Full wwPDB X-ray Structure Validation Report (i)

Nov 14, 2016 – 06:21 PM EST

PDB ID	:	5HNI
Title	:	CRYSTAL STRUCTURE OF CMET WT with compound 3
Authors	:	Vallee, F.; Houtmann, J.
Deposited on	:	2016-01-18
Resolution	:	1.71 Å(reported)

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

|		
MolProbity	:	4.02b-467
Mogul	:	1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20028320
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)	:	rb-20028320

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 1.71 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		0.235
Clashscore		12
Ramachandran outliers		0.2%
Sidechain outliers		2.5%
RSRZ outliers		22.4%

Worse   *Better*

■ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution
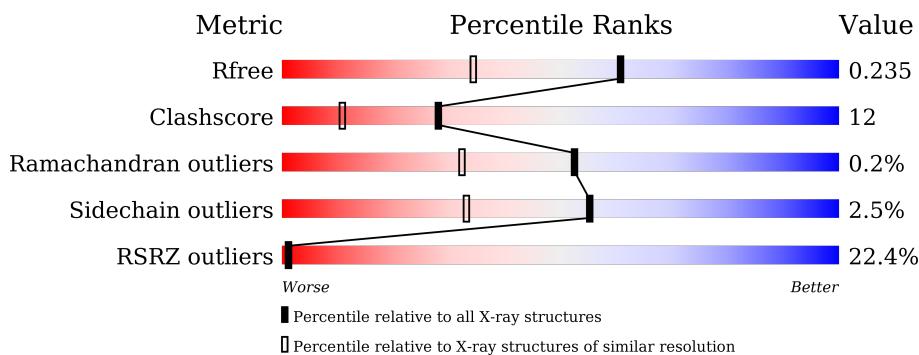
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R$_{free}$	91344	3998 (1.74-1.70)
Clashscore	102246	4425 (1.74-1.70)
Ramachandran outliers	100387	4360 (1.74-1.70)
Sidechain outliers	100360	4360 (1.74-1.70)
RSRZ outliers	91569	4010 (1.74-1.70)

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	X	312	17% 61% 16% • 21%
1	Y	312	19% 62% 15% • 21%
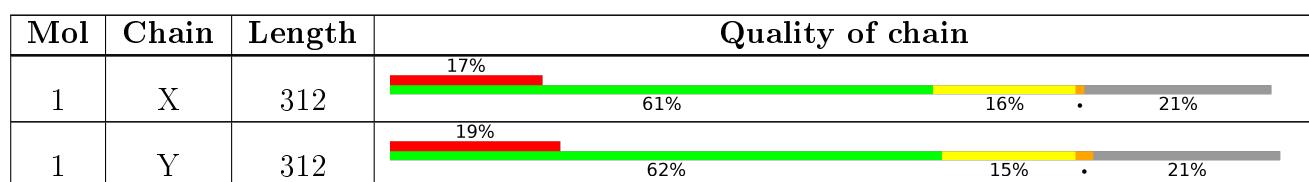
2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 4345 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 Hepatocyte growth factor receptor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	X	245	Total	C	N	O	S	0	0	0
			1952	1265	332	340	15			
1	Y	245	Total	C	N	O	S	0	0	0
			1952	1265	332	340	15			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
X	1194	PHE	TYR	conflict	UNP P08581
X	1234	PHE	TYR	conflict	UNP P08581
X	1235	ASP	TYR	conflict	UNP P08581
Y	1194	PHE	TYR	conflict	UNP P08581
Y	1234	PHE	TYR	conflict	UNP P08581
Y	1235	ASP	TYR	conflict	UNP P08581

- Molecule 2 is methyl (6-{[6-(4-fluorophenyl)[1,2,4]triazolo[4,3-b]pyridazin-3-yl]sulfanyl}-1H-benzimidazol-2-yl)carbamate (three-letter code: 63B) (formula: $C_{20}H_{14}FN_7O_2S$).
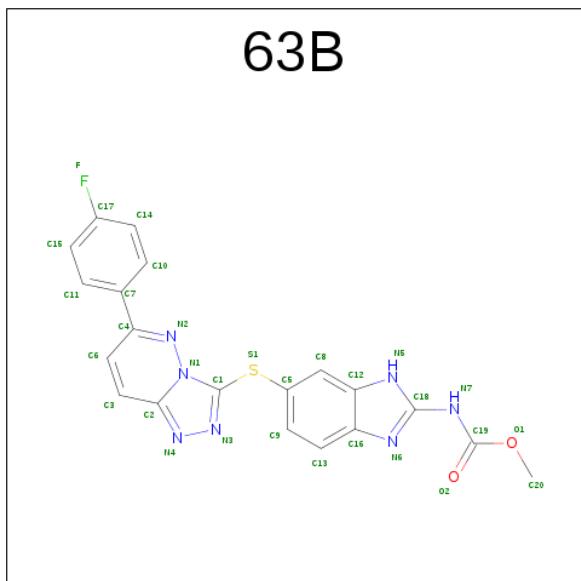
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	X	1	Total	C	F	N	O	S	0	0
			31	20	1	7	2	1		
2	Y	1	Total	C	F	N	O	S	0	0
			31	20	1	7	2	1		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	X	194	Total	O	0	0
			194	194		
3	Y	185	Total	O	0	0
			185	185		

3 Residue-property plots ⓘ

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: Hepatocyte growth factor receptor
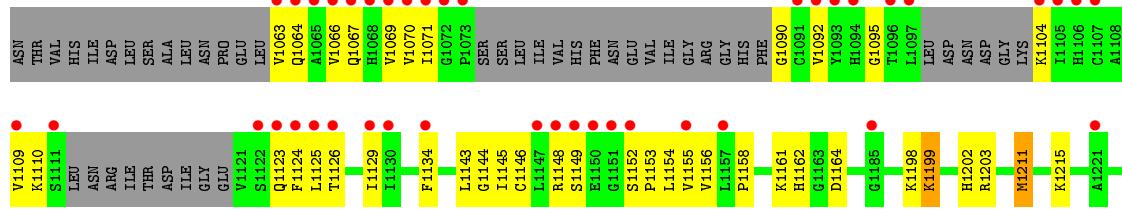
- Molecule 1: Hepatocyte growth factor receptor
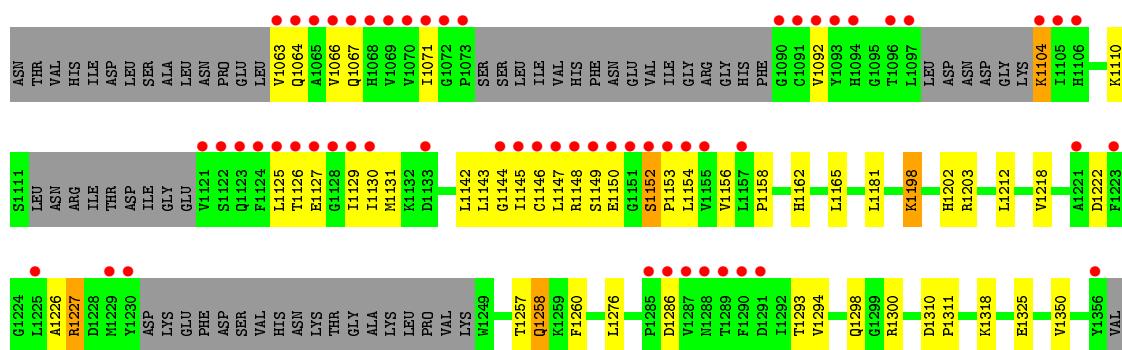
4   Data and refinement statistics $\textcircled{i}$

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	42.85Å 47.06Å 81.98Å 76.96° 76.96° 90.00°	Depositor
Resolution (Å)	77.70 – 1.71 25.42 – 1.60	Depositor EDS
% Data completeness (in resolution range)	77.1 (77.70-1.71) 64.4 (25.42-1.60)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.61 (at 1.60Å)	Xtriage
Refinement program	CNX	Depositor
R, R_{free}	0.227 , 0.245 0.241 , 0.235	Depositor DCC
R_{free} test set	2509 reflections (5.26%)	DCC
Wilson B-factor (Å^2)	13.3	Xtriage
Anisotropy	0.319	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.41 , 64.5	EDS
L-test for twinning[2]	$< |L| > = 0.48, < L^2 > = 0.31$	Xtriage
Estimated twinning fraction	0.147 for h,-k,h-l	Xtriage
F_o,F_c correlation	0.89	EDS
Total number of atoms	4345	wwPDB-VP
Average B, all atoms (Å^2)	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.14% of the height of the origin peak. No significant pseudotranslation is detected.*

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[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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: 63B

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	X	0.29	0/2000	0.46	0/2705
1	Y	0.29	0/2000	0.47	0/2705
All	All	0.29	0/4000	0.47	0/5410

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 (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	X	1952	0	1962	44	0
1	Y	1952	0	1962	48	0
2	X	31	0	0	0	0
2	Y	31	0	0	1	0
3	X	194	0	0	7	0
3	Y	185	0	0	5	0
All	All	4345	0	3924	92	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 12.

All (92) 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:Y:1127:GLU:HA	1:Y:1130:ILE:HB	1.48	0.93
1:Y:1152:SER:H	1:Y:1153:PRO:HA	1.33	0.92
1:X:1069:VAL:HG21	1:X:1129:ILE:HA	1.61	0.82
1:Y:1144:GLY:O	1:Y:1156:VAL:HG22	1.85	0.76
1:Y:1063:VAL:HG23	1:Y:1064:GLN:HG3	1.69	0.74
1:Y:1143:LEU:HB2	1:Y:1156:VAL:HG23	1.71	0.73
1:Y:1258:GLN:HA	1:Y:1258:GLN:HE21	1.55	0.71
1:X:1064:GLN:HA	1:X:1067:GLN:HE21	1.57	0.70
1:X:1144:GLY:O	1:X:1156:VAL:HG22	1.92	0.70
1:X:1152:SER:N	1:X:1153:PRO:HA	2.08	0.69
1:X:1063:VAL:HG23	1:X:1064:GLN:HG3	1.75	0.68
1:X:1066:VAL:HG21	1:X:1125:LEU:HD22	1.75	0.68
1:X:1066:VAL:HG11	1:X:1125:LEU:HD13	1.75	0.67
1:Y:1152:SER:N	1:Y:1153:PRO:HA	2.10	0.64
1:Y:1198:LYS:NZ	1:Y:1198:LYS:HA	2.13	0.64
1:Y:1146:CYS:HB3	1:Y:1154:LEU:HB2	1.79	0.63
1:X:1202:HIS:O	1:X:1203:ARG:HB3	1.99	0.63
1:X:1258:GLN:HE21	1:X:1258:GLN:HA	1.64	0.62
1:Y:1152:SER:H	1:Y:1153:PRO:CA	2.11	0.62
1:Y:1165:LEU:HD21	1:Y:1276:LEU:HD21	1.81	0.60
1:Y:1066:VAL:HG11	1:Y:1125:LEU:HD13	1.83	0.60
1:Y:1152:SER:HB3	1:Y:1153:PRO:O	2.02	0.60
1:Y:1148:ARG:HB2	1:Y:1149:SER:HB3	1.86	0.58
1:Y:1071:ILE:HG13	1:Y:1145:ILE:O	2.04	0.57
1:Y:1143:LEU:HG	1:Y:1158:PRO:HD3	1.87	0.56
1:X:1146:CYS:HB3	1:X:1154:LEU:HB2	1.88	0.56
1:X:1333:LEU:HA	3:X:1606:HOH:O	2.07	0.55
1:X:1066:VAL:HG22	1:X:1070:VAL:HG23	1.89	0.55
1:Y:1092:VAL:HG22	1:Y:1110:LYS:HD3	1.88	0.55
1:Y:1071:ILE:HD11	1:Y:1146:CYS:SG	2.47	0.55
1:X:1092:VAL:HG22	1:X:1110:LYS:HD3	1.87	0.55
1:X:1110:LYS:HB3	1:X:1155:VAL:HB	1.90	0.54
1:Y:1126:THR:O	1:Y:1130:ILE:HG13	2.09	0.53
1:X:1164:ASP:HA	1:X:1211:MET:HE3	1.90	0.53
1:X:1162:HIS:HD2	3:X:1656:HOH:O	1.92	0.52
1:X:1325:GLU:H	1:X:1325:GLU:CD	2.12	0.52
1:X:1148:ARG:HB2	1:X:1149:SER:HB3	1.90	0.52
1:X:1064:GLN:O	1:X:1067:GLN:HG2	2.09	0.52
1:Y:1198:LYS:HD2	1:Y:1198:LYS:N	2.25	0.51
1:Y:1318:LYS:HE2	3:Y:1640:HOH:O	2.11	0.51
1:X:1152:SER:N	1:X:1153:PRO:CA	2.74	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Y:1147:LEU:HA	1:Y:1153:PRO:HB3	1.93	0.51
1:X:1071:ILE:HD11	1:X:1156:VAL:HG21	1.91	0.50
1:Y:1310:ASP:N	1:Y:1311:PRO:HD2	2.27	0.50
1:Y:1203:ARG:HG3	1:Y:1260:PHE:CG	2.46	0.50
1:X:1226:ALA:HB3	3:X:1626:HOH:O	2.12	0.50
1:X:1070:VAL:HG22	1:X:1145:ILE:HD11	1.94	0.50
1:X:1336:ARG:HB2	3:X:1606:HOH:O	2.11	0.50
1:Y:1066:VAL:HG22	1:Y:1066:VAL:O	2.12	0.49
1:Y:1181:LEU:HD12	1:Y:1350:VAL:HG21	1.93	0.49
1:Y:1131:MET:HG2	1:Y:1142:LEU:HB2	1.95	0.49
1:Y:1325:GLU:CD	1:Y:1325:GLU:H	2.15	0.49
1:Y:1162:HIS:HE1	3:Y:1537:HOH:O	1.96	0.49
1:Y:1147:LEU:HD23	1:Y:1153:PRO:CG	2.43	0.49
1:Y:1198:LYS:HZ2	1:Y:1198:LYS:HA	1.78	0.48
1:X:1198:LYS:C	1:X:1199:LYS:HE3	2.33	0.48
1:X:1064:GLN:HA	1:X:1067:GLN:NE2	2.26	0.48
1:Y:1293:THR:HG23	1:Y:1294:VAL:N	2.29	0.48
1:Y:1162:HIS:HD2	3:Y:1655:HOH:O	1.96	0.48
1:Y:1152:SER:N	1:Y:1153:PRO:CA	2.75	0.47
1:X:1124:PHE:CZ	1:X:1153:PRO:HB2	2.49	0.47
1:X:1293:THR:HG23	1:X:1294:VAL:N	2.29	0.47
1:X:1143:LEU:HG	1:X:1158:PRO:HD3	1.97	0.47
1:X:1300:ARG:HD3	3:X:1546:HOH:O	2.14	0.47
1:Y:1064:GLN:HA	1:Y:1067:GLN:HE21	1.80	0.46
1:Y:1226:ALA:HB3	3:Y:1604:HOH:O	2.15	0.46
1:Y:1212:LEU:CD1	1:Y:1218:VAL:HG22	2.47	0.45
1:Y:1294:VAL:O	1:Y:1298:GLN:HG3	2.17	0.45
1:X:1066:VAL:O	1:X:1066:VAL:HG22	2.17	0.45
1:X:1095:GLY:HA3	1:X:1109:VAL:HG23	1.98	0.45
1:Y:1300:ARG:HD3	3:Y:1513:HOH:O	2.17	0.45
1:Y:1148:ARG:HA	1:Y:1149:SER:HA	1.71	0.44
1:X:1152:SER:HB3	1:X:1153:PRO:O	2.18	0.44
1:Y:1257:THR:O	1:Y:1258:GLN:HB2	2.18	0.44
1:Y:1064:GLN:O	1:Y:1067:GLN:HG2	2.19	0.43
1:X:1148:ARG:HA	1:X:1149:SER:HA	1.69	0.43
1:Y:1222:ASP:OD1	1:Y:1227:ARG:HA	2.19	0.43
1:Y:1202:HIS:O	1:Y:1203:ARG:CB	2.66	0.43
1:Y:1092:VAL:HG21	2:Y:1401:63B:S1	2.59	0.42
1:X:1253:GLU:HA	1:X:1256:GLN:HE21	1.82	0.42
1:X:1215:LYS:HB3	1:X:1215:LYS:HE2	1.83	0.42
1:X:1071:ILE:HG13	1:X:1071:ILE:O	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:1310:ASP:N	1:X:1311:PRO:HD2	2.35	0.41
1:Y:1104:LYS:O	1:Y:1104:LYS:HD2	2.21	0.41
1:Y:1149:SER:N	1:Y:1150:GLU:HA	2.34	0.41
1:Y:1125:LEU:O	1:Y:1129:ILE:HG13	2.21	0.41
1:X:1161:LYS:HB2	3:X:1625:HOH:O	2.20	0.41
1:X:1134:PHE:HE1	1:X:1198:LYS:HG3	1.85	0.41
1:X:1090:GLY:O	1:X:1110:LYS:HE3	2.21	0.41
1:X:1199:LYS:HA	3:X:1539:HOH:O	2.20	0.41
1:X:1123:GLN:O	1:X:1126:THR:HB	2.22	0.40
1:X:1228:ASP:HB3	1:X:1230:TYR:CZ	2.57	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	X	235/312 (75%)	225 (96%)	10 (4%)	0	100	100
1	Y	235/312 (75%)	226 (96%)	8 (3%)	1 (0%)	39	20
All	All	470/624 (75%)	451 (96%)	18 (4%)	1 (0%)	52	32

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	Y	1152	SER

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	X	216/277 (78%)	210 (97%)	6 (3%)	51	28
1	Y	216/277 (78%)	211 (98%)	5 (2%)	58	37
All	All	432/554 (78%)	421 (98%)	11 (2%)	55	33

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	X	1104	LYS
1	X	1199	LYS
1	X	1211	MET
1	X	1225	LEU
1	X	1258	GLN
1	X	1325	GLU
1	Y	1104	LYS
1	Y	1198	LYS
1	Y	1227	ARG
1	Y	1258	GLN
1	Y	1286	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	X	1067	GLN
1	X	1123	GLN
1	X	1162	HIS
1	X	1167	ASN
1	X	1256	GLN
1	X	1258	GLN
1	X	1304	GLN
1	Y	1067	GLN
1	Y	1162	HIS
1	Y	1167	ASN
1	Y	1256	GLN
1	Y	1258	GLN
1	Y	1304	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)

2 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	63B	X	1401	-	30,35,35	2.94	10 (33%)	31,50,50	2.68	6 (19%)
2	63B	Y	1401	-	30,35,35	2.96	10 (33%)	31,50,50	2.67	6 (19%)

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	63B	X	1401	-	-	2/10/14/14	0/5/5/5
2	63B	Y	1401	-	-	2/10/14/14	0/5/5/5

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	Y	1401	63B	N4-N3	-5.97	1.26	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	X	1401	63B	N4-N3	-5.89	1.26	1.37
2	X	1401	63B	C14-C10	2.14	1.43	1.38
2	X	1401	63B	C15-C17	2.22	1.41	1.37
2	Y	1401	63B	C14-C10	2.23	1.43	1.38
2	Y	1401	63B	C14-C17	2.38	1.41	1.37
2	X	1401	63B	C14-C17	2.40	1.41	1.37
2	Y	1401	63B	C15-C17	2.46	1.41	1.37
2	X	1401	63B	C13-C9	2.92	1.42	1.36
2	Y	1401	63B	C13-C9	3.10	1.43	1.36
2	Y	1401	63B	C8-C5	3.17	1.42	1.36
2	X	1401	63B	C8-C5	3.27	1.43	1.36
2	X	1401	63B	C4-N2	4.29	1.37	1.33
2	Y	1401	63B	C4-N2	4.36	1.37	1.33
2	Y	1401	63B	C3-C2	5.77	1.49	1.40
2	X	1401	63B	C6-C4	5.80	1.52	1.38
2	Y	1401	63B	C6-C4	5.82	1.52	1.38
2	X	1401	63B	C3-C2	5.83	1.49	1.40
2	Y	1401	63B	C18-N7	9.19	1.49	1.38
2	X	1401	63B	C18-N7	9.20	1.49	1.38

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	X	1401	63B	O1-C19-O2	-5.82	116.43	124.61
2	Y	1401	63B	O1-C19-O2	-5.75	116.53	124.61
2	X	1401	63B	C6-C4-N2	-4.24	117.42	121.58
2	Y	1401	63B	C6-C4-N2	-4.23	117.44	121.58
2	Y	1401	63B	O2-C19-N7	-2.10	121.41	126.14
2	X	1401	63B	O2-C19-N7	-2.03	121.55	126.14
2	Y	1401	63B	C1-S1-C5	3.79	109.44	103.18
2	X	1401	63B	C1-S1-C5	4.29	110.25	103.18
2	X	1401	63B	C20-O1-C19	5.39	122.38	115.65
2	Y	1401	63B	C20-O1-C19	5.53	122.55	115.65
2	X	1401	63B	O1-C19-N7	10.34	122.02	109.14
2	Y	1401	63B	O1-C19-N7	10.37	122.06	109.14

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	X	1401	63B	C20-O1-C19-O2
2	X	1401	63B	C20-O1-C19-N7

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Mol	Chain	Res	Type	Atoms
2	Y	1401	63B	C20-O1-C19-N7
2	Y	1401	63B	C20-O1-C19-O2

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	Y	1401	63B	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 (i)

6.1 Protein, DNA and RNA chains (i)

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	X	245/312 (78%)	1.42	52 (21%)	1	1	4, 16, 66, 102	0
1	Y	245/312 (78%)	1.86	58 (23%)	1	1	5, 16, 72, 98	0
All	All	490/624 (78%)	1.64	110 (22%)	1	1	4, 16, 70, 102	0

All (110) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	Y	1065	ALA	30.3
1	Y	1072	GLY	25.0
1	Y	1126	THR	22.8
1	X	1065	ALA	20.3
1	X	1063	VAL	18.4
1	Y	1151	GLY	15.5
1	Y	1149	SER	14.9
1	X	1073	PRO	14.1
1	X	1149	SER	13.8
1	Y	1122	SER	13.8
1	Y	1073	PRO	12.7
1	X	1072	GLY	11.7
1	Y	1129	ILE	11.0
1	Y	1121	VAL	10.8
1	Y	1070	VAL	10.3
1	X	1151	GLY	10.3
1	X	1290	PHE	10.2
1	Y	1064	GLN	9.6
1	Y	1123	GLN	9.4
1	Y	1148	ARG	8.8
1	Y	1130	ILE	8.3
1	Y	1127	GLU	8.2
1	Y	1071	ILE	8.1
1	X	1064	GLN	7.9

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Mol	Chain	Res	Type	RSRZ
1	X	1105	ILE	7.9
1	Y	1289	THR	7.7
1	Y	1125	LEU	7.6
1	X	1229	MET	7.6
1	X	1071	ILE	7.5
1	Y	1063	VAL	7.2
1	X	1091	CYS	7.1
1	Y	1150	GLU	6.8
1	X	1126	THR	6.7
1	Y	1069	VAL	6.6
1	Y	1152	SER	6.5
1	Y	1290	PHE	6.5
1	X	1230	TYR	6.5
1	Y	1229	MET	6.5
1	Y	1105	ILE	6.4
1	Y	1091	CYS	6.4
1	Y	1230	TYR	6.3
1	Y	1097	LEU	6.2
1	X	1150	GLU	6.2
1	X	1148	ARG	6.2
1	Y	1286	ASP	6.1
1	X	1067	GLN	6.0
1	Y	1067	GLN	6.0
1	X	1123	GLN	5.9
1	X	1096	THR	5.9
1	Y	1104	LYS	5.8
1	X	1152	SER	5.7
1	Y	1147	LEU	5.7
1	Y	1287	VAL	5.6
1	X	1097	LEU	5.2
1	Y	1225	LEU	5.2
1	Y	1094	HIS	5.2
1	X	1094	HIS	5.2
1	X	1069	VAL	5.1
1	Y	1124	PHE	5.1
1	X	1289	THR	5.1
1	Y	1066	VAL	5.1
1	X	1104	LYS	5.1
1	Y	1291	ASP	4.8
1	Y	1145	ILE	4.6
1	Y	1068	HIS	4.5
1	X	1125	LEU	4.4

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Mol	Chain	Res	Type	RSRZ
1	Y	1288	ASN	4.4
1	X	1356	TYR	4.3
1	X	1286	ASP	4.3
1	X	1291	ASP	4.2
1	X	1225	LEU	4.1
1	X	1147	LEU	4.1
1	Y	1146	CYS	4.1
1	X	1068	HIS	4.0
1	Y	1153	PRO	4.0
1	X	1070	VAL	3.9
1	X	1130	ILE	3.8
1	X	1106	HIS	3.6
1	X	1285	PRO	3.6
1	Y	1106	HIS	3.6
1	Y	1356	TYR	3.6
1	X	1066	VAL	3.5
1	X	1287	VAL	3.5
1	Y	1154	LEU	3.5
1	X	1107	CYS	3.4
1	X	1092	VAL	3.3
1	Y	1093	TYR	3.3
1	X	1288	ASN	3.0
1	Y	1133	ASP	2.9
1	X	1124	PHE	2.9
1	Y	1285	PRO	2.9
1	X	1157	LEU	2.8
1	Y	1155	VAL	2.8
1	X	1109	VAL	2.6
1	X	1185	GLY	2.6
1	Y	1090	GLY	2.6
1	X	1093	TYR	2.6
1	Y	1096	THR	2.5
1	Y	1223	PHE	2.5
1	Y	1128	GLY	2.5
1	Y	1144	GLY	2.4
1	X	1155	VAL	2.4
1	X	1129	ILE	2.4
1	X	1122	SER	2.4
1	X	1111	SER	2.3
1	Y	1092	VAL	2.3
1	X	1221	ALA	2.1
1	X	1134	PHE	2.1

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Mol	Chain	Res	Type	RSRZ
1	Y	1157	LEU	2.1
1	Y	1221	ALA	2.1

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

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

6.3 Carbohydrates (i)

There are no 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, 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	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
2	63B	Y	1401	31/31	0.67	0.24	1.18	22,33,36,37	0
2	63B	X	1401	31/31	0.72	0.21	0.83	22,30,36,38	0

6.5 Other polymers (i)

There are no such residues in this entry.