



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 24, 2017 – 05:35 PM EST

PDB ID : 1QS4
Title : Core domain of HIV-1 integrase complexed with Mg⁺⁺ and 1-(5-chloroindol-3-yl)-3-hydroxy-3-(2H-tetrazol-5-yl)-propenone
Authors : Goldgur, Y.; Craigie, R.; Fujiwara, T.; Yoshinaga, T.; Davies, D.R.
Deposited on : 1999-06-25
Resolution : 2.10 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 ⓘ symbol.

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

MolProbity	:	4.02b-467
Mogul	:	1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20028442

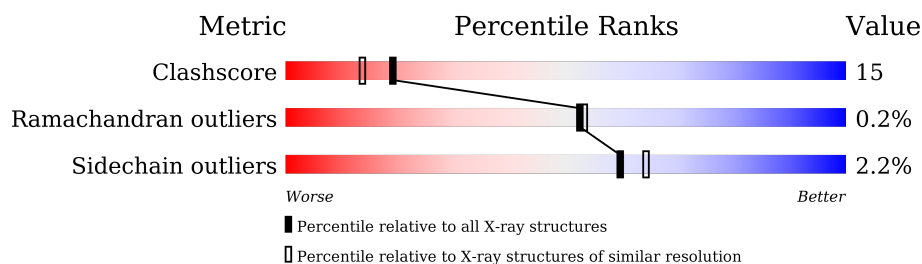
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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))
Clashscore	102246	4460 (2.10-2.10)
Ramachandran outliers	100387	4413 (2.10-2.10)
Sidechain outliers	100360	4414 (2.10-2.10)

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 $\leq 5\%$. 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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	154	
1	B	154	
1	C	154	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 4036 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 PROTEIN (HIV-1 INTEGRASE (E.C.2.7.7.49)).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	150	Total	C	N	O	S	0	0	0
			1147	726	200	216	5			
1	B	152	Total	C	N	O	S	0	0	0
			1167	739	203	220	5			
1	C	151	Total	C	N	O	S	0	0	0
			1155	730	202	218	5			

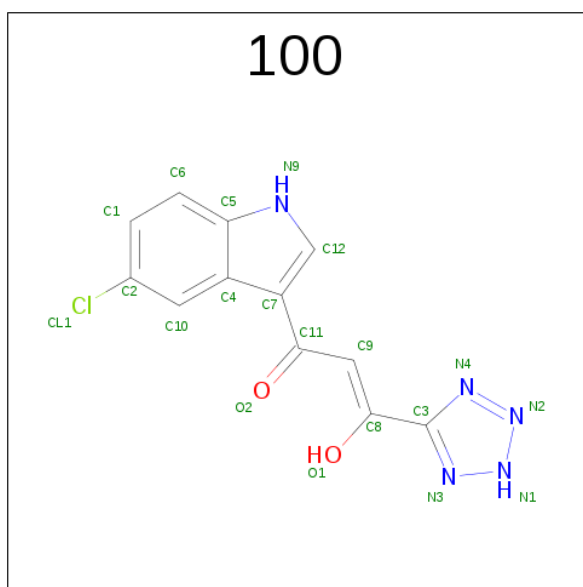
There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	131	GLU	TRP	ENGINEERED	UNP Q76353
A	133	GLY	ALA	CONFLICT	UNP Q76353
A	185	LYS	PHE	ENGINEERED	UNP Q76353
B	131	GLU	TRP	ENGINEERED	UNP Q76353
B	133	GLY	ALA	CONFLICT	UNP Q76353
B	185	LYS	PHE	ENGINEERED	UNP Q76353
C	131	GLU	TRP	ENGINEERED	UNP Q76353
C	133	GLY	ALA	CONFLICT	UNP Q76353
C	185	LYS	PHE	ENGINEERED	UNP Q76353

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Mg	0	0
			1	1		
2	A	1	Total	Mg	0	0
			1	1		
2	C	1	Total	Mg	0	0
			1	1		

- Molecule 3 is 1-(5-CHLOROINDOL-3-YL)-3-HYDROXY-3-(2H-TETRAZOL-5-YL)-PROP ENONE (three-letter code: 100) (formula: C₁₂H₈ClN₅O₂).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	Cl	N	O	0	0
			20	12	1	5	2		

- Molecule 4 is water.

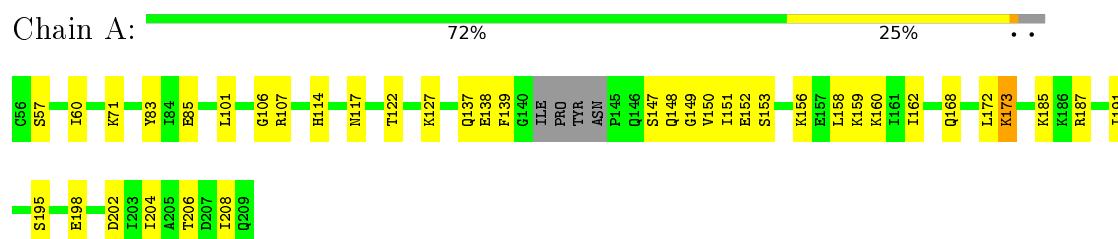
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	155	Total	O	0	0
			155	155		
4	B	187	Total	O	0	0
			187	187		
4	C	202	Total	O	0	0
			202	202		

3 Residue-property plots [i](#)

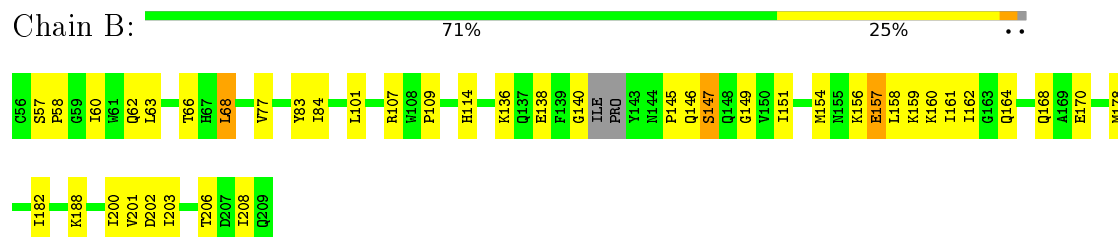
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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.

Note EDS was not executed.

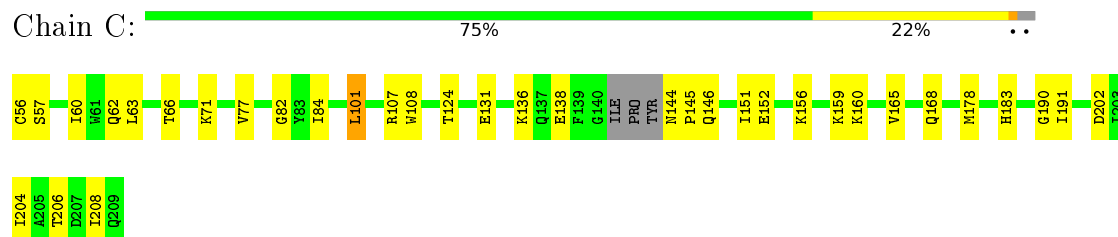
- Molecule 1: PROTEIN (HIV-1 INTEGRASE (E.C.2.7.7.49))



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- Molecule 1: PROTEIN (HIV-1 INTEGRASE (E.C.2.7.7.49))



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	76.23 Å 46.73 Å 141.36 Å 90.00° 105.55° 90.00°	Depositor
Resolution (Å)	38.07 – 2.10	Depositor
% Data completeness (in resolution range)	94.2 (38.07-2.10)	Depositor
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS	Depositor
R, R_{free}	0.209 , 0.255	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	4036	wwPDB-VP
Average B, all atoms (Å ²)	37.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 100, 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	0.30	0/1167	0.55	0/1573
1	B	0.33	0/1188	0.56	0/1603
1	C	0.34	0/1175	0.59	0/1585
All	All	0.32	0/3530	0.57	0/4761

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	1147	0	1155	39	0
1	B	1167	0	1169	48	0
1	C	1155	0	1160	35	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
3	A	20	0	7	1	0
4	A	155	0	0	7	0
4	B	187	0	0	16	0
4	C	202	0	0	12	0
All	All	4036	0	3491	106	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 15.

All (106) 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:A:173:LYS:HD2	4:B:1148:HOH:O	1.85	0.75
1:A:107:ARG:HD2	1:B:107:ARG:NE	2.03	0.73
1:B:154:MET:HE1	4:C:1194:HOH:O	1.89	0.72
1:C:202:ASP:O	1:C:206:THR:HG23	1.90	0.71
1:B:145:PRO:O	1:C:146:GLN:HA	1.91	0.71
1:A:160:LYS:HE3	4:A:1078:HOH:O	1.93	0.68
1:B:146:GLN:HB3	1:C:145:PRO:HB2	1.74	0.68
1:C:136:LYS:HE2	4:C:1139:HOH:O	1.94	0.67
1:B:140:GLY:HA2	4:B:1138:HOH:O	1.95	0.67
1:B:170:GLU:H	1:B:170:GLU:CD	1.99	0.66
1:B:145:PRO:HB2	1:C:146:GLN:HB2	1.78	0.66
1:A:85:GLU:OE1	1:B:107:ARG:HD3	1.96	0.66
1:B:146:GLN:CG	1:C:146:GLN:HB3	2.27	0.65
1:B:114:HIS:CD2	1:B:138:GLU:HB2	2.31	0.65
1:A:127:LYS:HA	1:A:137:GLN:HE22	1.61	0.64
1:B:156:LYS:HE2	1:C:156:LYS:NZ	2.13	0.63
1:C:66:THR:OG1	1:C:159:LYS:HE3	1.98	0.63
1:C:204:ILE:O	1:C:208:ILE:HG13	1.98	0.63
1:C:62:GLN:HE21	1:C:151:ILE:HB	1.63	0.62
1:B:188:LYS:HG2	4:B:1073:HOH:O	2.01	0.60
1:A:173:LYS:NZ	1:A:173:LYS:HB3	2.17	0.60
1:A:71:LYS:HE2	4:A:1137:HOH:O	2.01	0.59
1:A:147:SER:C	1:A:149:GLY:H	2.06	0.59
1:A:148:GLN:O	1:A:151:ILE:HG22	2.02	0.59
1:B:149:GLY:HA2	4:B:1106:HOH:O	2.02	0.58
1:B:68:LEU:HD22	4:B:1166:HOH:O	2.03	0.58
1:A:107:ARG:HD3	4:B:1053:HOH:O	2.02	0.58
1:C:152:GLU:HG3	4:C:1128:HOH:O	2.03	0.58
1:A:147:SER:HA	1:A:150:VAL:HG23	1.86	0.58
1:B:188:LYS:HD3	4:B:1101:HOH:O	2.04	0.58
1:B:146:GLN:HG2	1:C:146:GLN:HB3	1.86	0.58
1:B:158:LEU:O	1:B:162:ILE:HG13	2.04	0.57
1:B:138:GLU:HG3	4:B:1132:HOH:O	2.03	0.57
1:A:159:LYS:NZ	3:A:1004:100:HN1	2.02	0.57
1:C:82:GLY:O	1:C:183:HIS:HE1	1.88	0.57
1:B:168:GLN:HB2	1:B:178:MET:HE1	1.87	0.56
1:A:204:ILE:O	1:A:208:ILE:HG13	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:151:ILE:HG22	4:B:1106:HOH:O	2.04	0.56
1:C:168:GLN:HA	4:C:1193:HOH:O	2.06	0.56
1:B:202:ASP:O	1:B:206:THR:HG23	2.07	0.55
1:A:147:SER:O	1:A:149:GLY:N	2.38	0.55
1:B:57:SER:OG	1:B:60:ILE:HG13	2.05	0.55
1:C:62:GLN:HE22	1:C:151:ILE:H	1.55	0.55
1:C:57:SER:HB3	1:C:60:ILE:HG13	1.88	0.55
1:A:107:ARG:HD2	1:B:107:ARG:CD	2.38	0.54
1:B:109:PRO:HD2	4:B:1177:HOH:O	2.09	0.53
1:B:62:GLN:C	1:B:63:LEU:HD12	2.29	0.53
1:C:160:LYS:HE2	4:C:1154:HOH:O	2.08	0.53
1:B:57:SER:HB2	4:B:1110:HOH:O	2.08	0.53
1:C:144:ASN:HB2	1:C:145:PRO:HD2	1.91	0.52
1:C:71:LYS:HE2	4:C:1127:HOH:O	2.10	0.51
1:A:71:LYS:HE3	4:A:1084:HOH:O	2.10	0.50
1:C:107:ARG:HG2	1:C:108:TRP:CD1	2.46	0.50
1:A:127:LYS:HA	1:A:137:GLN:NE2	2.26	0.50
1:B:66:THR:OG1	1:B:159:LYS:HE3	2.12	0.50
1:A:57:SER:HB3	1:A:60:ILE:HG13	1.92	0.50
1:C:136:LYS:HZ3	1:C:138:GLU:HG2	1.77	0.50
1:C:56:CYS:HB3	1:C:146:GLN:OE1	2.12	0.50
1:A:185:LYS:HE3	4:B:1165:HOH:O	2.11	0.49
1:B:170:GLU:N	1:B:170:GLU:CD	2.65	0.49
1:C:56:CYS:HB3	1:C:146:GLN:CD	2.33	0.49
1:A:152:GLU:HG2	1:A:156:LYS:HE2	1.95	0.49
1:A:107:ARG:HG3	1:B:83:TYR:OH	2.12	0.49
1:A:114:HIS:ND1	1:A:138:GLU:HB2	2.27	0.49
1:A:187:ARG:HB3	4:A:1099:HOH:O	2.13	0.48
1:A:107:ARG:HD2	1:B:107:ARG:HD2	1.95	0.48
1:B:200:ILE:HG23	1:B:201:VAL:N	2.28	0.48
1:B:58:PRO:HB3	1:B:203:ILE:HG22	1.94	0.48
1:A:106:GLY:HA3	4:B:1023:HOH:O	2.14	0.47
1:B:136:LYS:HE2	4:B:1037:HOH:O	2.14	0.47
1:A:83:TYR:CE2	1:A:85:GLU:HG3	2.49	0.47
1:C:168:GLN:HG2	4:C:1061:HOH:O	2.14	0.47
1:A:152:GLU:CG	1:A:156:LYS:HE2	2.44	0.47
1:A:122:THR:HG22	1:A:139:PHE:CE2	2.50	0.46
1:B:182:ILE:HG23	4:B:1056:HOH:O	2.15	0.46
1:B:114:HIS:HD2	1:B:138:GLU:HB2	1.79	0.46
1:B:146:GLN:O	1:B:147:SER:HB3	2.14	0.46
1:A:202:ASP:O	1:A:206:THR:HG23	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:107:ARG:HD2	1:B:107:ARG:HE	1.81	0.46
1:B:146:GLN:HA	1:C:145:PRO:C	2.37	0.45
1:C:101:LEU:HG	4:C:1166:HOH:O	2.16	0.45
1:A:71:LYS:HD2	1:A:172:LEU:HD23	1.99	0.45
1:B:168:GLN:CB	1:B:178:MET:HE1	2.47	0.45
1:C:165:VAL:O	1:C:168:GLN:HB2	2.16	0.44
1:C:124:THR:HG23	4:C:1030:HOH:O	2.18	0.44
1:C:168:GLN:HG3	4:C:1193:HOH:O	2.17	0.44
1:A:195:SER:OG	1:A:198:GLU:HG3	2.17	0.44
1:B:146:GLN:HG3	1:C:146:GLN:HB3	1.98	0.44
1:B:208:ILE:O	1:B:208:ILE:HG22	2.16	0.44
1:B:140:GLY:HA3	4:C:1063:HOH:O	2.19	0.43
1:A:147:SER:C	1:A:149:GLY:N	2.71	0.43
1:A:107:ARG:CD	1:B:107:ARG:HD2	2.49	0.43
1:A:158:LEU:O	1:A:162:ILE:HG13	2.20	0.42
1:C:168:GLN:HB3	1:C:178:MET:CE	2.50	0.42
1:C:63:LEU:HD21	4:C:1166:HOH:O	2.18	0.42
1:B:156:LYS:CE	1:C:156:LYS:NZ	2.81	0.42
1:B:160:LYS:O	1:B:164:GLN:HG3	2.20	0.41
1:B:136:LYS:HB2	4:B:1133:HOH:O	2.20	0.41
1:C:77:VAL:HG22	1:C:84:ILE:HG22	2.03	0.41
1:A:153:SER:HB2	4:A:1117:HOH:O	2.20	0.41
1:A:173:LYS:NZ	1:A:173:LYS:CB	2.82	0.41
1:A:191:ILE:HA	4:A:1085:HOH:O	2.20	0.41
1:B:157:GLU:O	1:B:161:ILE:HG13	2.21	0.40
1:B:77:VAL:HG22	1:B:84:ILE:HG22	2.03	0.40
1:C:190:GLY:C	1:C:191:ILE:HG13	2.42	0.40
1:A:117:ASN:CG	4:A:1108:HOH:O	2.59	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	146/154 (95%)	139 (95%)	7 (5%)	0	100	100
1	B	148/154 (96%)	139 (94%)	8 (5%)	1 (1%)	26	21
1	C	147/154 (96%)	143 (97%)	4 (3%)	0	100	100
All	All	441/462 (96%)	421 (96%)	19 (4%)	1 (0%)	52	53

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	147	SER

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	121/125 (97%)	118 (98%)	3 (2%)	55	59
1	B	123/125 (98%)	120 (98%)	3 (2%)	57	61
1	C	122/125 (98%)	120 (98%)	2 (2%)	70	76
All	All	366/375 (98%)	358 (98%)	8 (2%)	60	64

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

Mol	Chain	Res	Type
1	A	101	LEU
1	A	168	GLN
1	A	173	LYS
1	B	68	LEU
1	B	101	LEU
1	B	157	GLU
1	C	101	LEU
1	C	131	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	95	GLN
1	A	137	GLN
1	B	62	GLN
1	B	95	GLN
1	B	114	HIS
1	B	137	GLN
1	B	144	ASN
1	C	62	GLN
1	C	67	HIS
1	C	95	GLN
1	C	114	HIS
1	C	144	ASN
1	C	148	GLN
1	C	183	HIS

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 4 ligands modelled in this entry, 3 are monoatomic - leaving 1 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	$\# Z > 2$
3	100	A	1004	-	20,22,22	3.17	8 (40%)	21,31,31	3.76	6 (28%)

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
3	100	A	1004	-	-	0/4/12/12	0/3/3/3

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1004	100	C7-C11	-9.00	1.40	1.50
3	A	1004	100	N3-N1	2.41	1.38	1.34
3	A	1004	100	C1-C2	2.82	1.43	1.38
3	A	1004	100	C10-C2	3.51	1.43	1.36
3	A	1004	100	C6-C1	3.55	1.44	1.36
3	A	1004	100	C9-C8	4.45	1.47	1.38
3	A	1004	100	N2-N1	4.64	1.39	1.32
3	A	1004	100	C7-C4	5.11	1.46	1.42

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1004	100	N3-N1-N2	-7.33	104.05	109.54
3	A	1004	100	N4-C3-N3	-6.52	102.59	111.31
3	A	1004	100	N4-N2-N1	-6.01	105.04	109.54
3	A	1004	100	C10-C4-C5	-2.61	119.31	120.34
3	A	1004	100	C3-N4-N2	8.53	113.97	104.89
3	A	1004	100	C3-N3-N1	8.87	114.34	104.89

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1004	100	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

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.