



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 02:05 PM UTC

PDB ID : 4PBG / pdb_00004pbg
Title : 6-PHOSPHO-BETA-GALACTOSIDASE FORM-CST
Authors : Wiesmann, C.; Schulz, G.E.
Deposited on : 1997-02-21
Resolution : 2.50 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) : 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

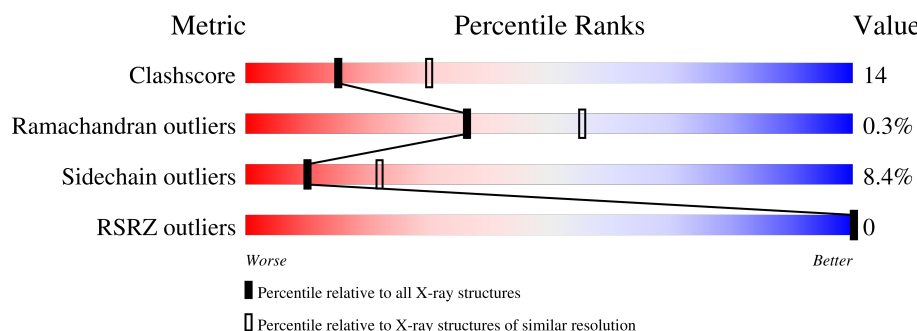
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

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	468	
1	B	468	

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 8057 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.

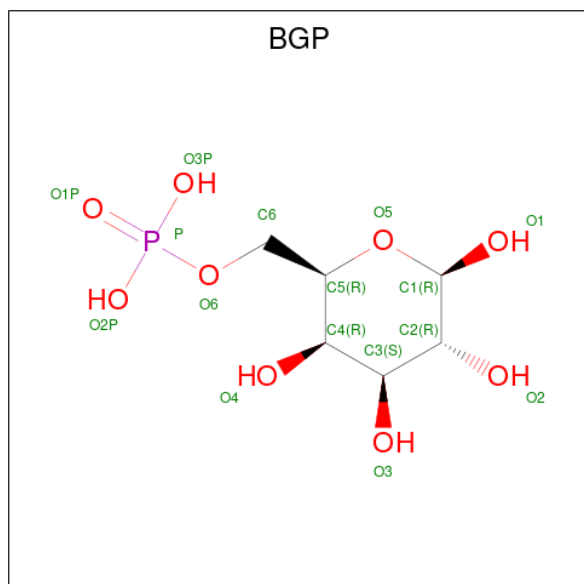
- Molecule 1 is a protein called 6-PHOSPHO-BETA-D-GALACTOSIDASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	468	Total	C	N	O	S	0	0	0
			3833	2473	624	725	11			
1	B	468	Total	C	N	O	S	0	0	0
			3833	2473	624	725	11			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	375	CYS	GLU	engineered mutation	UNP P11546
B	375	CYS	GLU	engineered mutation	UNP P11546

- Molecule 2 is 6-O-phosphono-beta-D-galactopyranose (CCD ID: BGP) (formula: C₆H₁₃O₉P).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	O	P	0	0
			16	6	9	1		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	B	1	Total	C	O	P	0	0
			16	6	9	1		

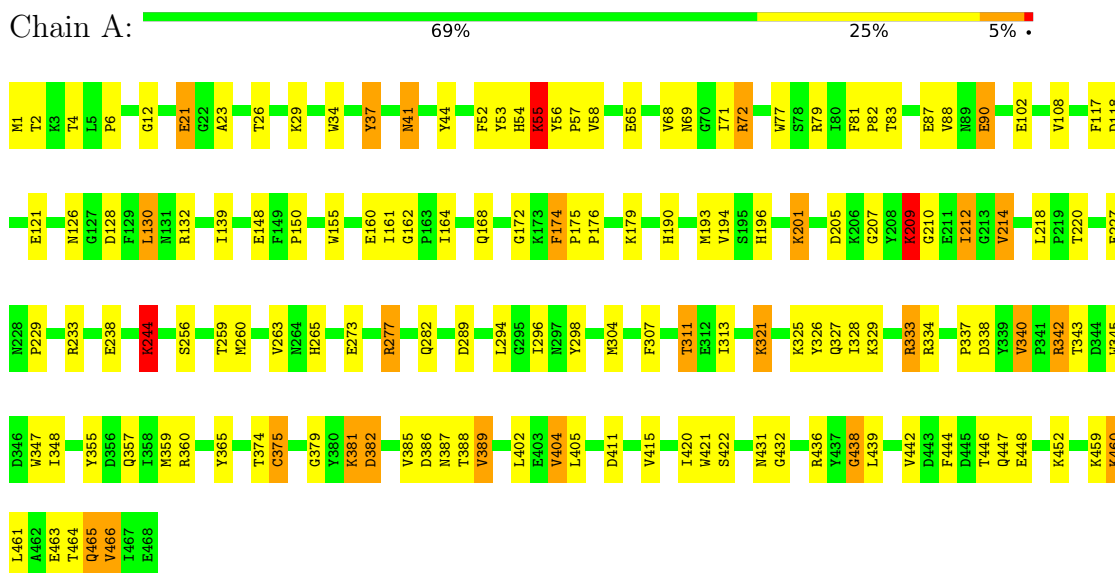
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	178	Total	O	0	0
			178	178		
3	B	181	Total	O	0	0
			181	181		

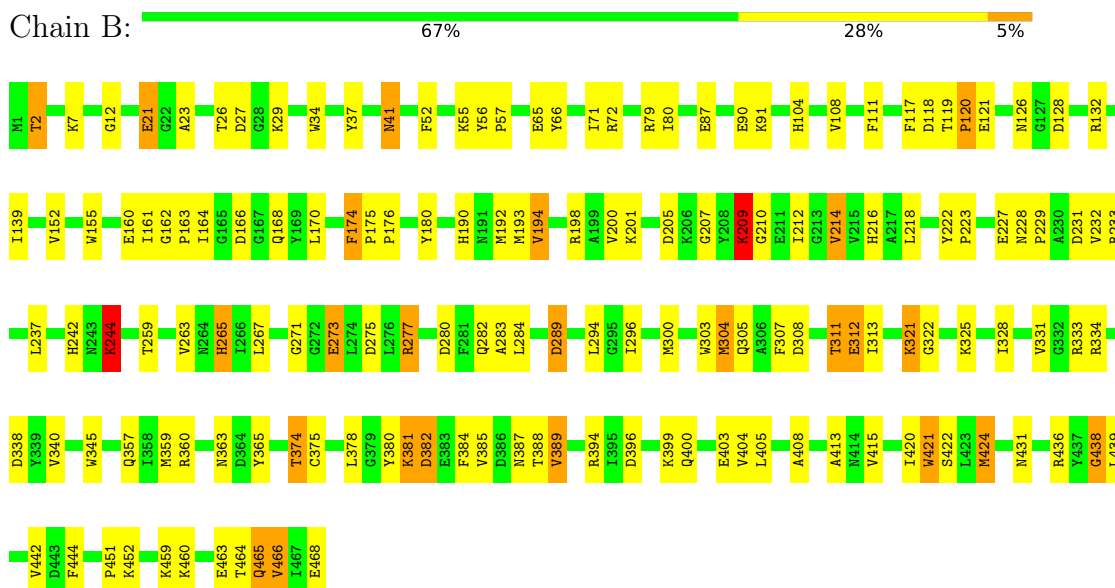
3 Residue-property plots

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: 6-PHOSPHO-BETA-D-GALACTOSIDASE



• Molecule 1: 6-PHOSPHO-BETA-D-GALACTOSIDASE



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	104.70Å 174.30Å 60.50Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	10.00 – 2.50 10.00 – 2.50	Depositor EDS
% Data completeness (in resolution range)	84.4 (10.00-2.50) 83.5 (10.00-2.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$	-	Xtriage
Refinement program	X-PLOR 3.1	Depositor
R, R_{free}	0.202 , (Not available) 0.201 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	13.2	Xtriage
Anisotropy	1.002	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 73.9	EDS
L-test for twinning ¹	$\langle L \rangle = 0.35$, $\langle L^2 \rangle = 0.19$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	8057	wwPDB-VP
Average B, all atoms (Å ²)	14.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 45.97 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.2245e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Theoretical 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: BGP

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	0.71	1/3953 (0.0%)	1.10	27/5363 (0.5%)
1	B	0.70	2/3953 (0.1%)	1.12	26/5363 (0.5%)
All	All	0.71	3/7906 (0.0%)	1.11	53/10726 (0.5%)

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	A	0	1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	304	MET	SD-CE	5.72	1.93	1.79
1	B	424	MET	SD-CE	-5.31	1.66	1.79
1	A	212	ILE	CA-CB	5.27	1.60	1.54

All (53) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	438	GLY	N-CA-C	14.37	128.46	111.93
1	A	438	GLY	N-CA-C	12.07	125.81	111.93
1	B	338	ASP	N-CA-C	11.62	123.50	111.07
1	B	209	LYS	N-CA-C	11.25	123.55	111.28
1	A	209	LYS	N-CA-C	11.20	123.56	111.36
1	A	338	ASP	N-CA-C	10.42	122.22	111.07
1	B	21	GLU	N-CA-C	9.47	122.58	111.02
1	B	389	VAL	N-CA-C	-7.58	98.34	108.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	439	LEU	N-CA-C	-7.51	103.57	112.89
1	A	439	LEU	N-CA-C	-7.04	103.36	112.23
1	B	162	GLY	CA-C-N	6.97	126.65	119.82
1	B	162	GLY	C-N-CA	6.97	126.65	119.82
1	B	242	HIS	N-CA-C	6.50	121.41	112.90
1	A	160	GLU	N-CA-C	6.49	118.50	110.91
1	A	201	LYS	N-CA-C	-6.46	104.16	111.07
1	B	201	LYS	N-CA-C	-6.43	104.19	111.07
1	A	342	ARG	N-CA-C	-6.05	100.22	109.41
1	B	244	LYS	N-CA-C	5.99	121.26	111.37
1	A	37	TYR	N-CA-C	5.90	117.41	110.97
1	B	282	GLN	N-CA-C	-5.87	104.96	111.36
1	B	118	ASP	N-CA-C	5.87	120.68	108.53
1	A	340	VAL	CA-C-N	-5.85	113.75	119.90
1	A	340	VAL	C-N-CA	-5.85	113.75	119.90
1	A	174	PHE	N-CA-C	-5.84	102.05	110.40
1	A	148	GLU	N-CA-C	5.79	118.53	111.82
1	B	365	TYR	CA-C-N	5.79	125.46	119.56
1	B	365	TYR	C-N-CA	5.79	125.46	119.56
1	B	216	HIS	N-CA-C	5.75	119.20	109.76
1	A	244	LYS	N-CA-C	5.71	120.79	111.37
1	A	118	ASP	N-CA-C	5.60	120.13	108.53
1	B	160	GLU	N-CA-C	5.49	117.88	111.02
1	B	174	PHE	N-CA-C	-5.46	103.29	110.39
1	A	21	GLU	N-CA-C	5.36	122.22	110.80
1	B	12	GLY	N-CA-C	5.35	119.91	112.57
1	B	214	VAL	CB-CA-C	-5.30	102.66	110.82
1	B	128	ASP	CB-CA-C	-5.23	110.53	116.54
1	B	152	VAL	N-CA-C	5.16	115.53	107.99
1	A	55	LYS	N-CA-C	5.14	118.70	112.23
1	B	421	TRP	N-CA-C	-5.13	100.80	108.96
1	A	389	VAL	N-CA-C	-5.13	101.25	108.27
1	A	72	ARG	N-CA-C	-5.12	101.36	109.96
1	A	162	GLY	CA-C-N	5.11	124.83	119.82
1	A	162	GLY	C-N-CA	5.11	124.83	119.82
1	B	111	PHE	N-CA-C	-5.10	98.96	107.99
1	B	194	VAL	N-CA-C	-5.10	105.57	110.72
1	A	128	ASP	CB-CA-C	-5.08	110.70	116.54
1	A	58	VAL	CB-CA-C	-5.07	105.48	111.97
1	B	80	ILE	N-CA-C	-5.07	106.73	111.45
1	A	365	TYR	CA-C-N	5.05	124.71	119.56
1	A	365	TYR	C-N-CA	5.05	124.71	119.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	130	LEU	N-CA-C	-5.05	105.87	112.23
1	A	348	ILE	N-CA-C	5.05	115.55	108.89
1	A	282	GLN	N-CA-C	-5.01	105.90	111.36

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	326	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	3833	0	3594	102	0
1	B	3833	0	3594	102	0
2	A	16	0	11	0	0
2	B	16	0	11	0	0
3	A	178	0	0	17	0
3	B	181	0	0	14	0
All	All	8057	0	7210	203	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 (203) 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:244:LYS:HG2	1:B:360:ARG:NH2	1.86	0.90
1:A:388:THR:HG22	1:A:389:VAL:H	1.37	0.88
1:A:244:LYS:HG2	1:A:360:ARG:NH2	1.91	0.85
1:A:161:ILE:HD12	1:A:193:MET:HE3	1.60	0.82
1:B:388:THR:HG22	1:B:389:VAL:H	1.45	0.81
1:B:283:ALA:HB1	3:B:510:HOH:O	1.81	0.79
1:A:29:LYS:HE3	3:A:634:HOH:O	1.82	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:161:ILE:HD12	1:B:193:MET:HE3	1.65	0.78
1:B:198:ARG:HG3	3:B:510:HOH:O	1.87	0.75
1:A:311:THR:HB	1:A:328:ILE:HA	1.69	0.74
1:B:37:TYR:CG	1:B:175:PRO:HG3	2.25	0.71
1:A:90:GLU:HG3	3:A:483:HOH:O	1.89	0.71
1:A:321:LYS:HD2	1:A:321:LYS:H	1.55	0.70
1:B:244:LYS:HG2	1:B:360:ARG:HH21	1.55	0.70
1:A:311:THR:HG22	1:A:329:LYS:H	1.57	0.69
1:A:307:PHE:HB2	1:A:333:ARG:HG2	1.74	0.69
1:B:168:GLN:HG3	1:B:175:PRO:O	1.93	0.68
1:B:307:PHE:CD2	1:B:333:ARG:HD2	2.29	0.68
1:B:308:ASP:HA	3:B:570:HOH:O	1.92	0.68
1:B:244:LYS:HD3	3:B:575:HOH:O	1.92	0.67
1:A:168:GLN:HG3	1:A:175:PRO:O	1.96	0.66
1:A:464:THR:O	1:A:465:GLN:HG2	1.96	0.66
1:B:259:THR:O	1:B:263:VAL:HG23	1.96	0.65
1:A:244:LYS:HG2	1:A:360:ARG:HH21	1.60	0.65
1:B:311:THR:HB	1:B:328:ILE:HA	1.78	0.65
1:A:23:ALA:HB3	1:A:79:ARG:HH22	1.61	0.65
1:A:102:GLU:HG2	3:A:630:HOH:O	1.97	0.65
1:A:37:TYR:CG	1:A:175:PRO:HG3	2.31	0.64
1:B:304:MET:SD	1:B:334:ARG:HG2	2.37	0.64
1:B:396:ASP:O	1:B:400:GLN:HG3	1.98	0.64
1:B:164:ILE:O	1:B:168:GLN:HB2	1.98	0.63
1:A:381:LYS:NZ	1:A:436:ARG:HD2	2.15	0.62
1:A:161:ILE:HD12	1:A:193:MET:CE	2.30	0.62
1:B:381:LYS:NZ	1:B:436:ARG:HD2	2.14	0.62
1:B:382:ASP:HB3	1:B:389:VAL:HG11	1.82	0.62
1:A:259:THR:O	1:A:263:VAL:HG23	2.00	0.62
1:B:209:LYS:HD2	1:B:210:GLY:N	2.15	0.62
1:B:2:THR:HA	3:B:501:HOH:O	1.99	0.61
1:A:209:LYS:HB3	3:B:514:HOH:O	2.00	0.61
1:A:345:TRP:CD1	1:A:431:ASN:HD22	2.18	0.60
1:A:382:ASP:HB3	1:A:389:VAL:HG11	1.83	0.60
1:B:23:ALA:HB1	1:B:26:THR:HB	1.84	0.59
1:A:132:ARG:NH2	1:A:277:ARG:HD3	2.18	0.59
1:A:405:LEU:HD22	1:A:415:VAL:HG11	1.84	0.59
1:A:381:LYS:HE2	1:A:382:ASP:O	2.04	0.58
1:A:164:ILE:O	1:A:168:GLN:HB2	2.04	0.58
1:B:384:PHE:CZ	1:B:387:ASN:HA	2.38	0.58
1:B:289:ASP:HB3	3:B:505:HOH:O	2.03	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:321:LYS:H	1:A:321:LYS:CD	2.17	0.57
1:A:386:ASP:O	1:A:387:ASN:HB2	2.03	0.57
1:B:117:PHE:CD1	1:B:164:ILE:HD11	2.39	0.57
1:B:190:HIS:O	1:B:194:VAL:HG23	2.04	0.57
1:B:244:LYS:HG2	1:B:360:ARG:HH22	1.68	0.57
1:A:260:MET:HG2	3:A:612:HOH:O	2.03	0.57
1:A:209:LYS:HD2	1:A:210:GLY:N	2.19	0.57
1:A:130:LEU:HB3	3:A:496:HOH:O	2.05	0.56
1:A:355:TYR:HB2	1:A:404:VAL:HG13	1.87	0.56
1:B:464:THR:O	1:B:465:GLN:HG2	2.05	0.56
1:A:464:THR:HG22	1:A:466:VAL:HB	1.87	0.56
1:B:168:GLN:HG2	1:B:176:PRO:HD2	1.87	0.56
1:A:381:LYS:HZ2	1:A:436:ARG:HD2	1.69	0.56
1:A:53:TYR:HB3	1:A:54:HIS:HD2	1.72	0.55
1:A:342:ARG:HH11	1:A:342:ARG:HG2	1.71	0.55
1:B:381:LYS:HA	1:B:381:LYS:HE3	1.89	0.55
1:B:55:LYS:HE2	3:B:619:HOH:O	2.06	0.55
1:A:343:THR:HB	3:A:513:HOH:O	2.05	0.55
1:A:168:GLN:HG2	1:A:176:PRO:HD2	1.88	0.55
1:B:438:GLY:O	1:B:452:LYS:HD2	2.07	0.54
1:B:312:GLU:HG2	1:B:325:LYS:HD3	1.90	0.54
1:B:307:PHE:HB2	1:B:333:ARG:HD2	1.88	0.54
1:B:381:LYS:HZ1	1:B:436:ARG:HD2	1.72	0.54
1:A:218:LEU:HD12	1:A:296:ILE:HG12	1.91	0.53
1:B:7:LYS:HB3	3:B:588:HOH:O	2.08	0.53
1:B:436:ARG:NH2	1:B:442:VAL:O	2.41	0.53
1:B:117:PHE:HD1	1:B:164:ILE:HD11	1.74	0.53
1:A:53:TYR:HB3	1:A:54:HIS:CD2	2.44	0.52
1:B:388:THR:HG23	1:B:451:PRO:O	2.08	0.52
1:B:345:TRP:CD1	1:B:431:ASN:HD22	2.27	0.52
1:B:117:PHE:HA	1:B:164:ILE:HD11	1.92	0.52
1:B:307:PHE:HD2	1:B:333:ARG:HD2	1.73	0.52
1:B:209:LYS:HD2	1:B:210:GLY:H	1.74	0.52
1:B:405:LEU:HD22	1:B:415:VAL:HG11	1.92	0.52
1:A:117:PHE:CD1	1:A:164:ILE:HD11	2.44	0.52
1:A:327:GLN:HB3	1:A:333:ARG:HB3	1.92	0.51
1:A:464:THR:C	1:A:465:GLN:HG2	2.35	0.51
1:A:381:LYS:HA	1:A:381:LYS:HE3	1.93	0.51
1:B:218:LEU:O	1:B:357:GLN:HG3	2.10	0.51
1:B:34:TRP:HH2	1:B:174:PHE:CD1	2.29	0.51
1:B:464:THR:C	1:B:465:GLN:HG2	2.36	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:81:PHE:CE1	1:A:88:VAL:HG22	2.45	0.51
1:B:27:ASP:HB3	1:B:91:LYS:HD3	1.92	0.50
1:A:359:MET:SD	3:A:568:HOH:O	2.60	0.50
1:A:34:TRP:HH2	1:A:174:PHE:CD1	2.29	0.50
1:A:117:PHE:HA	1:A:164:ILE:HD11	1.94	0.50
1:A:382:ASP:HB3	1:A:389:VAL:CG1	2.42	0.49
1:A:388:THR:HG22	1:A:389:VAL:N	2.17	0.49
1:A:205:ASP:C	1:A:207:GLY:H	2.20	0.49
1:B:161:ILE:HD12	1:B:193:MET:CE	2.38	0.49
1:A:256:SER:CB	3:A:608:HOH:O	2.60	0.49
1:A:244:LYS:HG2	1:A:360:ARG:HH22	1.73	0.49
1:B:328:ILE:HB	1:B:331:VAL:HB	1.94	0.49
1:A:256:SER:HB3	3:A:608:HOH:O	2.13	0.48
1:B:399:LYS:O	1:B:403:GLU:HG3	2.14	0.48
3:A:579:HOH:O	1:B:209:LYS:HB3	2.12	0.48
1:A:155:TRP:HB2	1:A:212:ILE:HD12	1.96	0.47
1:B:26:THR:HG22	1:B:27:ASP:OD2	2.15	0.47
1:B:322:GLY:HA2	3:B:599:HOH:O	2.14	0.47
1:A:311:THR:CG2	1:A:329:LYS:H	2.27	0.47
1:B:72:ARG:HD2	1:B:374:THR:HG22	1.95	0.47
1:B:198:ARG:N	3:B:510:HOH:O	2.48	0.47
1:A:72:ARG:HD2	1:A:374:THR:HG22	1.96	0.46
1:B:132:ARG:NH2	1:B:277:ARG:HD3	2.30	0.46
1:B:275:ASP:OD1	1:B:277:ARG:HD2	2.16	0.46
1:A:220:THR:HA	3:A:606:HOH:O	2.15	0.46
1:A:402:LEU:HD13	1:A:461:LEU:HD21	1.97	0.46
1:A:460:LYS:HE2	3:A:558:HOH:O	2.16	0.46
1:B:200:VAL:HG23	1:B:212:ILE:HG21	1.98	0.46
1:B:231:ASP:OD1	1:B:305:GLN:HA	2.15	0.46
1:B:381:LYS:HE2	1:B:382:ASP:O	2.14	0.46
1:B:382:ASP:HB3	1:B:389:VAL:CG1	2.44	0.46
1:B:466:VAL:HG12	1:B:468:GLU:HB2	1.98	0.46
1:A:436:ARG:NH2	1:A:442:VAL:O	2.48	0.46
1:A:459:LYS:O	1:A:463:GLU:HG2	2.15	0.46
1:A:375:CYS:SG	1:A:421:TRP:HB2	2.55	0.45
1:B:280:ASP:O	1:B:284:LEU:HG	2.15	0.45
1:A:190:HIS:O	1:A:194:VAL:HG23	2.16	0.45
1:A:196:HIS:CE1	1:A:214:VAL:HG22	2.51	0.45
1:B:56:TYR:CD1	1:B:57:PRO:HD3	2.52	0.45
1:B:378:LEU:HD23	1:B:380:TYR:CE2	2.51	0.45
1:A:201:LYS:HE3	1:A:205:ASP:OD2	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:56:TYR:N	1:B:57:PRO:HD2	2.32	0.45
1:A:209:LYS:HD2	1:A:210:GLY:H	1.82	0.45
1:A:446:THR:HB	1:A:448:GLU:HG3	1.98	0.45
1:B:205:ASP:C	1:B:207:GLY:H	2.25	0.45
1:B:209:LYS:HG3	3:B:512:HOH:O	2.16	0.45
1:B:222:TYR:O	1:B:303:TRP:HA	2.17	0.45
1:B:459:LYS:O	1:B:463:GLU:HG2	2.17	0.45
1:A:313:ILE:HA	1:A:325:LYS:O	2.17	0.44
1:A:238:GLU:HB2	1:A:304:MET:HE2	1.99	0.44
1:B:66:TYR:CD2	1:B:459:LYS:HE3	2.52	0.44
1:B:55:LYS:C	1:B:57:PRO:HD2	2.42	0.44
1:B:218:LEU:HD12	1:B:296:ILE:HG12	1.99	0.44
1:A:218:LEU:O	1:A:357:GLN:HG3	2.18	0.44
1:B:420:ILE:O	1:B:420:ILE:HG23	2.17	0.44
1:A:69:ASN:OD1	1:A:69:ASN:N	2.49	0.44
1:B:237:LEU:HD11	1:B:265:HIS:CD2	2.52	0.44
1:A:77:TRP:HD1	1:A:77:TRP:O	2.00	0.43
1:B:388:THR:HG22	1:B:389:VAL:N	2.24	0.43
1:A:311:THR:HG22	1:A:329:LYS:HB2	2.00	0.43
1:A:420:ILE:O	1:A:420:ILE:HG23	2.18	0.43
1:A:6:PRO:HG3	3:A:570:HOH:O	2.18	0.43
1:A:21:GLU:HA	1:A:52:PHE:HB3	2.00	0.43
1:B:228:ASN:O	1:B:231:ASP:HB2	2.19	0.43
1:B:155:TRP:HB2	1:B:212:ILE:HD12	2.00	0.43
1:A:307:PHE:HB2	1:A:333:ARG:CG	2.46	0.43
1:B:71:ILE:HG22	1:B:108:VAL:HG12	2.01	0.42
1:B:23:ALA:HB3	1:B:79:ARG:HH22	1.84	0.42
1:A:172:GLY:HA3	1:A:179:LYS:HG2	2.01	0.42
1:A:421:TRP:HA	1:A:422:SER:HA	1.86	0.42
1:A:298:TYR:CD1	1:A:298:TYR:C	2.96	0.42
1:A:1:MET:N	3:A:560:HOH:O	2.52	0.42
1:A:438:GLY:O	1:A:452:LYS:HD2	2.19	0.42
1:B:21:GLU:HA	1:B:52:PHE:HB3	2.01	0.42
1:B:421:TRP:HA	1:B:422:SER:HA	1.83	0.42
1:A:150:PRO:HG2	1:B:104:HIS:ND1	2.35	0.42
1:A:71:ILE:HG22	1:A:108:VAL:HG12	2.02	0.42
1:A:227:GLU:O	1:A:229:PRO:HD3	2.19	0.42
1:A:307:PHE:CD1	1:A:333:ARG:HG2	2.55	0.42
1:A:343:THR:CB	3:A:513:HOH:O	2.67	0.42
1:B:267:LEU:O	1:B:271:GLY:N	2.53	0.42
1:B:321:LYS:N	1:B:321:LYS:HD2	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:155:TRP:CB	1:A:212:ILE:HD12	2.49	0.42
1:B:29:LYS:HE2	3:B:621:HOH:O	2.20	0.42
1:B:313:ILE:HA	1:B:325:LYS:O	2.20	0.42
1:B:384:PHE:CE1	1:B:387:ASN:HA	2.55	0.42
1:A:41:ASN:HD22	1:A:41:ASN:N	2.18	0.41
1:B:41:ASN:N	1:B:41:ASN:ND2	2.68	0.41
1:A:81:PHE:C	1:A:83:THR:H	2.28	0.41
1:B:41:ASN:N	1:B:41:ASN:HD22	2.18	0.41
1:A:411:ASP:HB2	3:A:568:HOH:O	2.20	0.41
1:B:464:THR:HG22	1:B:466:VAL:HB	2.02	0.41
1:B:273:GLU:N	3:B:561:HOH:O	2.51	0.41
1:A:55:LYS:C	1:A:57:PRO:HD2	2.45	0.41
1:A:56:TYR:CD2	1:A:57:PRO:HD3	2.55	0.41
1:B:166:ASP:OD1	1:B:170:LEU:HD23	2.21	0.41
1:A:304:MET:SD	1:A:334:ARG:HG2	2.61	0.41
1:A:311:THR:HG22	1:A:329:LYS:CB	2.51	0.41
1:A:12:GLY:HA2	1:A:68:VAL:HG13	2.03	0.41
1:A:44:TYR:CZ	1:A:432:GLY:HA2	2.56	0.41
1:A:307:PHE:CB	1:A:333:ARG:HG2	2.49	0.41
1:B:155:TRP:CB	1:B:212:ILE:HD12	2.51	0.41
1:B:321:LYS:N	1:B:321:LYS:CD	2.83	0.41
1:B:223:PRO:HB3	1:B:232:VAL:HA	2.03	0.41
1:A:379:GLY:HA2	1:A:436:ARG:O	2.21	0.40
1:A:347:TRP:HE3	3:A:517:HOH:O	2.02	0.40
1:B:119:THR:O	1:B:120:PRO:C	2.63	0.40
1:A:4:THR:HA	1:A:465:GLN:O	2.21	0.40
1:B:164:ILE:HG21	1:B:192:MET:HE1	2.04	0.40
1:B:227:GLU:O	1:B:229:PRO:HD3	2.21	0.40
1:B:394:ARG:HH11	1:B:394:ARG:HD2	1.72	0.40
1:B:408:ALA:O	1:B:413:ALA:HB3	2.22	0.40
1:A:446:THR:O	1:A:447:GLN:HB2	2.21	0.40
1:B:359:MET:O	1:B:363:ASN:ND2	2.54	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	466/468 (100%)	432 (93%)	32 (7%)	2 (0%)	30	49
1	B	466/468 (100%)	434 (93%)	31 (7%)	1 (0%)	43	63
All	All	932/936 (100%)	866 (93%)	63 (7%)	3 (0%)	36	55

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	444	PHE
1	B	444	PHE
1	A	82	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	397/397 (100%)	365 (92%)	32 (8%)	11	23
1	B	397/397 (100%)	362 (91%)	35 (9%)	9	20
All	All	794/794 (100%)	727 (92%)	67 (8%)	10	22

All (67) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	THR
1	A	26	THR
1	A	41	ASN
1	A	55	LYS
1	A	65	GLU
1	A	87	GLU
1	A	90	GLU
1	A	121	GLU
1	A	126	ASN

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Mol	Chain	Res	Type
1	A	139	ILE
1	A	209	LYS
1	A	214	VAL
1	A	233	ARG
1	A	244	LYS
1	A	265	HIS
1	A	273	GLU
1	A	277	ARG
1	A	289	ASP
1	A	294	LEU
1	A	311	THR
1	A	321	LYS
1	A	333	ARG
1	A	337	PRO
1	A	340	VAL
1	A	375	CYS
1	A	381	LYS
1	A	382	ASP
1	A	385	VAL
1	A	404	VAL
1	A	460	LYS
1	A	465	GLN
1	A	466	VAL
1	B	2	THR
1	B	41	ASN
1	B	65	GLU
1	B	87	GLU
1	B	90	GLU
1	B	120	PRO
1	B	121	GLU
1	B	126	ASN
1	B	139	ILE
1	B	163	PRO
1	B	180	TYR
1	B	209	LYS
1	B	214	VAL
1	B	233	ARG
1	B	244	LYS
1	B	265	HIS
1	B	273	GLU
1	B	277	ARG
1	B	289	ASP

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Mol	Chain	Res	Type
1	B	294	LEU
1	B	300	MET
1	B	311	THR
1	B	312	GLU
1	B	321	LYS
1	B	340	VAL
1	B	374	THR
1	B	375	CYS
1	B	381	LYS
1	B	382	ASP
1	B	385	VAL
1	B	404	VAL
1	B	424	MET
1	B	460	LYS
1	B	465	GLN
1	B	466	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	25	HIS
1	A	41	ASN
1	A	54	HIS
1	A	126	ASN
1	A	242	HIS
1	A	264	ASN
1	A	265	HIS
1	A	291	ASN
1	A	315	HIS
1	B	25	HIS
1	B	41	ASN
1	B	54	HIS
1	B	89	ASN
1	B	242	HIS
1	B	264	ASN
1	B	265	HIS
1	B	327	GLN
1	B	363	ASN
1	B	414	ASN
1	B	456	HIS

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 ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

2 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	$\# Z > 2$
2	BGP	B	469	-	16,16,16	0.86	0	23,24,24	1.47	3 (13%)
2	BGP	A	469	-	16,16,16	0.86	0	23,24,24	1.46	3 (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
2	BGP	B	469	-	-	2/6/26/26	0/1/1/1
2	BGP	A	469	-	-	2/6/26/26	0/1/1/1

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	469	BGP	C1-C2-C3	-4.70	100.77	110.36
2	A	469	BGP	C1-C2-C3	-3.95	102.30	110.36
2	A	469	BGP	C3-C4-C5	3.52	116.62	110.23
2	B	469	BGP	O5-C5-C4	2.81	114.77	109.70
2	B	469	BGP	C3-C4-C5	2.62	114.98	110.23
2	A	469	BGP	O5-C5-C6	-2.44	101.87	106.69

There are no chirality outliers.

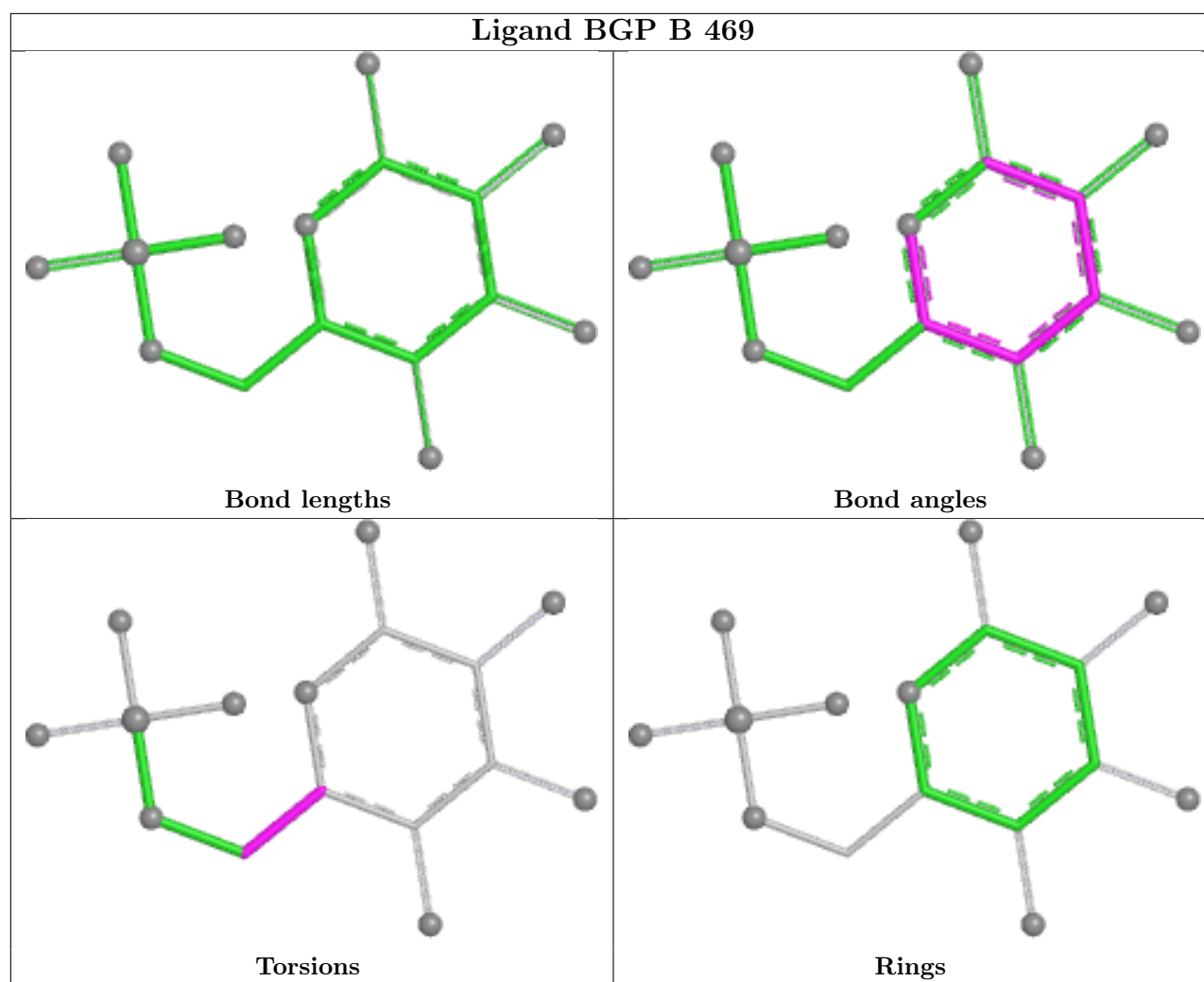
All (4) torsion outliers are listed below:

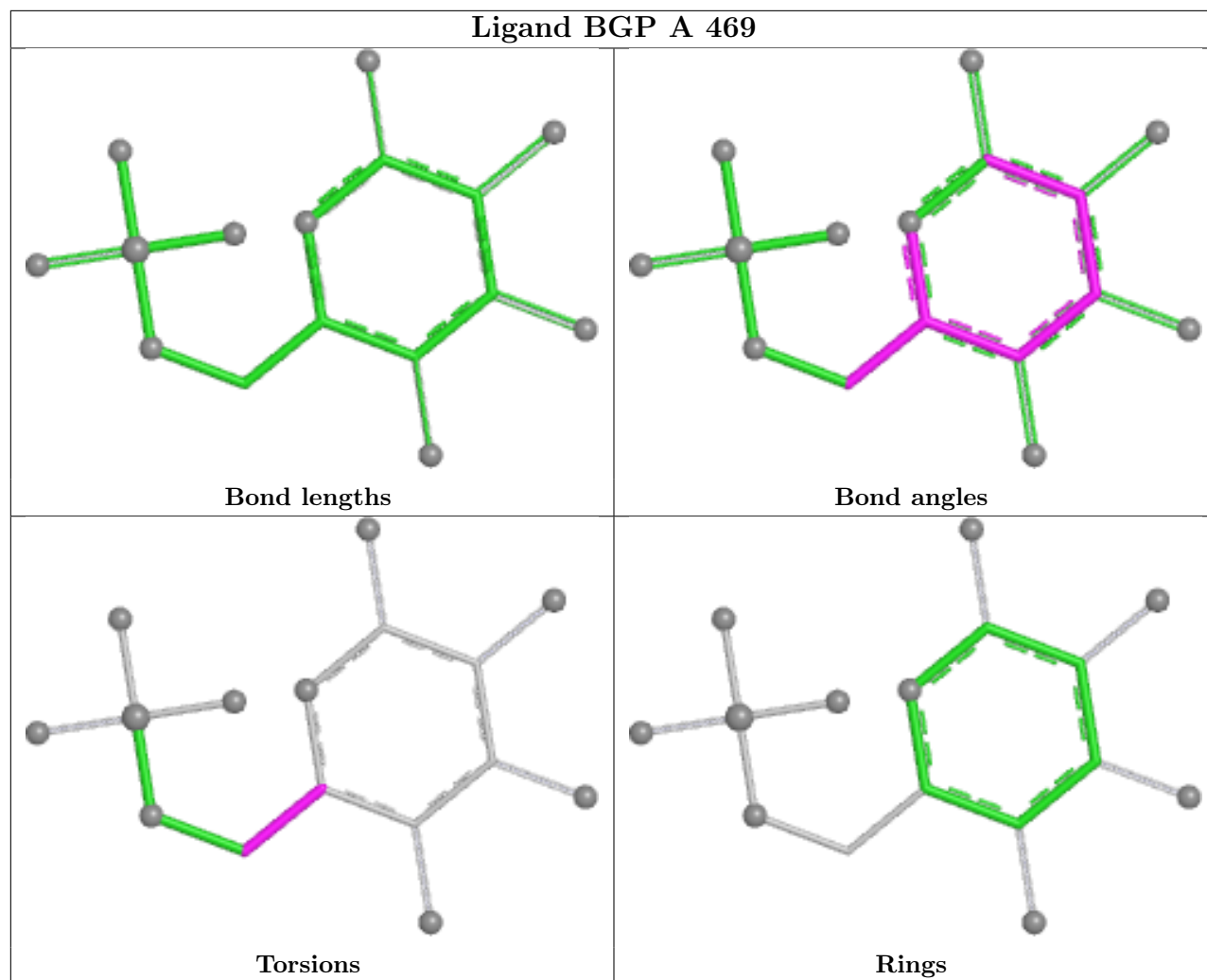
Mol	Chain	Res	Type	Atoms
2	A	469	BGP	C4-C5-C6-O6
2	A	469	BGP	O5-C5-C6-O6
2	B	469	BGP	C4-C5-C6-O6
2	B	469	BGP	O5-C5-C6-O6

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 [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	468/468 (100%)	-0.48	0 100 100	2, 12, 33, 64	0
1	B	468/468 (100%)	-0.40	0 100 100	2, 12, 31, 65	0
All	All	936/936 (100%)	-0.44	0 100 100	2, 12, 33, 65	0

There are no RSRZ outliers to report.

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](#)

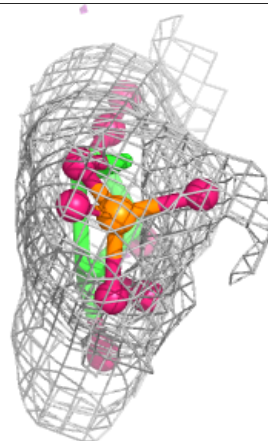
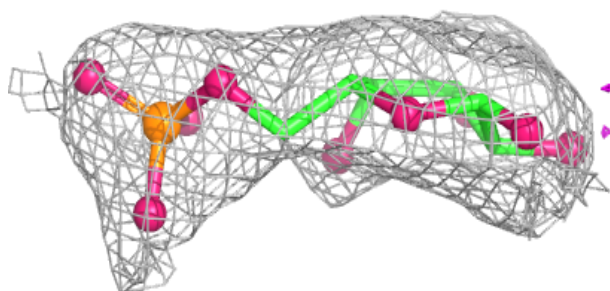
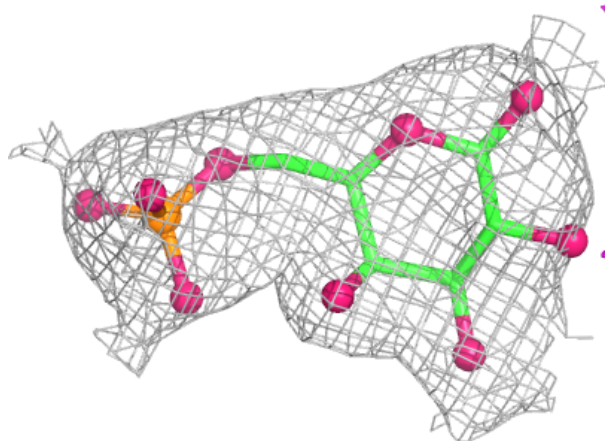
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	BGP	B	469	16/16	0.95	0.07	6,13,22,23	0
2	BGP	A	469	16/16	0.96	0.07	7,12,19,24	0

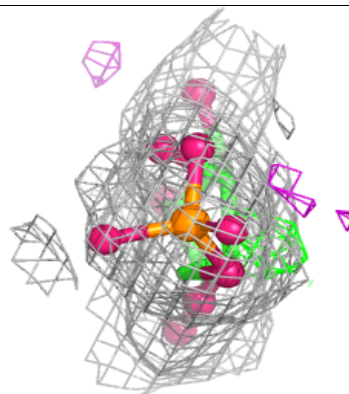
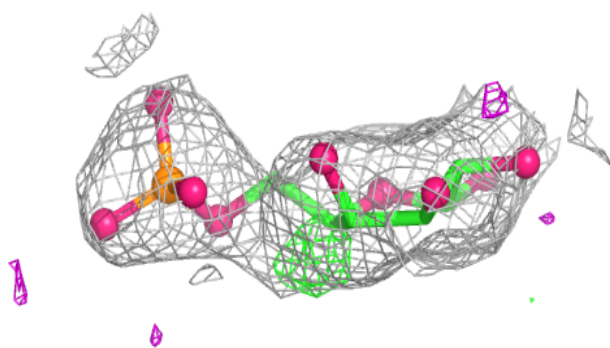
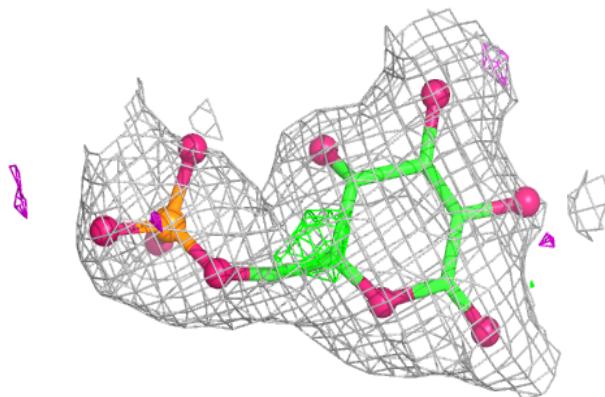
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around BGP B 469:

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

**Electron density around BGP A 469:**

$2mF_o-DF_c$ (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.