



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 01:10 AM UTC

PDB ID : 1FS5 / pdb_00001fs5
Title : A DISCOVERY OF THREE ALTERNATE CONFORMATIONS IN THE
ACTIVE SITE OF GLUCOSAMINE-6-PHOSPHATE ISOMERASE
Authors : Rudino-Pinera, E.; Morales-Arrieta, S.; Rojas-Trejo, S.P.; Horjales, E.
Deposited on : 2000-09-08
Resolution : 1.73 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

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

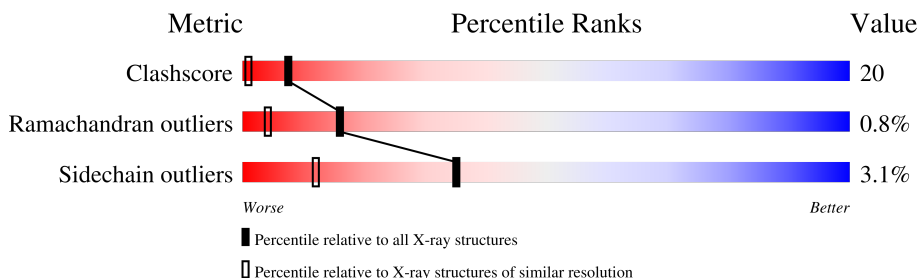
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.73 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	190562	1207 (1.74-1.74)
Ramachandran outliers	187476	1200 (1.74-1.74)
Sidechain outliers	187428	1200 (1.74-1.74)

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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. 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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	266	 76% 22% .
1	B	266	 70% 27% .

2 Entry composition [i](#)

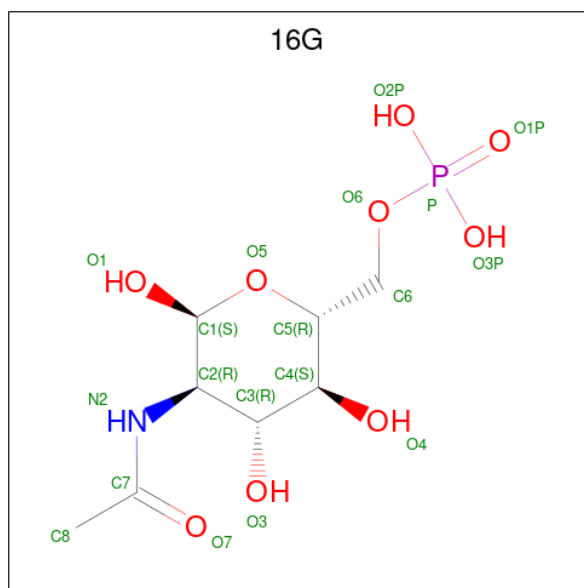
There are 4 unique types of molecules in this entry. The entry contains 6306 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 GLUCOSAMINE-6-PHOSPHATE DEAMINASE.

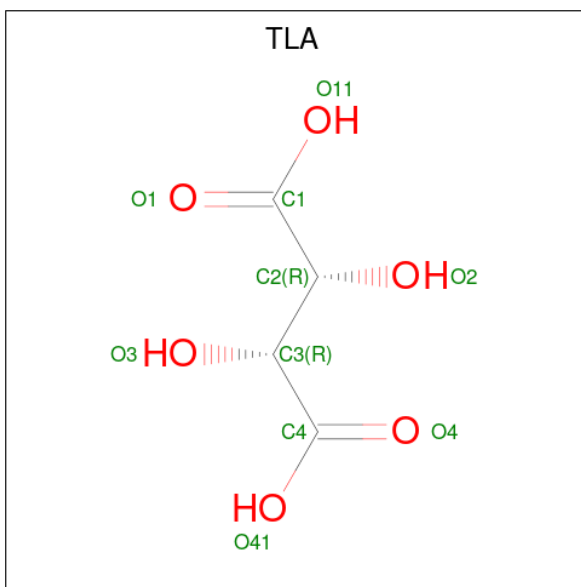
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	266	Total	C	N	O	S	0	9	0
			2246	1416	390	426	14			
1	B	266	Total	C	N	O	S	0	55	0
			2974	1878	520	562	14			

- Molecule 2 is 2-acetamido-2-deoxy-6-O-phosphono-alpha-D-glucopyranose (CCD ID: 16G) (formula: C₈H₁₆NO₉P).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			19	8	1	9	1		
2	B	1	Total	C	N	O	P	0	0
			19	8	1	9	1		

- Molecule 3 is L(+)-TARTARIC ACID (CCD ID: TLA) (formula: C₄H₆O₆).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			10	4	6		

- Molecule 4 is water.

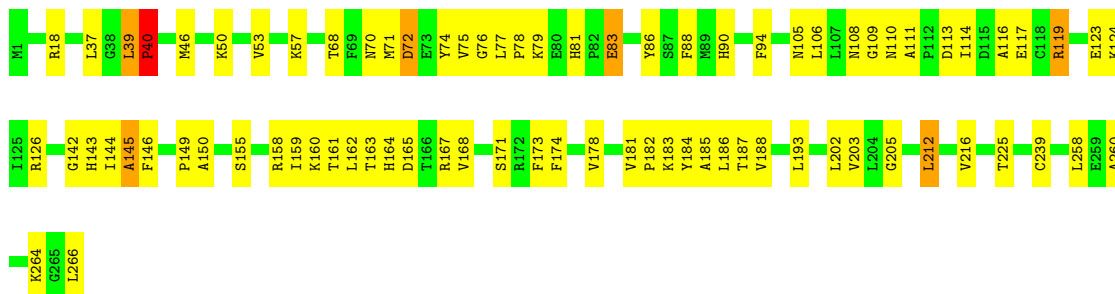
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	537	Total	O	0	0
			537	537		
4	B	501	Total	O	0	0
			501	501		

Note EDS was not executed.

Chain A: 76% 22% 2%



Chain B: 70% 27%



4 Data and refinement statistics

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

Property	Value	Source
Space group	H 3 2	Depositor
Cell constants a, b, c, α , β , γ	124.23Å 124.23Å 222.72Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	50.00 – 1.73	Depositor
% Data completeness (in resolution range)	95.9 (50.00-1.73)	Depositor
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS	Depositor
R, R_{free}	0.212 , 0.251	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	6306	wwPDB-VP
Average B, all atoms (Å ²)	25.0	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: 16G, TLA

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	1/2293 (0.0%)	0.88	10/3102 (0.3%)
1	B	0.39	0/3041	0.77	7/4118 (0.2%)
All	All	0.39	1/5334 (0.0%)	0.82	17/7220 (0.2%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	266	LEU	C-OXT	5.38	1.34	1.23

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	266	LEU	CA-C-O	-7.23	99.30	121.00
1	A	205	GLY	N-CA-C	6.78	121.22	112.68
1	A	144	ILE	N-CA-C	-6.45	99.14	108.17
1	A	245	MET	N-CA-C	6.22	118.86	111.71
1	A	216	VAL	N-CA-C	6.16	117.18	111.45
1	B	72	ASP	N-CA-C	6.11	116.62	108.38
1	B	216	VAL	N-CA-C	6.05	117.08	111.45
1	A	239	CYS	N-CA-C	5.89	119.14	109.72
1	B	71	MET	N-CA-C	5.82	118.57	111.82
1	A	114	ILE	N-CA-C	5.66	115.85	110.42
1	B	188	VAL	N-CA-C	-5.50	103.99	110.21
1	B	239	CYS	N-CA-C	5.40	118.39	109.85
1	A	188	VAL	N-CA-C	-5.21	102.87	109.80
1	A	72	ASP	N-CA-C	5.13	115.31	108.38
1	B	39	LEU	N-CA-C	5.12	117.92	109.58
1	B	205	GLY	N-CA-C	5.10	118.65	112.48
1	A	186	LEU	N-CA-C	-5.04	101.03	109.24

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	2246	0	2210	75	0
1	B	2974	0	2907	137	0
2	A	19	0	14	0	0
2	B	19	0	14	0	0
3	A	10	0	4	0	0
4	A	537	0	0	12	1
4	B	501	0	0	6	2
All	All	6306	0	5149	212	3

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 20.

All (212) 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:B:77[B]:LEU:HD21	1:B:174[B]:PHE:CE2	1.62	1.31
1:B:146[A]:PHE:CD1	1:B:162[A]:LEU:HD21	1.73	1.23
1:A:14[C]:LYS:NZ	1:A:266:LEU:HD23	1.59	1.16
1:A:14[C]:LYS:HZ1	1:A:266:LEU:HD23	1.21	0.97
1:B:77[B]:LEU:HG	1:B:182[B]:PRO:HG2	1.45	0.96
1:B:146[A]:PHE:HD1	1:B:162[A]:LEU:HD21	1.17	0.96
1:A:36:VAL:H	1:A:132:HIS:HD2	1.14	0.96
1:B:77[B]:LEU:HG	1:B:182[B]:PRO:CG	1.98	0.94
1:B:77[B]:LEU:HD21	1:B:174[B]:PHE:CZ	2.03	0.94
1:B:77[B]:LEU:HD11	1:B:174[B]:PHE:HZ	1.33	0.93
1:B:77[B]:LEU:N	1:B:182[B]:PRO:HG3	1.84	0.93
1:A:21:VAL:HG22	1:A:61:VAL:HG21	1.49	0.92
1:B:77[B]:LEU:HD21	1:B:174[B]:PHE:HE2	1.15	0.91
1:A:207[C]:GLN:NE2	1:A:207[C]:GLN:H	1.69	0.90
1:A:265:GLY:O	1:A:266:LEU:HB2	1.71	0.89
1:B:146[A]:PHE:HD1	1:B:162[A]:LEU:CD2	1.87	0.87

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:119:ARG:NH2	4:B:2586:HOH:O	2.10	0.84
1:A:14[C]:LYS:HZ3	1:A:266:LEU:HB3	1.42	0.83
1:A:172:ARG:NH1	4:A:1668:HOH:O	2.13	0.81
1:B:77[B]:LEU:HD11	1:B:174[B]:PHE:CZ	2.17	0.79
1:B:143:HIS:HA	1:B:225:THR:HG22	1.63	0.78
1:B:77[B]:LEU:CD2	1:B:174[B]:PHE:HE2	1.97	0.77
1:B:146[A]:PHE:CD1	1:B:162[A]:LEU:CD2	2.61	0.76
1:A:207[B]:GLN:HE21	1:A:207[B]:GLN:H	1.34	0.75
1:A:10[A]:GLU:O	1:A:14[A]:LYS:HD3	1.85	0.74
1:A:36:VAL:H	1:A:132:HIS:CD2	2.01	0.74
1:B:119:ARG:HH21	1:B:123[B]:GLU:CD	1.95	0.73
1:A:21:VAL:HG13	1:A:61:VAL:HG22	1.69	0.73
1:B:143:HIS:HA	1:B:225:THR:CG2	2.17	0.73
1:B:77[B]:LEU:HG	1:B:182[B]:PRO:CD	2.19	0.72
1:B:144[C]:ILE:HD13	1:B:193:LEU:HD13	1.72	0.71
1:A:266:LEU:HD22	4:A:1482:HOH:O	1.90	0.71
1:B:77[B]:LEU:CD2	1:B:174[B]:PHE:CE2	2.58	0.71
1:B:77[B]:LEU:N	1:B:182[B]:PRO:CG	2.54	0.71
1:A:14[C]:LYS:CE	1:A:266:LEU:HD23	2.21	0.71
1:B:75[B]:VAL:HB	1:B:184[B]:TYR:C	2.15	0.70
1:B:146[A]:PHE:CE1	1:B:162[A]:LEU:HD21	2.24	0.70
1:A:265:GLY:O	1:A:266:LEU:CB	2.39	0.70
1:B:146[A]:PHE:HE1	1:B:162[A]:LEU:HD11	1.54	0.70
1:B:167[B]:ARG:HH12	1:B:183[B]:LYS:HE2	1.57	0.69
1:B:144[B]:ILE:HD13	1:B:193:LEU:HD13	1.75	0.68
1:A:207[B]:GLN:H	1:A:207[B]:GLN:NE2	1.92	0.68
1:A:14[C]:LYS:HZ3	1:A:266:LEU:HD23	1.58	0.68
1:A:172:ARG:NH1	4:A:1538:HOH:O	2.28	0.67
1:B:114[B]:ILE:H	1:B:114[B]:ILE:HD12	1.60	0.67
1:A:50:LYS:O	1:A:54:GLU:HG3	1.95	0.67
1:B:258:LEU:C	1:B:258:LEU:HD23	2.18	0.67
1:B:75[B]:VAL:HG23	1:B:185[B]:ALA:HA	1.76	0.66
1:B:77[B]:LEU:H	1:B:182[B]:PRO:CG	2.08	0.66
1:B:114[B]:ILE:HG23	1:B:186:LEU:HD21	1.78	0.66
1:B:75[B]:VAL:HB	1:B:184[B]:TYR:HB2	1.77	0.66
1:A:265:GLY:O	1:A:266:LEU:HD13	1.96	0.66
1:B:159:ILE:HD11	1:B:184[B]:TYR:HB3	1.76	0.65
1:A:64[B]:LYS:NZ	1:A:98:ASP:HB2	2.11	0.65
1:B:108:ASN:ND2	1:B:110[C]:ASN:H	1.94	0.65
1:A:78:PRO:HG2	1:A:81:HIS:HB2	1.77	0.64
1:B:258:LEU:HD23	1:B:258:LEU:O	1.97	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:21:VAL:CG2	1:A:61:VAL:HG21	2.24	0.64
1:B:146[A]:PHE:HB2	1:B:187:THR:HB	1.79	0.64
1:A:77:LEU:HD23	1:A:78:PRO:HD2	1.78	0.64
1:B:119:ARG:NH2	1:B:123[B]:GLU:OE2	2.31	0.64
1:B:18:ARG:HD2	4:B:2357:HOH:O	1.98	0.63
1:B:146[A]:PHE:CE1	1:B:162[A]:LEU:HD11	2.34	0.63
1:B:75[B]:VAL:HB	1:B:184[B]:TYR:O	1.99	0.63
1:B:160[B]:LYS:HZ2	1:B:161[B]:THR:H	1.45	0.62
1:A:80:GLU:H	1:A:80:GLU:CD	2.08	0.62
1:B:114[C]:ILE:HD12	1:B:114[C]:ILE:N	2.16	0.61
1:B:77[B]:LEU:CD1	1:B:174[B]:PHE:HZ	2.12	0.61
1:B:114[B]:ILE:HG21	1:B:159:ILE:HD12	1.83	0.60
1:B:77[A]:LEU:HD12	1:B:78[A]:PRO:HD2	1.83	0.60
1:B:77[B]:LEU:CG	1:B:182[B]:PRO:HG2	2.27	0.59
1:B:108:ASN:ND2	1:B:110[A]:ASN:H	1.99	0.59
1:B:146[A]:PHE:HB2	1:B:187:THR:CB	2.33	0.59
1:A:253:ARG:O	1:A:257:GLU:HG3	2.02	0.59
1:B:108:ASN:HB3	1:B:117[B]:GLU:OE1	2.01	0.59
1:B:109[B]:GLY:C	1:B:111[B]:ALA:H	2.10	0.59
1:B:75[B]:VAL:HG23	1:B:185[B]:ALA:CA	2.32	0.59
1:B:119:ARG:O	1:B:123[C]:GLU:HG3	2.02	0.59
1:A:241:GLU:HB3	1:A:242:PRO:HD3	1.85	0.58
1:A:14[C]:LYS:NZ	1:A:266:LEU:CD2	2.51	0.58
1:A:108:ASN:ND2	1:A:110:ASN:H	2.00	0.58
1:A:207[C]:GLN:H	1:A:207[C]:GLN:HE21	1.46	0.58
1:A:116:ALA:O	1:A:120[B]:GLN:HG3	2.04	0.58
1:B:142:GLY:O	1:B:225:THR:HG22	2.04	0.57
1:A:207[A]:GLN:H	1:A:207[A]:GLN:CD	2.13	0.57
1:B:18:ARG:NH1	4:B:2357:HOH:O	2.36	0.57
1:B:167[A]:ARG:HH12	1:B:183[A]:LYS:HE2	1.68	0.57
1:A:265:GLY:O	1:A:266:LEU:CD1	2.52	0.57
1:B:146[A]:PHE:HE1	1:B:162[A]:LEU:CD1	2.18	0.57
1:A:265:GLY:C	1:A:266:LEU:CD1	2.78	0.56
1:B:77[C]:LEU:HG	1:B:182[C]:PRO:HG2	1.87	0.56
1:B:53:VAL:O	1:B:57:LYS:HG2	2.05	0.56
1:B:119:ARG:NE	1:B:123[C]:GLU:OE2	2.38	0.56
1:B:83[B]:GLU:HG3	1:B:173[B]:PHE:HB3	1.88	0.56
1:B:168[C]:VAL:HG22	1:B:178[C]:VAL:HG21	1.86	0.56
1:B:114[B]:ILE:HD12	1:B:114[B]:ILE:N	2.20	0.56
1:B:75[B]:VAL:N	1:B:184[B]:TYR:O	2.38	0.55
1:B:119:ARG:NE	4:B:2618:HOH:O	2.40	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:114[C]:ILE:HG23	1:B:186:LEU:HD21	1.87	0.55
1:A:77:LEU:CD2	1:A:78:PRO:HD2	2.36	0.55
1:A:116:ALA:O	1:A:120[C]:GLN:HG3	2.07	0.55
1:A:106:LEU:HB3	4:A:1404:HOH:O	2.06	0.55
1:A:108:ASN:C	1:A:108:ASN:HD22	2.14	0.55
1:B:167[B]:ARG:NH1	1:B:183[B]:LYS:HE2	2.22	0.54
1:B:149:PRO:O	1:B:150:ALA:HB3	2.08	0.53
1:B:76[B]:GLY:HA3	1:B:182[B]:PRO:HB3	1.91	0.53
1:B:108:ASN:HB3	1:B:117[B]:GLU:CD	2.33	0.53
1:A:14[B]:LYS:NZ	1:A:266:LEU:HD23	2.22	0.53
1:B:119:ARG:CZ	1:B:123[B]:GLU:OE2	2.57	0.53
1:A:229:LEU:HB2	4:A:1506:HOH:O	2.09	0.52
1:B:167[B]:ARG:CZ	1:B:183[B]:LYS:HG2	2.39	0.52
1:A:14[C]:LYS:HZ3	1:A:266:LEU:CB	2.18	0.52
1:B:18:ARG:CZ	4:B:2735:HOH:O	2.58	0.52
1:B:114[A]:ILE:HD13	1:B:159:ILE:HD12	1.92	0.51
1:A:143:HIS:HD1	1:A:143:HIS:C	2.19	0.51
1:B:81[A]:HIS:CE1	1:B:83[A]:GLU:HB2	2.46	0.51
1:B:163[C]:THR:HG22	1:B:165[C]:ASP:H	1.75	0.51
1:B:203:VAL:HG11	1:B:212:LEU:HG	1.92	0.51
1:B:163[C]:THR:O	1:B:167[C]:ARG:HG3	2.10	0.51
1:B:258:LEU:C	1:B:258:LEU:CD2	2.84	0.51
1:B:160[B]:LYS:NZ	1:B:161[B]:THR:H	2.09	0.50
1:B:46:MET:HE3	1:B:50:LYS:NZ	2.25	0.50
1:B:119:ARG:NE	1:B:123[B]:GLU:OE2	2.45	0.50
1:B:159:ILE:HD11	1:B:184[C]:TYR:HB3	1.94	0.50
1:B:76[B]:GLY:C	1:B:182[B]:PRO:HG3	2.36	0.50
1:A:205:GLY:HA3	1:A:207[C]:GLN:OE1	2.12	0.50
1:B:77[B]:LEU:CD2	1:B:174[B]:PHE:CZ	2.88	0.50
1:A:53:VAL:O	1:A:57:LYS:HG2	2.12	0.49
1:B:74[A]:TYR:CE1	1:B:182[A]:PRO:HB2	2.47	0.49
1:B:75[B]:VAL:HB	1:B:184[B]:TYR:CB	2.41	0.49
1:B:144[A]:ILE:HG13	1:B:225:THR:HG23	1.94	0.49
1:B:184[A]:TYR:O	1:B:185[A]:ALA:HB2	2.12	0.49
1:A:172:ARG:NH2	4:A:1751:HOH:O	2.46	0.49
1:A:163[A]:THR:HG22	1:A:165:ASP:H	1.77	0.49
1:B:164[A]:HIS:O	1:B:168[A]:VAL:HG23	2.12	0.49
1:B:146[A]:PHE:CE2	1:B:185[A]:ALA:CB	2.96	0.49
1:B:114[B]:ILE:H	1:B:114[B]:ILE:CD1	2.25	0.48
1:B:164[B]:HIS:O	1:B:168[B]:VAL:HG23	2.13	0.48
1:A:64[B]:LYS:HZ2	1:A:98:ASP:HB2	1.78	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:88:PHE:CD1	1:A:88:PHE:C	2.91	0.48
1:B:90:HIS:HA	1:B:94:PHE:HB2	1.94	0.47
1:B:74[A]:TYR:O	1:B:109[A]:GLY:HA3	2.15	0.47
1:A:117:GLU:O	1:A:120[A]:GLN:HG2	2.14	0.47
1:B:266[A]:LEU:N	1:B:266[A]:LEU:HD12	2.30	0.47
1:A:56:HIS:HD2	1:A:61:VAL:O	1.99	0.46
1:A:149:PRO:O	1:A:150:ALA:HB3	2.15	0.46
1:A:265:GLY:C	1:A:266:LEU:HD12	2.40	0.46
1:A:90:HIS:HA	1:A:94:PHE:HB2	1.96	0.46
1:B:75[B]:VAL:CB	1:B:184[B]:TYR:O	2.63	0.46
1:B:83[C]:GLU:OE1	1:B:173[C]:PHE:HB3	2.16	0.46
1:B:18:ARG:CZ	4:B:2357:HOH:O	2.64	0.46
1:B:113[A]:ASP:HB3	1:B:116[A]:ALA:HB3	1.98	0.46
1:B:68:THR:O	1:B:105:ASN:HB2	2.14	0.45
1:A:70:ASN:HB2	1:A:106:LEU:HD23	1.99	0.45
1:B:168[C]:VAL:HG22	1:B:178[C]:VAL:CG2	2.47	0.45
1:A:64[C]:LYS:HG2	1:A:98:ASP:OD2	2.17	0.45
1:B:108:ASN:HD22	1:B:110[C]:ASN:H	1.60	0.45
1:B:159:ILE:HD11	1:B:184[C]:TYR:CG	2.52	0.45
1:B:143:HIS:HA	1:B:225:THR:HG21	1.98	0.45
1:B:72:ASP:HB2	1:B:146[A]:PHE:CE2	2.52	0.45
1:B:163[B]:THR:HG22	1:B:165[B]:ASP:H	1.82	0.45
1:A:236:ILE:HD11	4:A:1560:HOH:O	2.17	0.44
1:B:77[B]:LEU:CG	1:B:182[B]:PRO:CG	2.83	0.44
1:B:260:ALA:O	1:B:264[C]:LYS:HG3	2.16	0.44
1:A:10[B]:GLU:OE1	1:A:10[B]:GLU:HA	2.16	0.44
1:A:207[C]:GLN:NE2	1:A:207[C]:GLN:N	2.52	0.44
1:B:74[C]:TYR:HB3	1:B:182[C]:PRO:HG2	2.00	0.44
1:B:167[C]:ARG:O	1:B:171[C]:SER:HB3	2.18	0.44
1:B:159:ILE:HD11	1:B:184[C]:TYR:CB	2.47	0.44
1:B:144[C]:ILE:O	1:B:145[C]:ALA:HB3	2.18	0.44
1:A:20:ILE:HD13	4:A:1775:HOH:O	2.18	0.44
1:B:109[B]:GLY:C	1:B:111[B]:ALA:N	2.76	0.44
1:B:146[A]:PHE:CE2	1:B:185[A]:ALA:HB1	2.53	0.44
1:B:167[A]:ARG:NH1	1:B:183[A]:LYS:HE2	2.33	0.44
1:B:126[A]:ARG:HH11	1:B:126[A]:ARG:HG3	1.82	0.43
1:B:260:ALA:O	1:B:264[B]:LYS:HG3	2.17	0.43
1:B:75[B]:VAL:CB	1:B:184[B]:TYR:HB2	2.46	0.43
1:A:21:VAL:HG13	1:A:61:VAL:CG2	2.44	0.43
1:B:119:ARG:HH21	1:B:123[C]:GLU:CD	2.27	0.43
1:A:108:ASN:HD22	1:A:110:ASN:H	1.66	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:151:SER:O	1:A:222:HIS:HB2	2.19	0.43
1:B:77[B]:LEU:HD23	1:B:77[B]:LEU:HA	1.45	0.43
1:A:56:HIS:HE1	4:A:1514:HOH:O	2.02	0.43
1:A:80:GLU:CD	1:A:80:GLU:N	2.76	0.43
1:A:3:LEU:C	1:A:3:LEU:HD23	2.44	0.42
1:B:70:ASN:HB2	1:B:106:LEU:HD23	2.01	0.42
1:A:259:GLU:O	1:A:263:ILE:HG23	2.19	0.42
1:A:177:ASP:CG	1:A:180:GLN:HG3	2.45	0.42
1:B:72:ASP:OD2	1:B:145[A]:ALA:HB1	2.20	0.42
1:B:88:PHE:CD1	1:B:88:PHE:C	2.98	0.42
1:B:167[B]:ARG:HA	1:B:181[B]:VAL:HG11	2.00	0.42
1:B:146[A]:PHE:O	1:B:160[A]:LYS:HG2	2.20	0.42
1:B:174[B]:PHE:CD1	1:B:174[B]:PHE:N	2.86	0.42
1:A:21:VAL:CG1	1:A:61:VAL:HG22	2.46	0.41
1:A:120[A]:GLN:HG3	4:A:1675:HOH:O	2.20	0.41
1:A:207[C]:GLN:HE21	1:A:207[C]:GLN:N	2.15	0.41
1:A:3:LEU:O	1:A:5:PRO:HD3	2.21	0.41
1:B:39:LEU:HA	1:B:40:PRO:HD3	1.95	0.41
1:B:119:ARG:NH2	1:B:123[B]:GLU:CD	2.68	0.41
1:A:130:LYS:HE2	4:A:1450:HOH:O	2.20	0.41
1:B:77[B]:LEU:H	1:B:182[B]:PRO:HG2	1.83	0.41
1:A:108:ASN:ND2	1:A:108:ASN:C	2.74	0.41
1:A:143:HIS:C	1:A:143:HIS:ND1	2.78	0.41
1:B:146[A]:PHE:HB2	1:B:187:THR:CG2	2.51	0.41
1:B:144[A]:ILE:O	1:B:145[A]:ALA:HB3	2.21	0.40
1:B:146[A]:PHE:CZ	1:B:185[A]:ALA:CB	3.03	0.40
1:B:155:SER:HB2	1:B:158:ARG:CZ	2.51	0.40
1:A:257:GLU:HB2	4:A:1532:HOH:O	2.22	0.40
1:B:79[A]:LYS:HD2	1:B:86:TYR:CE2	2.56	0.40
1:B:167[A]:ARG:NH1	1:B:183[A]:LYS:HG2	2.35	0.40
1:B:162[C]:LEU:HD12	1:B:182[C]:PRO:O	2.20	0.40
1:B:163[C]:THR:HG22	1:B:164[C]:HIS:N	2.36	0.40

All (3) 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)
4:B:2660:HOH:O	4:B:2660:HOH:O[3_555]	2.00	0.20
4:B:2273:HOH:O	4:B:2273:HOH:O[18_445]	2.09	0.11
4:A:1472:HOH:O	4:A:1472:HOH:O[6_555]	2.15	0.05

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	282/266 (106%)	271 (96%)	9 (3%)	2 (1%)	18	6
1	B	372/266 (140%)	338 (91%)	30 (8%)	4 (1%)	11	2
All	All	654/532 (123%)	609 (93%)	39 (6%)	6 (1%)	16	3

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	265	GLY
1	A	40	PRO
1	B	145[A]	ALA
1	B	145[B]	ALA
1	B	145[C]	ALA
1	B	40	PRO

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	245/227 (108%)	238 (97%)	7 (3%)	37	14
1	B	321/227 (141%)	312 (97%)	9 (3%)	38	15
All	All	566/454 (125%)	550 (97%)	16 (3%)	35	15

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	37	LEU
1	A	40	PRO
1	A	77	LEU
1	A	80	GLU
1	A	124	LYS
1	A	143	HIS
1	A	212	LEU
1	B	37	LEU
1	B	40	PRO
1	B	83[A]	GLU
1	B	83[B]	GLU
1	B	83[C]	GLU
1	B	119	ARG
1	B	124	LYS
1	B	202	LEU
1	B	212	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	22	ASN
1	A	56	HIS
1	A	108	ASN
1	A	110	ASN
1	A	132	HIS
1	A	140	ASN
1	A	176	ASN
1	A	180	GLN
1	B	22	ASN
1	B	108	ASN
1	B	143	HIS
1	B	262	ASN

5.3.3 RNA ⓘ

There are no RNA molecules 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 [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

3 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
3	TLA	A	1268	-	9,9,9	2.42	5 (55%)	12,12,12	2.68	6 (50%)
2	16G	A	1267	-	19,19,19	1.48	5 (26%)	27,28,28	1.68	9 (33%)
2	16G	B	2267	-	19,19,19	1.45	5 (26%)	27,28,28	1.59	7 (25%)

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	TLA	A	1268	-	-	2/12/12/12	-
2	16G	A	1267	-	-	4/10/30/30	0/1/1/1
2	16G	B	2267	-	-	4/10/30/30	0/1/1/1

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1268	TLA	O1-C1	4.22	1.34	1.22
3	A	1268	TLA	O41-C4	-3.65	1.19	1.30
2	A	1267	16G	O6-C6	-3.49	1.31	1.44
2	B	2267	16G	O6-C6	-3.27	1.32	1.44
3	A	1268	TLA	O3-C3	3.04	1.48	1.42
2	B	2267	16G	C4-C5	2.51	1.58	1.53
2	A	1267	16G	C4-C5	2.49	1.58	1.53
2	A	1267	16G	P-O3P	-2.48	1.45	1.54

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	2267	16G	P-O3P	-2.37	1.46	1.54
3	A	1268	TLA	O4-C4	2.25	1.28	1.22
2	B	2267	16G	C1-C2	2.24	1.55	1.52
2	B	2267	16G	P-O2P	-2.19	1.46	1.54
2	A	1267	16G	C1-C2	2.12	1.55	1.52
3	A	1268	TLA	O11-C1	-2.07	1.24	1.30
2	A	1267	16G	P-O2P	-2.03	1.47	1.54

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1268	TLA	O1-C1-C2	-4.47	109.73	121.62
3	A	1268	TLA	O4-C4-C3	-4.25	110.31	121.62
3	A	1268	TLA	O41-C4-C3	4.22	125.03	113.31
2	B	2267	16G	C1-C2-C3	-3.54	105.72	110.54
3	A	1268	TLA	O2-C2-C1	-3.53	103.15	110.69
2	A	1267	16G	C1-C2-C3	-3.38	105.94	110.54
2	B	2267	16G	O6-P-O1P	-3.14	97.96	106.44
2	A	1267	16G	O6-P-O1P	-3.06	98.18	106.44
2	A	1267	16G	O5-C5-C6	-2.94	100.86	106.69
3	A	1268	TLA	O11-C1-C2	2.86	121.27	113.31
2	A	1267	16G	O2P-P-O6	2.85	114.10	106.67
2	B	2267	16G	O5-C5-C6	-2.72	101.30	106.69
2	A	1267	16G	C1-O5-C5	2.49	118.46	113.65
2	B	2267	16G	O3P-P-O2P	2.47	117.06	107.80
2	A	1267	16G	O3P-P-O2P	2.44	116.97	107.80
2	B	2267	16G	O2P-P-O6	2.36	112.81	106.67
2	A	1267	16G	C6-C5-C4	2.34	116.98	112.07
2	B	2267	16G	C6-C5-C4	2.31	116.92	112.07
2	B	2267	16G	C1-O5-C5	2.28	118.06	113.65
3	A	1268	TLA	O11-C1-O1	2.17	129.00	124.08
2	A	1267	16G	O3P-P-O6	-2.13	101.13	106.67
2	A	1267	16G	C1-C2-N2	-2.01	108.40	110.73

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1267	16G	C6-O6-P-O1P
2	A	1267	16G	C6-O6-P-O2P
2	A	1267	16G	C6-O6-P-O3P
2	B	2267	16G	C6-O6-P-O1P

Continued on next page...

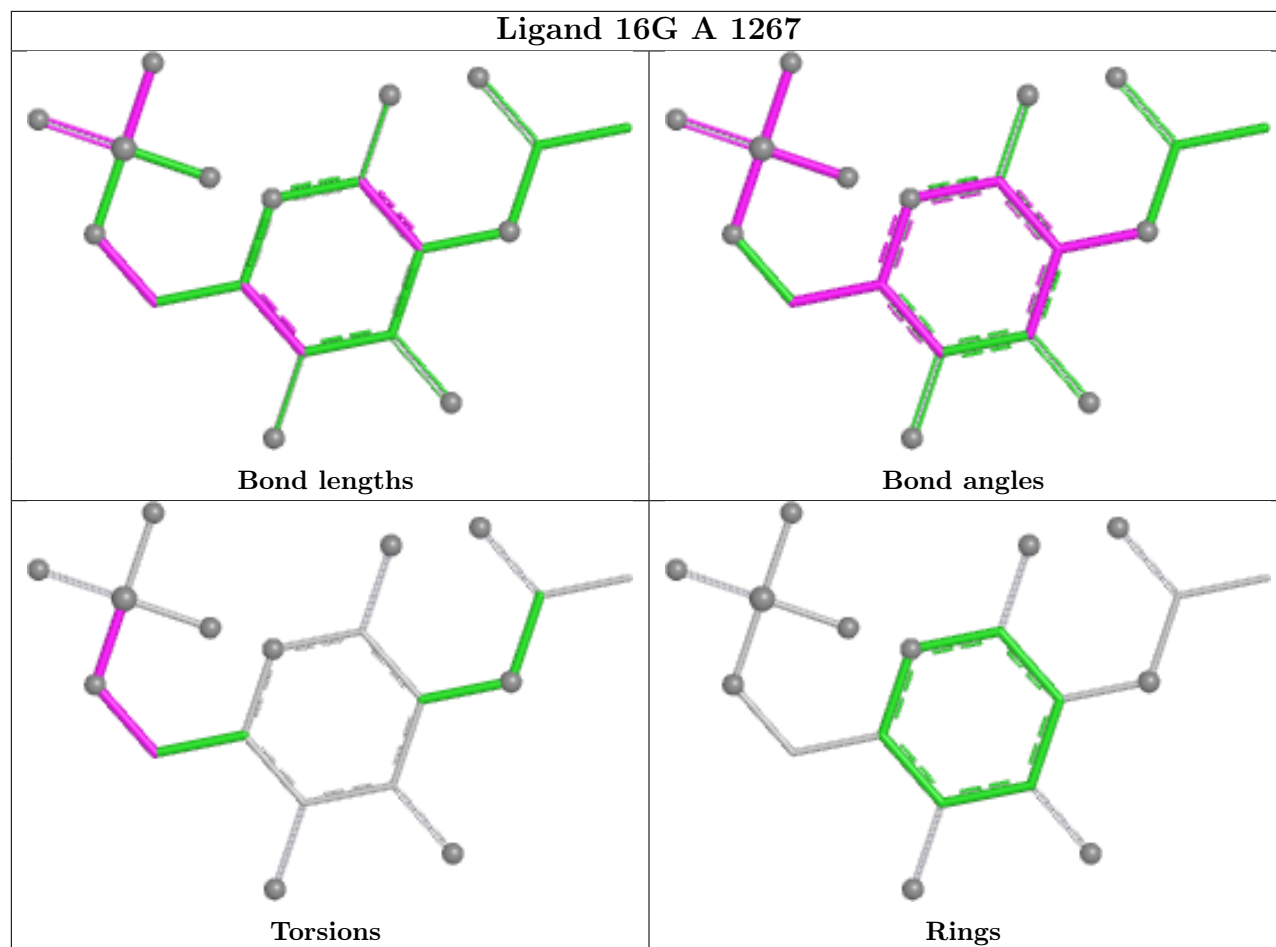
Continued from previous page...

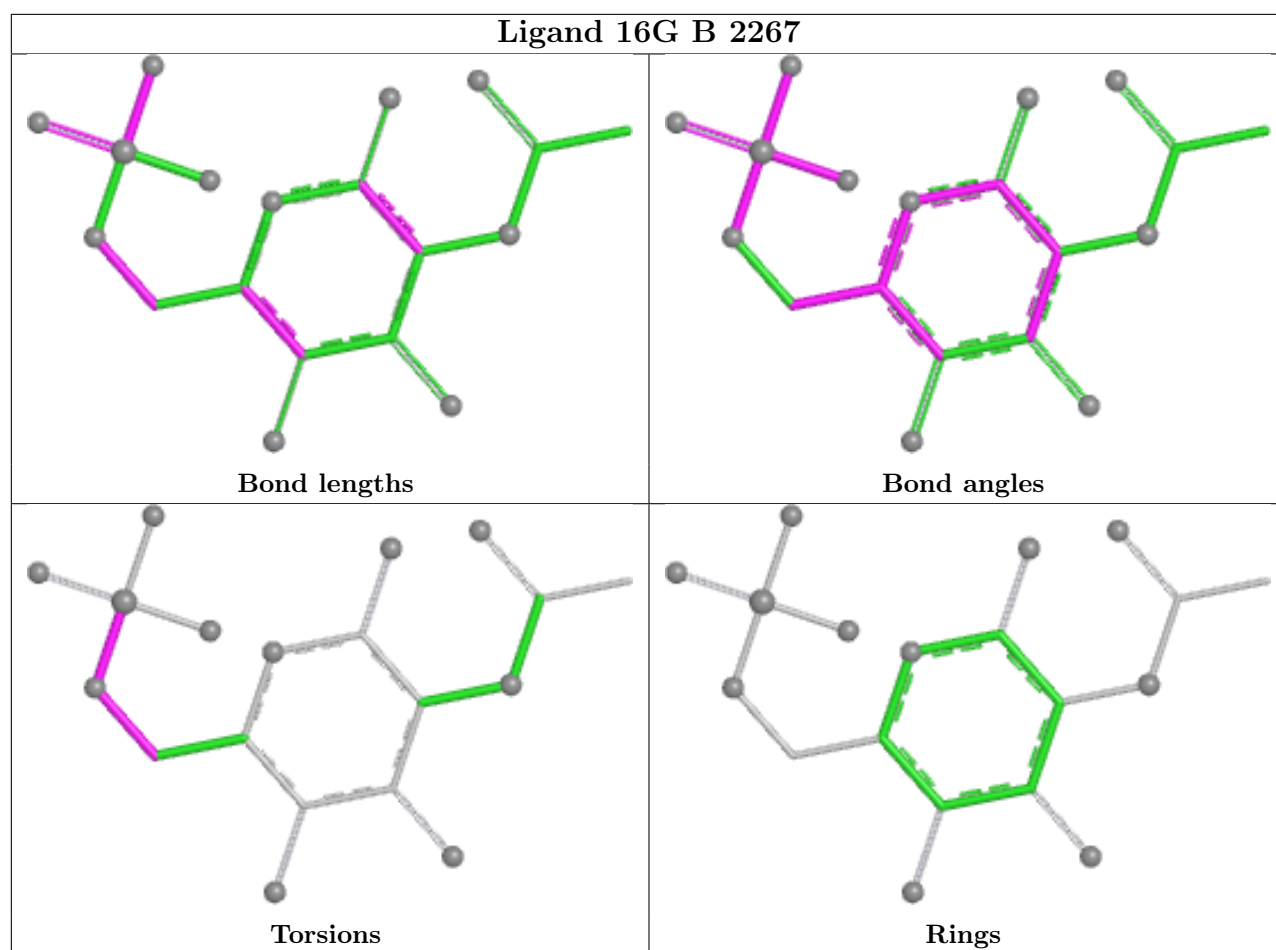
Mol	Chain	Res	Type	Atoms
2	B	2267	16G	C6-O6-P-O2P
2	B	2267	16G	C6-O6-P-O3P
3	A	1268	TLA	O3-C3-C4-O4
3	A	1268	TLA	O3-C3-C4-O41
2	A	1267	16G	C5-C6-O6-P
2	B	2267	16G	C5-C6-O6-P

There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





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 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.