



Full wwPDB X-ray Structure Validation Report ⓘ

May 29, 2020 – 06:50 pm BST

PDB ID : 3DYF
Title : T. Brucei Farnesyl Diphosphate Synthase Complexed with Bisphosphonate BPH-461 and Isopentyl Diphosphate
Authors : Cao, R.; Gao, Y.; Robinson, H.; Goddard, A.; Oldfield, E.
Deposited on : 2008-07-27
Resolution : 2.65 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

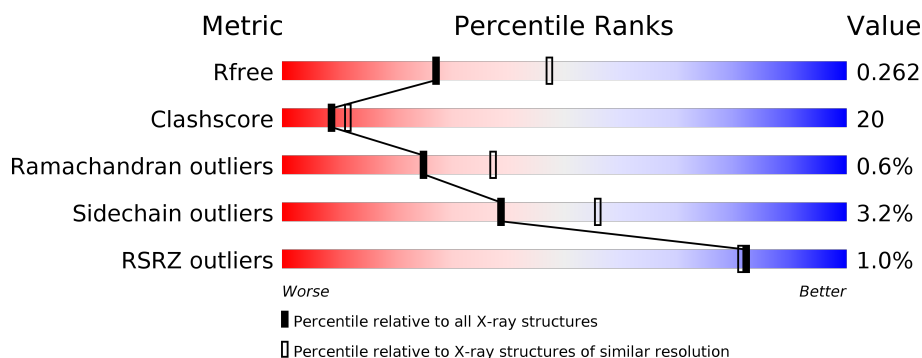
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.65 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}	130704	1332 (2.68-2.64)
Clashscore	141614	1374 (2.68-2.64)
Ramachandran outliers	138981	1349 (2.68-2.64)
Sidechain outliers	138945	1349 (2.68-2.64)
RSRZ outliers	127900	1318 (2.68-2.64)

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 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 $\leq 5\%$. 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	390	<div> <div>%</div> <div> <div></div> <div>59%</div> <div>31%</div> <div>• 8%</div> </div> </div>
1	B	390	<div> <div>%</div> <div> <div></div> <div>59%</div> <div>31%</div> <div>• 8%</div> </div> </div>

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 6117 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 FARNESYL PYROPHOSPHATE SYNTHASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	357	Total	C	N	O	S	0	0	0
			2862	1823	472	539	28			
1	B	358	Total	C	N	O	S	0	0	0
			2871	1829	473	541	28			

There are 46 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-22	MET	-	EXPRESSION TAG	UNP Q86C09
A	-21	GLY	-	EXPRESSION TAG	UNP Q86C09
A	-20	SER	-	EXPRESSION TAG	UNP Q86C09
A	-19	SER	-	EXPRESSION TAG	UNP Q86C09
A	-18	HIS	-	EXPRESSION TAG	UNP Q86C09
A	-17	HIS	-	EXPRESSION TAG	UNP Q86C09
A	-16	HIS	-	EXPRESSION TAG	UNP Q86C09
A	-15	HIS	-	EXPRESSION TAG	UNP Q86C09
A	-14	HIS	-	EXPRESSION TAG	UNP Q86C09
A	-13	HIS	-	EXPRESSION TAG	UNP Q86C09
A	-12	SER	-	EXPRESSION TAG	UNP Q86C09
A	-11	SER	-	EXPRESSION TAG	UNP Q86C09
A	-10	GLY	-	EXPRESSION TAG	UNP Q86C09
A	-9	LEU	-	EXPRESSION TAG	UNP Q86C09
A	-8	VAL	-	EXPRESSION TAG	UNP Q86C09
A	-7	PRO	-	EXPRESSION TAG	UNP Q86C09
A	-6	ARG	-	EXPRESSION TAG	UNP Q86C09
A	-5	GLY	-	EXPRESSION TAG	UNP Q86C09
A	-4	SER	-	EXPRESSION TAG	UNP Q86C09
A	-3	HIS	-	EXPRESSION TAG	UNP Q86C09
A	-2	MET	-	EXPRESSION TAG	UNP Q86C09
A	-1	ALA	-	EXPRESSION TAG	UNP Q86C09
A	0	SER	-	EXPRESSION TAG	UNP Q86C09
B	-22	MET	-	EXPRESSION TAG	UNP Q86C09
B	-21	GLY	-	EXPRESSION TAG	UNP Q86C09

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-20	SER	-	EXPRESSION TAG	UNP Q86C09
B	-19	SER	-	EXPRESSION TAG	UNP Q86C09
B	-18	HIS	-	EXPRESSION TAG	UNP Q86C09
B	-17	HIS	-	EXPRESSION TAG	UNP Q86C09
B	-16	HIS	-	EXPRESSION TAG	UNP Q86C09
B	-15	HIS	-	EXPRESSION TAG	UNP Q86C09
B	-14	HIS	-	EXPRESSION TAG	UNP Q86C09
B	-13	HIS	-	EXPRESSION TAG	UNP Q86C09
B	-12	SER	-	EXPRESSION TAG	UNP Q86C09
B	-11	SER	-	EXPRESSION TAG	UNP Q86C09
B	-10	GLY	-	EXPRESSION TAG	UNP Q86C09
B	-9	LEU	-	EXPRESSION TAG	UNP Q86C09
B	-8	VAL	-	EXPRESSION TAG	UNP Q86C09
B	-7	PRO	-	EXPRESSION TAG	UNP Q86C09
B	-6	ARG	-	EXPRESSION TAG	UNP Q86C09
B	-5	GLY	-	EXPRESSION TAG	UNP Q86C09
B	-4	SER	-	EXPRESSION TAG	UNP Q86C09
B	-3	HIS	-	EXPRESSION TAG	UNP Q86C09
B	-2	MET	-	EXPRESSION TAG	UNP Q86C09
B	-1	ALA	-	EXPRESSION TAG	UNP Q86C09
B	0	SER	-	EXPRESSION TAG	UNP Q86C09

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

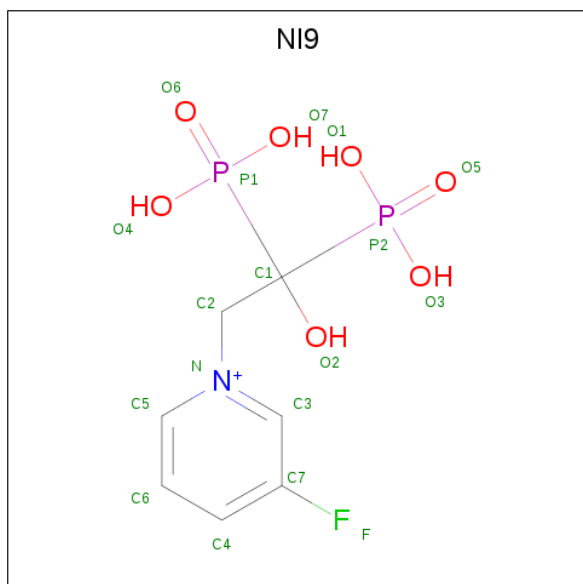
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	B	3	Total Mg 3 3	0	0
2	A	3	Total Mg 3 3	0	0

- Molecule 3 is ACETATE ION (three-letter code: ACT) (formula: C₂H₃O₂).



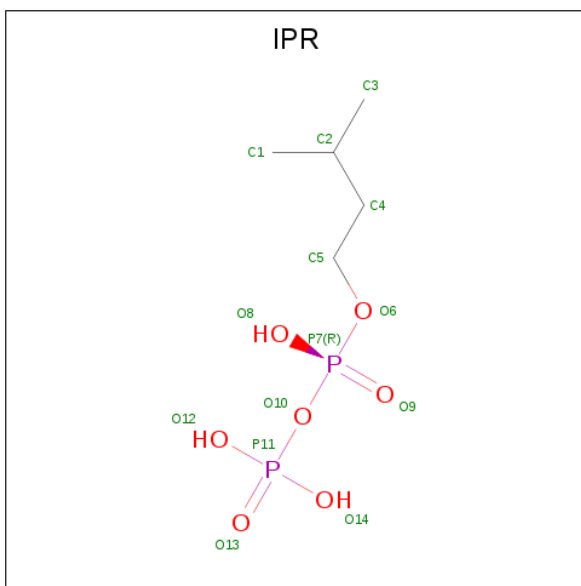
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			4	2	2		

- Molecule 4 is 3-FLUORO-1-(2-HYDROXY-2,2-DIPHOSPHONOETHYL)PYRIDINIUM (three-letter code: NI9) (formula: $C_7H_{11}FNO_7P_2$).



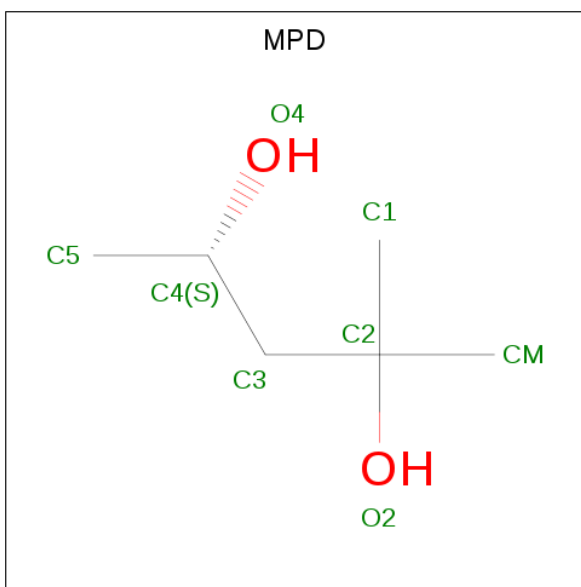
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
4	A	1	Total	C	F	N	O	P	0	0
			18	7	1	1	7	2		
4	B	1	Total	C	F	N	O	P	0	0
			18	7	1	1	7	2		

- Molecule 5 is ISOPENTYL PYROPHOSPHATE (three-letter code: IPR) (formula: $C_5H_{14}O_7P_2$).



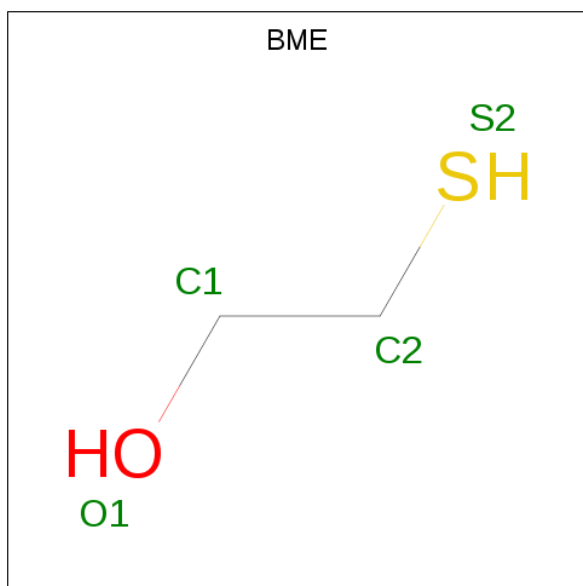
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	O	P	0	0
			14	5	7	2		
5	B	1	Total	C	O	P	0	0
			14	5	7	2		

- Molecule 6 is (4S)-2-METHYL-2,4-PENTANEDIOL (three-letter code: MPD) (formula: $C_6H_{14}O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			8	6	2		

- Molecule 7 is BETA-MERCAPTOETHANOL (three-letter code: BME) (formula: C_2H_6OS).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	B	1	Total	C	O	S	0	0
			4	2	1	1		

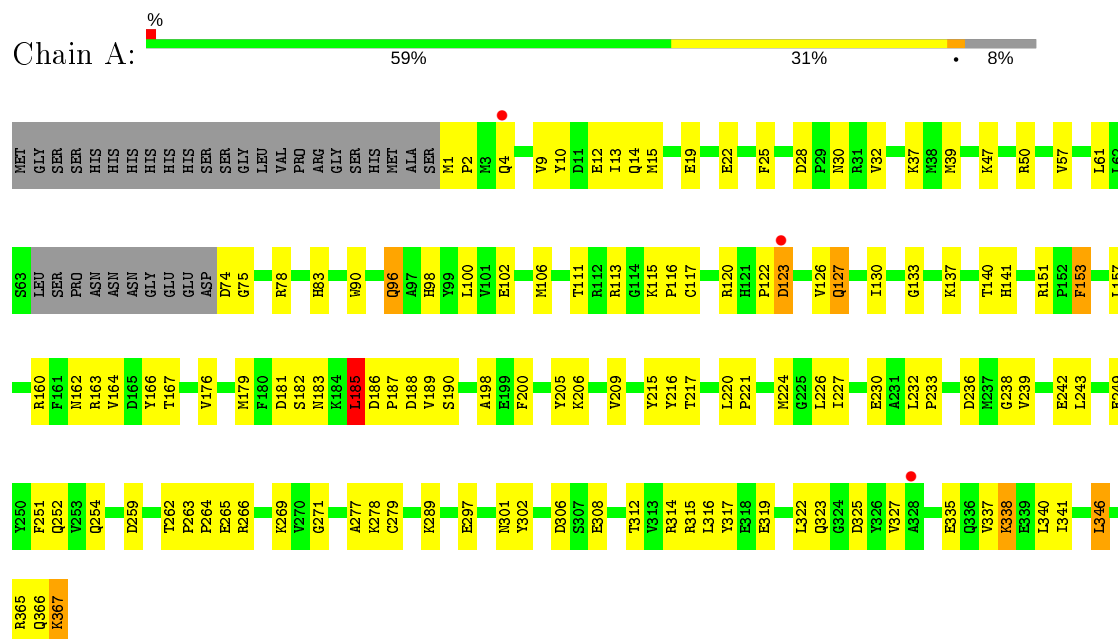
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	143	Total	O	0	0
			143	143		
8	B	155	Total	O	0	0
			155	155		

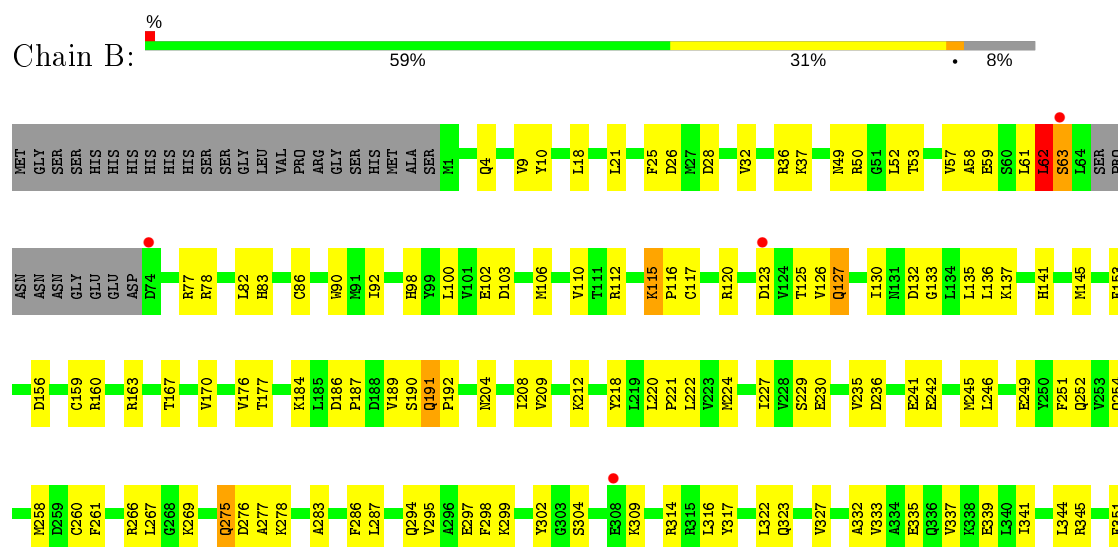
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes 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: FARNESYL PYROPHOSPHATE SYNTHASE



• Molecule 1: FARNESYL PYROPHOSPHATE SYNTHASE





4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	133.94Å 117.90Å 63.27Å 90.00° 111.27° 90.00°	Depositor
Resolution (Å)	29.48 – 2.65 29.48 – 2.64	Depositor EDS
% Data completeness (in resolution range)	95.5 (29.48-2.65) 94.8 (29.48-2.64)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.89 (at 2.64Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.201 , 0.268 0.196 , 0.262	Depositor DCC
R_{free} test set	1293 reflections (4.84%)	wwPDB-VP
Wilson B-factor (Å ²)	35.2	Xtriage
Anisotropy	0.510	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 60.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	6117	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 6.73% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 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: MG, BME, MPD, IPR, NI9, ACT

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	0.33	0/2921	0.53	0/3950
1	B	0.33	0/2930	0.53	0/3961
All	All	0.33	0/5851	0.53	0/7911

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	2862	0	2821	127	0
1	B	2871	0	2832	130	0
2	A	3	0	0	0	0
2	B	3	0	0	0	0
3	A	4	0	3	0	0
4	A	18	0	7	1	0
4	B	18	0	7	1	0
5	A	14	0	10	1	0
5	B	14	0	10	1	0
6	A	8	0	14	2	0
7	B	4	0	6	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	A	143	0	0	13	0
8	B	155	0	0	19	0
All	All	6117	0	5710	236	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 20.

All (236) 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:365:ARG:HB2	1:A:367:LYS:HE2	1.42	0.99
1:B:127:GLN:H	1:B:127:GLN:HE21	0.96	0.96
1:A:367:LYS:HZ2	1:A:367:LYS:HA	1.32	0.92
1:B:127:GLN:N	1:B:127:GLN:HE21	1.75	0.84
1:B:127:GLN:H	1:B:127:GLN:NE2	1.75	0.83
1:B:191:GLN:HG3	1:B:192:PRO:HD2	1.63	0.81
1:A:1:MET:O	1:A:4:GLN:HG2	1.81	0.81
1:A:123:ASP:HB2	1:B:186:ASP:O	1.82	0.79
1:A:37:LYS:HD2	1:B:187:PRO:HD2	1.63	0.78
1:A:47:LYS:HE3	1:A:367:LYS:HE3	1.65	0.77
1:A:367:LYS:NZ	1:A:367:LYS:HA	1.99	0.77
1:A:127:GLN:H	1:A:127:GLN:NE2	1.84	0.75
1:A:301:ASN:ND2	1:A:312:THR:HG21	2.02	0.75
1:A:187:PRO:HG3	1:B:37:LYS:HG2	1.66	0.75
1:A:230:GLU:HA	8:A:5246:HOH:O	1.87	0.73
1:A:1:MET:N	1:A:2:PRO:HD2	2.02	0.73
1:A:189:VAL:O	1:B:123:ASP:HB2	1.88	0.73
1:A:167:THR:HG22	1:B:25:PHE:CE1	2.24	0.72
1:A:306:ASP:OD1	1:A:308:GLU:HG2	1.88	0.72
1:A:297:GLU:HG2	1:A:316:LEU:HD11	1.71	0.71
1:B:115:LYS:HB3	1:B:116:PRO:HD2	1.73	0.71
1:B:176:VAL:HG13	1:B:177:THR:HG23	1.72	0.70
1:A:25:PHE:HE1	1:B:167:THR:HG22	1.56	0.70
1:A:15:MET:O	1:A:19:GLU:HG3	1.92	0.69
1:B:163:ARG:O	1:B:167:THR:HG23	1.92	0.69
1:A:127:GLN:H	1:A:127:GLN:HE21	1.40	0.69
8:A:5068:HOH:O	1:B:106:MET:HE1	1.92	0.68
1:B:156:ASP:O	1:B:160:ARG:HG3	1.92	0.68
1:B:159:CYS:HG	7:B:9001:BME:HS2	0.70	0.68
1:A:122:PRO:HB3	1:B:190:SER:HB3	1.76	0.67
1:B:10:TYR:HB2	1:B:90:TRP:CZ2	2.30	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:28:ASP:O	1:B:32:VAL:HG23	1.96	0.66
1:A:167:THR:HG22	1:B:25:PHE:HE1	1.60	0.66
1:A:232:LEU:HB3	1:A:233:PRO:HD3	1.77	0.65
1:A:187:PRO:CG	1:B:37:LYS:HG2	2.26	0.65
1:A:151:ARG:HH11	1:A:151:ARG:HG2	1.61	0.65
1:B:125:THR:HB	1:B:127:GLN:HE22	1.62	0.65
1:B:83:HIS:HD2	8:B:5163:HOH:O	1.80	0.64
1:B:220:LEU:HB3	1:B:221:PRO:HD3	1.78	0.64
1:A:186:ASP:O	1:B:123:ASP:HB2	1.96	0.64
1:A:12:GLU:OE1	1:A:83:HIS:HE1	1.81	0.63
1:A:157:LEU:HD21	1:A:224:MET:HE2	1.79	0.63
1:A:10:TYR:HB2	1:A:90:TRP:CZ2	2.33	0.63
1:A:209:VAL:HG22	1:A:252:GLN:HG2	1.82	0.62
1:B:267:LEU:HG	1:B:269:LYS:HG2	1.81	0.61
1:A:338:LYS:HE2	8:A:5279:HOH:O	1.99	0.61
1:A:366:GLN:O	1:A:367:LYS:HB2	2.00	0.61
1:B:266:ARG:HD3	8:B:5292:HOH:O	2.00	0.61
1:A:163:ARG:O	1:A:167:THR:HG23	2.00	0.61
1:B:254:GLN:O	1:B:258:MET:HG3	2.00	0.61
1:B:332:ALA:O	1:B:335:GLU:HB3	2.01	0.61
1:B:117:CYS:HB2	1:B:120:ARG:HG3	1.81	0.61
1:A:367:LYS:HD2	1:A:367:LYS:N	2.15	0.61
1:A:187:PRO:HA	1:B:123:ASP:HB3	1.83	0.60
1:A:243:LEU:HD21	1:A:340:LEU:HB2	1.84	0.59
1:A:317:TYR:O	1:A:322:LEU:HD23	2.02	0.59
1:B:52:LEU:HD12	8:B:5295:HOH:O	2.03	0.59
1:B:186:ASP:HA	8:B:5286:HOH:O	2.01	0.59
1:A:50:ARG:HD3	1:A:217:THR:HA	1.84	0.59
1:B:209:VAL:HG11	1:B:249:GLU:HA	1.85	0.58
1:A:176:VAL:HG21	1:B:127:GLN:HG2	1.85	0.58
1:A:106:MET:HA	1:B:127:GLN:HB2	1.84	0.58
1:B:323:GLN:O	1:B:327:VAL:HG23	2.03	0.58
1:A:22:GLU:CG	1:A:32:VAL:HG21	2.34	0.58
1:B:62:LEU:HD23	1:B:78:ARG:NH1	2.19	0.58
1:A:25:PHE:CE1	1:B:167:THR:HG22	2.37	0.58
1:B:102:GLU:C	1:B:106:MET:HE2	2.24	0.58
1:A:37:LYS:HE3	8:B:5286:HOH:O	2.02	0.57
1:B:145:MET:HE3	8:B:5058:HOH:O	2.05	0.57
1:A:167:THR:HG21	6:A:7001:MPD:H12	1.86	0.57
1:A:166:TYR:OH	1:B:21:LEU:HD21	2.05	0.57
1:B:50:ARG:HH21	5:B:6002:IPR:HC12	1.70	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:141:HIS:HB3	8:B:5175:HOH:O	2.04	0.56
1:A:242:GLU:HB3	8:A:5272:HOH:O	2.06	0.55
1:B:98:HIS:HD2	1:B:133:GLY:O	1.88	0.55
1:A:1:MET:H2	1:A:2:PRO:HD2	1.69	0.55
1:A:200:PHE:CE2	1:A:279:CYS:HA	2.40	0.55
1:B:49:ASN:HB2	8:B:5275:HOH:O	2.05	0.55
1:B:304:SER:OG	1:B:309:LYS:HD2	2.06	0.55
1:B:4:GLN:HG3	8:B:5191:HOH:O	2.06	0.55
1:A:209:VAL:HG11	1:A:249:GLU:HA	1.88	0.55
1:B:160:ARG:HD3	1:B:227:ILE:HD11	1.87	0.55
1:A:365:ARG:HD2	1:A:367:LYS:CE	2.36	0.55
1:B:62:LEU:O	1:B:63:SER:HB3	2.06	0.54
1:A:315:ARG:HD3	1:A:319:GLU:OE2	2.07	0.54
1:B:339:GLU:HG3	8:B:5204:HOH:O	2.08	0.54
1:A:115:LYS:HG2	1:A:116:PRO:HD2	1.91	0.53
1:A:314:ARG:HD2	8:A:5257:HOH:O	2.08	0.53
1:A:126:VAL:O	1:A:130:ILE:HG13	2.08	0.53
1:A:1:MET:N	1:A:2:PRO:CD	2.72	0.53
1:A:117:CYS:O	1:A:120:ARG:HB2	2.09	0.52
1:A:1:MET:H3	1:A:2:PRO:HD2	1.74	0.52
1:A:259:ASP:OD1	1:A:271:GLY:HA2	2.09	0.52
1:B:277:ALA:HA	1:B:302:TYR:CE2	2.44	0.52
1:A:182:SER:HA	1:A:185:LEU:HB2	1.92	0.52
1:A:186:ASP:O	1:B:123:ASP:CB	2.58	0.52
1:A:151:ARG:HG2	1:A:151:ARG:NH1	2.24	0.51
1:B:184:LYS:HG2	1:B:191:GLN:OE1	2.10	0.51
1:A:209:VAL:CG1	1:A:249:GLU:HA	2.41	0.51
1:A:236:ASP:CG	1:A:239:VAL:HG23	2.31	0.51
1:B:59:GLU:HG3	1:B:82:LEU:HD21	1.92	0.51
1:B:242:GLU:HG2	8:B:5145:HOH:O	2.11	0.51
1:B:351:PHE:O	1:B:355:VAL:HG23	2.11	0.51
1:A:78:ARG:HD2	8:A:5269:HOH:O	2.10	0.51
1:B:261:PHE:HE1	1:B:314:ARG:HG3	1.75	0.51
1:B:159:CYS:SG	7:B:9001:BME:S2	2.72	0.51
1:A:266:ARG:HH11	1:A:266:ARG:HG2	1.77	0.50
1:B:283:ALA:O	1:B:287:LEU:HG	2.10	0.50
1:B:103:ASP:HA	1:B:106:MET:HE3	1.94	0.50
1:B:125:THR:HB	1:B:127:GLN:NE2	2.25	0.50
1:B:133:GLY:HA2	1:B:136:LEU:HD12	1.93	0.50
1:B:62:LEU:O	1:B:63:SER:CB	2.60	0.50
1:B:295:VAL:O	1:B:298:PHE:HB3	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:167:THR:HG21	6:A:7001:MPD:C1	2.42	0.50
1:B:9:VAL:HG21	1:B:86:CYS:CB	2.41	0.50
1:B:126:VAL:HG12	8:B:5090:HOH:O	2.10	0.50
1:B:317:TYR:HB3	1:B:322:LEU:HD12	1.94	0.50
8:A:5070:HOH:O	1:B:26:ASP:HB2	2.11	0.50
1:A:206:LYS:HG2	1:A:249:GLU:OE2	2.12	0.49
1:A:236:ASP:OD1	1:A:239:VAL:HG23	2.12	0.49
1:A:238:GLY:O	1:A:242:GLU:HG3	2.13	0.49
1:A:365:ARG:NH1	1:A:367:LYS:HD3	2.27	0.49
1:A:96:GLN:O	1:A:100:LEU:HG	2.12	0.49
1:B:208:ILE:O	1:B:212:LYS:HG2	2.13	0.49
1:A:366:GLN:C	1:A:367:LYS:HD2	2.33	0.49
1:B:241:GLU:O	1:B:245:MET:HG2	2.12	0.49
1:A:365:ARG:CB	1:A:367:LYS:HE2	2.30	0.49
1:B:102:GLU:O	1:B:106:MET:HE2	2.13	0.49
1:B:358:LEU:O	1:B:358:LEU:HD22	2.12	0.49
1:A:9:VAL:O	1:A:13:ILE:HG13	2.13	0.49
1:B:209:VAL:HG13	1:B:252:GLN:CB	2.42	0.49
1:A:289:LYS:HB3	8:A:5176:HOH:O	2.13	0.49
1:A:337:VAL:O	1:A:341:ILE:HG13	2.13	0.48
1:A:83:HIS:HD2	8:A:5071:HOH:O	1.96	0.48
1:B:209:VAL:CG1	1:B:249:GLU:HA	2.42	0.48
1:B:61:LEU:O	1:B:63:SER:N	2.47	0.48
1:A:220:LEU:HB3	1:A:221:PRO:HD3	1.94	0.48
1:B:286:PHE:HZ	1:B:294:GLN:HB3	1.78	0.48
1:B:57:VAL:O	1:B:61:LEU:HD23	2.13	0.48
1:B:254:GLN:OE1	1:B:365:ARG:HD3	2.14	0.48
1:B:258:MET:CE	1:B:367:LYS:HA	2.44	0.48
1:A:57:VAL:O	1:A:61:LEU:HD13	2.14	0.48
1:B:295:VAL:HG12	1:B:299:LYS:HE3	1.96	0.47
1:A:123:ASP:CB	1:B:189:VAL:O	2.63	0.47
1:A:323:GLN:O	1:A:327:VAL:HG23	2.14	0.47
1:A:365:ARG:HD2	1:A:367:LYS:HE2	1.96	0.47
1:B:230:GLU:HA	8:B:5062:HOH:O	2.14	0.47
1:B:53:THR:O	1:B:57:VAL:HG23	2.14	0.47
1:A:226:LEU:HB3	1:A:232:LEU:HA	1.96	0.47
1:B:62:LEU:HD23	1:B:78:ARG:HG3	1.96	0.47
1:A:266:ARG:HG2	1:A:266:ARG:NH1	2.28	0.47
1:B:98:HIS:CD2	1:B:137:LYS:HB2	2.49	0.47
1:B:58:ALA:HA	1:B:229:SER:OG	2.15	0.47
1:A:102:GLU:O	1:A:106:MET:HG3	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:190:SER:HB3	8:A:5106:HOH:O	2.15	0.47
1:A:164:VAL:HG13	1:A:215:TYR:HB3	1.97	0.47
1:B:126:VAL:O	1:B:130:ILE:HG13	2.15	0.46
1:A:367:LYS:NZ	1:A:367:LYS:CA	2.76	0.46
1:A:98:HIS:HD2	1:A:133:GLY:O	1.98	0.46
1:B:36:ARG:HG2	1:B:36:ARG:HH11	1.80	0.46
1:B:98:HIS:O	1:B:102:GLU:HG2	2.16	0.46
1:A:160:ARG:HD2	1:A:227:ILE:HD11	1.97	0.46
1:A:102:GLU:OE2	1:A:133:GLY:HA3	2.16	0.46
1:B:260:CYS:SG	1:B:314:ARG:HD3	2.56	0.46
1:A:12:GLU:OE1	1:A:83:HIS:CE1	2.65	0.46
1:B:59:GLU:O	1:B:62:LEU:N	2.49	0.46
1:A:47:LYS:HB2	8:A:5022:HOH:O	2.15	0.45
1:B:275:GLN:NE2	8:B:5179:HOH:O	2.44	0.45
1:A:113:ARG:HA	8:A:5244:HOH:O	2.16	0.45
1:A:153:PHE:CD1	1:A:153:PHE:C	2.90	0.45
1:A:123:ASP:HB2	1:B:189:VAL:O	2.17	0.45
1:B:62:LEU:CD2	1:B:78:ARG:HG3	2.47	0.45
1:A:187:PRO:CA	1:B:123:ASP:HB3	2.47	0.45
1:A:123:ASP:CB	1:B:186:ASP:O	2.60	0.45
1:A:98:HIS:CD2	1:A:137:LYS:HB2	2.53	0.44
1:A:160:ARG:CD	1:A:227:ILE:HD11	2.48	0.44
1:A:74:ASP:CG	1:A:75:GLY:N	2.70	0.44
1:B:218:TYR:CD2	1:B:358:LEU:HD11	2.51	0.44
1:A:137:LYS:O	1:A:140:THR:OG1	2.33	0.44
1:B:235:VAL:HG23	8:B:5194:HOH:O	2.17	0.44
1:B:235:VAL:HG22	1:B:236:ASP:N	2.32	0.44
1:B:21:LEU:HA	1:B:25:PHE:HB2	1.99	0.44
1:A:9:VAL:O	1:A:12:GLU:HB3	2.17	0.44
1:A:162:ASN:HD22	1:B:141:HIS:CG	2.35	0.44
1:B:323:GLN:HG2	8:B:5250:HOH:O	2.18	0.44
1:B:160:ARG:CD	1:B:227:ILE:HD11	2.48	0.43
1:B:229:SER:O	1:B:230:GLU:HB2	2.18	0.43
1:B:9:VAL:HG21	1:B:86:CYS:HB3	1.99	0.43
1:A:96:GLN:HG3	1:A:216:TYR:HE2	1.83	0.43
4:A:3001:NI9:H21	5:A:6001:IPR:HC42	2.00	0.43
1:B:246:LEU:HD11	1:B:333:VAL:HG13	2.00	0.43
1:B:145:MET:HB2	1:B:145:MET:HE3	1.81	0.43
1:B:110:VAL:HA	1:B:120:ARG:HD3	2.00	0.43
1:B:261:PHE:CE1	1:B:314:ARG:HG3	2.54	0.43
1:A:14:GLN:HG3	1:A:39:MET:SD	2.59	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:153:PHE:CD1	1:B:153:PHE:C	2.92	0.43
1:A:179:MET:CE	1:A:278:LYS:HD3	2.48	0.43
1:A:1:MET:HG3	1:A:2:PRO:CD	2.49	0.43
1:B:258:MET:HE2	1:B:367:LYS:HA	2.01	0.42
1:A:181:ASP:OD1	1:A:183:ASN:HB2	2.20	0.42
1:A:28:ASP:OD1	1:A:30:ASN:HB2	2.19	0.42
1:A:346:LEU:HA	1:A:346:LEU:HD12	1.88	0.42
1:B:137:LYS:HE3	8:B:5267:HOH:O	2.19	0.42
1:B:92:ILE:HD11	1:B:224:MET:SD	2.59	0.42
1:A:1:MET:HG3	1:A:2:PRO:HD3	2.02	0.42
1:A:262:THR:HA	1:A:263:PRO:HD2	1.91	0.42
1:A:96:GLN:HE21	1:A:96:GLN:HB3	1.55	0.42
1:B:345:ARG:NH1	8:B:5092:HOH:O	2.44	0.42
1:B:112:ARG:NH2	4:B:4001:NI9:O1	2.42	0.42
1:A:98:HIS:CE1	1:A:137:LYS:HE3	2.54	0.42
1:B:141:HIS:HB3	8:B:5058:HOH:O	2.19	0.42
1:B:286:PHE:CZ	1:B:294:GLN:HB3	2.55	0.42
1:A:209:VAL:HG22	1:A:252:GLN:CG	2.48	0.42
1:A:123:ASP:OD2	1:B:189:VAL:O	2.37	0.42
1:A:10:TYR:HB2	1:A:90:TRP:CE2	2.55	0.41
1:B:297:GLU:HG2	1:B:316:LEU:HD11	2.01	0.41
1:A:327:VAL:HG13	8:A:5049:HOH:O	2.20	0.41
1:B:132:ASP:HA	1:B:135:LEU:HD12	2.01	0.41
1:B:251:PHE:CE1	1:B:365:ARG:CZ	3.03	0.41
1:A:176:VAL:O	1:A:176:VAL:HG22	2.21	0.41
1:A:263:PRO:HA	1:A:264:PRO:HD2	1.91	0.41
1:A:277:ALA:HA	1:A:302:TYR:CE2	2.55	0.41
1:B:344:LEU:O	1:B:345:ARG:C	2.59	0.41
1:A:205:TYR:CZ	1:A:209:VAL:HG21	2.55	0.41
1:B:156:ASP:OD1	1:B:160:ARG:NH1	2.53	0.41
1:A:111:THR:OG1	1:A:269:LYS:HA	2.22	0.40
1:B:133:GLY:O	1:B:136:LEU:HB2	2.21	0.40
1:B:18:LEU:HD11	1:B:36:ARG:HB2	2.03	0.40
1:B:337:VAL:O	1:B:341:ILE:HG13	2.22	0.40
1:A:239:VAL:HG13	1:A:340:LEU:HD22	2.04	0.40
1:B:204:ASN:O	1:B:208:ILE:HG13	2.22	0.40
1:B:218:TYR:O	1:B:222:LEU:HG	2.22	0.40
1:A:251:PHE:HA	1:A:254:GLN:OE1	2.21	0.40
1:B:276:ASP:HB3	1:B:278:LYS:HE2	2.04	0.40
1:A:50:ARG:NH1	1:A:216:TYR:CE2	2.89	0.40
1:B:167:THR:O	1:B:170:VAL:HB	2.20	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	353/390 (90%)	334 (95%)	17 (5%)	2 (1%)	25	37
1	B	354/390 (91%)	330 (93%)	22 (6%)	2 (1%)	25	37
All	All	707/780 (91%)	664 (94%)	39 (6%)	4 (1%)	25	37

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	63	SER
1	A	185	LEU
1	B	62	LEU
1	A	198	ALA

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	312/340 (92%)	300 (96%)	12 (4%)	33	49
1	B	313/340 (92%)	305 (97%)	8 (3%)	46	64
All	All	625/680 (92%)	605 (97%)	20 (3%)	39	56

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

Mol	Chain	Res	Type
1	A	96	GLN
1	A	123	ASP
1	A	127	GLN
1	A	153	PHE
1	A	185	LEU
1	A	188	ASP
1	A	265	GLU
1	A	325	ASP
1	A	335	GLU
1	A	338	LYS
1	A	346	LEU
1	A	367	LYS
1	B	62	LEU
1	B	77	ARG
1	B	100	LEU
1	B	115	LYS
1	B	127	GLN
1	B	191	GLN
1	B	275	GLN
1	B	358	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	4	GLN
1	A	49	ASN
1	A	83	HIS
1	A	96	GLN
1	A	98	HIS
1	A	127	GLN
1	A	141	HIS
1	A	146	HIS
1	A	162	ASN
1	A	172	GLN
1	A	183	ASN
1	A	204	ASN
1	A	252	GLN
1	A	301	ASN
1	A	323	GLN
1	A	336	GLN
1	B	30	ASN
1	B	49	ASN
1	B	83	HIS

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Mol	Chain	Res	Type
1	B	98	HIS
1	B	127	GLN
1	B	204	ASN
1	B	275	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 13 ligands modelled in this entry, 6 are monoatomic - leaving 7 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	$\# Z > 2$
7	BME	B	9001	-	3,3,3	0.47	0	1,2,2	0.16	0
4	NI9	A	3001	2	17,18,18	1.43	3 (17%)	25,29,29	1.40	3 (12%)
5	IPR	A	6001	-	11,13,13	1.24	2 (18%)	16,19,19	1.70	5 (31%)
3	ACT	A	8001	-	1,3,3	1.71	0	0,3,3	0.00	-
5	IPR	B	6002	-	11,13,13	1.27	2 (18%)	16,19,19	1.69	5 (31%)
6	MPD	A	7001	-	7,7,7	0.55	0	9,10,10	0.41	0
4	NI9	B	4001	2	17,18,18	1.28	3 (17%)	25,29,29	1.62	5 (20%)

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
7	BME	B	9001	-	-	0/1/1/1	-
4	NI9	A	3001	2	-	12/23/23/23	0/1/1/1
5	IPR	A	6001	-	-	4/13/13/13	-
5	IPR	B	6002	-	-	4/13/13/13	-
6	MPD	A	7001	-	-	0/5/5/5	-
4	NI9	B	4001	2	-	12/23/23/23	0/1/1/1

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	3001	NI9	P2-C1	4.08	1.88	1.85
4	B	4001	NI9	P2-C1	2.68	1.87	1.85
5	B	6002	IPR	C3-C2	-2.64	1.37	1.51
5	A	6001	IPR	C3-C2	-2.62	1.37	1.51
5	B	6002	IPR	P11-O14	-2.13	1.46	1.54
5	A	6001	IPR	P11-O14	-2.09	1.46	1.54
4	A	3001	NI9	C5-N	2.08	1.39	1.34
4	B	4001	NI9	C5-N	2.03	1.39	1.34
4	A	3001	NI9	P2-O5	-2.03	1.47	1.50
4	B	4001	NI9	P2-O5	-2.03	1.47	1.50

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	4001	NI9	C2-N-C3	-5.36	115.20	119.54
4	A	3001	NI9	C2-N-C3	-4.49	115.90	119.54
5	B	6002	IPR	O12-P11-O14	3.36	120.48	107.64
5	A	6001	IPR	C3-C2-C1	3.32	125.83	110.51
5	A	6001	IPR	O12-P11-O14	3.32	120.32	107.64
5	B	6002	IPR	C3-C2-C1	3.31	125.76	110.51
4	B	4001	NI9	P2-C1-P1	-2.89	107.64	112.81
4	B	4001	NI9	C2-N-C5	2.66	121.75	119.62
5	B	6002	IPR	O6-C5-C4	-2.60	100.17	109.09
5	A	6001	IPR	O6-C5-C4	-2.48	100.59	109.09
5	A	6001	IPR	C3-C2-C4	2.35	126.05	111.54
4	A	3001	NI9	P2-C1-P1	-2.33	108.64	112.81
5	B	6002	IPR	C3-C2-C4	2.32	125.87	111.54
4	B	4001	NI9	P1-C1-O2	2.29	112.50	107.30
4	B	4001	NI9	C5-N-C3	2.09	123.06	121.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	3001	NI9	P1-C1-O2	2.09	112.05	107.30
5	B	6002	IPR	O12-P11-O13	2.06	118.74	110.68
5	A	6001	IPR	O12-P11-O13	2.05	118.70	110.68

There are no chirality outliers.

All (32) torsion outliers are listed below:

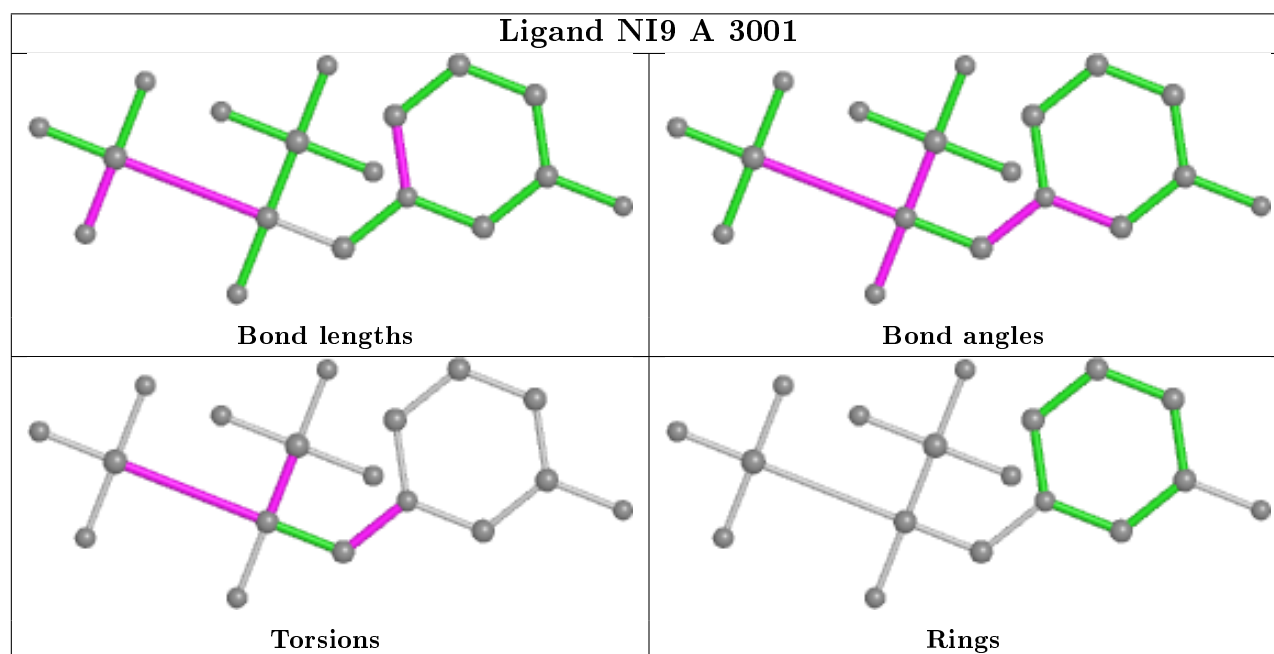
Mol	Chain	Res	Type	Atoms
5	A	6001	IPR	P7-O10-P11-O12
4	A	3001	NI9	O2-C1-P2-O1
4	A	3001	NI9	O2-C1-P2-O3
4	A	3001	NI9	O2-C1-P2-O5
4	A	3001	NI9	C2-C1-P2-O1
4	A	3001	NI9	C2-C1-P2-O3
4	A	3001	NI9	C2-C1-P2-O5
4	A	3001	NI9	P1-C1-P2-O1
4	A	3001	NI9	P1-C1-P2-O3
4	A	3001	NI9	P1-C1-P2-O5
4	A	3001	NI9	C1-C2-N-C3
4	A	3001	NI9	C1-C2-N-C5
5	B	6002	IPR	P7-O10-P11-O12
4	B	4001	NI9	O2-C1-P2-O1
4	B	4001	NI9	O2-C1-P2-O3
4	B	4001	NI9	O2-C1-P2-O5
4	B	4001	NI9	C2-C1-P2-O1
4	B	4001	NI9	C2-C1-P2-O3
4	B	4001	NI9	C2-C1-P2-O5
4	B	4001	NI9	P1-C1-P2-O1
4	B	4001	NI9	P1-C1-P2-O3
4	B	4001	NI9	P1-C1-P2-O5
5	A	6001	IPR	C1-C2-C4-C5
5	B	6002	IPR	C1-C2-C4-C5
4	B	4001	NI9	C1-C2-N-C3
4	B	4001	NI9	C1-C2-N-C5
5	A	6001	IPR	P7-O10-P11-O13
5	B	6002	IPR	P7-O10-P11-O13
5	A	6001	IPR	P7-O10-P11-O14
5	B	6002	IPR	P7-O10-P11-O14
4	A	3001	NI9	C2-C1-P1-O6
4	B	4001	NI9	C2-C1-P1-O6

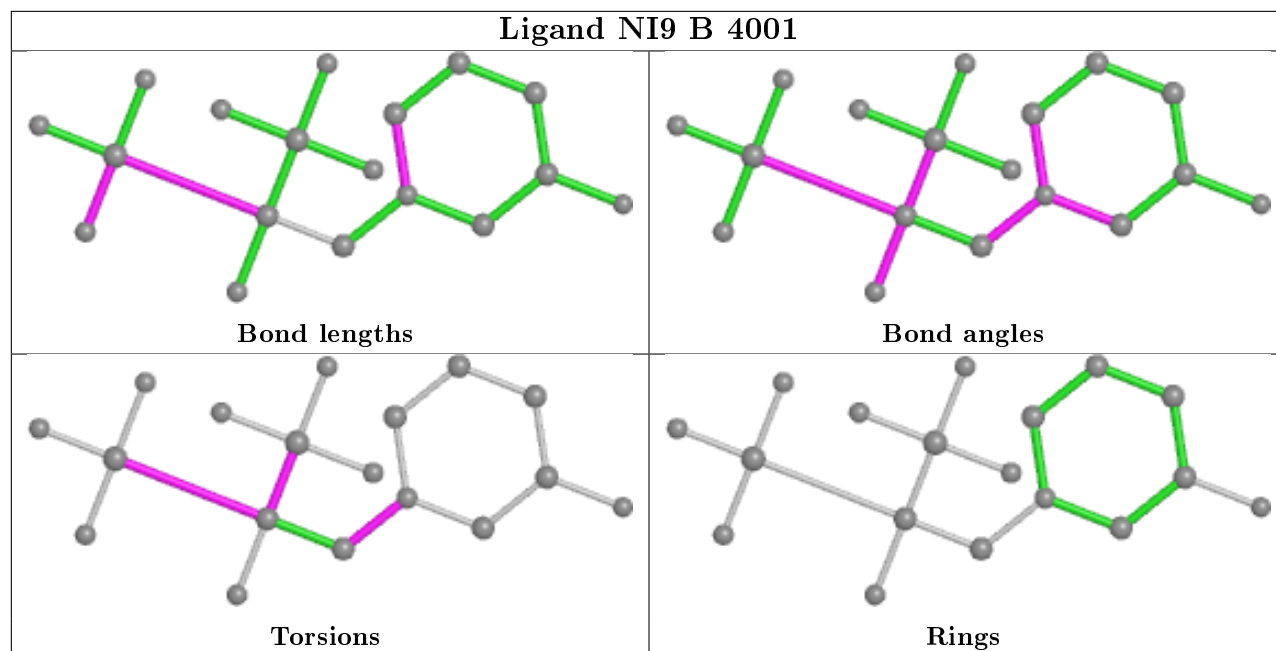
There are no ring outliers.

6 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	B	9001	BME	2	0
4	A	3001	NI9	1	0
5	A	6001	IPR	1	0
5	B	6002	IPR	1	0
6	A	7001	MPD	2	0
4	B	4001	NI9	1	0

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 [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	A	357/390 (91%)	-0.05	3 (0%) 86 85	20, 41, 60, 73	0
1	B	358/390 (91%)	-0.18	4 (1%) 80 79	21, 40, 57, 75	0
All	All	715/780 (91%)	-0.11	7 (0%) 82 81	20, 41, 58, 75	0

All (7) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	308	GLU	2.8
1	B	123	ASP	2.8
1	A	123	ASP	2.6
1	A	4	GLN	2.3
1	B	63	SER	2.3
1	B	74	ASP	2.1
1	A	328	ALA	2.0

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](#)

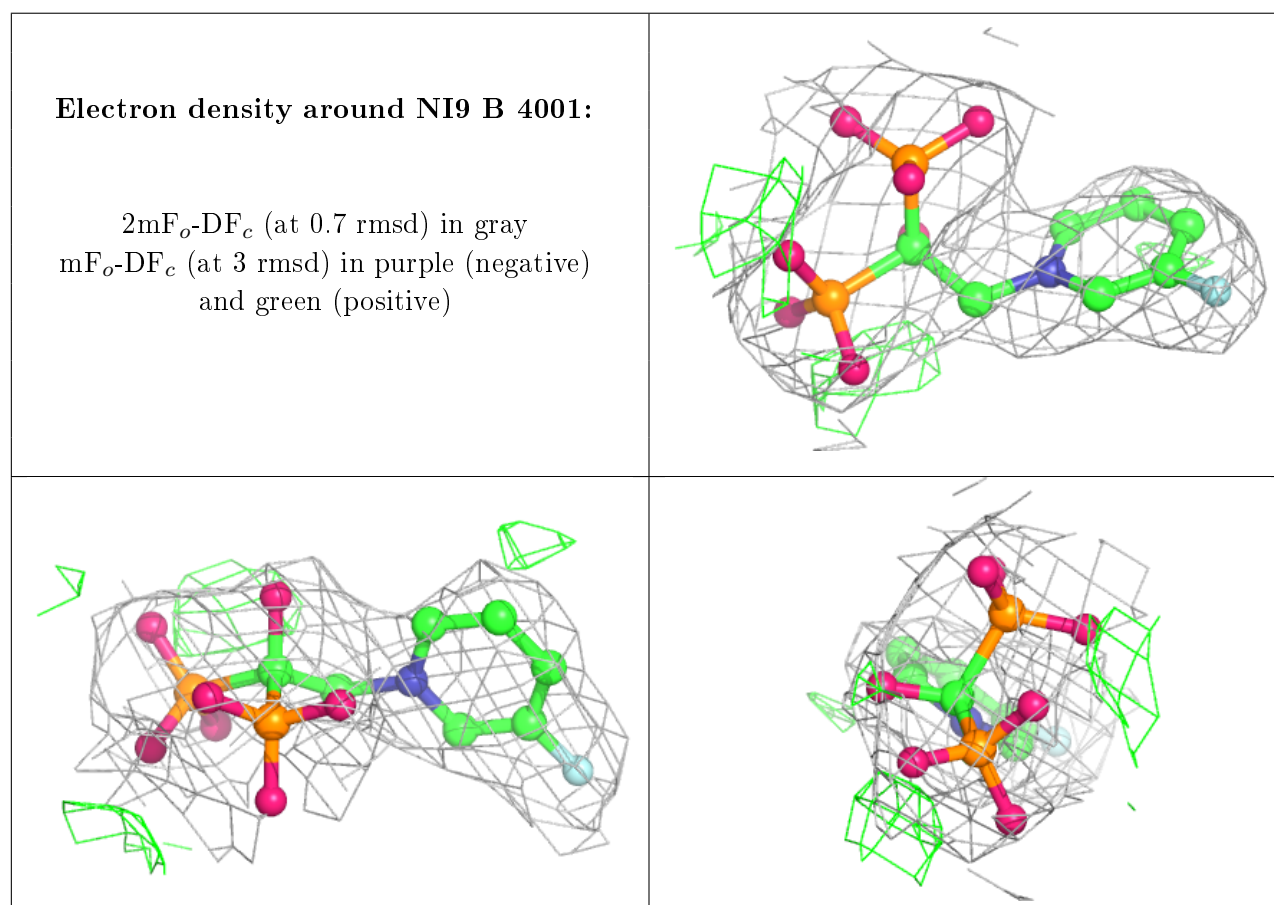
There are no carbohydrates in this entry.

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. 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.

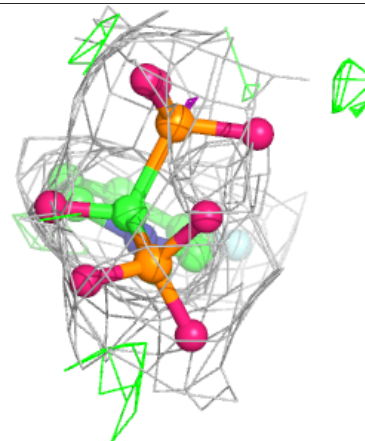
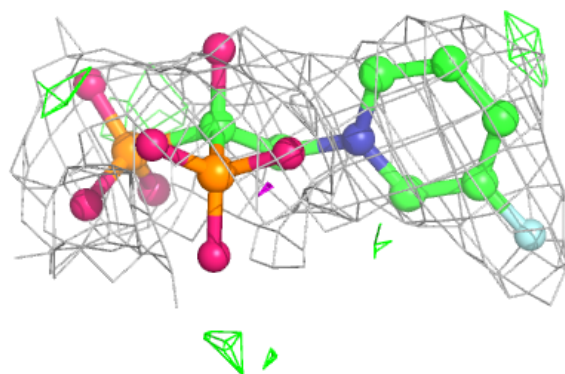
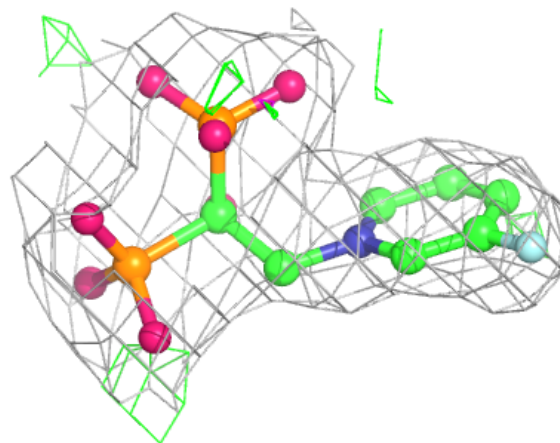
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	MG	A	3003	1/1	0.76	0.19	21,21,21,21	0
2	MG	B	4003	1/1	0.79	0.12	23,23,23,23	0
6	MPD	A	7001	8/8	0.81	0.25	33,53,57,57	0
7	BME	B	9001	4/4	0.88	0.23	44,47,56,60	0
2	MG	A	3004	1/1	0.89	0.23	41,41,41,41	0
2	MG	B	4002	1/1	0.91	0.30	36,36,36,36	0
2	MG	B	4004	1/1	0.91	0.46	27,27,27,27	0
3	ACT	A	8001	4/4	0.95	0.26	49,49,56,63	0
2	MG	A	3002	1/1	0.96	0.18	42,42,42,42	0
4	NI9	B	4001	18/18	0.96	0.25	36,50,58,67	0
4	NI9	A	3001	18/18	0.97	0.20	21,43,52,62	0
5	IPR	B	6002	14/14	0.97	0.15	24,37,52,54	0
5	IPR	A	6001	14/14	0.97	0.15	15,33,43,43	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.



Electron density around NI9 A 3001:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers [i](#)

There are no such residues in this entry.