



Full wwPDB X-ray Structure Validation Report

Mar 12, 2014 – 04:22 PM GMT

PDB ID : 4G0V
Title : Human topoisomerase iibeta in complex with DNA and mitoxantrone
Authors : Wu, C.C.; Li, T.K.; Li, Y.C.; Chan, N.L.
Deposited on : 2012-07-10
Resolution : 2.55 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

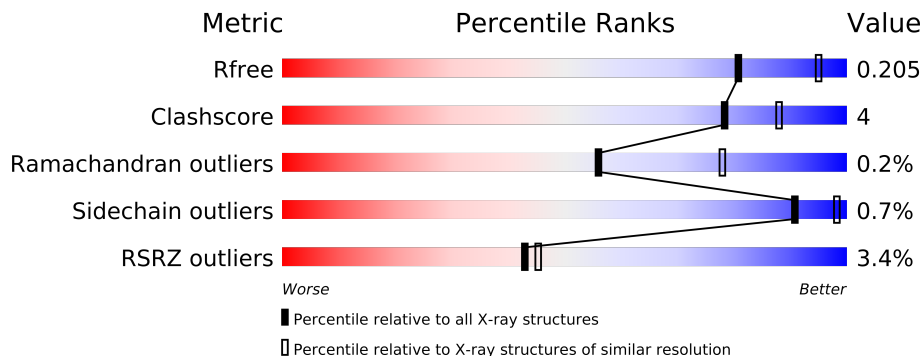
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.16 November 2013
Xtriage (Phenix) : dev-1323
EDS : trunk22714
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : trunk22714

1 Overall quality at a glance

The reported resolution of this entry is 2.55 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}	66092	3413 (2.58-2.50)
Clashscore	79885	4284 (2.58-2.50)
Ramachandran outliers	78287	4193 (2.58-2.50)
Sidechain outliers	78261	4195 (2.58-2.50)
RSRZ outliers	66119	3414 (2.58-2.50)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	803	
1	B	803	
2	C	8	
2	E	8	
3	D	12	
3	F	12	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
5	MG	A	1303	-	X

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 12243 atoms, of which 0 are hydrogen and 0 are deuterium.

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 DNA topoisomerase 2-beta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	663	Total	C	N	O	S	0	8	0
			5391	3432	932	1003	24			
1	B	666	Total	C	N	O	S	0	4	0
			5403	3438	939	1002	24			

There are 92 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	419	MET	-	EXPRESSION TAG	UNP Q02880
A	420	ALA	-	EXPRESSION TAG	UNP Q02880
A	421	SER	-	EXPRESSION TAG	UNP Q02880
A	422	TRP	-	EXPRESSION TAG	UNP Q02880
A	423	SER	-	EXPRESSION TAG	UNP Q02880
A	424	HIS	-	EXPRESSION TAG	UNP Q02880
A	425	PRO	-	EXPRESSION TAG	UNP Q02880
A	426	GLN	-	EXPRESSION TAG	UNP Q02880
A	427	PHE	-	EXPRESSION TAG	UNP Q02880
A	428	GLU	-	EXPRESSION TAG	UNP Q02880
A	429	LYS	-	EXPRESSION TAG	UNP Q02880
A	430	GLY	-	EXPRESSION TAG	UNP Q02880
A	431	ALA	-	EXPRESSION TAG	UNP Q02880
A	432	ASP	-	EXPRESSION TAG	UNP Q02880
A	433	ASP	-	EXPRESSION TAG	UNP Q02880
A	434	ASP	-	EXPRESSION TAG	UNP Q02880
A	435	ASP	-	EXPRESSION TAG	UNP Q02880
A	436	LYS	-	EXPRESSION TAG	UNP Q02880
A	437	VAL	-	EXPRESSION TAG	UNP Q02880
A	438	PRO	-	EXPRESSION TAG	UNP Q02880
A	439	ASP	-	EXPRESSION TAG	UNP Q02880
A	440	PRO	-	EXPRESSION TAG	UNP Q02880
A	441	THR	-	EXPRESSION TAG	UNP Q02880
A	442	SER	-	EXPRESSION TAG	UNP Q02880
A	443	VAL	-	EXPRESSION TAG	UNP Q02880

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
A	444	ASP	-	EXPRESSION TAG	UNP Q02880
A	1202	GLY	-	EXPRESSION TAG	UNP Q02880
A	1203	ALA	-	EXPRESSION TAG	UNP Q02880
A	1204	PRO	-	EXPRESSION TAG	UNP Q02880
A	1205	GLY	-	EXPRESSION TAG	UNP Q02880
A	1206	PHE	-	EXPRESSION TAG	UNP Q02880
A	1207	SER	-	EXPRESSION TAG	UNP Q02880
A	1208	SER	-	EXPRESSION TAG	UNP Q02880
A	1209	ILE	-	EXPRESSION TAG	UNP Q02880
A	1210	SER	-	EXPRESSION TAG	UNP Q02880
A	1211	ALA	-	EXPRESSION TAG	UNP Q02880
A	1212	HIS	-	EXPRESSION TAG	UNP Q02880
A	1213	HIS	-	EXPRESSION TAG	UNP Q02880
A	1214	HIS	-	EXPRESSION TAG	UNP Q02880
A	1215	HIS	-	EXPRESSION TAG	UNP Q02880
A	1216	HIS	-	EXPRESSION TAG	UNP Q02880
A	1217	HIS	-	EXPRESSION TAG	UNP Q02880
A	1218	HIS	-	EXPRESSION TAG	UNP Q02880
A	1219	HIS	-	EXPRESSION TAG	UNP Q02880
A	1220	HIS	-	EXPRESSION TAG	UNP Q02880
A	1221	HIS	-	EXPRESSION TAG	UNP Q02880
B	419	MET	-	EXPRESSION TAG	UNP Q02880
B	420	ALA	-	EXPRESSION TAG	UNP Q02880
B	421	SER	-	EXPRESSION TAG	UNP Q02880
B	422	TRP	-	EXPRESSION TAG	UNP Q02880
B	423	SER	-	EXPRESSION TAG	UNP Q02880
B	424	HIS	-	EXPRESSION TAG	UNP Q02880
B	425	PRO	-	EXPRESSION TAG	UNP Q02880
B	426	GLN	-	EXPRESSION TAG	UNP Q02880
B	427	PHE	-	EXPRESSION TAG	UNP Q02880
B	428	GLU	-	EXPRESSION TAG	UNP Q02880
B	429	LYS	-	EXPRESSION TAG	UNP Q02880
B	430	GLY	-	EXPRESSION TAG	UNP Q02880
B	431	ALA	-	EXPRESSION TAG	UNP Q02880
B	432	ASP	-	EXPRESSION TAG	UNP Q02880
B	433	ASP	-	EXPRESSION TAG	UNP Q02880
B	434	ASP	-	EXPRESSION TAG	UNP Q02880
B	435	ASP	-	EXPRESSION TAG	UNP Q02880
B	436	LYS	-	EXPRESSION TAG	UNP Q02880
B	437	VAL	-	EXPRESSION TAG	UNP Q02880
B	438	PRO	-	EXPRESSION TAG	UNP Q02880
B	439	ASP	-	EXPRESSION TAG	UNP Q02880

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	440	PRO	-	EXPRESSION TAG	UNP Q02880
B	441	THR	-	EXPRESSION TAG	UNP Q02880
B	442	SER	-	EXPRESSION TAG	UNP Q02880
B	443	VAL	-	EXPRESSION TAG	UNP Q02880
B	444	ASP	-	EXPRESSION TAG	UNP Q02880
B	1202	GLY	-	EXPRESSION TAG	UNP Q02880
B	1203	ALA	-	EXPRESSION TAG	UNP Q02880
B	1204	PRO	-	EXPRESSION TAG	UNP Q02880
B	1205	GLY	-	EXPRESSION TAG	UNP Q02880
B	1206	PHE	-	EXPRESSION TAG	UNP Q02880
B	1207	SER	-	EXPRESSION TAG	UNP Q02880
B	1208	SER	-	EXPRESSION TAG	UNP Q02880
B	1209	ILE	-	EXPRESSION TAG	UNP Q02880
B	1210	SER	-	EXPRESSION TAG	UNP Q02880
B	1211	ALA	-	EXPRESSION TAG	UNP Q02880
B	1212	HIS	-	EXPRESSION TAG	UNP Q02880
B	1213	HIS	-	EXPRESSION TAG	UNP Q02880
B	1214	HIS	-	EXPRESSION TAG	UNP Q02880
B	1215	HIS	-	EXPRESSION TAG	UNP Q02880
B	1216	HIS	-	EXPRESSION TAG	UNP Q02880
B	1217	HIS	-	EXPRESSION TAG	UNP Q02880
B	1218	HIS	-	EXPRESSION TAG	UNP Q02880
B	1219	HIS	-	EXPRESSION TAG	UNP Q02880
B	1220	HIS	-	EXPRESSION TAG	UNP Q02880
B	1221	HIS	-	EXPRESSION TAG	UNP Q02880

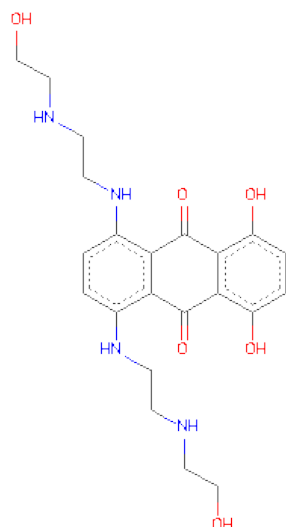
- Molecule 2 is a DNA chain called DNA (5'-D(P*AP*GP*CP*CP*GP*AP*GP*C)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	8	Total 165	C 77	N 34	O 46	P 8	0	0	0
2	E	8	Total 165	C 77	N 34	O 46	P 8	0	0	0

- Molecule 3 is a DNA chain called DNA (5'-D(P*TP*GP*CP*AP*GP*CP*TP*CP*GP*GP*CP*T)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	12	Total 245	C 116	N 43	O 74	P 12	0	0	0
3	F	12	Total 245	C 116	N 43	O 74	P 12	0	0	0

- Molecule 4 is 1,4-DIHYDROXY-5,8-BIS({2-[(2-HYDROXYETHYL)AMINO]ETHYL}AMINO)-9,10-ANTHRACENEDIONE (three-letter code: MIX) (formula: C₂₂H₂₈N₄O₆).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			32	22	4	6		
4	D	1	Total	C	N	O	0	0
			32	22	4	6		

- Molecule 5 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	2	Total	Mg	0	0
			2	2		
5	A	2	Total	Mg	0	0
			2	2		
5	D	1	Total	Mg	0	0
			1	1		
5	F	1	Total	Mg	0	0
			1	1		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	210	Total	O	0	0
			210	210		
6	B	242	Total	O	0	0
			242	242		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	C	17	Total 17	O 17	0	0
6	D	43	Total 43	O 43	0	0
6	E	14	Total 14	O 14	0	0
6	F	33	Total 33	O 33	0	0



- Molecule 2: DNA (5'-D(P*AP*GP*CP*CP*GP*AP*GP*C)-3')

Chain C:



- Molecule 2: DNA (5'-D(P*AP*GP*CP*CP*GP*AP*GP*C)-3')

Chain E:



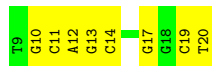
- Molecule 3: DNA (5'-D(P*TP*GP*CP*AP*GP*CP*TP*CP*GP*GP*CP*T)-3')

Chain D:



- Molecule 3: DNA (5'-D(P*TP*GP*CP*AP*GP*CP*TP*CP*GP*GP*CP*T)-3')

Chain F:



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	80.55Å 176.61Å 93.76Å 90.00° 111.53° 90.00°	Depositor
Resolution (Å)	27.94 – 2.55 27.94 – 2.55	Depositor EDS
% Data completeness (in resolution range)	99.3 (27.94-2.55) 95.0 (27.94-2.55)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.96 (at 2.54Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.1069)	Depositor
R, R_{free}	0.161 , 0.206 0.161 , 0.205	Depositor DCC
R_{free} test set	3785 reflections (5.02%)	DCC
Wilson B-factor (Å ²)	40.4	Xtriage
Anisotropy	0.064	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 27.9	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 78798 reflections	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	12243	wwPDB-VP
Average B, all atoms (Å ²)	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.86% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality

5.1 Standard geometry

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

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	0.39	0/5516	0.54	0/7430
1	B	0.40	0/5515	0.53	0/7421
2	C	0.77	0/185	1.47	4/283 (1.4%)
2	E	0.81	0/185	1.40	4/283 (1.4%)
3	D	0.72	0/273	1.70	10/419 (2.4%)
3	F	0.77	0/273	1.58	8/419 (1.9%)
All	All	0.43	0/11947	0.69	26/16255 (0.2%)

There are no bond length outliers.

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	10	DG	O4'-C1'-N9	9.97	114.98	108.00
3	F	10	DG	O4'-C1'-N9	9.87	114.91	108.00
2	C	8	DC	O4'-C1'-N1	8.98	114.28	108.00
3	D	14	DC	C4'-C3'-C2'	-8.15	95.77	103.10
3	F	14	DC	O4'-C4'-C3'	-7.97	101.22	106.00
3	F	14	DC	C4'-C3'-C2'	-7.91	95.98	103.10
3	D	14	DC	C1'-O4'-C4'	-6.97	103.13	110.10
2	E	1	DA	C1'-O4'-C4'	-6.89	103.21	110.10
2	E	8	DC	O4'-C1'-N1	6.88	112.81	108.00
3	D	19	DC	C1'-O4'-C4'	-6.71	103.39	110.10
3	F	19	DC	C1'-O4'-C4'	-6.37	103.73	110.10
3	D	20	DT	O4'-C4'-C3'	-6.34	101.96	104.50
3	D	16	DC	O4'-C1'-N1	5.94	112.16	108.00
3	F	14	DC	C1'-O4'-C4'	-5.89	104.21	110.10
3	D	14	DC	O4'-C4'-C3'	-5.35	102.36	104.50
2	E	1	DA	C3'-C2'-C1'	-5.35	96.08	102.50
3	D	17	DG	C5-C6-O6	-5.34	125.40	128.60
3	F	17	DG	O4'-C1'-N9	-5.31	104.28	108.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	20	DT	C1'-O4'-C4'	-5.29	104.81	110.10
3	F	20	DT	N3-C4-O4	5.28	123.07	119.90
2	E	1	DA	O4'-C1'-N9	5.26	111.69	108.00
2	C	2	DG	C3'-C2'-C1'	-5.26	96.19	102.50
2	C	2	DG	O4'-C1'-N9	5.25	111.67	108.00
3	D	19	DC	O4'-C4'-C3'	-5.15	102.44	104.50
2	C	4	DC	C1'-O4'-C4'	-5.10	105.00	110.10
3	F	19	DC	P-O5'-C5'	-5.07	112.79	120.90

There are no chirality outliers.

There are no planarity outliers.

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5391	0	5438	40	0
1	B	5403	0	5449	39	0
2	C	165	0	89	0	0
2	E	165	0	89	0	0
3	D	245	0	136	2	0
3	F	245	0	136	2	0
4	A	32	0	26	3	0
4	D	32	0	28	4	0
5	A	2	0	0	0	0
5	B	2	0	0	0	0
5	D	1	0	0	0	0
5	F	1	0	0	0	0
6	A	210	0	0	3	0
6	B	242	0	0	1	0
6	C	17	0	0	0	0
6	D	43	0	0	0	0
6	E	14	0	0	0	0
6	F	33	0	0	0	0
All	All	12243	0	11391	82	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 4.

All (82) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:732:PRO:HG2	1:B:869:ALA:HB1	1.71	0.70
1:A:482:LYS:HG2	1:A:499:VAL:HG12	1.79	0.64
1:A:778[A]:GLN:HG3	6:A:1531:HOH:O	1.98	0.62
1:A:1076:GLN:OE1	1:A:1078:LYS:NZ	2.33	0.61
1:B:757:GLU:HB2	1:B:823:PHE:HB3	1.84	0.59
1:A:551:LYS:NZ	6:A:1566:HOH:O	2.34	0.58
4:D:101:MIX:OAB	4:D:101:MIX:NAV	2.31	0.57
1:B:1170:ASP:OD1	1:B:1173[B]:ARG:NH2	2.37	0.56
1:B:1080:THR:O	1:B:1084:ARG:NH1	2.37	0.56
1:B:507:LEU:HD13	3:D:14:DC:H5"	1.88	0.56
1:A:1002:HIS:HB3	1:A:1008:GLN:HG3	1.88	0.56
1:A:560:GLN:HB3	1:A:722:PHE:HA	1.89	0.54
1:B:1082:GLU:OE1	1:B:1082:GLU:N	2.33	0.53
1:A:485:ALA:O	1:A:489:LEU:HB2	2.07	0.53
1:A:457:LEU:HD22	1:A:529:ILE:HG12	1.89	0.53
1:A:482:LYS:HG2	1:A:499:VAL:CG1	2.39	0.53
3:D:13:DG:O6	4:D:101:MIX:HAN1	2.09	0.53
1:A:752:ARG:HD3	1:A:754:ASP:OD2	2.09	0.52
1:B:461:ASN:HB2	1:B:495:ASP:HA	1.91	0.52
1:A:757:GLU:HB2	1:A:823:PHE:HB3	1.90	0.52
1:A:773:TYR:CE1	1:A:775:HIS:HB2	2.46	0.51
1:A:820:ARG:HH21	1:B:820[B]:ARG:NH2	2.09	0.51
1:B:637:ALA:HB3	1:B:639:GLU:HG3	1.93	0.50
1:A:460:ALA:HB3	1:A:463:ALA:HB2	1.93	0.50
1:A:503:ARG:HD3	6:A:1413:HOH:O	2.10	0.50
1:B:752:ARG:HD3	1:B:754:ASP:OD2	2.11	0.50
1:A:646:ASP:HA	1:A:649:ARG:NH2	2.27	0.49
1:B:673:LYS:NZ	6:B:1451:HOH:O	2.43	0.49
1:B:810:LEU:HD12	1:B:948:THR:HB	1.94	0.49
1:A:762[A]:GLN:NE2	1:B:765:GLY:HA3	2.28	0.49
1:B:846:TYR:CZ	1:B:851:ARG:HG3	2.48	0.49
1:B:759:LYS:HG3	1:B:823:PHE:CE2	2.48	0.48
1:A:846:TYR:CZ	1:A:851:ARG:HG3	2.48	0.48
1:B:673:LYS:HD2	1:B:676:ASP:OD1	2.14	0.48
1:B:482:LYS:HD2	1:B:501:PRO:HD3	1.96	0.47
1:B:587:GLU:HG2	1:B:653:LEU:HG	1.97	0.47
1:B:1084:ARG:CZ	1:B:1092:MET:HE1	2.45	0.47
1:B:976:TYR:HB2	1:B:983:LYS:HD3	1.97	0.47
1:B:858:ILE:HG13	1:B:1042:ARG:HD2	1.96	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:560:GLN:HB3	1:B:722:PHE:HA	1.98	0.46
1:A:1150:THR:O	1:A:1154:VAL:HG23	2.16	0.46
1:A:472:THR:HB	1:A:497:TYR:CD2	2.50	0.45
4:A:1301:MIX:NAV	4:A:1301:MIX:OAB	2.42	0.45
1:B:1084:ARG:NE	1:B:1092:MET:HE1	2.32	0.45
1:A:768:ALA:HA	1:A:773:TYR:HB3	1.99	0.45
1:A:858:ILE:HG13	1:A:1042:ARG:HD2	1.98	0.45
1:A:777:GLU:OE1	1:B:820[B]:ARG:NH1	2.51	0.44
4:D:101:MIX:OAA	4:D:101:MIX:NAU	2.49	0.44
4:A:1301:MIX:HAK1	3:F:13:DG:O6	2.17	0.44
1:A:1026:LYS:HB3	1:A:1026:LYS:HE2	1.70	0.44
1:B:881:PRO:HB3	1:B:1011:LEU:HD21	2.00	0.43
1:B:457:LEU:HD22	1:B:529:ILE:HG12	1.99	0.43
1:B:480:SER:O	1:B:484:LEU:HG	2.17	0.43
1:A:503:ARG:O	4:A:1301:MIX:HAP1	2.18	0.43
1:A:524:ASN:O	1:A:528:LYS:HD3	2.18	0.43
1:B:731:ILE:HA	1:B:732:PRO:HD3	1.75	0.42
1:A:807:GLY:HA3	1:A:813:GLY:HA2	2.01	0.42
1:A:469:LEU:HD21	1:A:544:LEU:O	2.19	0.42
1:A:818:SER:C	1:A:820:ARG:H	2.23	0.42
3:F:11:DC:H2'	3:F:12:DA:C8	2.53	0.42
1:A:456:LYS:HE2	1:A:479:ASP:OD2	2.19	0.42
1:A:939:ILE:HB	1:A:984:PHE:HB2	2.01	0.42
1:A:773:TYR:CZ	1:A:775:HIS:HB2	2.54	0.42
1:B:768:ALA:HA	1:B:773:TYR:HB3	2.01	0.42
1:B:460:ALA:HB3	1:B:463:ALA:HB2	2.01	0.42
1:A:844:PHE:HA	1:A:854:PRO:HA	2.01	0.42
1:A:883:TYR:CZ	1:A:1031:VAL:HG21	2.54	0.42
1:B:842:LEU:HD21	1:B:858:ILE:HG22	2.02	0.42
1:B:807:GLY:HA3	1:B:813:GLY:HA2	2.01	0.42
1:B:1145:SER:OG	1:B:1147:TRP:HB2	2.20	0.41
1:A:680:TRP:CE2	1:A:720:ILE:HD12	2.55	0.41
1:A:969:LEU:HD12	1:A:969:LEU:O	2.20	0.41
1:A:869:ALA:HB3	1:A:880:LEU:HB2	2.03	0.41
1:A:731:ILE:HA	1:A:732:PRO:HD3	1.87	0.41
1:B:1080:THR:OG1	1:B:1084:ARG:NH1	2.54	0.41
1:A:842:LEU:HD21	1:A:858:ILE:HG22	2.02	0.41
1:B:1056:MET:O	1:B:1060:GLU:HG3	2.21	0.41
1:B:492:ILE:HG13	1:B:492:ILE:H	1.71	0.40
1:B:522:GLU:OE1	4:D:101:MIX:HAK1	2.22	0.40
1:A:762[A]:GLN:HA	1:A:762[A]:GLN:NE2	2.37	0.40
1:B:654:PHE:HB3	1:B:711:TYR:CZ	2.56	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:539:ASP:OD1	1:B:540:ASP:N	2.52	0.40

There are no symmetry-related clashes.

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	663/803 (83%)	637 (96%)	25 (4%)	1 (0%)	56	78
1	B	660/803 (82%)	639 (97%)	19 (3%)	2 (0%)	50	71
All	All	1323/1606 (82%)	1276 (96%)	44 (3%)	3 (0%)	56	78

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	852	VAL
1	B	852	VAL
1	B	1101	ASP

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	591/704 (84%)	587 (99%)	4 (1%)	91	98
1	B	588/704 (84%)	584 (99%)	4 (1%)	91	98
All	All	1179/1408 (84%)	1171 (99%)	8 (1%)	91	98

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

Mol	Chain	Res	Type
1	A	523	ILE
1	A	653	LEU
1	A	766	SER
1	A	1092	MET
1	B	480	SER
1	B	848	ASP
1	B	880	LEU
1	B	905	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	811	HIS
1	A	922	GLN
1	B	1076	GLN

5.3.3 RNA ⓘ

There are no RNA chains 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 carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 8 ligands modelled in this entry, 6 are monoatomic - leaving 2 for Mogul analysis.

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
4	MIX	A	1301	-	34,34,34	1.18	4 (11%)	46,46,46	0.89	1 (2%)
4	MIX	D	101	-	34,34,34	1.17	4 (11%)	46,46,46	0.84	1 (2%)

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
4	MIX	A	1301	-	-	0/14/30/30	0/3/3/3
4	MIX	D	101	-	-	0/14/30/30	0/3/3/3

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	101	MIX	CBF-CBB	-3.19	1.39	1.47
4	A	1301	MIX	CBC-CBA	-3.19	1.39	1.47
4	A	1301	MIX	CBF-CBB	-2.97	1.40	1.47
4	A	1301	MIX	CBD-CBB	-2.91	1.40	1.47
4	A	1301	MIX	CBE-CBA	-2.90	1.40	1.47
4	D	101	MIX	CBE-CBA	-2.79	1.40	1.47
4	D	101	MIX	CBD-CBB	-2.70	1.40	1.47
4	D	101	MIX	CBC-CBA	-2.48	1.41	1.47

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	101	MIX	CAN-NAT-CAP	2.07	120.47	113.25
4	A	1301	MIX	CAN-NAT-CAP	2.03	120.31	113.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

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	663/803 (82%)	-0.16	27 (4%) 35 38	14, 31, 63, 91	0
1	B	666/803 (82%)	-0.18	18 (2%) 52 55	13, 29, 62, 106	0
2	C	8/8 (100%)	-0.18	1 (12%) 5 4	20, 22, 48, 69	0
2	E	8/8 (100%)	-0.39	1 (12%) 5 4	17, 20, 40, 70	0
3	D	12/12 (100%)	-0.79	0 100 100	19, 24, 29, 33	0
3	F	12/12 (100%)	-0.72	0 100 100	21, 26, 36, 53	0
All	All	1369/1646 (83%)	-0.18	47 (3%) 43 45	13, 30, 63, 106	0

All (47) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	643	TYR	6.2
1	B	638	LYS	5.4
1	A	541	ALA	5.3
1	B	644	PHE	5.2
1	B	642	GLU	5.0
1	A	491	VAL	4.9
1	B	641	LYS	4.1
1	A	848	ASP	4.0
1	B	849	ASN	4.0
1	B	645	ALA	3.9
1	A	490	GLY	3.8
1	A	568	LEU	3.8
1	A	849	ASN	3.5
1	A	696	LEU	3.3
1	B	640	ALA	3.2
1	A	692	ARG	3.1
1	B	848	ASP	3.0
1	A	569	LEU	2.9
2	C	1	DA	2.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	491	VAL	2.9
1	B	568	LEU	2.9
1	A	466	LYS	2.8
1	A	539	ASP	2.8
1	B	692	ARG	2.8
1	A	695	GLY	2.8
1	A	453	GLY	2.7
1	B	693	LEU	2.6
1	A	452	LYS	2.6
1	A	514	HIS	2.5
1	A	552	ILE	2.5
1	A	567	GLY	2.5
1	B	639	GLU	2.5
1	A	492	ILE	2.5
1	A	646	ASP	2.5
1	B	846	TYR	2.3
1	A	484	LEU	2.2
1	B	637	ALA	2.2
1	A	542	GLU	2.2
1	B	545	LYS	2.2
1	B	492	ILE	2.1
2	E	1	DA	2.1
1	A	846	TYR	2.1
1	A	487	SER	2.1
1	A	540	ASP	2.1
1	A	570	ILE	2.0
1	A	518	MET	2.0
1	A	535	LYS	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, 95th 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	RSR	LLDF	B-factors(Å ²)	Q<0.9
5	MG	A	1303	1/1	0.35	7.00	39,39,39,39	0
5	MG	B	1301	1/1	0.10	0.71	25,25,25,25	0
5	MG	D	102	1/1	0.14	0.44	39,39,39,39	0
5	MG	A	1302	1/1	0.10	0.21	27,27,27,27	0
5	MG	F	101	1/1	0.13	-0.23	38,38,38,38	0
4	MIX	D	101	32/32	0.12	-0.40	14,23,38,40	0
4	MIX	A	1301	32/32	0.13	-0.50	17,26,41,41	0
5	MG	B	1302	1/1	0.14	-0.78	46,46,46,46	0

6.5 Other polymers ⓘ

There are no such residues in this entry.