



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 03:06 PM UTC

PDB ID : 1QHI / pdb_00001qhi
Title : HERPES SIMPLEX VIRUS TYPE-I THYMIDINE KINASE COMPLEXED
WITH A NOVEL NON-SUBSTRATE INHIBITOR, 9-(4-HYDROXYBUTY
L)-N2-PHENYLGUANINE
Authors : Bennett, M.S.; Wien, F.; Champness, J.N.; Batuwangala, T.; Rutherford, T.;
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Deposited on : 1999-05-12
Resolution : 1.90 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](#) ①) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

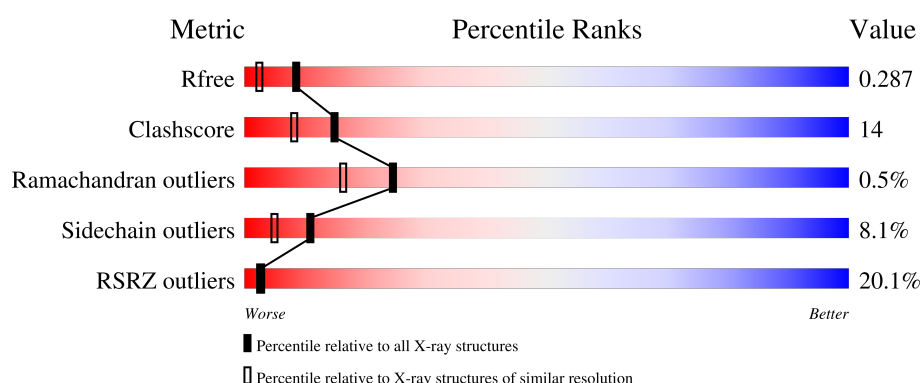
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 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}	180053	7789 (1.90-1.90)
Clashscore	190562	8410 (1.90-1.90)
Ramachandran outliers	187476	8333 (1.90-1.90)
Sidechain outliers	187428	8333 (1.90-1.90)
RSRZ outliers	180081	7790 (1.90-1.90)

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 $\leq 5\%$. 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	366	20% 57% 21% • • 17%
1	B	366	13% 57% 23% • • 16%

2 Entry composition [i](#)

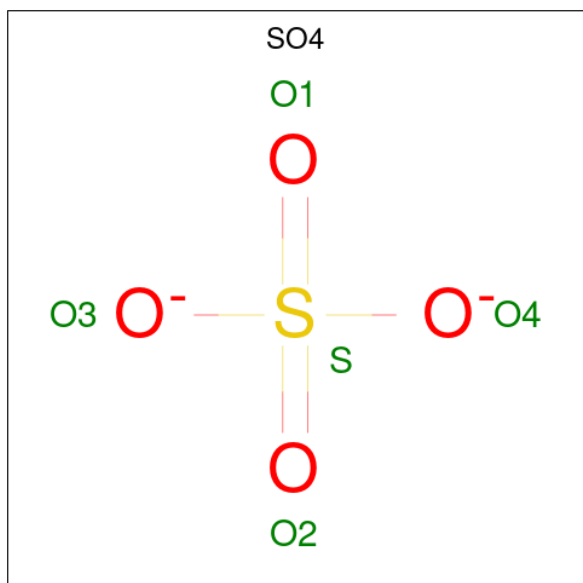
There are 4 unique types of molecules in this entry. The entry contains 4953 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 (THYMIDINE KINASE).

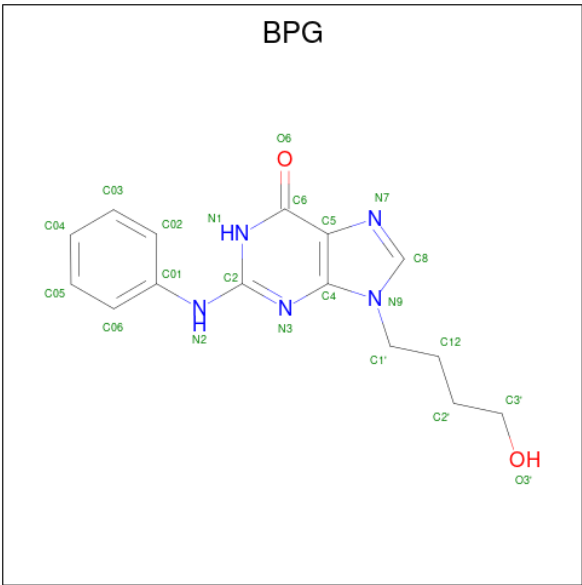
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	304	Total	C	N	O	S	0	0	4
			2304	1467	406	416	15			
1	B	308	Total	C	N	O	S	0	0	4
			2323	1482	407	419	15			

- Molecule 2 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		

- Molecule 3 is 9-(4-HYDROXYBUTYL)-N2-PHENYLGUANINE (CCD ID: BPG) (formula: C₁₅H₁₇N₅O₂).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			22	15	5	2		
3	B	1	Total	C	N	O	0	0
			22	15	5	2		

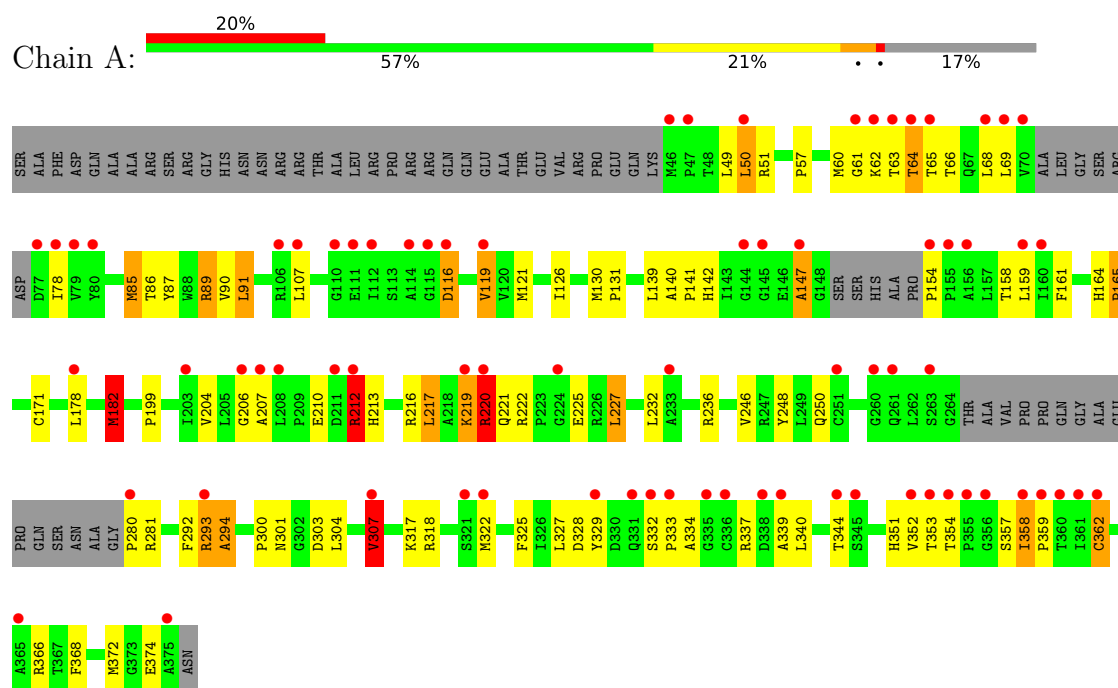
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	136	Total	O	0	0
			136	136		
4	B	136	Total	O	0	0
			136	136		

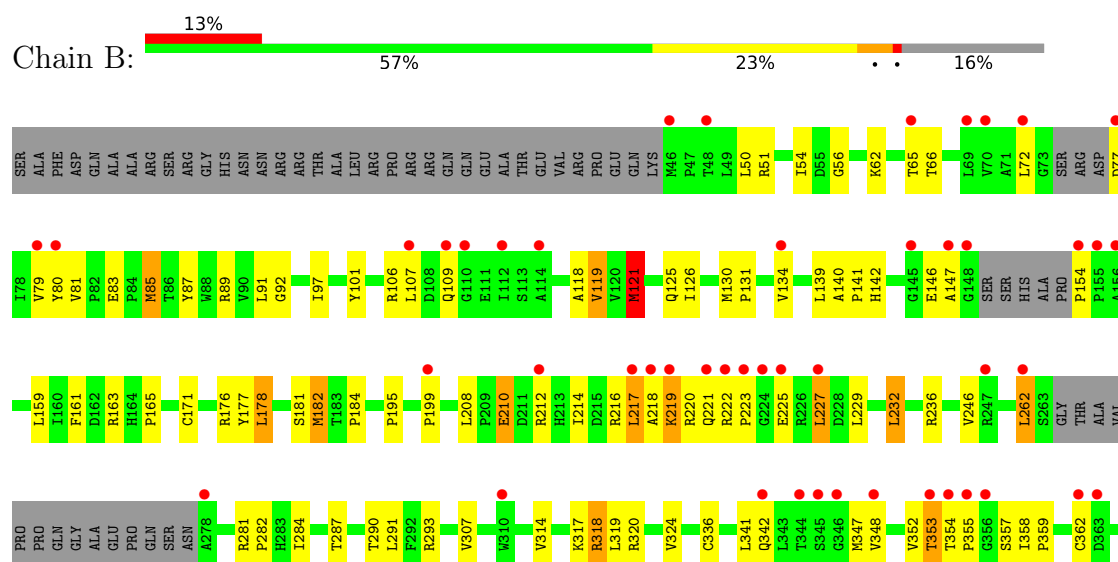
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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: PROTEIN (THYMIDINE KINASE)



• Molecule 1: PROTEIN (THYMIDINE KINASE)





4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	113.40Å 118.00Å 109.00Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	12.00 – 1.90 12.00 – 1.90	Depositor EDS
% Data completeness (in resolution range)	88.5 (12.00-1.90) 84.3 (12.00-1.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.04	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.51 (at 1.71Å)	Xtriage
Refinement program	X-PLOR 3.1F	Depositor
R, R_{free}	0.227 , 0.291 (Not available) , 0.287	Depositor DCC
R_{free} test set	6514 reflections (9.37%)	wwPDB-VP
Wilson B-factor (Å ²)	13.9	Xtriage
Anisotropy	0.050	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.40 , 87.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.42$, $\langle L^2 \rangle = 0.25$	Xtriage
Estimated twinning fraction	0.166 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.85	EDS
Total number of atoms	4953	wwPDB-VP
Average B, all atoms (Å ²)	20.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.26% 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: SO4, BPG

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	0.85	4/2355 (0.2%)	1.09	19/3215 (0.6%)
1	B	0.86	8/2375 (0.3%)	1.05	11/3245 (0.3%)
All	All	0.85	12/4730 (0.3%)	1.07	30/6460 (0.5%)

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	85	MET	SD-CE	-8.11	1.59	1.79
1	B	182	MET	SD-CE	-7.87	1.59	1.79
1	A	358	ILE	CA-CB	7.36	1.57	1.54
1	B	121	MET	SD-CE	-6.50	1.63	1.79
1	B	374	GLU	C-N	-6.00	1.25	1.33
1	A	182	MET	SD-CE	-5.79	1.65	1.79
1	B	195	PRO	CA-C	5.75	1.55	1.51
1	B	72	LEU	C-N	-5.68	1.25	1.33
1	A	147	ALA	C-N	-5.42	1.25	1.33
1	B	262	LEU	C-N	-5.32	1.25	1.33
1	B	134	VAL	CA-CB	5.16	1.60	1.54
1	B	147	ALA	C-N	-5.13	1.26	1.33

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	293	ARG	N-CA-C	-8.06	100.20	111.81
1	A	307	VAL	CB-CA-C	-7.92	101.66	112.04
1	B	171	CYS	N-CA-C	7.57	119.22	110.97
1	B	91	LEU	N-CA-C	7.41	119.36	111.28
1	A	210	GLU	N-CA-C	6.81	119.28	111.11
1	A	91	LEU	N-CA-C	6.74	118.28	111.07
1	B	81	VAL	N-CA-C	-6.65	101.56	108.15

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	154	PRO	N-CA-CB	6.23	109.86	103.00
1	A	280	PRO	N-CA-CB	6.11	109.72	103.00
1	A	171	CYS	N-CA-C	6.09	117.58	111.07
1	B	154	PRO	N-CA-CB	6.04	109.65	103.00
1	A	332	SER	CA-C-N	5.86	126.27	119.47
1	A	332	SER	C-N-CA	5.86	126.27	119.47
1	B	320	ARG	N-CA-C	5.85	119.67	112.54
1	A	212	ARG	N-CA-C	-5.66	105.26	111.82
1	A	222	ARG	N-CA-C	-5.64	103.64	110.13
1	B	372	MET	N-CA-C	5.59	120.99	113.72
1	B	319	LEU	N-CA-C	5.39	118.07	111.82
1	A	220	ARG	N-CA-C	5.38	119.66	108.53
1	A	116	ASP	N-CA-C	-5.31	105.57	111.36
1	B	66	THR	N-CA-C	-5.29	105.59	111.36
1	A	294	ALA	CA-C-N	5.27	125.59	119.47
1	A	294	ALA	C-N-CA	5.27	125.59	119.47
1	B	210	GLU	N-CA-C	5.23	116.98	111.28
1	A	334	ALA	N-CA-C	-5.22	105.50	111.14
1	B	140	ALA	N-CA-C	5.20	121.31	109.81
1	A	90	VAL	N-CA-C	5.17	120.10	109.34
1	A	307	VAL	N-CA-CB	5.07	116.81	110.47
1	B	293	ARG	N-CA-C	-5.06	104.62	111.55
1	A	64	THR	N-CA-C	-5.04	105.79	111.28

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	2304	0	2310	65	0
1	B	2323	0	2332	68	0
2	A	5	0	0	0	0
2	B	5	0	0	0	0
3	A	22	0	17	2	0
3	B	22	0	17	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	136	0	0	2	0
4	B	136	0	0	4	0
All	All	4953	0	4676	129	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 14.

All (129) 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:89:ARG:NH1	1:B:223:PRO:HB2	1.85	0.91
1:A:372:MET:SD	1:B:307:VAL:HG11	2.12	0.88
1:A:362:CYS:HB3	1:A:366:ARG:HH12	1.39	0.87
1:B:208:LEU:HD11	1:B:212:ARG:HD3	1.58	0.83
1:B:65:THR:HG21	1:B:336:CYS:HB2	1.66	0.77
1:B:121:MET:HG3	1:B:181:SER:HB2	1.67	0.75
1:B:353:THR:HG23	1:B:354:THR:HG23	1.68	0.73
1:B:176:ARG:HB2	1:B:182:MET:HE3	1.69	0.73
1:A:61:GLY:O	1:A:65:THR:HG23	1.90	0.71
1:B:347:MET:HA	4:B:657:HOH:O	1.92	0.69
1:A:353:THR:HG23	1:A:354:THR:HG23	1.74	0.69
1:B:176:ARG:CB	1:B:182:MET:HE3	2.23	0.68
1:B:89:ARG:HH12	1:B:223:PRO:HB2	1.59	0.66
1:A:362:CYS:HB3	1:A:366:ARG:NH1	2.12	0.65
1:A:159:LEU:HD13	1:A:161:PHE:CZ	2.31	0.65
1:A:62:LYS:HG2	1:A:329:TYR:OH	1.99	0.63
1:B:210:GLU:HG2	1:B:214:ILE:HD13	1.80	0.62
1:A:362:CYS:SG	1:A:366:ARG:NH2	2.73	0.62
1:B:287:THR:O	1:B:290:THR:HG22	1.99	0.62
1:A:219:LYS:NZ	1:A:220:ARG:HB2	2.14	0.61
1:B:77:ASP:N	4:B:687:HOH:O	2.34	0.61
1:B:56:GLY:O	1:B:163:ARG:NH2	2.33	0.61
1:B:142:HIS:HD2	1:B:357:SER:OG	1.85	0.60
1:B:219:LYS:N	1:B:219:LYS:HD2	2.15	0.60
3:A:1:BPG:N3	3:A:1:BPG:H061	2.17	0.60
1:B:85:MET:HE1	1:B:97:ILE:HD12	1.84	0.60
1:B:358:ILE:HB	1:B:359:PRO:HD3	1.82	0.60
1:B:85:MET:HE3	1:B:222:ARG:HD2	1.83	0.59
3:B:2:BPG:H061	3:B:2:BPG:N3	2.18	0.59
1:A:126:ILE:HD11	1:B:126:ILE:HD11	1.85	0.58
1:A:86:THR:OG1	1:A:374:GLU:HG2	2.04	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:177:TYR:CE1	1:B:184:PRO:HD3	2.39	0.57
1:B:121:MET:HE3	1:B:121:MET:HA	1.86	0.57
1:A:147:ALA:HA	1:A:351:HIS:CE1	2.40	0.56
1:A:212:ARG:CZ	1:A:216:ARG:HH21	2.18	0.56
1:A:85:MET:HB3	1:A:374:GLU:HG3	1.87	0.56
1:A:217:LEU:HD13	1:A:227:LEU:HD23	1.88	0.56
1:A:51:ARG:NH2	1:A:199:PRO:O	2.38	0.56
4:A:645:HOH:O	1:B:317:LYS:HE2	2.06	0.56
1:A:51:ARG:HD3	1:A:139:LEU:HD21	1.87	0.55
1:B:246:VAL:HG21	1:B:324:VAL:HG21	1.88	0.55
1:A:221:GLN:NE2	1:A:225:GLU:HG2	2.22	0.55
1:A:372:MET:SD	1:B:307:VAL:CG1	2.91	0.54
1:A:63:THR:HA	1:A:66:THR:OG1	2.07	0.54
1:B:159:LEU:HD13	1:B:161:PHE:CZ	2.42	0.54
1:A:64:THR:O	1:A:68:LEU:HG	2.08	0.54
1:B:210:GLU:O	1:B:214:ILE:HD13	2.08	0.54
1:A:207:ALA:HB3	1:A:328:ASP:HA	1.88	0.53
1:B:51:ARG:NH2	1:B:199:PRO:O	2.42	0.53
1:A:358:ILE:HB	1:A:359:PRO:HD3	1.90	0.53
1:A:119:VAL:HG13	1:B:119:VAL:HG13	1.91	0.52
1:A:217:LEU:HD13	1:A:227:LEU:CD2	2.39	0.52
1:B:262:LEU:HD21	1:B:284:ILE:HD13	1.89	0.52
1:B:222:ARG:HD3	1:B:223:PRO:HD2	1.91	0.52
1:A:66:THR:O	1:A:69:LEU:HB2	2.09	0.51
1:A:246:VAL:O	1:A:250:GLN:HG3	2.10	0.51
1:A:307:VAL:HG22	1:B:371:GLU:OE1	2.10	0.51
1:A:327:LEU:HD11	1:A:339:ALA:HB3	1.92	0.51
1:B:118:ALA:HA	1:B:181:SER:O	2.11	0.51
1:A:87:TYR:HA	1:A:91:LEU:HB2	1.94	0.50
1:B:101:TYR:CD1	1:B:225:GLU:HA	2.47	0.50
1:A:307:VAL:HG13	1:B:372:MET:HE1	1.92	0.50
1:A:221:GLN:HE22	1:A:225:GLU:HG2	1.77	0.50
1:A:60:MET:HE1	1:A:206:GLY:HA3	1.94	0.49
1:A:164:HIS:CD2	1:A:165:PRO:HD2	2.47	0.49
1:B:85:MET:CE	1:B:222:ARG:HD2	2.41	0.49
1:B:216:ARG:O	1:B:219:LYS:HB2	2.12	0.49
1:A:140:ALA:HB3	1:A:141:PRO:HD3	1.93	0.49
1:B:121:MET:CE	1:B:125:GLN:HE21	2.26	0.49
1:B:236:ARG:NH1	4:B:671:HOH:O	2.46	0.49
1:B:353:THR:CG2	1:B:354:THR:HG23	2.40	0.48
1:A:62:LYS:O	1:A:66:THR:HG23	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:354:THR:HB	1:B:355:PRO:HD2	1.95	0.48
1:B:141:PRO:O	1:B:353:THR:HG21	2.14	0.48
1:A:142:HIS:HA	1:A:353:THR:HG22	1.96	0.47
1:A:85:MET:HE3	1:A:89:ARG:HG2	1.96	0.47
1:A:219:LYS:HZ2	1:A:220:ARG:HB2	1.78	0.47
1:B:87:TYR:CE2	1:B:92:GLY:HA3	2.50	0.47
1:B:178:LEU:HD11	1:B:291:LEU:HD22	1.95	0.46
1:B:212:ARG:NH1	4:B:593:HOH:O	2.48	0.46
1:A:68:LEU:HB2	1:A:337:ARG:HG3	1.98	0.46
1:B:218:ALA:C	1:B:219:LYS:HD2	2.40	0.46
1:A:119:VAL:HG13	1:B:119:VAL:CG1	2.46	0.46
1:B:51:ARG:HD3	1:B:139:LEU:HD21	1.97	0.45
1:B:232:LEU:HD13	1:B:236:ARG:HD2	1.97	0.45
1:A:340:LEU:HD12	1:A:340:LEU:O	2.16	0.45
1:B:83:GLU:OE2	1:B:163:ARG:HD2	2.16	0.45
1:A:219:LYS:HZ3	1:A:220:ARG:HB2	1.79	0.45
1:A:78:ILE:HA	1:A:158:THR:O	2.18	0.44
3:A:1:BPG:N3	3:A:1:BPG:C06	2.75	0.44
1:A:147:ALA:HA	1:A:351:HIS:HE1	1.81	0.44
1:A:49:LEU:HG	1:A:50:LEU:N	2.33	0.44
1:A:116:ASP:O	1:A:119:VAL:HG12	2.17	0.44
1:B:79:VAL:HG12	1:B:80:TYR:N	2.33	0.43
1:A:57:PRO:HB2	1:A:213:HIS:HE1	1.82	0.43
1:A:307:VAL:HG13	1:B:372:MET:CE	2.48	0.43
1:A:62:LYS:HG2	1:A:329:TYR:CZ	2.53	0.43
1:A:292:PHE:C	1:A:294:ALA:H	2.26	0.43
1:B:85:MET:HB3	1:B:374:GLU:HB3	2.01	0.43
1:A:204:VAL:HA	1:A:325:PHE:O	2.18	0.43
1:A:317:LYS:HE3	1:A:318:ARG:NH2	2.34	0.43
1:B:146:GLU:HG3	1:B:199:PRO:HB3	2.00	0.43
1:A:333:PRO:O	1:A:337:ARG:HB2	2.19	0.43
1:A:164:HIS:CE1	1:A:322:MET:HE1	2.54	0.42
1:A:352:VAL:HB	1:A:357:SER:CB	2.50	0.42
1:B:222:ARG:H	1:B:225:GLU:HB3	1.85	0.42
1:A:57:PRO:HD2	1:A:60:MET:CE	2.49	0.42
1:A:60:MET:CE	1:A:206:GLY:HA3	2.49	0.42
1:B:54:ILE:HD12	1:B:54:ILE:N	2.35	0.42
1:B:121:MET:HE3	1:B:121:MET:CA	2.49	0.42
1:B:146:GLU:CD	1:B:348:VAL:HG11	2.44	0.42
3:B:2:BPG:N3	3:B:2:BPG:C06	2.79	0.42
1:A:130:MET:HB3	1:A:131:PRO:HD3	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:248:TYR:CD1	1:A:281:ARG:HD3	2.55	0.42
1:A:121:MET:HG3	1:A:182:MET:HE1	2.02	0.42
1:A:368:PHE:C	1:A:368:PHE:CD2	2.98	0.42
1:B:281:ARG:HA	1:B:282:PRO:HD3	1.92	0.41
1:B:79:VAL:HG12	1:B:80:TYR:H	1.85	0.41
1:B:130:MET:HB3	1:B:131:PRO:HD3	2.02	0.41
1:B:222:ARG:HB2	1:B:225:GLU:OE2	2.20	0.41
1:B:217:LEU:C	1:B:219:LYS:N	2.77	0.41
1:A:236:ARG:HA	4:A:614:HOH:O	2.21	0.41
1:B:121:MET:CE	1:B:125:GLN:NE2	2.84	0.41
1:B:222:ARG:HB3	1:B:225:GLU:HB2	2.03	0.41
1:B:227:LEU:HD11	1:B:229:LEU:HD21	2.02	0.41
1:B:106:ARG:HA	1:B:106:ARG:HD3	1.95	0.41
1:B:314:VAL:O	1:B:318:ARG:HG2	2.21	0.40
1:A:85:MET:CE	1:A:89:ARG:CG	2.99	0.40
1:A:301:ASN:OD1	1:A:303:ASP:HB2	2.20	0.40

There are no symmetry-related clashes.

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	296/366 (81%)	282 (95%)	14 (5%)	0	100	100
1	B	300/366 (82%)	284 (95%)	13 (4%)	3 (1%)	12	5
All	All	596/732 (81%)	566 (95%)	27 (4%)	3 (0%)	24	16

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	374	GLU
1	B	220	ARG

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Mol	Chain	Res	Type
1	B	221	GLN

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	241/293 (82%)	222 (92%)	19 (8%)	11	5
1	B	242/293 (83%)	222 (92%)	20 (8%)	10	4
All	All	483/586 (82%)	444 (92%)	39 (8%)	11	5

All (39) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	50	LEU
1	A	89	ARG
1	A	107	LEU
1	A	119	VAL
1	A	165	PRO
1	A	178	LEU
1	A	182	MET
1	A	212	ARG
1	A	217	LEU
1	A	219	LYS
1	A	220	ARG
1	A	227	LEU
1	A	232	LEU
1	A	293	ARG
1	A	300	PRO
1	A	304	LEU
1	A	307	VAL
1	A	344	THR
1	A	362	CYS
1	B	50	LEU
1	B	62	LYS
1	B	85	MET

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Mol	Chain	Res	Type
1	B	107	LEU
1	B	109	GLN
1	B	119	VAL
1	B	121	MET
1	B	165	PRO
1	B	178	LEU
1	B	217	LEU
1	B	219	LYS
1	B	227	LEU
1	B	232	LEU
1	B	318	ARG
1	B	341	LEU
1	B	342	GLN
1	B	352	VAL
1	B	353	THR
1	B	362	CYS
1	B	374	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	67	GLN
1	A	142	HIS
1	A	221	GLN
1	B	109	GLN
1	B	142	HIS
1	B	323	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 oligosaccharides in this entry.

5.6 Ligand geometry

4 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	BPG	A	1	-	24,24,24	1.05	1 (4%)	30,32,32	1.10	2 (6%)
2	SO4	A	3	-	4,4,4	0.84	0	6,6,6	0.65	0
2	SO4	B	4	-	4,4,4	0.83	0	6,6,6	0.86	0
3	BPG	B	2	-	24,24,24	0.88	1 (4%)	30,32,32	1.25	4 (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	BPG	A	1	-	-	0/9/9/9	0/3/3/3
3	BPG	B	2	-	-	0/9/9/9	0/3/3/3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1	BPG	C4-N9	3.82	1.43	1.37
3	B	2	BPG	C4-N9	2.40	1.41	1.37

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1	BPG	C8-N9-C4	-2.98	102.67	105.89
3	B	2	BPG	N9-C8-N7	2.80	116.44	113.52
3	B	2	BPG	O3'-C3'-C2'	-2.77	93.84	111.44
3	A	1	BPG	N9-C8-N7	2.77	116.41	113.52
3	B	2	BPG	C8-N9-C4	-2.44	103.25	105.89
3	B	2	BPG	C12-C1'-N9	-2.26	104.86	112.25

There are no chirality outliers.

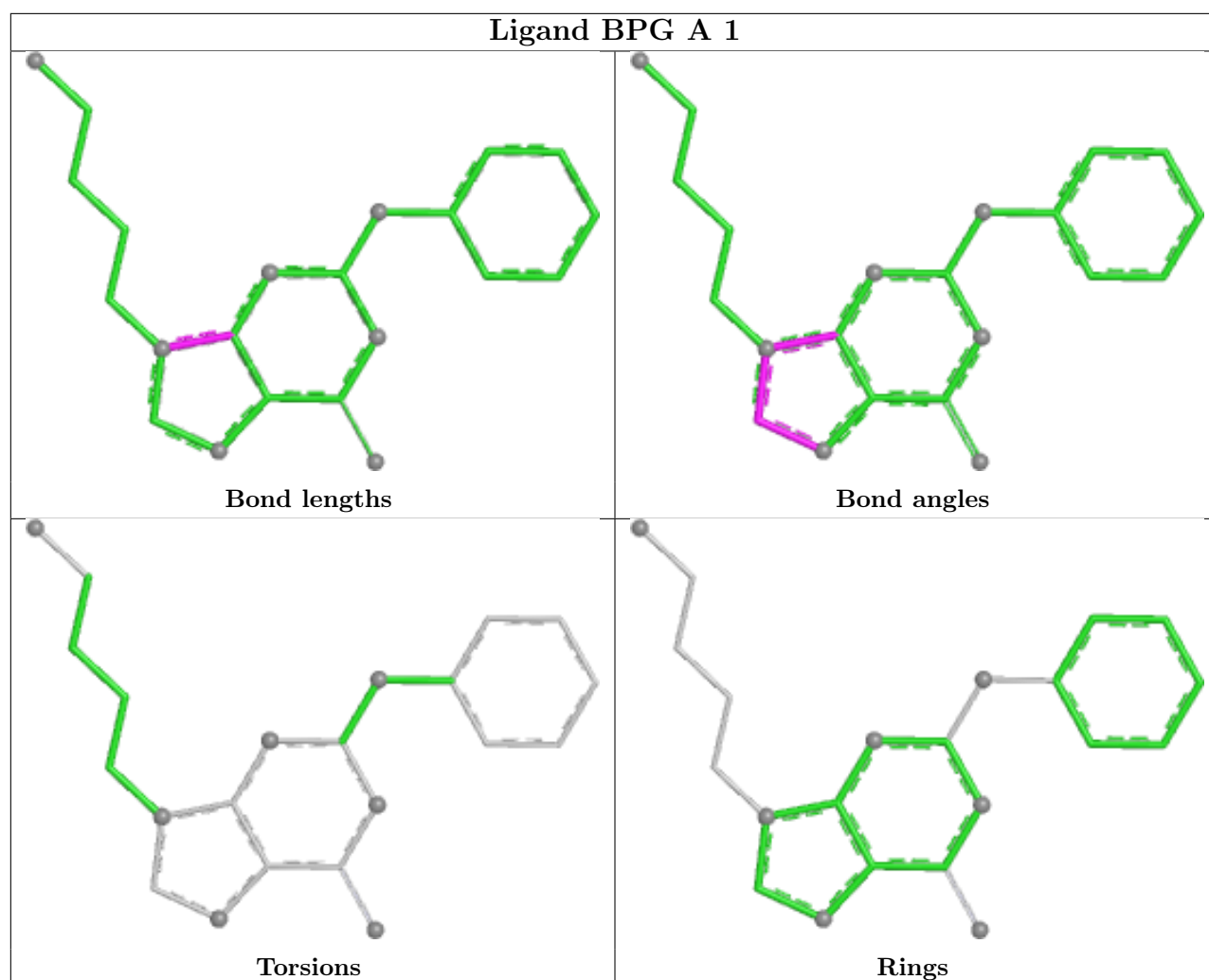
There are no torsion outliers.

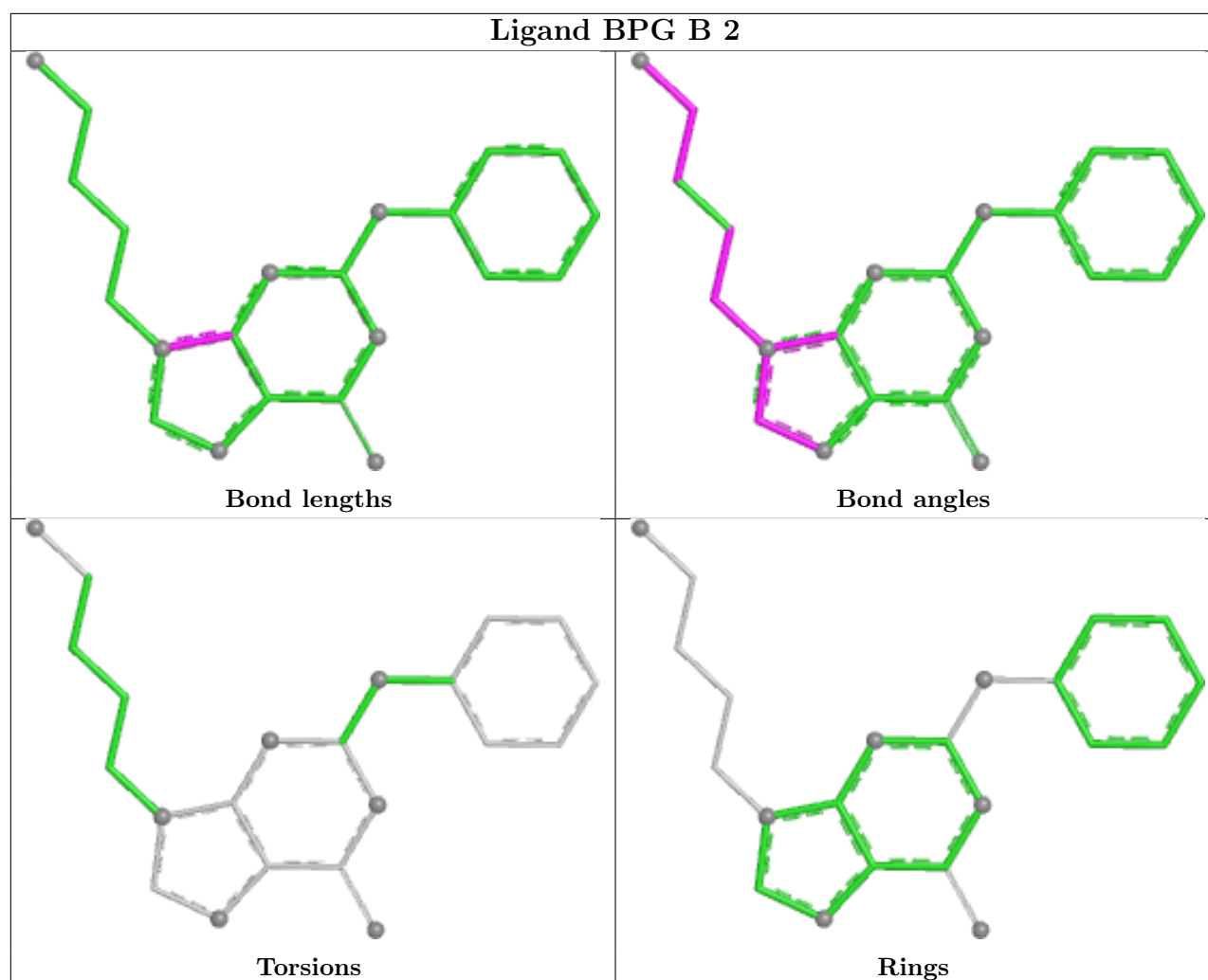
There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1	BPG	2	0
3	B	2	BPG	2	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	304/366 (83%)	1.36	74 (24%) 2 1	8, 19, 37, 49	0
1	B	308/366 (84%)	1.24	49 (15%) 5 5	8, 17, 37, 45	0
All	All	612/732 (83%)	1.30	123 (20%) 3 2	8, 18, 37, 49	0

All (123) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	147	ALA	6.5
1	B	218	ALA	6.2
1	A	375	ALA	6.0
1	A	280	PRO	5.5
1	B	155	PRO	5.0
1	B	345	SER	4.8
1	A	68	LEU	4.7
1	B	148	GLY	4.6
1	B	46	MET	4.6
1	A	70	VAL	4.6
1	A	78	ILE	4.5
1	B	212	ARG	4.1
1	A	356	GLY	4.1
1	B	346	GLY	4.0
1	A	260	GLY	4.0
1	A	77	ASP	3.9
1	A	110	GLY	3.8
1	A	219	LYS	3.8
1	B	356	GLY	3.7
1	A	333	PRO	3.7
1	A	115	GLY	3.6
1	B	80	TYR	3.5
1	A	344	THR	3.5
1	B	353	THR	3.5

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Mol	Chain	Res	Type	RSRZ
1	B	225	GLU	3.4
1	B	154	PRO	3.4
1	A	307	VAL	3.3
1	A	154	PRO	3.3
1	A	79	VAL	3.2
1	A	353	THR	3.2
1	A	211	ASP	3.2
1	A	63	THR	3.2
1	B	79	VAL	3.2
1	B	221	GLN	3.2
1	B	354	THR	3.1
1	A	156	ALA	3.1
1	A	339	ALA	3.1
1	A	329	TYR	3.1
1	A	147	ALA	3.1
1	B	110	GLY	3.1
1	A	69	LEU	3.0
1	A	112	ILE	3.0
1	A	208	LEU	3.0
1	B	363	ASP	3.0
1	B	199	PRO	3.0
1	A	220	ARG	3.0
1	B	223	PRO	2.9
1	B	355	PRO	2.9
1	A	332	SER	2.9
1	B	70	VAL	2.9
1	B	344	THR	2.9
1	A	207	ALA	2.8
1	B	77	ASP	2.8
1	A	145	GLY	2.8
1	A	178	LEU	2.8
1	A	345	SER	2.8
1	B	114	ALA	2.7
1	B	262	LEU	2.7
1	A	263	SER	2.7
1	A	354	THR	2.7
1	A	352	VAL	2.7
1	B	227	LEU	2.7
1	A	111	GLU	2.6
1	B	219	LYS	2.6
1	A	64	THR	2.6
1	A	50	LEU	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	107	LEU	2.6
1	A	65	THR	2.6
1	B	65	THR	2.5
1	B	217	LEU	2.5
1	A	47	PRO	2.5
1	A	335	GLY	2.5
1	B	72	LEU	2.5
1	A	106	ARG	2.5
1	A	203	ILE	2.5
1	B	342	GLN	2.5
1	A	155	PRO	2.5
1	A	61	GLY	2.4
1	A	206	GLY	2.4
1	A	355	PRO	2.4
1	B	348	VAL	2.4
1	A	360	THR	2.4
1	A	358	ILE	2.4
1	B	134	VAL	2.4
1	A	62	LYS	2.4
1	B	107	LEU	2.3
1	B	224	GLY	2.3
1	B	247	ARG	2.3
1	A	365	ALA	2.3
1	B	375	ALA	2.3
1	B	145	GLY	2.3
1	A	212	ARG	2.3
1	A	46	MET	2.3
1	A	233	ALA	2.3
1	A	336	CYS	2.3
1	B	362	CYS	2.3
1	B	310	TRP	2.2
1	A	224	GLY	2.2
1	A	361	ILE	2.2
1	A	119	VAL	2.2
1	A	331	GLN	2.2
1	A	338	ASP	2.2
1	A	80	TYR	2.2
1	B	69	LEU	2.2
1	A	322	MET	2.1
1	A	160	ILE	2.1
1	B	109	GLN	2.1
1	A	116	ASP	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	321	SER	2.1
1	A	359	PRO	2.1
1	B	222	ARG	2.1
1	A	114	ALA	2.1
1	B	48	THR	2.1
1	A	144	GLY	2.1
1	A	362	CYS	2.1
1	A	261	GLN	2.1
1	B	156	ALA	2.1
1	B	374	GLU	2.1
1	B	278	ALA	2.1
1	B	112	ILE	2.0
1	A	159	LEU	2.0
1	A	251	CYS	2.0
1	A	293	ARG	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

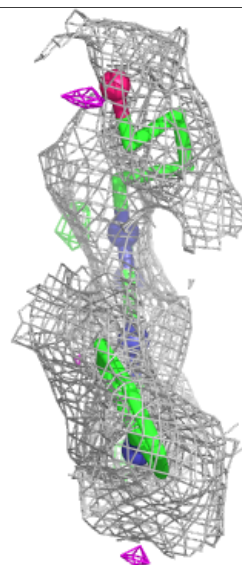
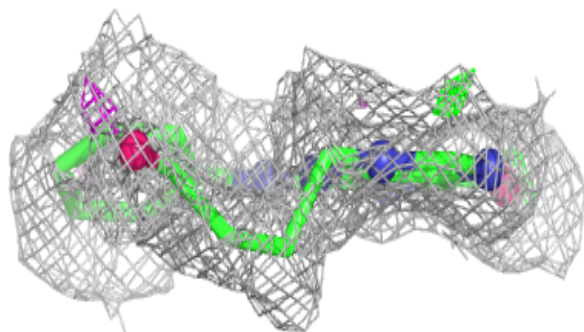
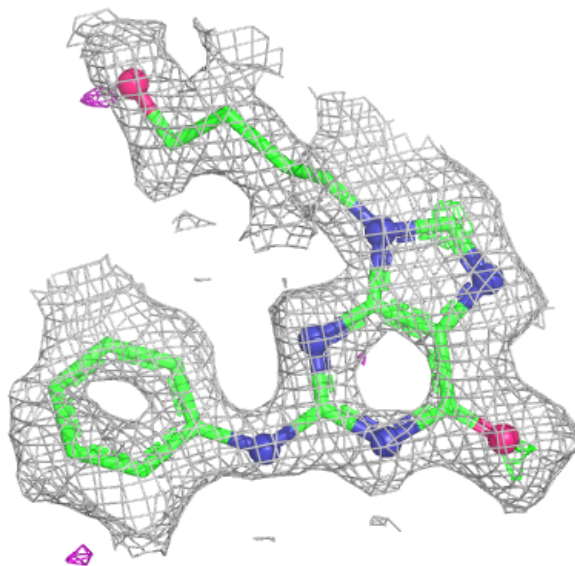
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

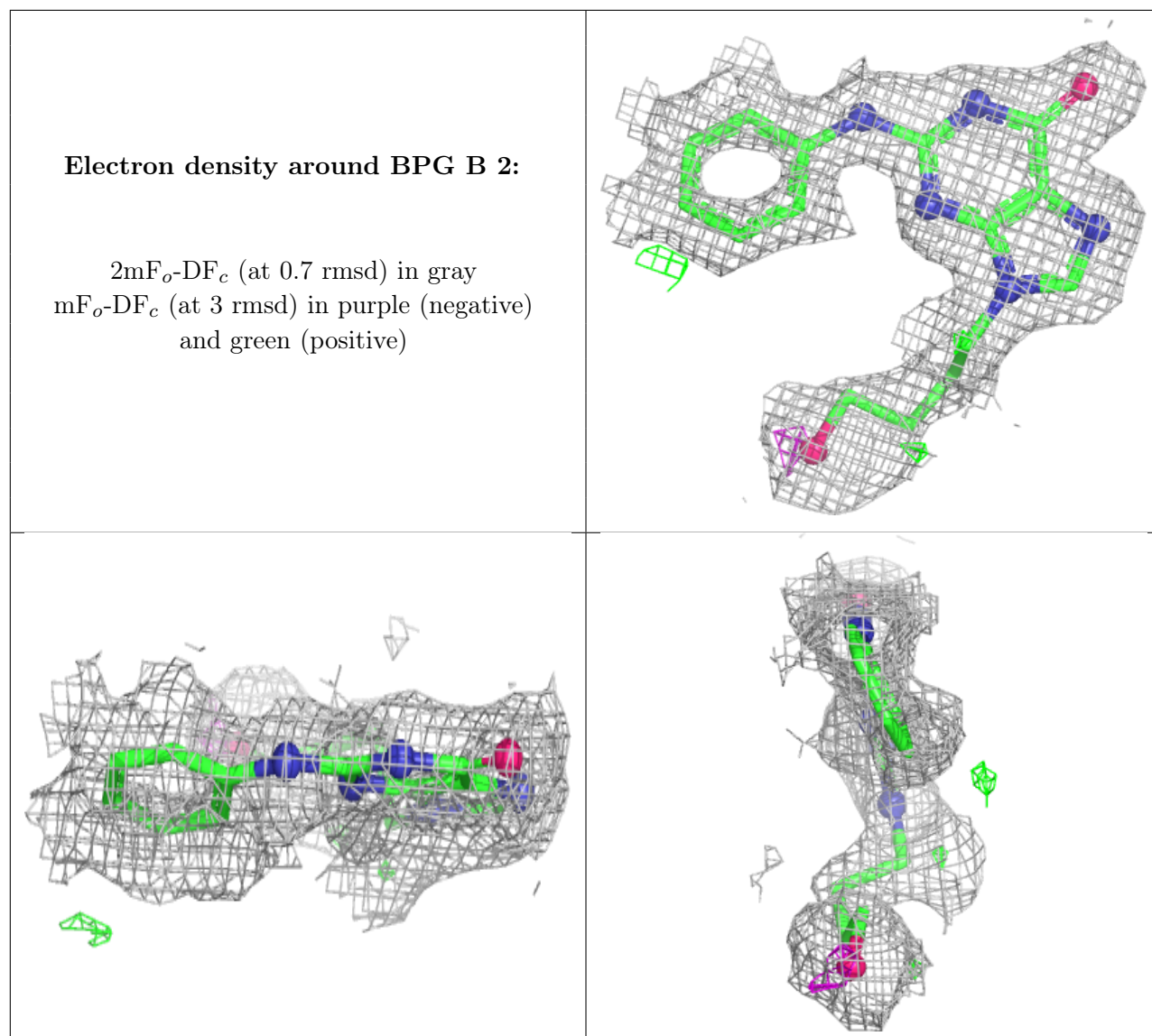
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	SO4	A	3	5/5	0.89	0.13	26,28,30,30	0
3	BPG	A	1	22/22	0.89	0.11	12,15,17,21	0
3	BPG	B	2	22/22	0.91	0.09	8,13,22,30	0
2	SO4	B	4	5/5	0.94	0.11	21,22,24,27	0

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 BPG A 1:

$2mF_o-DF_c$ (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.