



wwPDB X-ray Structure Validation Summary Report ⓘ

Jan 31, 2016 – 08:46 PM GMT

PDB ID : 1LV8
Title : Crystal structure of calf spleen purine nucleoside phosphorylase in a new space group with full trimer in the asymmetric unit
Authors : Bzowska, A.; Koellner, G.; Wielgus-Kutrowska, B.; Stroh, A.; Raszewski, G.; Holy, A.; Steiner, T.; Frank, J.
Deposited on : 2002-05-27
Resolution : 2.30 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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 (RC4), CSD as536be (2015)
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) : trunk26865

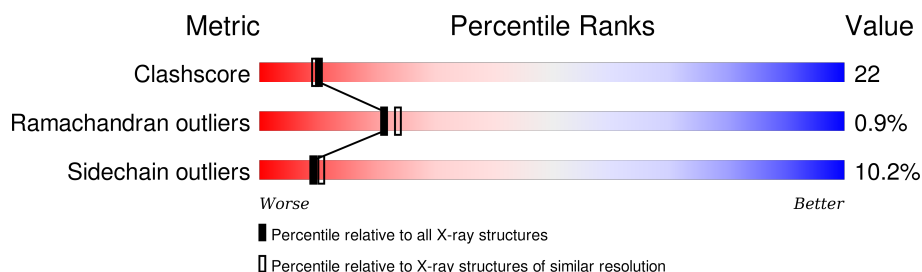
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	4452 (2.30-2.30)
Ramachandran outliers	100387	4410 (2.30-2.30)
Sidechain outliers	100360	4409 (2.30-2.30)

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	289	 61% 26% 5% 8%
1	B	289	 61% 24% 7% 8%
1	C	289	 61% 24% 7% 8%
1	D	289	 58% 29% 5% 8%
1	E	289	 61% 26% 8%
1	F	289	 60% 26% 6% 8%

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 13315 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 PURINE NUCLEOSIDE PHOSPHORYLASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	265	Total	C	N	O	S	0	0	0
			2074	1317	365	377	15			
1	B	265	Total	C	N	O	S	0	0	0
			2074	1317	365	377	15			
1	C	267	Total	C	N	O	S	0	0	0
			2087	1325	368	379	15			
1	D	265	Total	C	N	O	S	0	0	0
			2074	1317	365	377	15			
1	E	265	Total	C	N	O	S	0	0	0
			2074	1317	365	377	15			
1	F	266	Total	C	N	O	S	0	0	0
			2082	1323	367	377	15			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	144	GLN	GLU	CONFLICT	UNP P55859
B	1144	GLN	GLU	CONFLICT	UNP P55859
C	2144	GLN	GLU	CONFLICT	UNP P55859
D	144	GLN	GLU	CONFLICT	UNP P55859
E	1144	GLN	GLU	CONFLICT	UNP P55859
F	2144	GLN	GLU	CONFLICT	UNP P55859

- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

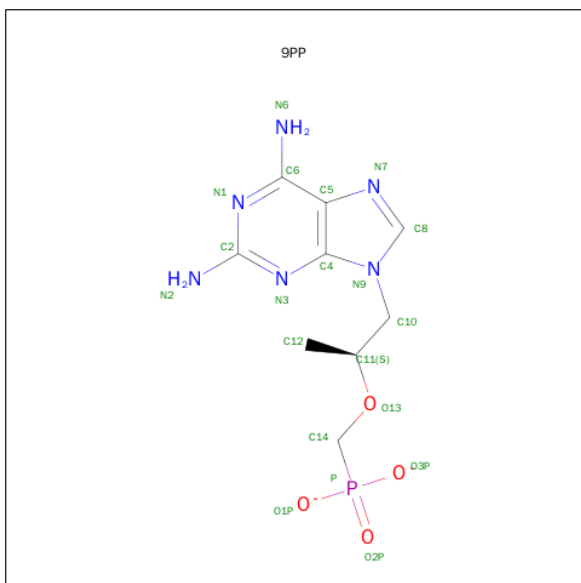
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	D	1	Total	Ca	0	0
			1	1		
2	E	1	Total	Ca	0	0
			1	1		
2	B	1	Total	Ca	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	C	1	Total	Ca	0	0
			1	1		
2	A	1	Total	Ca	0	0
			1	1		
2	F	1	Total	Ca	0	0
			1	1		

- Molecule 3 is 2,6-DIAMINO-(S)-9-[2-(PHOSPHONOMETHOXY)PROPYL]PURINE (three-letter code: 9PP) (formula: $C_9H_{13}N_6O_4P$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			20	9	6	4	1		
3	B	1	Total	C	N	O	P	0	0
			20	9	6	4	1		
3	C	1	Total	C	N	O	P	0	0
			20	9	6	4	1		
3	E	1	Total	C	N	O	P	0	0
			20	9	6	4	1		
3	F	1	Total	C	N	O	P	0	0
			20	9	6	4	1		
3	D	1	Total	C	N	O	P	0	0
			20	9	6	4	1		

- Molecule 4 is water.

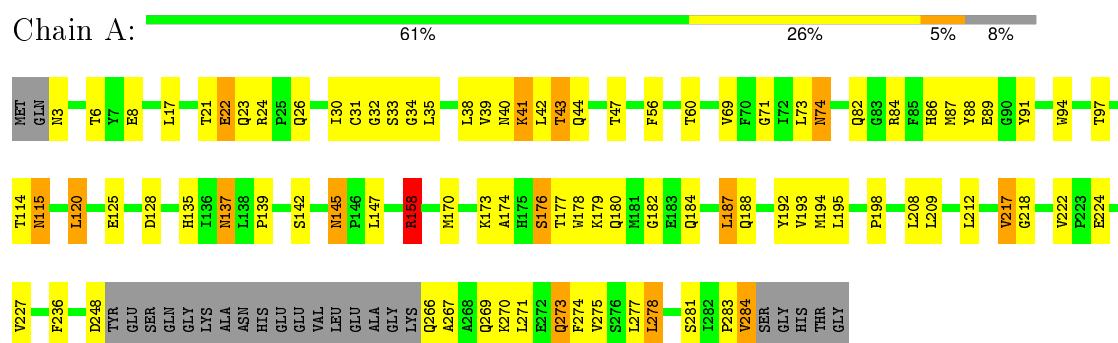
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	120	Total 120	O 120	0	0
4	B	134	Total 134	O 134	0	0
4	C	147	Total 147	O 147	0	0
4	D	99	Total 99	O 99	0	0
4	E	87	Total 87	O 87	0	0
4	F	137	Total 137	O 137	0	0

3 Residue-property plots

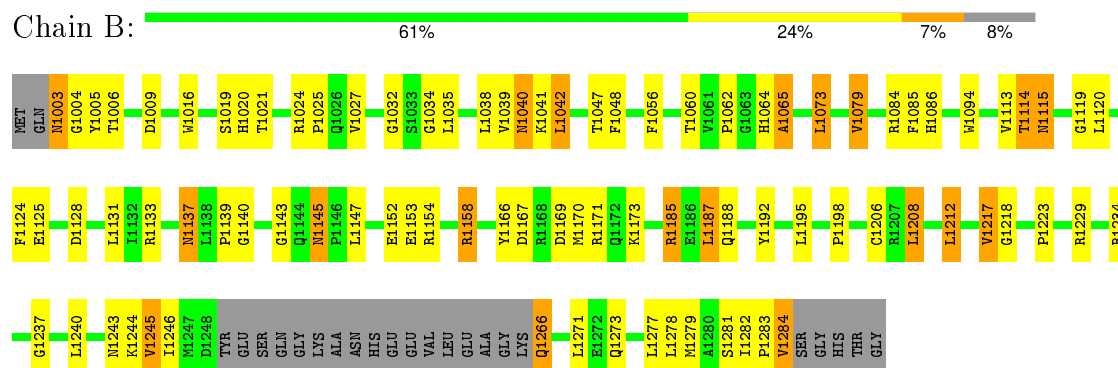
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according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

Note EDS was not executed.

• Molecule 1: PURINE NUCLEOSIDE PHOSPHORYLASE



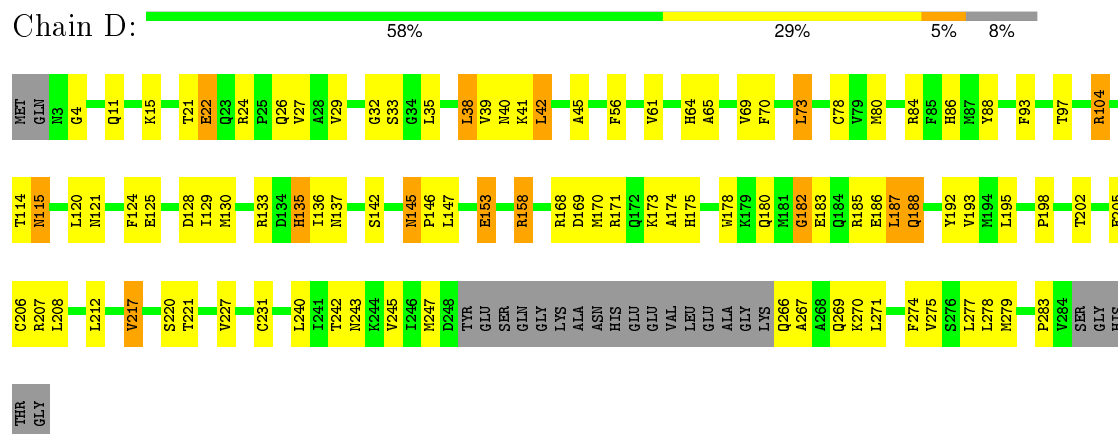
• Molecule 1: PURINE NUCLEOSIDE PHOSPHORYLASE



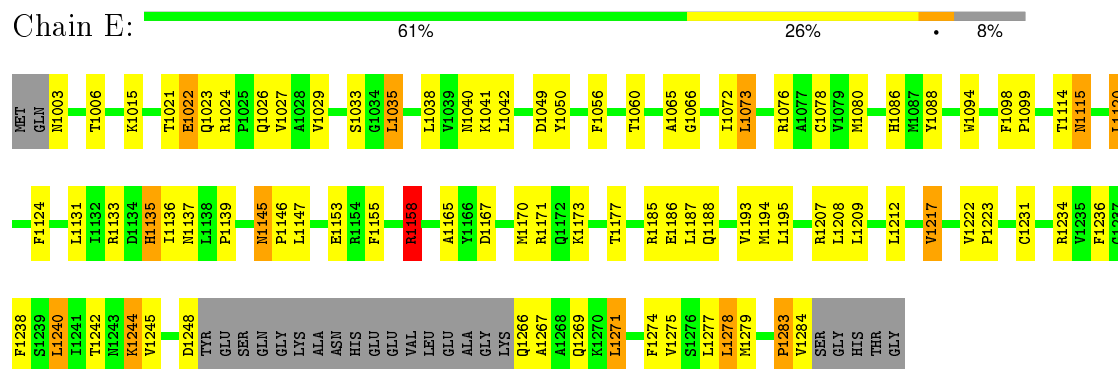
• Molecule 1: PURINE NUCLEOSIDE PHOSPHORYLASE



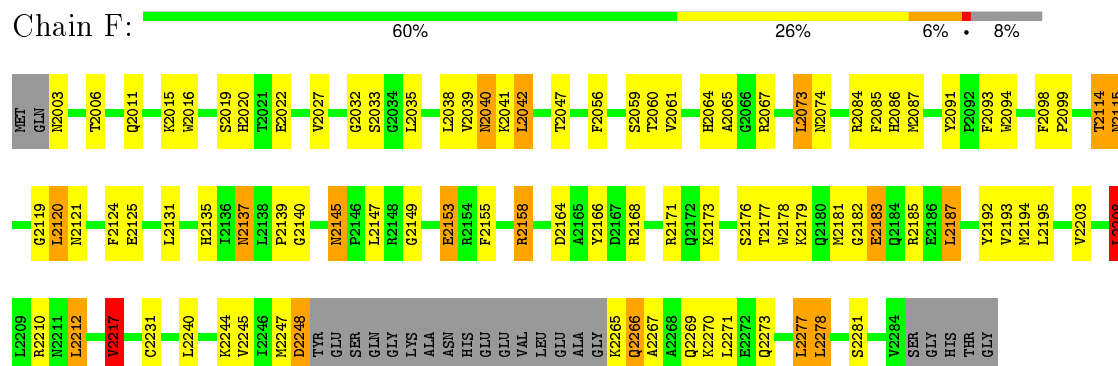
● Molecule 1: PURINE NUCLEOSIDE PHOSPHORYLASE



● Molecule 1: PURINE NUCLEOSIDE PHOSPHORYLASE



- Molecule 1: PURINE NUCLEOSIDE PHOSPHORYLASE



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	79.14Å 134.24Å 177.15Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.85 – 2.30	Depositor
% Data completeness (in resolution range)	99.7 (19.85-2.30)	Depositor
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS	Depositor
R, R_{free}	0.189 , 0.258	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	13315	wwPDB-VP
Average B, all atoms (Å ²)	42.0	wwPDB-VP

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: CA, 9PP

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	0.59	0/2121	0.79	1/2871 (0.0%)
1	B	0.62	0/2121	0.87	5/2871 (0.2%)
1	C	0.67	1/2134 (0.0%)	0.84	2/2887 (0.1%)
1	D	0.61	0/2121	0.78	1/2871 (0.0%)
1	E	0.54	0/2121	0.79	1/2871 (0.0%)
1	F	0.64	0/2129	0.85	4/2881 (0.1%)
All	All	0.61	1/12747 (0.0%)	0.82	14/17252 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	D	0	1
1	E	0	1
All	All	0	2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	2231	CYS	CB-SG	-6.40	1.71	1.82

The worst 5 of 14 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	1217	VAL	CB-CA-C	-7.79	96.61	111.40
1	F	2208	LEU	CA-CB-CG	6.61	130.49	115.30
1	F	2040	ASN	N-CA-C	-6.10	94.53	111.00
1	F	2042	LEU	CA-CB-CG	6.08	129.29	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	1040	ASN	N-CA-C	-5.92	95.02	111.00

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	88	TYR	Sidechain
1	E	1088	TYR	Sidechain

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	2074	0	2041	104	0
1	B	2074	0	2041	87	0
1	C	2087	0	2057	82	0
1	D	2074	0	2041	94	0
1	E	2074	0	2041	97	0
1	F	2082	0	2054	94	1
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
2	E	1	0	0	0	0
2	F	1	0	0	0	0
3	A	20	0	13	2	0
3	B	20	0	11	2	0
3	C	20	0	13	2	0
3	D	20	0	13	2	0
3	E	20	0	13	1	0
3	F	20	0	13	2	0
4	A	120	0	0	8	0
4	B	134	0	0	9	0
4	C	147	0	0	3	0
4	D	99	0	0	3	1
4	E	87	0	0	7	0
4	F	137	0	0	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	13315	0	12351	543	1

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 22.

The worst 5 of 543 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:C:2173:LYS:HD3	1:C:2281:SER:HB3	1.23	1.16
1:B:1125:GLU:HG2	1:B:1185:ARG:HH21	1.15	1.09
1:E:1267:ALA:HA	1:E:1269:GLN:HE22	1.12	1.08
1:D:39:VAL:HA	1:D:80:MET:HE1	1.36	1.06
1:B:1145:ASN:HD22	1:B:1147:LEU:H	1.06	1.00

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:2073:LEU:O	4:D:7002:HOH:O[4_448]	2.06	0.14

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	261/289 (90%)	241 (92%)	16 (6%)	4 (2%)	13	12
1	B	261/289 (90%)	247 (95%)	13 (5%)	1 (0%)	39	48
1	C	263/289 (91%)	247 (94%)	13 (5%)	3 (1%)	17	18
1	D	261/289 (90%)	245 (94%)	13 (5%)	3 (1%)	17	18
1	E	261/289 (90%)	244 (94%)	16 (6%)	1 (0%)	39	48

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	F	262/289 (91%)	250 (95%)	10 (4%)	2 (1%)	24	27
All	All	1569/1734 (90%)	1474 (94%)	81 (5%)	14 (1%)	21	24

5 of 14 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	74	ASN
1	B	1065	ALA
1	C	2065	ALA
1	D	65	ALA
1	A	182	GLY

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	221/239 (92%)	200 (90%)	21 (10%)	11	12
1	B	221/239 (92%)	196 (89%)	25 (11%)	7	8
1	C	222/239 (93%)	197 (89%)	25 (11%)	7	8
1	D	221/239 (92%)	198 (90%)	23 (10%)	9	10
1	E	221/239 (92%)	201 (91%)	20 (9%)	12	14
1	F	222/239 (93%)	200 (90%)	22 (10%)	10	11
All	All	1328/1434 (93%)	1192 (90%)	136 (10%)	9	10

5 of 136 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	2194	MET
1	D	104	ARG
1	F	2187	LEU
1	C	2208	LEU
1	C	2277	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 58 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	2199	ASN
1	D	144	GLN
1	F	2145	ASN
1	C	2266	GLN
1	D	86	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 12 ligands modelled in this entry, 6 are monoatomic - leaving 6 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	9PP	A	3001	-	17,21,21	5.13	8 (47%)	15,31,31	1.53	4 (26%)
3	9PP	B	3002	-	17,21,21	5.00	7 (41%)	15,31,31	1.53	3 (20%)
3	9PP	C	3003	-	17,21,21	5.13	6 (35%)	15,31,31	1.45	3 (20%)
3	9PP	D	3006	-	17,21,21	5.62	8 (47%)	15,31,31	1.51	3 (20%)
3	9PP	E	3004	-	17,21,21	5.86	7 (41%)	15,31,31	1.63	3 (20%)
3	9PP	F	3005	-	17,21,21	5.19	9 (52%)	15,31,31	1.48	2 (13%)

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	9PP	A	3001	-	-	0/6/10/10	0/2/2/2
3	9PP	B	3002	-	-	0/6/10/10	0/2/2/2
3	9PP	C	3003	-	-	0/6/10/10	0/2/2/2
3	9PP	D	3006	-	-	0/6/10/10	0/2/2/2
3	9PP	E	3004	-	-	0/6/10/10	0/2/2/2
3	9PP	F	3005	-	-	0/6/10/10	0/2/2/2

The worst 5 of 45 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	3004	9PP	P-C14	-20.83	1.53	1.79
3	D	3006	9PP	P-C14	-19.25	1.55	1.79
3	A	3001	9PP	P-C14	-18.14	1.56	1.79
3	F	3005	9PP	P-C14	-18.02	1.56	1.79
3	B	3002	9PP	P-C14	-17.70	1.57	1.79

The worst 5 of 18 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	3004	9PP	C14-O13-C11	-3.48	111.56	114.35
3	B	3002	9PP	N3-C2-N1	-3.16	122.62	127.44
3	E	3004	9PP	N3-C2-N1	-3.09	122.74	127.44
3	D	3006	9PP	N3-C2-N1	-2.96	122.94	127.44
3	A	3001	9PP	N3-C2-N1	-2.90	123.03	127.44

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

6 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	3001	9PP	2	0
3	B	3002	9PP	2	0
3	C	3003	9PP	2	0
3	D	3006	9PP	2	0
3	E	3004	9PP	1	0
3	F	3005	9PP	2	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 ⓘ

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates ⓘ

EDS was not executed - this section will therefore be empty.

6.4 Ligands ⓘ

EDS was not executed - this section will therefore be empty.

6.5 Other polymers ⓘ

EDS was not executed - this section will therefore be empty.