3
2	B	28	THR	5.3
1	C	80	GLY	5.2
2	H	99	LEU	4.5
2	D	100	ILE	4.5
1	E	163	ARG	4.5
1	A	119	LEU	4.5
2	B	33	ARG	4.4
2	F	153	VAL	4.3
1	A	56	ILE	4.3
2	F	100	ILE	4.2
2	B	30	PRO	4.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	D	98	THR	4.0
2	B	99	LEU	3.9
1	C	164	LYS	3.9
1	E	59	ILE	3.9
2	B	97	VAL	3.8
1	E	56	ILE	3.7
1	G	56	ILE	3.7
2	F	25	ALA	3.7
1	E	164	LYS	3.6
2	F	98	THR	3.5
2	H	114	ASN	3.4
1	A	53	ALA	3.4
2	B	29	LYS	3.3
2	B	96	ILE	3.3
2	F	102	PHE	3.3
2	D	102	PHE	3.2
2	B	114	ASN	3.2
2	H	112	THR	3.2
2	D	97	VAL	3.2
1	C	82	VAL	3.2
1	E	80	GLY	3.2
1	C	38	ASP	3.1
1	E	58	ALA	3.1
1	C	79	ALA	3.1
1	A	121	LYS	3.0
1	A	52	ALA	3.0
2	F	97	VAL	3.0
1	G	55	ILE	3.0
2	H	102	PHE	3.0
1	C	127	GLU	2.9
1	E	85	ASP	2.9
2	B	98	THR	2.9
1	E	131	ARG	2.8
2	B	100	ILE	2.8
1	G	52	ALA	2.8
2	D	27	ASP	2.7
1	E	87	LEU	2.7
2	F	99	LEU	2.7
1	C	81	LEU	2.7
1	E	55	ILE	2.7
2	F	96	ILE	2.6
1	A	35	LEU	2.6

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	G	167	SER	2.6
2	B	126	ILE	2.6
1	A	51	TYR	2.6
1	E	84	SER	2.6
1	C	56	ILE	2.6
2	B	34	SER	2.6
2	H	100	ILE	2.6
1	C	6	LYS	2.6
2	F	81	VAL	2.6
2	H	97	VAL	2.6
1	C	59	ILE	2.5
2	H	81	VAL	2.5
1	G	59	ILE	2.5
1	C	92	ARG	2.5
1	E	6	LYS	2.5
2	H	98	THR	2.5
1	A	54	ALA	2.4
1	G	53	ALA	2.4
1	C	121	LYS	2.4
2	D	99	LEU	2.4
2	D	96	ILE	2.4
2	B	25	ALA	2.4
2	D	103	GLY	2.4
2	D	63	MET	2.4
2	D	153	VAL	2.3
1	A	58	ALA	2.3
2	B	102	PHE	2.3
1	C	84	SER	2.3
1	E	89	ALA	2.3
2	H	152	HIS	2.3
1	A	120	ASP	2.3
1	A	123	ASN	2.3
1	C	163	ARG	2.2
1	E	60	GLY	2.2
1	C	55	ILE	2.2
2	B	153	VAL	2.2
2	H	23	THR	2.2
2	H	78	LEU	2.2
1	A	126	GLU	2.2
1	A	60	GLY	2.2
2	F	61	GLN	2.1
2	F	152	HIS	2.1

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	B	65	ARG	2.1
2	D	101	SER	2.1
1	G	51	TYR	2.1
2	D	60	PHE	2.1
1	E	130	ASP	2.1
2	D	82	MET	2.1
1	G	54	ALA	2.0
1	G	80	GLY	2.0
1	A	59	ILE	2.0
1	G	124	GLY	2.0
1	C	85	ASP	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

6.4 Ligands ⓘ

There are no ligands in this entry.

6.5 Other polymers ⓘ

There are no such residues in this entry.