Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 03:13 PM GMT

PDB ID	:	4BUL
Title	:	Novel hydroxyl tricyclics (e.g. GSK966587) as potent inhibitors of bacterial type IIA topoisomerases
Authors	:	Miles, T.J.; Hennessy, A.J.; Bax, B.; Brooks, G.; Brown, B.S.; Brown, P.; Cailleau, N.; Chen, D.; Dabbs, S.; Davies, D.T.; Esken, J.M.; Giordano, I.; Hoover, J.L.; Huang, J.; Jones, G.E.; Sukmar, S.K.K.; Spitzfaden, C.; Markwell, R.E.; Minthorn, E.A.; Rittenhouse, S.; Gwynn, M.N.; Pearson, N.D.
Deposited on	:	2013-06-20
Resolution	:	2.60 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:

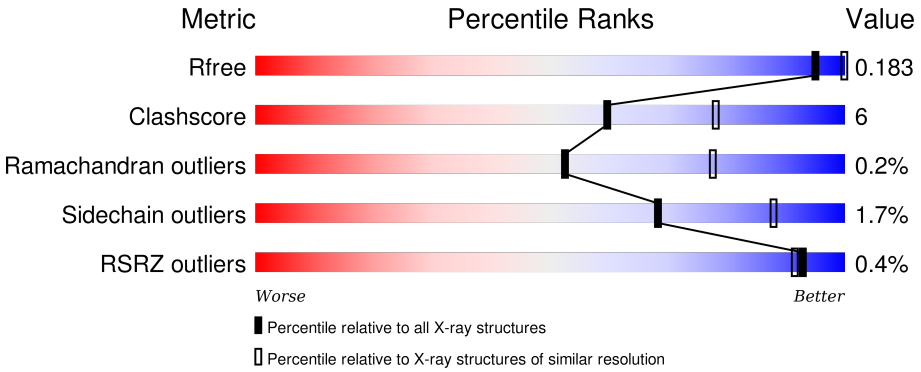
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 2.60 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	2328 (2.60-2.60)
Clashscore	102246	2679 (2.60-2.60)
Ramachandran outliers	100387	2635 (2.60-2.60)
Sidechain outliers	100360	2635 (2.60-2.60)
RSRZ outliers	91569	2334 (2.60-2.60)

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	692	87% 10% •
1	C	692	87% 10% •
2	E	20	30% 70%
2	G	20	55% 40% 5%
3	F	20	50% 45% 5%

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Mol	Chain	Length	Quality of chain
3	H	20	45% 55%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	AE8	F	1020[A]	-	-	-	X
5	AE8	F	1020[B]	-	-	-	X

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 12809 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 DNA GYRASE SUBUNIT B, DNA GYRASE SUBUNIT A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	675	Total	C	N	O	S	0	4	1
			5367	3342	969	1031	25			
1	C	672	Total	C	N	O	S	0	3	1
			5335	3323	963	1024	25			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	409	MET	-	EXPRESSION TAG	UNP P66937
A	544	THR	-	LINKER	UNP P66937
A	545	GLY	-	LINKER	UNP P66937
A	1123	PHE	TYR	ENGINEERED MUTATION	UNP Q99XG5
C	409	MET	-	EXPRESSION TAG	UNP P66937
C	544	THR	-	LINKER	UNP P66937
C	545	GLY	-	LINKER	UNP P66937
C	1123	PHE	TYR	ENGINEERED MUTATION	UNP Q99XG5

- Molecule 2 is a DNA chain called 5'-D(*TP*GP*TP*GP*CP*GP*GP*TP*GP*TP*AP*CP*CP*TP *AP*CP*GP*GP*CP*T)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	20	Total	C	N	O	P	0	20	0
			408	195	72	122	19			
2	G	19	Total	C	N	O	P	0	19	0
			388	185	70	115	18			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	F	19	Total	C	N	O	P	0	19	0
			385	183	75	109	18			

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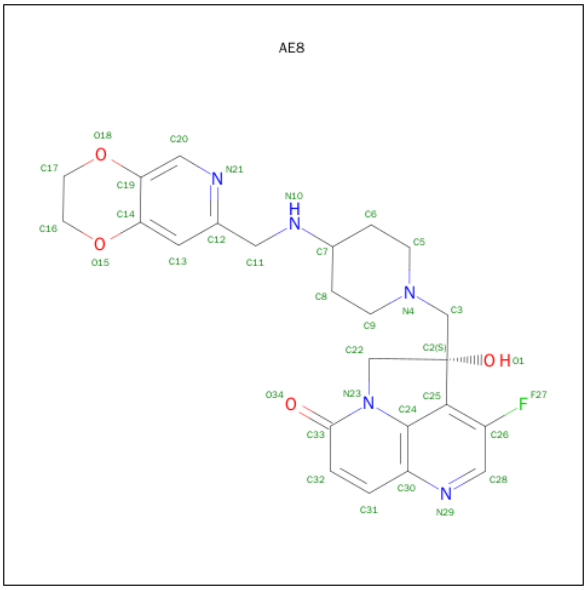
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	H	20	Total	C	N	O	P	0	20	0
			406	193	80	114	19			

- Molecule 4 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	2	Total	Mn	0	0
			2	2		
4	C	1	Total	Mn	0	0
			1	1		
4	E	1	Total	Mn	0	0
			1	1		

- Molecule 5 is (S)-4-((4-(((2,3-DIHYDRO-[1,4]DIOXINO[2,3-C]PYRIDIN-7-YL)METHYL) AMINO)PIPERIDIN-1-YL)METHYL)-3-FLUORO-4-HYDROXY-4H-PYRROLO[3,2,1-D E][1,5]NAPHTHYRIDIN-7(5H)-ONE (three-letter code: AE8) (formula: $C_{24}H_{26}FN_5O_4$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	F	1	Total	C	F	N	O	0	1
			68	48	2	10	8		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	230	Total	O	0	0
			230	230		

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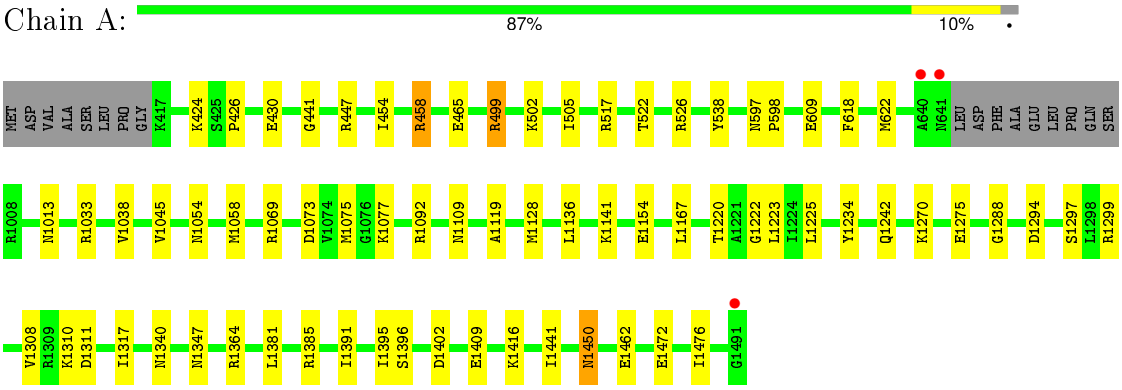
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	C	197	Total O 197 197	0	0
6	E	20	Total O 20 20	0	0
6	F	1	Total O 1 1	0	0

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.

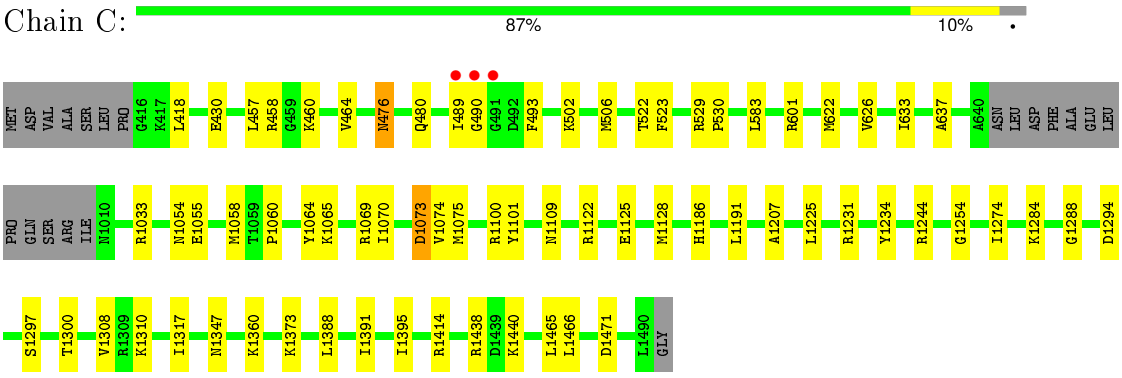
• Molecule 1: DNA GYRASE SUBUNIT B, DNA GYRASE SUBUNIT A

Chain A:



• Molecule 1: DNA GYRASE SUBUNIT B, DNA GYRASE SUBUNIT A

Chain C:



• Molecule 2: 5'-D(*TP*GP*TP*GP*CP*GP*GP*TP*GP*TP*AP*CP*CP*TP *AP*CP*GP*GP*CP*T)-3'

Chain E:

• Molecule 2: 5'-D(*TP*GP*TP*GP*CP*GP*GP*TP*GP*TP*AP*CP*CP*TP *AP*CP*GP*GP*CP*T)-3'

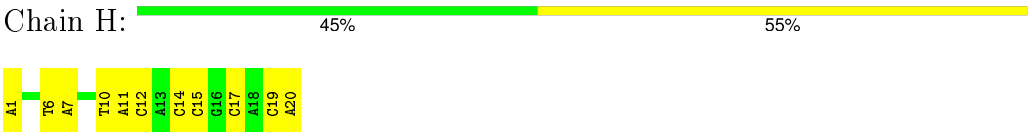
Chain G:

• Molecule 3: 5'-D(*AP*GP*CP*CP*GP*TP*AP*GP*GP*TP*AP*CP*AP*CP *CP*GP*CP*AP*C)-3'

Chain F:

• Molecule 3: 5'-D(*AP*GP*CP*CP*GP*TP*AP*GP*GP*TP*AP*CP*AP*CP *CP*GP*CP*AP*C)-3'

Chain H:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 61	Depositor
Cell constants a, b, c, α, β, γ	93.87Å 93.87Å 416.44Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	24.79 – 2.60 24.79 – 2.60	Depositor EDS
% Data completeness (in resolution range)	95.8 (24.79-2.60) 95.7 (24.79-2.60)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.12 (at 2.60Å)	Xtriage
Refinement program	REFMAC 5.7.0032	Depositor
R, R_{free}	0.144 , 0.183 0.145 , 0.183	Depositor DCC
R_{free} test set	1845 reflections (3.14%)	DCC
Wilson B-factor (Å^2)	42.2	Xtriage
Anisotropy	0.248	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 16.3	EDS
Estimated twinning fraction	0.803 for H, K, L 0.197 for K, H, -L 0.206 for h,-h-k,-l	Xtriage
Reported twinning fraction	0.803 for H, K, L 0.197 for K, H, -L	Depositor
L-test for twinning[2]	$< \|L\| > = 0.40$, $< L^2 > = 0.22$	Xtriage
Outliers	0 of 60660 reflections	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	12809	wwPDB-VP
Average B, all atoms (Å^2)	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.69% 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: AE8, MN

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	0.43	0/5439	0.61	0/7327
1	C	0.43	0/5407	0.61	0/7288
2	E	0.33	0/456	0.75	0/703
2	G	0.34	0/434	0.72	0/669
3	F	0.38	0/432	0.80	0/664
3	H	0.33	0/456	0.76	0/701
All	All	0.42	0/12624	0.64	0/17352

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5367	0	5394	57	0
1	C	5335	0	5361	36	0
2	E	408	0	207	21	0
2	G	388	0	199	10	0
3	F	385	0	193	15	0
3	H	406	0	204	13	0
4	A	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	C	1	0	0	0	0
4	E	1	0	0	0	0
5	F	68	0	52	2	0
6	A	230	0	0	6	0
6	C	197	0	0	1	0
6	E	20	0	0	0	0
6	F	1	0	0	0	0
All	All	12809	0	11610	136	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 6.

All (136) 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)
3:F:14[A]:DC:C2'	3:F:15[A]:DC:H5'	1.99	0.91
3:F:14[A]:DC:H2"	3:F:15[A]:DC:H5'	1.54	0.89
2:E:1[A]:DT:HO5'	2:E:1[A]:DT:H6	1.18	0.87
2:E:19[A]:DC:H2"	2:E:20[A]:DT:O5'	1.75	0.84
1:A:458:ARG:HH11	1:A:458:ARG:CG	1.91	0.83
2:E:19[A]:DC:C2'	2:E:20[A]:DT:O5'	2.28	0.81
2:E:11[A]:DA:H2"	2:E:12[A]:DC:H5"	1.63	0.79
1:A:1058:MET:HE2	1:A:1069:ARG:HH12	1.50	0.77
1:C:1207:ALA:HB2	1:C:1231:ARG:HH22	1.51	0.76
3:H:20[B]:DA:H2'	3:H:20[B]:DA:N3	1.98	0.75
1:A:458:ARG:HH11	1:A:458:ARG:HG3	1.53	0.72
3:H:1[B]:DA:H8	3:H:1[B]:DA:O5'	1.72	0.71
1:A:424:LYS:O	1:A:426:PRO:HD3	1.92	0.70
1:A:499:ARG:HH11	1:A:499:ARG:HG3	1.57	0.69
1:A:1058:MET:CE	1:A:1069:ARG:NH1	2.55	0.69
1:A:502:LYS:HG2	1:A:538:TYR:CE1	2.28	0.69
1:A:1092[A]:ARG:NH1	2:E:5[A]:DC:OP1	2.26	0.68
1:A:458:ARG:NH1	1:A:458:ARG:HG3	2.08	0.67
2:E:19[A]:DC:H3'	2:E:19[A]:DC:H6	1.58	0.67
2:G:12[B]:DC:H2"	2:G:13[B]:DC:OP2	1.93	0.67
1:C:1471:ASP:OD2	6:C:2188:HOH:O	2.13	0.66
1:A:1054:ASN:HA	1:A:1128:MET:HE2	1.76	0.65
1:C:430:GLU:HB3	1:C:502:LYS:HB2	1.77	0.65
1:A:1092[B]:ARG:NH1	3:H:6[B]:DT:OP2	2.31	0.64
1:C:1075:MET:HE1	5:F:1020[A]:AE8:H20	1.80	0.63
3:H:14[B]:DC:H2"	3:H:15[B]:DC:H5'	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1360:LYS:HE3	1:C:1466:LEU:HD13	1.79	0.63
3:H:6[B]:DT:H2"	3:H:7[B]:DA:H5"	1.81	0.62
3:F:14[A]:DC:H2'	3:F:15[A]:DC:H5'	1.79	0.62
1:A:499:ARG:HH11	1:A:499:ARG:CG	2.12	0.62
1:A:1058:MET:HE2	1:A:1069:ARG:NH1	2.13	0.61
1:A:1058:MET:HE1	1:A:1069:ARG:NH1	2.16	0.60
1:C:457:LEU:O	1:C:458:ARG:NH1	2.34	0.60
1:A:1310:LYS:HB2	6:A:2188:HOH:O	2.02	0.60
1:A:1058:MET:CE	1:A:1069:ARG:HH12	2.13	0.59
3:H:19[B]:DC:C4	3:H:20[B]:DA:N6	2.70	0.59
3:H:1[B]:DA:C8	3:H:1[B]:DA:O5'	2.53	0.59
1:A:441:GLY:HA3	1:C:1109:ASN:ND2	2.18	0.59
2:E:1[A]:DT:H2"	2:E:2[A]:DG:O5'	2.02	0.59
2:E:14[A]:DT:H2"	2:E:15[A]:DA:H5'	1.85	0.58
2:G:13[B]:DC:H5"	2:G:13[B]:DC:H6	1.68	0.57
2:G:7[B]:DG:N2	3:H:14[B]:DC:O2	2.30	0.57
1:A:1077:LYS:HB3	1:A:1154:GLU:HG3	1.86	0.57
1:A:1288:GLY:HA3	1:A:1317:ILE:HD11	1.87	0.57
2:G:2[B]:DG:H2"	2:G:3[B]:DT:OP2	2.04	0.57
2:E:19[A]:DC:C6	2:E:19[A]:DC:H3'	2.39	0.56
1:C:1207:ALA:HB2	1:C:1231:ARG:NH2	2.20	0.56
1:C:1297:SER:HB3	1:C:1300:THR:OG1	2.05	0.55
1:A:447:ARG:HD3	1:A:454:ILE:HD11	1.88	0.55
1:C:1391:ILE:O	1:C:1395:ILE:HG12	2.07	0.55
1:A:597:ASN:HD22	1:A:598:PRO:HD2	1.72	0.55
1:C:1225:LEU:HD21	1:C:1244:ARG:HD2	1.89	0.55
1:A:1234:TYR:O	1:A:1347:ASN:HB2	2.07	0.55
1:A:1054:ASN:CA	1:A:1128:MET:HE2	2.38	0.54
2:E:7[A]:DG:N2	3:F:14[A]:DC:O2	2.39	0.54
2:E:19[A]:DC:H2"	2:E:20[A]:DT:C5'	2.37	0.53
1:C:1070:ILE:O	1:C:1074:VAL:HG23	2.08	0.53
1:A:1069:ARG:HD2	6:A:2077:HOH:O	2.08	0.53
1:C:464:VAL:HG21	1:C:523:PHE:HA	1.90	0.53
1:A:1396:SER:HB3	6:A:2209:HOH:O	2.08	0.53
3:F:12[A]:DC:H2"	3:F:13[A]:DA:OP2	2.08	0.53
1:C:1388:LEU:HD13	1:C:1438:ARG:HG2	1.90	0.53
1:A:1450:ASN:HD22	1:A:1450:ASN:N	2.07	0.52
2:E:19[A]:DC:C6	2:E:19[A]:DC:C3'	2.92	0.52
1:C:493:PHE:CE1	1:C:530:PRO:HB2	2.44	0.52
2:E:5[A]:DC:N3	3:F:16[A]:DG:N1	2.57	0.52
1:A:1275[B]:GLU:HG3	6:A:2178:HOH:O	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1060:PRO:HD3	1:C:1128:MET:HB2	1.92	0.52
1:C:1308:VAL:HG13	1:C:1317:ILE:HD12	1.91	0.51
1:C:1064:TYR:HB3	1:C:1125:GLU:HB3	1.91	0.51
1:C:633:ILE:O	1:C:637:ALA:HB2	2.11	0.51
1:C:1288:GLY:HA3	1:C:1317:ILE:HD11	1.91	0.51
1:C:1274:ILE:HD13	1:C:1294:ASP:HB2	1.92	0.51
1:C:506:MET:HG2	1:C:583:LEU:HD11	1.93	0.51
1:A:609:GLU:HG3	1:A:1013:ASN:HD22	1.76	0.51
2:E:17[A]:DG:N2	3:F:4[A]:DC:O2	2.44	0.51
1:A:1054:ASN:HA	1:A:1128:MET:CE	2.41	0.50
1:A:1364:ARG:NH2	1:A:1462:GLU:OE1	2.36	0.50
1:A:1391:ILE:O	1:A:1395:ILE:HG12	2.12	0.50
1:A:458:ARG:HH11	1:A:458:ARG:HG2	1.74	0.49
1:A:465:GLU:HG3	1:A:622:MET:HB2	1.95	0.49
2:G:13[B]:DC:C4	2:G:14[B]:DT:C4	3.01	0.49
3:H:14[B]:DC:C2'	3:H:15[B]:DC:H5'	2.43	0.48
1:C:1254:GLY:O	1:C:1310:LYS:HE2	2.14	0.48
3:F:14[A]:DC:C2'	3:F:15[A]:DC:C5'	2.83	0.48
1:A:430:GLU:HB3	1:A:502:LYS:HB2	1.95	0.48
1:A:1310:LYS:O	1:A:1311:ASP:HB2	2.13	0.48
3:F:14[A]:DC:H2"	3:F:15[A]:DC:C5'	2.35	0.48
1:A:1270:LYS:NZ	1:A:1294:ASP:OD2	2.39	0.48
2:E:5[A]:DC:N4	3:F:16[A]:DG:O6	2.47	0.48
2:G:13[B]:DC:C6	2:G:13[B]:DC:H5"	2.48	0.48
1:A:1054:ASN:HB2	1:A:1136:LEU:HD13	1.96	0.47
3:F:12[A]:DC:C2'	3:F:13[A]:DA:OP2	2.61	0.47
1:C:626:VAL:HG11	2:E:17[A]:DG:H3'	1.97	0.47
2:E:17[A]:DG:N1	3:F:4[A]:DC:N3	2.62	0.47
1:A:1308:VAL:HG13	1:A:1317:ILE:HD12	1.96	0.47
3:F:7[A]:DA:H2'	3:F:8[A]:DG:C8	2.50	0.47
1:A:1472:GLU:O	1:A:1476:ILE:HG12	2.15	0.46
1:A:1038:VAL:HA	1:A:1167:LEU:HD22	1.98	0.46
2:G:13[B]:DC:N4	2:G:14[B]:DT:O4	2.48	0.46
1:A:465:GLU:OE2	1:A:526:ARG:NE	2.48	0.46
1:C:1069:ARG:O	1:C:1073:ASP:HB2	2.16	0.46
1:A:1222:GLY:C	1:A:1223:LEU:HD12	2.36	0.45
1:C:1186:HIS:HB2	1:C:1191:LEU:HD11	1.97	0.45
1:A:1381:LEU:HD22	1:A:1441:ILE:HG23	1.98	0.45
2:E:19[A]:DC:H2'	2:E:20[A]:DT:C6	2.51	0.45
1:A:1075:MET:HE1	5:F:1020[B]:AE8:H20	1.99	0.45
1:C:1055:GLU:OE1	1:C:1055:GLU:HA	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:430:GLU:OE2	1:C:601:ARG:NH1	2.39	0.44
2:G:4[B]:DG:O6	3:H:17[B]:DC:N4	2.50	0.44
2:E:16[A]:DC:N4	3:F:5[A]:DG:O6	2.51	0.43
1:A:1141:LYS:NZ	6:A:2116:HOH:O	2.51	0.43
1:C:1100:ARG:HG3	1:C:1101:TYR:CE2	2.53	0.43
1:C:460:LYS:HG2	3:F:8[A]:DG:H1'	2.00	0.43
1:A:1045:VAL:HG11	2:E:6[A]:DG:H5'	2.00	0.43
3:H:20[B]:DA:C2'	3:H:20[B]:DA:N3	2.76	0.43
1:C:476:ASN:ND2	1:C:480:GLN:HE21	2.17	0.43
1:A:505:ILE:HG21	1:A:517:ARG:HG3	2.01	0.42
1:C:1234:TYR:O	1:C:1347:ASN:HB2	2.19	0.42
2:G:13[B]:DC:N4	2:G:14[B]:DT:C4	2.88	0.42
1:A:597:ASN:HA	1:A:598:PRO:HD2	1.93	0.42
1:C:1054:ASN:HA	1:C:1128:MET:CE	2.49	0.42
1:A:1340[B]:ASN:CG	1:A:1340[B]:ASN:O	2.58	0.42
1:A:1225:LEU:HB2	1:A:1242:GLN:HB2	2.00	0.42
2:G:11[B]:DA:N1	3:H:10[B]:DT:N3	2.67	0.42
1:A:499:ARG:NH1	1:A:499:ARG:CG	2.78	0.42
1:A:1416:LYS:HE2	1:A:1416:LYS:HB3	1.87	0.42
1:A:1109:ASN:HB3	1:A:1119:ALA:HB2	2.02	0.42
1:C:522:THR:OG1	1:C:622:MET:HG3	2.20	0.42
3:H:11[B]:DA:H2"	3:H:12[B]:DC:OP2	2.20	0.41
1:A:441:GLY:HA3	1:C:1109:ASN:HD21	1.86	0.41
2:E:12[A]:DC:C2	2:E:13[A]:DC:C5	3.09	0.41
1:A:609:GLU:HG3	1:A:1013:ASN:ND2	2.36	0.41
1:C:1058:MET:HG2	1:C:1065:LYS:HG3	2.04	0.40
1:A:522:THR:HA	1:A:618:PHE:CE1	2.56	0.40
1:A:1409:GLU:HB2	6:A:2211:HOH:O	2.22	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	675/692 (98%)	652 (97%)	22 (3%)	1 (0%)	56 81
1	C	671/692 (97%)	651 (97%)	18 (3%)	2 (0%)	46 72
All	All	1346/1384 (97%)	1303 (97%)	40 (3%)	3 (0%)	52 77

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1033	ARG
1	C	490	GLY
1	C	1033	ARG

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	577/591 (98%)	568 (98%)	9 (2%)	70 89
1	C	574/591 (97%)	563 (98%)	11 (2%)	65 86
All	All	1151/1182 (97%)	1131 (98%)	20 (2%)	68 88

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	458	ARG
1	A	499	ARG
1	A	1073	ASP
1	A	1220	THR
1	A	1297	SER
1	A	1299	ARG
1	A	1385	ARG
1	A	1402	ASP
1	A	1450	ASN
1	C	418	LEU
1	C	476	ASN
1	C	489	ILE
1	C	529	ARG

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Mol	Chain	Res	Type
1	C	1073	ASP
1	C	1122	ARG
1	C	1284	LYS
1	C	1373	LYS
1	C	1414	ARG
1	C	1440	LYS
1	C	1465	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	474	ASN
1	A	597	ASN
1	A	1010	ASN
1	A	1054	ASN
1	A	1334	ASN
1	A	1368	GLN
1	A	1450	ASN
1	C	476	ASN
1	C	1334	ASN
1	C	1368	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains (i)

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

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

Of 6 ligands modelled in this entry, 4 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	$\#\|Z\| > 2$
5	AE8	F	1020[A]	-	34,39,39	1.11	3 (8%)	33,58,58	1.22	3 (9%)
5	AE8	F	1020[B]	-	34,39,39	1.16	2 (5%)	33,58,58	1.28	5 (15%)

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
5	AE8	F	1020[A]	-	-	0/10/38/38	0/5/6/6
5	AE8	F	1020[B]	-	-	0/10/38/38	0/5/6/6

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	F	1020[B]	AE8	C24-C30	-4.31	1.35	1.42
5	F	1020[A]	AE8	C24-C30	-3.87	1.36	1.42
5	F	1020[B]	AE8	C28-N29	2.02	1.35	1.31
5	F	1020[A]	AE8	C31-C30	2.16	1.45	1.41
5	F	1020[A]	AE8	C28-N29	2.18	1.35	1.31

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	F	1020[B]	AE8	O15-C14-C19	-2.54	119.64	121.97
5	F	1020[B]	AE8	C6-C5-N4	-2.39	107.06	110.96
5	F	1020[A]	AE8	O15-C14-C19	-2.11	120.04	121.97
5	F	1020[B]	AE8	O18-C19-C20	2.35	120.16	116.74
5	F	1020[A]	AE8	C31-C30-N29	2.54	122.73	118.52
5	F	1020[B]	AE8	C31-C30-N29	2.60	122.84	118.52
5	F	1020[A]	AE8	O15-C14-C13	2.94	121.02	116.72
5	F	1020[B]	AE8	O15-C14-C13	3.02	121.14	116.72

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	F	1020[A]	AE8	1	0
5	F	1020[B]	AE8	1	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	675/692 (97%)	-0.35	3 (0%)	93	91	26, 41, 60, 83	0
1	C	672/692 (97%)	-0.36	3 (0%)	93	91	25, 41, 62, 84	0
2	E	20/20 (100%)	-0.44	0	100	100	30, 41, 65, 69	20 (100%)
2	G	19/20 (95%)	-0.56	0	100	100	31, 40, 58, 71	19 (100%)
3	F	19/20 (95%)	-0.54	0	100	100	33, 41, 64, 68	19 (100%)
3	H	20/20 (100%)	-0.51	0	100	100	30, 37, 61, 72	20 (100%)
All	All	1425/1464 (97%)	-0.36	6 (0%)	93	91	25, 41, 61, 84	78 (5%)

All (6) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	491	GLY	3.6
1	A	640	ALA	2.5
1	A	1491	GLY	2.4
1	A	641	ASN	2.3
1	C	490	GLY	2.1
1	C	489	ILE	2.1

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 (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. 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
5	AE8	F	1020[B]	34/34	0.98	0.21	3.44	38,39,43,43	34
5	AE8	F	1020[A]	34/34	0.98	0.21	3.35	32,35,36,37	34
4	MN	A	2493	1/1	1.00	0.13	-0.51	34,34,34,34	0
4	MN	C	2491	1/1	0.99	0.12	-0.72	34,34,34,34	0
4	MN	A	2492	1/1	0.97	0.12	-1.27	55,55,55,55	0
4	MN	E	1021	1/1	0.95	0.05	-	64,64,64,64	0

6.5 Other polymers (i)

There are no such residues in this entry.