Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 10:52 PM GMT

PDB ID	:	4ZBI
Title	:	Mcl-1 complexed with small molecules
Authors	:	Zhao, B.
Deposited on	:	2015-04-14
Resolution	:	2.50 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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

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

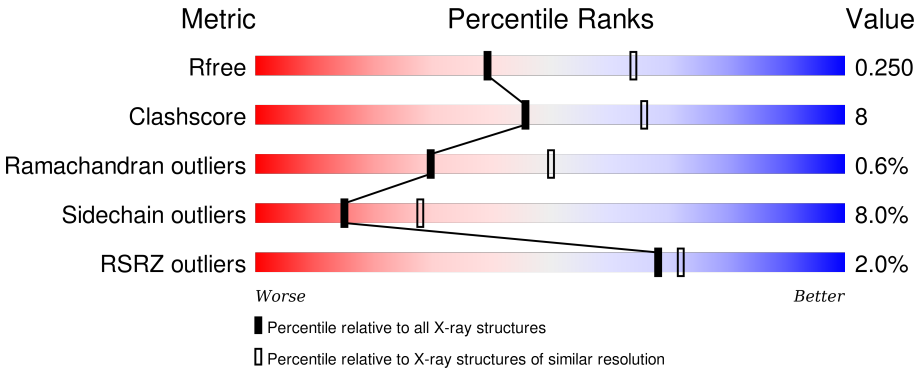
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

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 2.50 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.



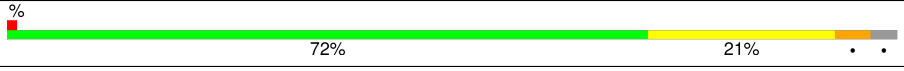
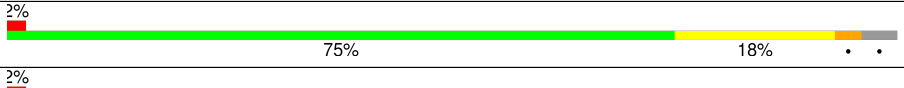
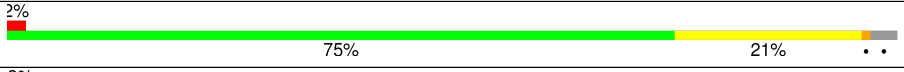
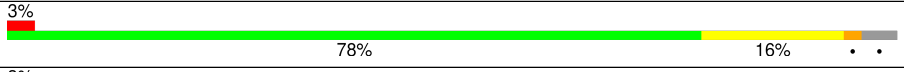
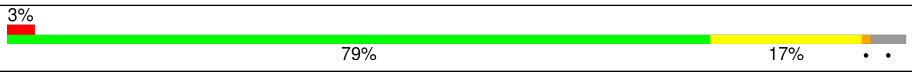
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	3553 (2.50-2.50)
Clashscore	102246	4242 (2.50-2.50)
Ramachandran outliers	100387	4156 (2.50-2.50)
Sidechain outliers	100360	4158 (2.50-2.50)
RSRZ outliers	91569	3562 (2.50-2.50)

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 on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. 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	157	3% 72% 22%
1	B	157	3% 80% 15%
1	C	157	3% 77% 18%
1	D	157	77% 15% 5%
1	E	157	% 72% 24%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	F	157	
1	G	157	
1	H	157	
1	I	157	
1	J	157	
1	K	157	
1	L	157	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 15009 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 Induced myeloid leukemia cell differentiation protein Mcl-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	152	Total	C	N	O	S	0	0	0
			1215	762	225	224	4			
1	B	153	Total	C	N	O	S	0	0	0
			1218	763	224	227	4			
1	C	151	Total	C	N	O	S	0	0	0
			1198	752	219	223	4			
1	D	152	Total	C	N	O	S	0	0	0
			1221	766	225	226	4			
1	E	152	Total	C	N	O	S	0	0	0
			1215	762	224	225	4			
1	F	151	Total	C	N	O	S	0	0	0
			1202	753	222	223	4			
1	G	152	Total	C	N	O	S	0	0	0
			1211	759	224	224	4			
1	H	151	Total	C	N	O	S	0	0	0
			1208	758	223	223	4			
1	I	151	Total	C	N	O	S	0	0	0
			1206	757	223	222	4			
1	J	152	Total	C	N	O	S	0	0	0
			1199	752	220	223	4			
1	K	150	Total	C	N	O	S	0	0	0
			1195	748	221	222	4			
1	L	151	Total	C	N	O	S	0	0	0
			1196	750	219	223	4			

There are 12 discrepancies between the modelled and reference sequences:

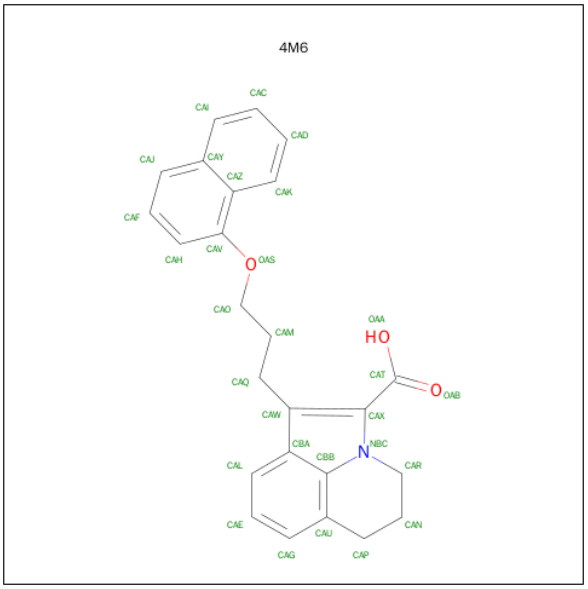
Chain	Residue	Modelled	Actual	Comment	Reference
A	171	GLY	-	expression tag	UNP Q07820
B	171	GLY	-	expression tag	UNP Q07820
C	171	GLY	-	expression tag	UNP Q07820
D	171	GLY	-	expression tag	UNP Q07820
E	171	GLY	-	expression tag	UNP Q07820

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
F	171	GLY	-	expression tag	UNP Q07820
G	171	GLY	-	expression tag	UNP Q07820
H	171	GLY	-	expression tag	UNP Q07820
I	171	GLY	-	expression tag	UNP Q07820
J	171	GLY	-	expression tag	UNP Q07820
K	171	GLY	-	expression tag	UNP Q07820
L	171	GLY	-	expression tag	UNP Q07820

- Molecule 2 is 1-[3-(naphthalen-1-yloxy)propyl]-5,6-dihydro-4H-pyrrolo[3,2,1-ij]quinoline-2-carboxylic acid (three-letter code: 4M6) (formula: $C_{25}H_{23}NO_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C N O 29 25 1 3	0	0
2	B	1	Total C N O 29 25 1 3	0	0
2	C	1	Total C N O 29 25 1 3	0	0
2	D	1	Total C N O 29 25 1 3	0	0
2	E	1	Total C N O 29 25 1 3	0	0
2	F	1	Total C N O 29 25 1 3	0	0
2	G	1	Total C N O 29 25 1 3	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	H	1	Total C N O 29 25 1 3	0	0
2	I	1	Total C N O 29 25 1 3	0	0
2	J	1	Total C N O 29 25 1 3	0	0
2	K	1	Total C N O 29 25 1 3	0	0
2	L	1	Total C N O 29 25 1 3	0	0

- Molecule 3 is water.

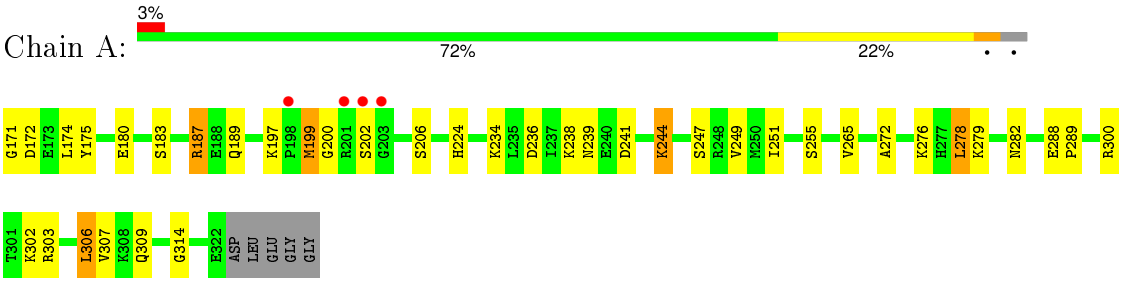
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	16	Total O 16 16	0	0
3	B	17	Total O 17 17	0	0
3	C	16	Total O 16 16	0	0
3	D	25	Total O 25 25	0	0
3	E	19	Total O 19 19	0	0
3	F	6	Total O 6 6	0	0
3	G	8	Total O 8 8	0	0
3	H	13	Total O 13 13	0	0
3	I	23	Total O 23 23	0	0
3	J	12	Total O 12 12	0	0
3	K	11	Total O 11 11	0	0
3	L	11	Total O 11 11	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

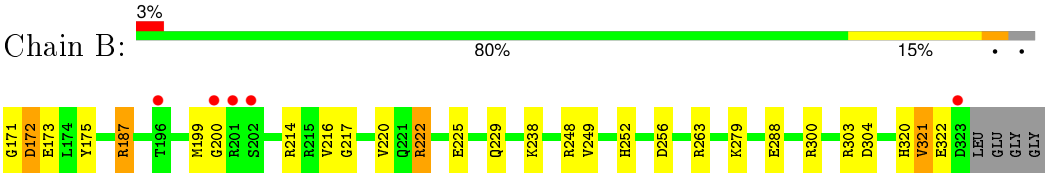
- Molecule 1: Induced myeloid leukemia cell differentiation protein Mcl-1

Chain A:



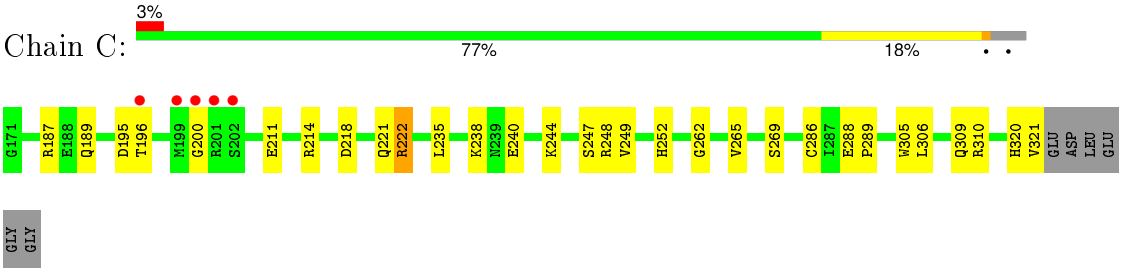
- Molecule 1: Induced myeloid leukemia cell differentiation protein Mcl-1

Chain B:



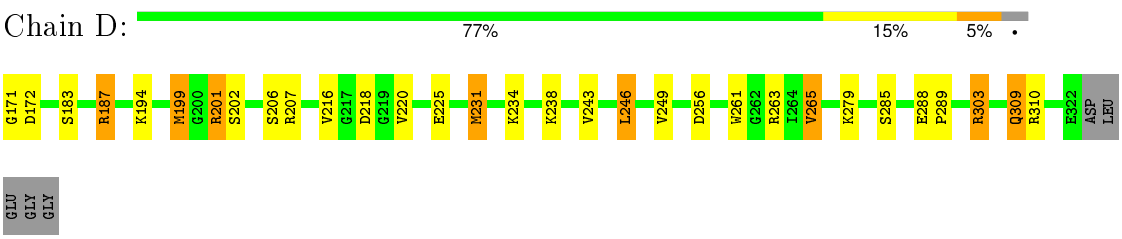
- Molecule 1: Induced myeloid leukemia cell differentiation protein Mcl-1

Chain C:



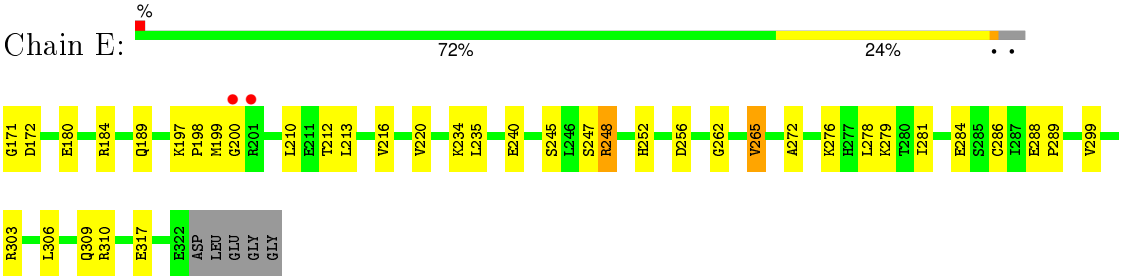
- Molecule 1: Induced myeloid leukemia cell differentiation protein Mcl-1

Chain D:



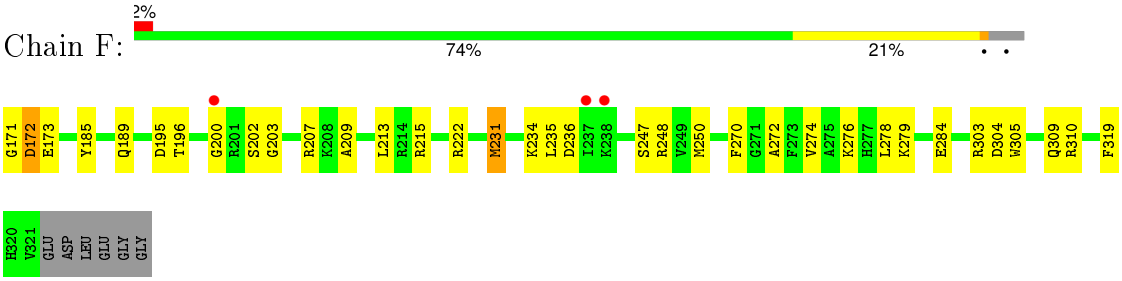
- Molecule 1: Induced myeloid leukemia cell differentiation protein Mcl-1

Chain E:



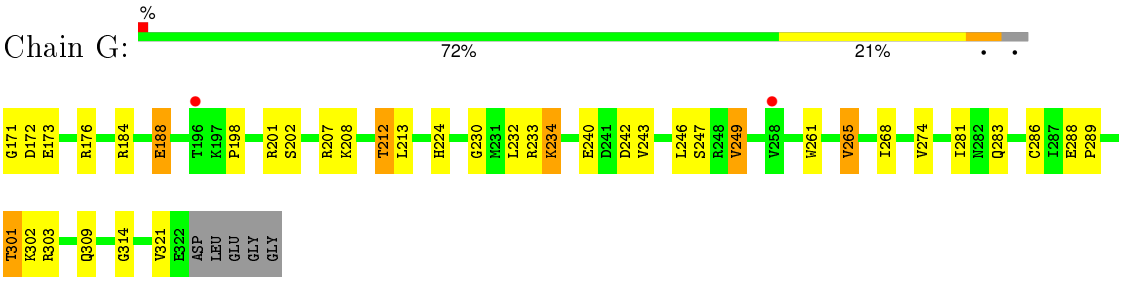
• Molecule 1: Induced myeloid leukemia cell differentiation protein Mcl-1

Chain F:



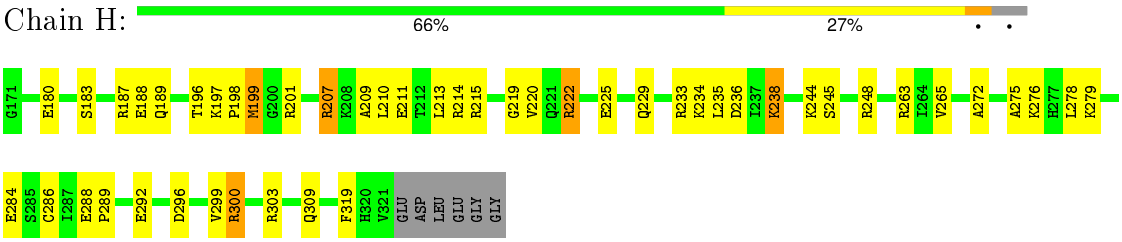
• Molecule 1: Induced myeloid leukemia cell differentiation protein Mcl-1

Chain G:



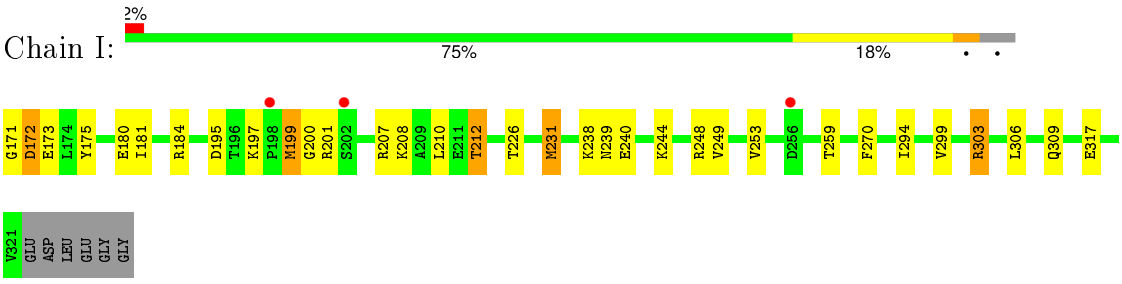
• Molecule 1: Induced myeloid leukemia cell differentiation protein Mcl-1

Chain H:



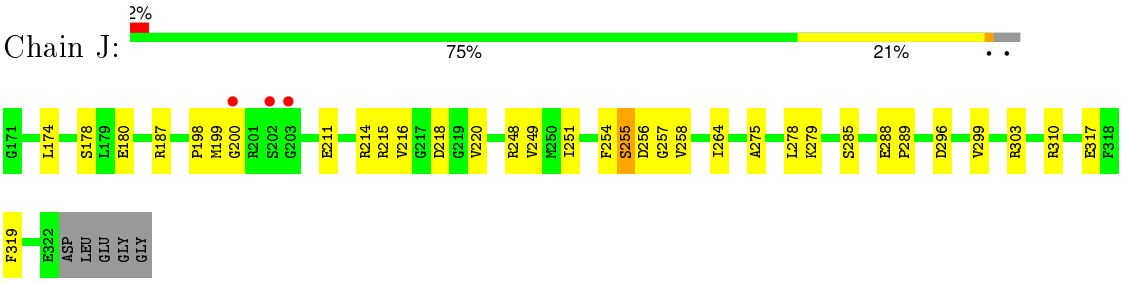
• Molecule 1: Induced myeloid leukemia cell differentiation protein Mcl-1

Chain I:



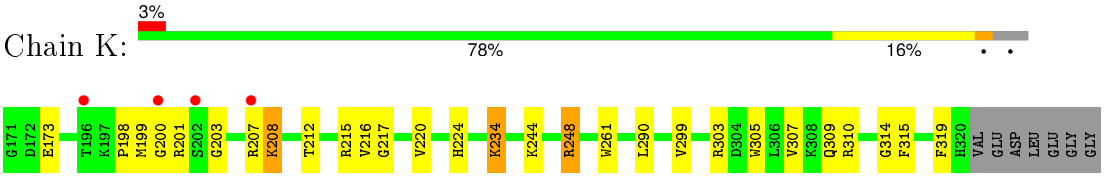
• Molecule 1: Induced myeloid leukemia cell differentiation protein Mcl-1

Chain J:



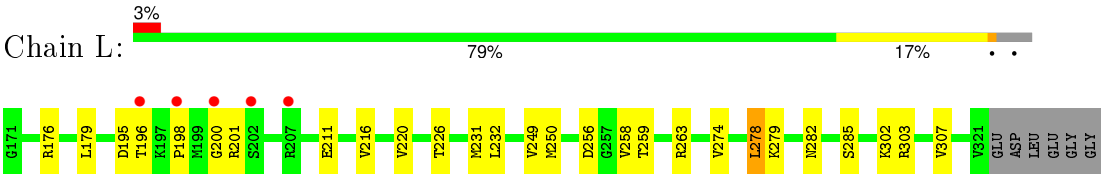
• Molecule 1: Induced myeloid leukemia cell differentiation protein Mcl-1

Chain K:



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

Chain L:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	62.26Å 134.01Å 135.93Å 90.00° 99.65° 90.00°	Depositor
Resolution (Å)	29.97 – 2.50 33.96 – 2.50	Depositor EDS
% Data completeness (in resolution range)	90.4 (29.97-2.50) 90.1 (33.96-2.50)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	0.05	Depositor
$< I/\sigma(I) >$ [1]	2.82 (at 2.51Å)	Xtriage
Refinement program	PHENIX (phenix.refine: dev_1951)	Depositor
R, R_{free}	0.182 , 0.239 0.195 , 0.250	Depositor DCC
R_{free} test set	1988 reflections (2.99%)	DCC
Wilson B-factor (Å^2)	36.9	Xtriage
Anisotropy	0.379	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 42.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Outliers	0 of 68717 reflections	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	15009	wwPDB-VP
Average B, all atoms (Å^2)	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.71% 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, 0.375 respectively for untwinned datasets, and 0.333, 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: 4M6

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	0.48	0/1235	0.71	1/1660 (0.1%)
1	B	0.51	0/1238	0.71	1/1667 (0.1%)
1	C	0.49	0/1218	0.73	0/1641
1	D	0.55	0/1241	0.70	1/1668 (0.1%)
1	E	0.49	0/1235	0.70	1/1661 (0.1%)
1	F	0.45	0/1222	0.72	1/1645 (0.1%)
1	G	0.51	0/1230	0.66	1/1654 (0.1%)
1	H	0.49	0/1228	0.69	0/1652
1	I	0.46	0/1226	0.72	1/1649 (0.1%)
1	J	0.46	0/1218	0.66	1/1640 (0.1%)
1	K	0.46	0/1214	0.71	1/1633 (0.1%)
1	L	0.44	0/1215	0.67	1/1636 (0.1%)
All	All	0.48	0/14720	0.70	10/19806 (0.1%)

There are no bond length outliers.

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	303	ARG	NE-CZ-NH2	-6.63	116.99	120.30
1	E	213	LEU	CB-CG-CD2	-6.40	100.12	111.00
1	G	198	PRO	N-CA-CB	6.06	110.58	103.30
1	J	198	PRO	N-CA-CB	5.94	110.43	103.30
1	L	198	PRO	N-CA-CB	5.94	110.42	103.30
1	K	198	PRO	N-CA-CB	5.79	110.25	103.30
1	A	278	LEU	CA-CB-CG	5.63	128.24	115.30
1	B	217	GLY	N-CA-C	5.28	126.30	113.10
1	F	284	GLU	OE1-CD-OE2	5.19	129.52	123.30
1	I	303	ARG	NE-CZ-NH2	-5.13	117.73	120.30

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	A	1215	0	1218	21	0
1	B	1218	0	1209	21	0
1	C	1198	0	1190	18	0
1	D	1221	0	1229	20	0
1	E	1215	0	1213	22	0
1	F	1202	0	1194	29	0
1	G	1211	0	1208	20	0
1	H	1208	0	1212	32	0
1	I	1206	0	1207	22	0
1	J	1199	0	1181	15	0
1	K	1195	0	1186	19	0
1	L	1196	0	1184	9	0
2	A	29	0	22	1	0
2	B	29	0	22	0	0
2	C	29	0	22	1	0
2	D	29	0	22	4	0
2	E	29	0	22	0	0
2	F	29	0	22	0	0
2	G	29	0	22	1	0
2	H	29	0	22	0	0
2	I	29	0	22	3	0
2	J	29	0	22	0	0
2	K	29	0	22	1	0
2	L	29	0	22	1	0
3	A	16	0	0	0	0
3	B	17	0	0	3	0
3	C	16	0	0	1	0
3	D	25	0	0	2	0
3	E	19	0	0	1	0
3	F	6	0	0	0	0
3	G	8	0	0	1	0
3	H	13	0	0	1	0
3	I	23	0	0	1	0
3	J	12	0	0	2	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	K	11	0	0	0	0
3	L	11	0	0	0	0
All	All	15009	0	14695	226	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 8.

All (226) 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:I:171:GLY:HA2	1:I:303:ARG:HH22	1.10	1.11
1:A:171:GLY:HA2	1:A:303:ARG:HH22	1.29	0.98
1:E:171:GLY:HA2	1:E:303:ARG:HH22	1.29	0.94
1:F:171:GLY:HA2	1:F:303:ARG:HH22	1.32	0.94
1:B:171:GLY:HA2	1:B:303:ARG:HH22	1.32	0.93
1:A:187:ARG:HH21	1:A:288:GLU:HG2	1.37	0.89
1:B:187:ARG:NH1	3:B:501:HOH:O	2.06	0.89
1:D:172:ASP:N	3:D:501:HOH:O	2.03	0.86
1:G:171:GLY:HA3	1:G:303:ARG:HH22	1.36	0.86
1:I:171:GLY:HA2	1:I:303:ARG:NH2	1.91	0.85
1:D:171:GLY:CA	1:D:303:ARG:HH22	1.89	0.85
1:E:248:ARG:NH2	1:F:235:LEU:O	2.11	0.84
1:C:235:LEU:O	1:H:248:ARG:NH2	2.15	0.79
1:D:256:ASP:O	1:D:263:ARG:NH1	2.16	0.79
1:F:171:GLY:HA2	1:F:303:ARG:NH2	1.98	0.78
1:H:199:MET:HE1	1:H:207:ARG:HG2	1.66	0.77
1:H:197:LYS:HG3	1:H:198:PRO:HD2	1.65	0.77
1:B:256:ASP:O	1:B:263:ARG:NH1	2.18	0.76
1:F:189:GLN:HG2	1:F:272:ALA:HB1	1.68	0.76
1:A:189:GLN:HG2	1:A:272:ALA:HB1	1.69	0.75
1:J:303:ARG:NH1	3:J:502:HOH:O	2.20	0.74
1:J:211:GLU:OE1	1:J:214:ARG:NH1	2.20	0.74
1:C:248:ARG:NH2	1:H:235:LEU:O	2.21	0.74
1:D:171:GLY:HA2	1:D:303:ARG:HH22	1.53	0.72
1:H:236:ASP:OD2	1:H:238:LYS:NZ	2.22	0.72
1:H:211:GLU:OE2	1:H:215:ARG:NH2	2.18	0.72
1:J:251:ILE:O	1:J:255:SER:HB2	1.91	0.71
1:E:171:GLY:CA	1:E:303:ARG:HH22	2.04	0.68
1:C:189:GLN:OE1	1:C:221:GLN:NE2	2.22	0.68
1:H:300:ARG:NH1	3:H:501:HOH:O	2.26	0.68
1:G:173:GLU:OE2	1:G:176:ARG:NH1	2.27	0.67

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:171:GLY:HA2	1:A:303:ARG:NH2	2.07	0.66
1:D:243:VAL:HA	1:D:246:LEU:HD22	1.77	0.66
1:A:244:LYS:HE3	1:A:289:PRO:HB2	1.78	0.66
1:G:171:GLY:HA3	1:G:303:ARG:NH2	2.09	0.66
1:B:320:HIS:O	1:B:321:VAL:HG22	1.96	0.66
1:E:235:LEU:O	1:F:248:ARG:NH2	2.29	0.65
1:I:171:GLY:CA	1:I:303:ARG:HH22	1.99	0.65
1:J:215:ARG:NH1	1:J:319:PHE:O	2.23	0.64
1:H:199:MET:CE	1:H:207:ARG:HG2	2.26	0.64
1:F:189:GLN:HG3	1:F:276:LYS:HE3	1.79	0.64
1:H:180:GLU:HG2	1:H:199:MET:HG2	1.79	0.64
1:F:171:GLY:CA	1:F:303:ARG:HH22	2.09	0.64
1:B:171:GLY:HA2	1:B:303:ARG:NH2	2.09	0.64
1:A:183:SER:OG	1:A:288:GLU:OE2	2.15	0.64
1:H:225:GLU:O	1:H:229:GLN:HG3	1.97	0.64
1:K:199:MET:HB2	1:K:203:GLY:HA2	1.80	0.64
1:I:253:VAL:HG11	2:I:400:4M6:H23	1.81	0.63
1:K:248:ARG:HG3	1:K:248:ARG:HH11	1.64	0.63
1:I:173:GLU:OE1	1:I:201:ARG:NH1	2.32	0.62
1:E:262:GLY:O	1:E:265:VAL:HG12	1.99	0.62
1:J:310:ARG:NH2	1:J:317:GLU:OE1	2.35	0.60
1:I:249:VAL:O	1:I:253:VAL:HG12	2.02	0.60
1:E:220:VAL:HG21	1:E:265:VAL:HG13	1.84	0.60
1:H:201:ARG:HB3	1:I:317:GLU:OE1	2.02	0.59
1:H:279:LYS:HD2	1:H:284:GLU:OE2	2.02	0.59
1:I:180:GLU:O	1:I:184:ARG:HG2	2.03	0.59
1:H:244:LYS:NZ	1:H:289:PRO:HB3	2.17	0.59
1:F:247:SER:HA	1:F:250:MET:HE2	1.85	0.58
1:I:240:GLU:HG2	1:I:244:LYS:HZ3	1.69	0.58
1:B:222:ARG:CZ	1:K:234:LYS:HG3	2.35	0.57
1:E:245:SER:OG	1:F:248:ARG:NH1	2.38	0.56
1:E:252:HIS:CE1	1:F:234:LYS:HE3	2.40	0.56
1:G:213:LEU:HD21	1:G:268:ILE:HG21	1.88	0.56
1:J:299:VAL:O	1:J:303:ARG:HB2	2.05	0.56
1:H:189:GLN:HG3	1:H:276:LYS:HE2	1.88	0.55
1:H:188:GLU:OE2	1:H:214:ARG:NE	2.36	0.55
1:G:261:TRP:O	1:G:265:VAL:HG12	2.07	0.55
1:E:189:GLN:HG2	1:E:272:ALA:HB1	1.88	0.55
1:I:231:MET:HG3	2:I:400:4M6:CAG	2.36	0.55
1:E:212:THR:O	1:E:216:VAL:HG22	2.07	0.54
1:F:195:ASP:OD1	1:F:196:THR:N	2.40	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:288:GLU:OE1	3:B:501:HOH:O	2.18	0.54
1:D:263:ARG:HH21	2:D:400:4M6:CAT	2.19	0.54
1:C:211:GLU:OE1	1:C:214:ARG:HD2	2.07	0.54
1:C:195:ASP:OD1	1:C:196:THR:N	2.39	0.54
1:D:183:SER:OG	1:D:187:ARG:NH1	2.41	0.54
1:C:252:HIS:HA	1:H:234:LYS:HE3	1.90	0.54
1:B:222:ARG:NH1	1:K:234:LYS:HG3	2.22	0.54
1:E:189:GLN:HG3	1:E:276:LYS:HE2	1.90	0.54
1:G:301:THR:HG23	1:G:302:LYS:HG2	1.90	0.53
1:J:285:SER:OG	3:J:501:HOH:O	2.19	0.53
1:D:263:ARG:NH2	2:D:400:4M6:OAB	2.27	0.53
1:G:230:GLY:O	1:G:234:LYS:HD2	2.09	0.52
1:A:302:LYS:O	1:A:306:LEU:HD22	2.10	0.52
1:A:199:MET:HG2	1:A:206:SER:HB2	1.90	0.52
1:L:256:ASP:O	1:L:263:ARG:NH1	2.31	0.52
1:L:259:THR:HG21	1:L:302:LYS:HD2	1.90	0.52
1:C:240:GLU:HG2	1:C:244:LYS:HE3	1.91	0.52
1:B:171:GLY:HA3	1:B:175:TYR:HB2	1.91	0.51
1:F:215:ARG:NH2	1:F:319:PHE:O	2.43	0.51
1:G:301:THR:CG2	1:G:302:LYS:HG2	2.40	0.51
1:A:171:GLY:HA3	1:A:175:TYR:HB2	1.93	0.51
1:A:189:GLN:HG3	1:A:276:LYS:HE3	1.93	0.51
1:D:261:TRP:O	1:D:265:VAL:HG12	2.10	0.50
1:L:176:ARG:NH2	1:L:201:ARG:O	2.44	0.50
1:E:288:GLU:HB3	1:E:289:PRO:HD3	1.93	0.50
1:D:171:GLY:HA2	1:D:303:ARG:NH2	2.23	0.50
1:B:303:ARG:HB3	1:F:172:ASP:HB2	1.93	0.50
1:G:233:ARG:HD2	3:G:502:HOH:O	2.11	0.50
1:A:234:LYS:HE3	1:B:252:HIS:CE1	2.47	0.50
1:B:304:ASP:OD2	1:F:172:ASP:HB3	2.11	0.50
1:K:299:VAL:O	1:K:303:ARG:HB2	2.12	0.50
1:J:275:ALA:HA	1:J:278:LEU:HD12	1.92	0.49
1:G:249:VAL:HG22	2:G:400:4M6:H22	1.93	0.49
1:D:172:ASP:OD2	3:D:502:HOH:O	2.19	0.49
1:H:219:GLY:O	1:H:222:ARG:HG2	2.13	0.49
1:B:216:VAL:O	1:B:220:VAL:HG23	2.13	0.49
1:H:288:GLU:HB3	1:H:289:PRO:HD3	1.94	0.49
1:L:303:ARG:O	1:L:307:VAL:HG13	2.13	0.49
1:A:239:ASN:OD1	1:A:241:ASP:HB2	2.12	0.48
1:H:286:CYS:C	1:H:289:PRO:HD2	2.32	0.48
1:J:254:PHE:HZ	1:J:264:ILE:HD13	1.78	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:208:LYS:O	1:G:212:THR:HG23	2.12	0.48
1:I:253:VAL:HG13	2:I:400:4M6:H15	1.96	0.48
1:F:274:VAL:O	1:F:278:LEU:HD13	2.13	0.48
1:A:309:GLN:O	1:A:314:GLY:HA3	2.13	0.48
1:E:299:VAL:O	1:E:303:ARG:HB2	2.14	0.48
1:A:234:LYS:HE2	1:B:256:ASP:OD2	2.13	0.48
1:L:249:VAL:HG12	2:L:400:4M6:H22	1.95	0.48
1:K:303:ARG:O	1:K:307:VAL:HG23	2.14	0.47
1:H:279:LYS:HA	1:H:284:GLU:OE2	2.14	0.47
1:L:274:VAL:HG12	1:L:278:LEU:HD22	1.96	0.47
1:E:310:ARG:HD2	3:E:514:HOH:O	2.13	0.47
1:H:244:LYS:HZ1	1:H:289:PRO:HB3	1.78	0.47
1:B:300:ARG:HE	1:F:171:GLY:N	2.13	0.47
1:I:259:THR:O	3:I:501:HOH:O	2.21	0.47
1:H:209:ALA:O	1:H:213:LEU:HB2	2.14	0.47
1:G:288:GLU:HB3	1:G:289:PRO:HD3	1.96	0.47
1:I:299:VAL:O	1:I:303:ARG:HB2	2.14	0.47
2:D:400:4M6:H14	2:D:400:4M6:OAB	2.15	0.47
1:J:187:ARG:HH22	1:J:288:GLU:HB2	1.79	0.47
1:I:208:LYS:O	1:I:212:THR:HG23	2.15	0.47
1:G:208:LYS:HD3	1:G:208:LYS:HA	1.66	0.46
1:J:256:ASP:HA	1:J:257:GLY:HA2	1.63	0.46
1:C:305:TRP:CZ2	1:C:309:GLN:HG3	2.50	0.46
1:K:309:GLN:O	1:K:310:ARG:HB2	2.14	0.46
1:E:252:HIS:O	1:F:234:LYS:NZ	2.38	0.46
1:H:180:GLU:CG	1:H:199:MET:HG2	2.45	0.46
1:E:256:ASP:OD2	1:F:234:LYS:HE2	2.16	0.46
1:D:171:GLY:HA3	1:D:303:ARG:HH22	1.76	0.46
1:H:215:ARG:NH1	1:H:319:PHE:O	2.49	0.46
1:I:199:MET:HE3	1:I:207:ARG:HG2	1.97	0.46
1:A:244:LYS:HD2	1:A:244:LYS:HA	1.57	0.46
1:B:321:VAL:O	1:B:322:GLU:HB2	2.15	0.46
1:J:288:GLU:HB3	1:J:289:PRO:HD3	1.98	0.46
1:K:215:ARG:HH22	1:K:319:PHE:HB3	1.81	0.46
1:H:183:SER:O	1:H:187:ARG:HG2	2.16	0.45
1:H:299:VAL:O	1:H:303:ARG:HB2	2.15	0.45
1:C:321:VAL:N	3:C:504:HOH:O	2.49	0.45
1:F:247:SER:HA	1:F:250:MET:CE	2.46	0.45
1:K:212:THR:O	1:K:216:VAL:HG22	2.16	0.45
1:G:201:ARG:O	1:G:202:SER:OG	2.33	0.45
1:K:261:TRP:CH2	1:K:315:PHE:HB2	2.52	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:171:GLY:CA	1:D:303:ARG:NH2	2.70	0.45
1:D:171:GLY:HA2	1:D:303:ARG:HH12	1.82	0.45
1:K:305:TRP:O	1:K:309:GLN:HG2	2.17	0.45
1:J:180:GLU:HG2	1:J:199:MET:HE3	1.99	0.45
1:D:231:MET:HG3	2:D:400:4M6:CAG	2.47	0.45
1:C:221:GLN:HG3	1:C:269:SER:HB3	1.98	0.45
1:D:199:MET:HE3	1:D:206:SER:HB2	1.98	0.44
1:K:215:ARG:NH2	1:K:319:PHE:O	2.51	0.44
1:K:309:GLN:O	1:K:314:GLY:HA3	2.17	0.44
1:E:180:GLU:CD	1:E:199:MET:HG2	2.38	0.44
1:F:209:ALA:O	1:F:213:LEU:HB2	2.17	0.44
1:K:208:LYS:H	1:K:208:LYS:HG2	1.56	0.44
1:I:171:GLY:HA3	1:I:175:TYR:HB2	1.99	0.44
1:C:262:GLY:HA2	1:C:265:VAL:HG12	1.99	0.44
1:H:189:GLN:HG2	1:H:272:ALA:HB1	2.00	0.43
1:J:174:LEU:O	1:J:178:SER:OG	2.27	0.43
1:C:249:VAL:HG12	2:C:400:4M6:H22	1.98	0.43
1:C:286:CYS:C	1:C:289:PRO:HD2	2.39	0.43
1:K:173:GLU:OE1	1:K:201:ARG:NH2	2.42	0.43
1:A:249:VAL:HG12	2:A:400:4M6:H22	2.00	0.43
1:I:231:MET:HB3	1:I:270:PHE:CZ	2.53	0.43
1:E:184:ARG:NH2	1:E:197:LYS:O	2.52	0.43
1:J:216:VAL:O	1:J:220:VAL:HG23	2.19	0.43
1:F:185:TYR:O	1:F:189:GLN:HB2	2.18	0.43
1:A:303:ARG:O	1:A:307:VAL:HG23	2.18	0.43
1:C:305:TRP:CH2	1:C:309:GLN:HG3	2.53	0.43
1:K:220:VAL:HG23	1:K:224:HIS:CE1	2.53	0.43
1:F:203:GLY:O	1:F:207:ARG:HG3	2.18	0.43
1:E:240:GLU:HG3	1:E:286:CYS:SG	2.59	0.43
1:E:197:LYS:HA	1:E:198:PRO:HD3	1.87	0.42
1:G:243:VAL:HG21	1:G:286:CYS:HB3	2.01	0.42
1:C:248:ARG:NH1	1:H:245:SER:OG	2.52	0.42
1:A:251:ILE:O	1:A:255:SER:HB2	2.19	0.42
1:L:216:VAL:O	1:L:220:VAL:HG23	2.18	0.42
1:D:201:ARG:HD3	1:E:317:GLU:OE2	2.19	0.42
1:F:231:MET:HB3	1:F:270:PHE:CZ	2.54	0.42
1:I:195:ASP:OD1	1:I:197:LYS:HD2	2.20	0.42
1:B:172:ASP:HB3	1:F:304:ASP:OD2	2.18	0.42
1:K:199:MET:HB2	1:K:203:GLY:CA	2.48	0.42
1:I:210:LEU:HD12	1:I:210:LEU:HA	1.83	0.42
1:E:256:ASP:CG	1:F:234:LYS:HE2	2.40	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:251:ILE:HD11	1:A:300:ARG:HH22	1.85	0.42
1:B:171:GLY:CA	1:B:303:ARG:HH22	2.14	0.42
1:F:305:TRP:CH2	1:F:309:GLN:HG3	2.55	0.42
1:L:250:MET:HB3	1:L:250:MET:HE2	1.69	0.41
1:H:219:GLY:HA2	1:H:222:ARG:HD2	2.02	0.41
1:C:288:GLU:HB3	1:C:289:PRO:HD3	2.00	0.41
1:L:195:ASP:O	1:L:196:THR:OG1	2.30	0.41
1:D:288:GLU:HB3	1:D:289:PRO:HD3	2.02	0.41
1:H:220:VAL:HG21	1:H:265:VAL:CG1	2.50	0.41
1:I:172:ASP:HB3	1:I:173:GLU:H	1.67	0.41
1:B:214:ARG:HD2	3:B:502:HOH:O	2.20	0.41
1:D:309:GLN:O	1:D:310:ARG:HB2	2.20	0.41
1:G:232:LEU:HD23	1:G:274:VAL:HG22	2.03	0.41
1:F:172:ASP:HB3	1:F:173:GLU:H	1.60	0.41
1:C:262:GLY:O	1:C:265:VAL:HG12	2.20	0.41
1:F:310:ARG:HH11	1:F:310:ARG:HG3	1.86	0.41
1:D:216:VAL:O	1:D:220:VAL:HG23	2.22	0.41
1:A:197:LYS:HB2	1:A:197:LYS:HE3	1.95	0.40
1:H:201:ARG:HA	1:I:317:GLU:O	2.22	0.40
1:B:172:ASP:HB3	1:B:173:GLU:H	1.63	0.40
1:K:290:LEU:HD11	2:K:400:4M6:H19	2.03	0.40
1:C:218:ASP:O	1:C:222:ARG:HG2	2.20	0.40
1:G:184:ARG:O	1:G:188:GLU:HB3	2.21	0.40
1:I:181:ILE:HG23	1:I:210:LEU:HD13	2.04	0.40
1:H:275:ALA:HA	1:H:278:LEU:HD12	2.02	0.40
1:G:242:ASP:O	1:G:246:LEU:HG	2.22	0.40
1:G:281:ILE:HG13	1:G:283:GLN:HG2	2.03	0.40
1:F:231:MET:O	1:F:235:LEU:HG	2.22	0.40
1:A:234:LYS:HE2	1:B:256:ASP:CG	2.42	0.40
1:K:217:GLY:HA2	1:K:220:VAL:HG12	2.03	0.40
1:G:309:GLN:O	1:G:314:GLY:HA3	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	Percentiles	
1	A	150/157 (96%)	145 (97%)	4 (3%)	1 (1%)	26	46
1	B	151/157 (96%)	146 (97%)	3 (2%)	2 (1%)	15	26
1	C	149/157 (95%)	145 (97%)	2 (1%)	2 (1%)	15	26
1	D	150/157 (96%)	148 (99%)	2 (1%)	0	100	100
1	E	150/157 (96%)	146 (97%)	3 (2%)	1 (1%)	26	46
1	F	149/157 (95%)	147 (99%)	1 (1%)	1 (1%)	26	46
1	G	150/157 (96%)	148 (99%)	2 (1%)	0	100	100
1	H	149/157 (95%)	146 (98%)	3 (2%)	0	100	100
1	I	149/157 (95%)	145 (97%)	3 (2%)	1 (1%)	26	46
1	J	150/157 (96%)	145 (97%)	4 (3%)	1 (1%)	26	46
1	K	148/157 (94%)	143 (97%)	4 (3%)	1 (1%)	26	46
1	L	149/157 (95%)	146 (98%)	2 (1%)	1 (1%)	26	46
All	All	1794/1884 (95%)	1750 (98%)	33 (2%)	11 (1%)	30	50

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	321	VAL
1	E	200	GLY
1	K	200	GLY
1	B	200	GLY
1	C	200	GLY
1	F	200	GLY
1	J	200	GLY
1	C	320	HIS
1	A	200	GLY
1	I	200	GLY
1	L	200	GLY

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	130/135 (96%)	114 (88%)	16 (12%)	6 11
1	B	130/135 (96%)	120 (92%)	10 (8%)	16 30
1	C	128/135 (95%)	122 (95%)	6 (5%)	32 56
1	D	132/135 (98%)	115 (87%)	17 (13%)	5 10
1	E	130/135 (96%)	118 (91%)	12 (9%)	11 21
1	F	128/135 (95%)	122 (95%)	6 (5%)	32 56
1	G	129/135 (96%)	117 (91%)	12 (9%)	11 21
1	H	130/135 (96%)	118 (91%)	12 (9%)	11 21
1	I	129/135 (96%)	118 (92%)	11 (8%)	13 25
1	J	126/135 (93%)	119 (94%)	7 (6%)	26 47
1	K	127/135 (94%)	122 (96%)	5 (4%)	39 66
1	L	127/135 (94%)	117 (92%)	10 (8%)	15 28
All	All	1546/1620 (95%)	1422 (92%)	124 (8%)	15 28

All (124) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	172	ASP
1	A	174	LEU
1	A	180	GLU
1	A	187	ARG
1	A	199	MET
1	A	202	SER
1	A	224	HIS
1	A	236	ASP
1	A	238	LYS
1	A	244	LYS
1	A	247	SER
1	A	265	VAL
1	A	278	LEU
1	A	279	LYS
1	A	282	ASN
1	A	306	LEU
1	B	172	ASP
1	B	187	ARG
1	B	199	MET
1	B	222	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	225	GLU
1	B	229	GLN
1	B	238	LYS
1	B	248	ARG
1	B	249	VAL
1	B	279	LYS
1	C	187	ARG
1	C	222	ARG
1	C	238	LYS
1	C	247	SER
1	C	306	LEU
1	C	310	ARG
1	D	187	ARG
1	D	194	LYS
1	D	199	MET
1	D	201	ARG
1	D	202	SER
1	D	207	ARG
1	D	218	ASP
1	D	225	GLU
1	D	231	MET
1	D	234	LYS
1	D	238	LYS
1	D	246	LEU
1	D	249	VAL
1	D	265	VAL
1	D	279	LYS
1	D	285	SER
1	D	309	GLN
1	E	172	ASP
1	E	210	LEU
1	E	234	LYS
1	E	247	SER
1	E	248	ARG
1	E	265	VAL
1	E	278	LEU
1	E	279	LYS
1	E	281	ILE
1	E	284	GLU
1	E	306	LEU
1	E	309	GLN
1	F	172	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	F	202	SER
1	F	222	ARG
1	F	231	MET
1	F	236	ASP
1	F	279	LYS
1	G	172	ASP
1	G	188	GLU
1	G	207	ARG
1	G	212	THR
1	G	224	HIS
1	G	234	LYS
1	G	240	GLU
1	G	247	SER
1	G	249	VAL
1	G	265	VAL
1	G	301	THR
1	G	321	VAL
1	H	196	THR
1	H	199	MET
1	H	207	ARG
1	H	210	LEU
1	H	222	ARG
1	H	233	ARG
1	H	238	LYS
1	H	263	ARG
1	H	292	GLU
1	H	296	ASP
1	H	300	ARG
1	H	309	GLN
1	I	172	ASP
1	I	199	MET
1	I	212	THR
1	I	226	THR
1	I	231	MET
1	I	238	LYS
1	I	239	ASN
1	I	248	ARG
1	I	294	ILE
1	I	306	LEU
1	I	309	GLN
1	J	218	ASP
1	J	248	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	J	249	VAL
1	J	255	SER
1	J	258	VAL
1	J	279	LYS
1	J	296	ASP
1	K	207	ARG
1	K	208	LYS
1	K	234	LYS
1	K	244	LYS
1	K	248	ARG
1	L	179	LEU
1	L	211	GLU
1	L	226	THR
1	L	231	MET
1	L	232	LEU
1	L	258	VAL
1	L	278	LEU
1	L	279	LYS
1	L	282	ASN
1	L	285	SER

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

Mol	Chain	Res	Type
1	C	177	GLN
1	C	320	HIS
1	E	252	HIS
1	E	277	HIS
1	G	277	HIS
1	L	223	ASN

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 (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

12 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	4M6	A	400	-	27,33,33	1.29	4 (14%)	32,47,47	1.06	3 (9%)
2	4M6	B	400	-	27,33,33	1.23	3 (11%)	32,47,47	1.08	3 (9%)
2	4M6	C	400	-	27,33,33	1.20	3 (11%)	32,47,47	1.13	1 (3%)
2	4M6	D	400	-	27,33,33	1.22	3 (11%)	32,47,47	1.01	2 (6%)
2	4M6	E	400	-	27,33,33	1.17	3 (11%)	32,47,47	1.33	4 (12%)
2	4M6	F	400	-	27,33,33	1.16	3 (11%)	32,47,47	1.25	4 (12%)
2	4M6	G	400	-	27,33,33	1.15	3 (11%)	32,47,47	1.30	4 (12%)
2	4M6	H	400	-	27,33,33	1.14	3 (11%)	32,47,47	1.34	3 (9%)
2	4M6	I	400	-	27,33,33	1.24	3 (11%)	32,47,47	1.30	6 (18%)
2	4M6	J	400	-	27,33,33	1.22	3 (11%)	32,47,47	1.16	4 (12%)
2	4M6	K	400	-	27,33,33	1.18	3 (11%)	32,47,47	1.08	2 (6%)
2	4M6	L	400	-	27,33,33	1.20	3 (11%)	32,47,47	1.23	2 (6%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	4M6	A	400	-	-	0/7/17/17	0/4/5/5
2	4M6	B	400	-	-	0/7/17/17	0/4/5/5
2	4M6	C	400	-	-	0/7/17/17	0/4/5/5
2	4M6	D	400	-	-	0/7/17/17	0/4/5/5
2	4M6	E	400	-	-	0/7/17/17	0/4/5/5

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	4M6	F	400	-	-	0/7/17/17	0/4/5/5
2	4M6	G	400	-	-	0/7/17/17	0/4/5/5
2	4M6	H	400	-	-	0/7/17/17	0/4/5/5
2	4M6	I	400	-	-	0/7/17/17	0/4/5/5
2	4M6	J	400	-	-	0/7/17/17	0/4/5/5
2	4M6	K	400	-	-	0/7/17/17	0/4/5/5
2	4M6	L	400	-	-	0/7/17/17	0/4/5/5

All (37) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	400	4M6	CAZ-CAY	-3.21	1.36	1.42
2	B	400	4M6	CAU-CBB	-3.17	1.36	1.42
2	F	400	4M6	CAU-CBB	-2.98	1.36	1.42
2	I	400	4M6	CAU-CBB	-2.94	1.37	1.42
2	L	400	4M6	CAZ-CAY	-2.92	1.37	1.42
2	J	400	4M6	CAU-CBB	-2.87	1.37	1.42
2	D	400	4M6	CAU-CBB	-2.87	1.37	1.42
2	B	400	4M6	CAZ-CAY	-2.83	1.37	1.42
2	J	400	4M6	CAZ-CAY	-2.66	1.37	1.42
2	E	400	4M6	CAU-CBB	-2.65	1.37	1.42
2	A	400	4M6	CAZ-CAY	-2.61	1.37	1.42
2	I	400	4M6	CAZ-CAY	-2.59	1.38	1.42
2	H	400	4M6	CAU-CBB	-2.57	1.37	1.42
2	E	400	4M6	CAZ-CAY	-2.44	1.38	1.42
2	C	400	4M6	CAU-CBB	-2.42	1.37	1.42
2	F	400	4M6	CAZ-CAY	-2.39	1.38	1.42
2	L	400	4M6	CAU-CBB	-2.36	1.38	1.42
2	K	400	4M6	CAU-CBB	-2.32	1.38	1.42
2	G	400	4M6	CAU-CBB	-2.31	1.38	1.42
2	G	400	4M6	CAZ-CAY	-2.28	1.38	1.42
2	K	400	4M6	CAZ-CAY	-2.28	1.38	1.42
2	C	400	4M6	CAZ-CAY	-2.21	1.38	1.42
2	A	400	4M6	CAU-CBB	-2.19	1.38	1.42
2	H	400	4M6	CAZ-CAY	-2.18	1.38	1.42
2	D	400	4M6	CAG-CAU	2.06	1.41	1.37
2	A	400	4M6	CAE-CAL	2.09	1.41	1.36
2	B	400	4M6	CAG-CAU	2.16	1.41	1.37
2	C	400	4M6	CAG-CAU	2.33	1.41	1.37
2	F	400	4M6	CAG-CAU	2.38	1.42	1.37
2	G	400	4M6	CAG-CAU	2.43	1.42	1.37
2	L	400	4M6	CAG-CAU	2.43	1.42	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	400	4M6	CAG-CAU	2.48	1.42	1.37
2	J	400	4M6	CAG-CAU	2.48	1.42	1.37
2	H	400	4M6	CAG-CAU	2.53	1.42	1.37
2	I	400	4M6	CAG-CAU	2.57	1.42	1.37
2	K	400	4M6	CAG-CAU	2.58	1.42	1.37
2	A	400	4M6	CAG-CAU	3.28	1.43	1.37

All (38) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	I	400	4M6	CAE-CAL-CBA	-2.79	116.93	120.88
2	I	400	4M6	CAM-CAQ-CAW	-2.51	108.46	112.16
2	E	400	4M6	OAS-CAV-CAH	-2.46	118.54	124.34
2	B	400	4M6	CAE-CAL-CBA	-2.37	117.52	120.88
2	H	400	4M6	CAM-CAQ-CAW	-2.33	108.72	112.16
2	J	400	4M6	OAS-CAV-CAH	-2.30	118.91	124.34
2	I	400	4M6	CAW-CBA-CBB	-2.19	104.88	109.48
2	J	400	4M6	CAE-CAL-CBA	-2.11	117.89	120.88
2	A	400	4M6	CAW-CBA-CBB	-2.04	105.20	109.48
2	D	400	4M6	CAE-CAL-CBA	-2.02	118.02	120.88
2	F	400	4M6	OAS-CAV-CAH	-2.00	119.61	124.34
2	F	400	4M6	CAV-CAZ-CAY	2.03	120.28	118.01
2	J	400	4M6	OAS-CAV-CAZ	2.03	120.55	114.91
2	H	400	4M6	CAR-CAN-CAP	2.10	119.17	112.15
2	F	400	4M6	OAS-CAV-CAZ	2.13	120.81	114.91
2	A	400	4M6	CAN-CAR-NBC	2.13	113.39	109.65
2	K	400	4M6	CAV-CAZ-CAY	2.14	120.40	118.01
2	E	400	4M6	CAR-CAN-CAP	2.16	119.37	112.15
2	I	400	4M6	CAN-CAR-NBC	2.17	113.46	109.65
2	G	400	4M6	OAS-CAV-CAZ	2.18	120.97	114.91
2	L	400	4M6	CAR-CAN-CAP	2.23	119.61	112.15
2	B	400	4M6	CAK-CAZ-CAY	2.23	120.83	117.91
2	A	400	4M6	CAV-CAZ-CAY	2.24	120.51	118.01
2	G	400	4M6	CAR-CAN-CAP	2.24	119.65	112.15
2	D	400	4M6	CAV-CAZ-CAY	2.28	120.56	118.01
2	G	400	4M6	CAV-CAZ-CAY	2.30	120.57	118.01
2	I	400	4M6	CAK-CAZ-CAY	2.35	120.99	117.91
2	E	400	4M6	OAS-CAV-CAZ	2.39	121.53	114.91
2	J	400	4M6	CAN-CAR-NBC	2.39	113.86	109.65
2	I	400	4M6	CAL-CBA-CBB	2.47	122.14	117.03
2	B	400	4M6	CAN-CAR-NBC	2.50	114.05	109.65
2	C	400	4M6	CAV-CAZ-CAY	2.62	120.94	118.01

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	K	400	4M6	CAN-CAR-NBC	2.90	114.75	109.65
2	F	400	4M6	CAN-CAR-NBC	3.38	115.59	109.65
2	L	400	4M6	CAN-CAR-NBC	3.62	116.02	109.65
2	G	400	4M6	CAN-CAR-NBC	3.64	116.06	109.65
2	E	400	4M6	CAN-CAR-NBC	3.84	116.40	109.65
2	H	400	4M6	CAN-CAR-NBC	4.02	116.72	109.65

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

7 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	400	4M6	1	0
2	C	400	4M6	1	0
2	D	400	4M6	4	0
2	G	400	4M6	1	0
2	I	400	4M6	3	0
2	K	400	4M6	1	0
2	L	400	4M6	1	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	A	152/157 (96%)	-0.24	4 (2%) 59 63	26, 47, 85, 129	0
1	B	153/157 (97%)	-0.22	5 (3%) 50 55	28, 41, 83, 118	0
1	C	151/157 (96%)	-0.23	5 (3%) 50 55	28, 52, 99, 127	0
1	D	152/157 (96%)	-0.37	0 100 100	22, 38, 62, 89	0
1	E	152/157 (96%)	-0.36	2 (1%) 79 82	26, 46, 76, 110	0
1	F	151/157 (96%)	-0.17	3 (1%) 68 72	31, 52, 88, 102	0
1	G	152/157 (96%)	-0.32	2 (1%) 79 82	24, 47, 83, 101	0
1	H	151/157 (96%)	-0.32	0 100 100	26, 48, 78, 95	0
1	I	151/157 (96%)	-0.35	3 (1%) 68 72	26, 47, 80, 104	0
1	J	152/157 (96%)	-0.07	3 (1%) 68 72	28, 51, 95, 134	0
1	K	150/157 (95%)	-0.00	4 (2%) 58 62	31, 56, 105, 119	0
1	L	151/157 (96%)	-0.06	5 (3%) 50 55	33, 55, 92, 119	0
All	All	1818/1884 (96%)	-0.23	36 (1%) 68 72	22, 48, 89, 134	0

All (36) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	202	SER	6.6
1	B	202	SER	6.2
1	K	196	THR	5.7
1	A	202	SER	5.7
1	C	201	ARG	5.4
1	K	202	SER	4.8
1	C	200	GLY	4.5
1	J	203	GLY	4.2
1	K	200	GLY	4.1
1	B	201	ARG	4.1
1	A	201	ARG	3.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	200	GLY	3.7
1	B	196	THR	3.7
1	L	200	GLY	3.7
1	E	200	GLY	3.7
1	B	323	ASP	3.3
1	L	202	SER	3.1
1	A	203	GLY	3.1
1	C	196	THR	2.9
1	K	207	ARG	2.9
1	F	237	ILE	2.8
1	G	258	VAL	2.7
1	F	200	GLY	2.7
1	L	196	THR	2.6
1	J	202	SER	2.6
1	J	200	GLY	2.5
1	F	238	LYS	2.5
1	A	198	PRO	2.3
1	C	199	MET	2.2
1	I	256	ASP	2.2
1	I	202	SER	2.1
1	E	201	ARG	2.1
1	L	198	PRO	2.1
1	I	198	PRO	2.1
1	G	196	THR	2.0
1	L	207	ARG	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 carbohydrates in this entry.

6.4 Ligands

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å^2)	Q<0.9
2	4M6	F	400	29/29	0.97	0.14	0.41	31,52,69,70	0
2	4M6	B	400	29/29	0.98	0.14	0.35	13,37,56,74	0
2	4M6	E	400	29/29	0.96	0.14	0.15	29,58,70,82	0
2	4M6	C	400	29/29	0.97	0.12	0.13	17,47,70,76	0
2	4M6	H	400	29/29	0.96	0.13	-0.05	20,47,61,64	0
2	4M6	K	400	29/29	0.97	0.12	-0.10	17,39,78,79	0
2	4M6	G	400	29/29	0.98	0.11	-0.26	16,29,42,47	0
2	4M6	D	400	29/29	0.98	0.13	-0.26	15,31,43,49	0
2	4M6	J	400	29/29	0.95	0.13	-0.35	27,40,58,68	0
2	4M6	I	400	29/29	0.97	0.11	-0.75	15,43,59,70	0
2	4M6	L	400	29/29	0.97	0.11	-0.99	20,44,75,75	0
2	4M6	A	400	29/29	0.97	0.09	-1.34	16,38,52,59	0

6.5 Other polymers

There are no such residues in this entry.