



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 04:21 PM UTC

PDB ID : 3APF / pdb_00003apf
Title : Crystal structure of human PI3K-gamma in complex with CH5039699
Authors : Nakamura, M.; Fukami, T.A.; Miyazaki, T.; Yoshida, M.
Deposited on : 2010-10-14
Resolution : 2.82 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

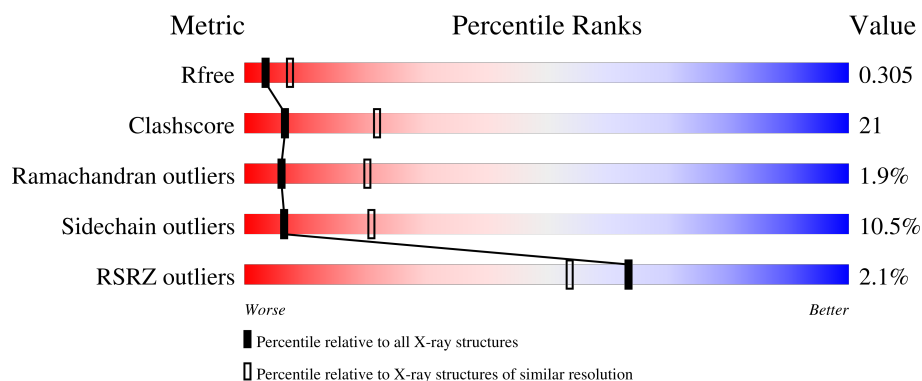
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.82 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	4591 (2.84-2.80)
Clashscore	190562	5010 (2.84-2.80)
Ramachandran outliers	187476	4916 (2.84-2.80)
Sidechain outliers	187428	4918 (2.84-2.80)
RSRZ outliers	180081	4594 (2.84-2.80)

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	966	

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 6611 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.

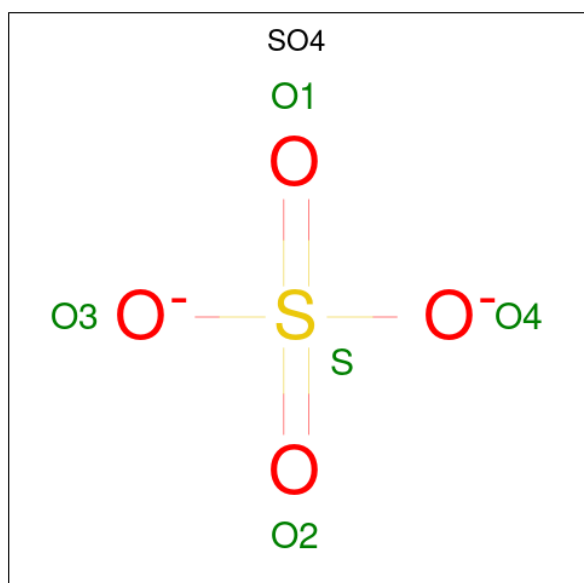
- Molecule 1 is a protein called Phosphatidylinositol-4,5-bisphosphate 3-kinase catalytic subunit gamma isoform.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	840	Total	C	N	O	S	0	0	0
			6567	4211	1116	1206	34			

There are 7 discrepancies between the modelled and reference sequences:

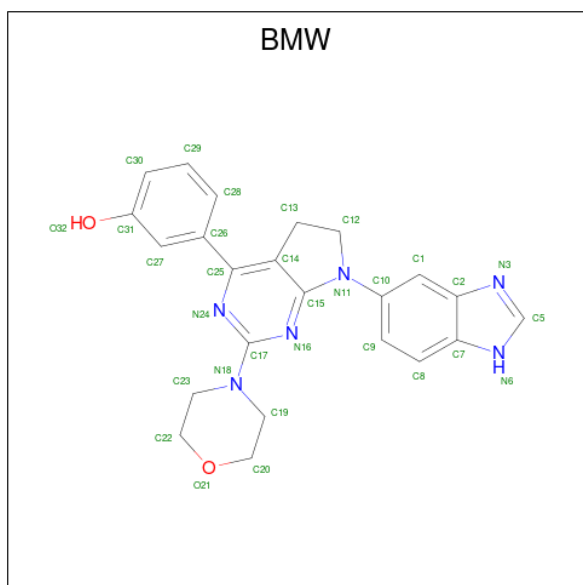
Chain	Residue	Modelled	Actual	Comment	Reference
A	137	GLY	-	expression tag	UNP P48736
A	138	PRO	-	expression tag	UNP P48736
A	139	LEU	-	expression tag	UNP P48736
A	140	HIS	-	expression tag	UNP P48736
A	141	MET	-	expression tag	UNP P48736
A	142	GLY	-	expression tag	UNP P48736
A	143	SER	-	expression tag	UNP P48736

- 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	A	1	Total	O	S	0	0
			5	4	1		

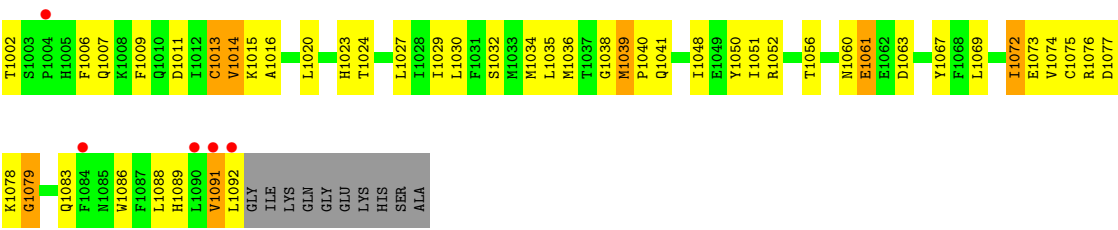
- Molecule 3 is 3-[7-(1H-benzimidazol-5-yl)-2-(morpholin-4-yl)-6,7-dihydro-5H-pyrrolo[2,3-d]pyrimidin-4-yl]phenol (CCD ID: BMW) (formula: C₂₃H₂₂N₆O₂).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			31	23	6	2		

- Molecule 4 is water.

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



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	144.22Å 67.87Å 106.60Å 90.00° 95.38° 90.00°	Depositor
Resolution (Å)	62.23 – 2.82 62.23 – 2.82	Depositor EDS
% Data completeness (in resolution range)	100.0 (62.23-2.82) 99.4 (62.23-2.82)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	0.05	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.95 (at 2.81Å)	Xtriage
Refinement program	REFMAC refmac_5.5.0109	Depositor
R, R_{free}	0.241 , 0.315 0.231 , 0.305	Depositor DCC
R_{free} test set	1271 reflections (5.09%)	wwPDB-VP
Wilson B-factor (Å ²)	77.0	Xtriage
Anisotropy	0.053	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 57.6	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	0.93	EDS
Total number of atoms	6611	wwPDB-VP
Average B, all atoms (Å ²)	67.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.21% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: SO4, BMW

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	0.78	0/6707	0.98	10/9111 (0.1%)

There are no bond length outliers.

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	412	VAL	N-CA-C	6.07	116.67	108.17
1	A	988	THR	CA-C-N	5.69	126.95	119.84
1	A	988	THR	C-N-CA	5.69	126.95	119.84
1	A	516	ILE	CB-CA-C	-5.36	103.19	110.90
1	A	153	GLN	N-CA-C	-5.31	105.14	111.03
1	A	808	LYS	N-CA-C	-5.27	102.19	110.36
1	A	1067	TYR	N-CA-C	-5.22	104.53	112.04
1	A	478	GLY	N-CA-C	5.21	117.78	110.38
1	A	175	PHE	N-CA-C	-5.09	105.17	111.33
1	A	683	LYS	N-CA-C	-5.05	105.46	110.97

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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	6567	0	6378	278	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	10	0	0	1	0
3	A	31	0	22	2	0
4	A	3	0	0	0	0
All	All	6611	0	6400	279	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 21.

All (279) 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:729:LEU:O	1:A:733:THR:HG23	1.62	0.99
1:A:861:ASP:C	1:A:862:LEU:HD23	1.89	0.98
1:A:429:LEU:HB2	1:A:468:LEU:HD21	1.49	0.94
1:A:887:THR:HG22	1:A:953:MET:HE2	1.53	0.89
1:A:767:LEU:HD22	1:A:803:VAL:HG23	1.57	0.87
1:A:482:LEU:HB2	1:A:516:ILE:HD12	1.57	0.85
1:A:564:LEU:HD11	1:A:1048:ILE:HG22	1.59	0.84
1:A:395:CYS:HB2	1:A:418:ILE:HD11	1.60	0.83
1:A:167:ASN:HD22	1:A:711:GLN:HE22	1.28	0.81
1:A:829:GLY:C	1:A:881:ILE:HD12	2.06	0.80
1:A:922:GLN:HE21	1:A:922:GLN:HA	1.46	0.80
1:A:168:VAL:HG13	1:A:170:ASP:H	1.46	0.80
1:A:767:LEU:HD22	1:A:803:VAL:CG2	2.13	0.79
1:A:464:VAL:HG11	1:A:516:ILE:HD11	1.66	0.77
1:A:861:ASP:O	1:A:862:LEU:HD23	1.84	0.77
1:A:167:ASN:ND2	1:A:711:GLN:HE22	1.83	0.76
1:A:174:GLU:HB3	1:A:178:ARG:NH1	2.01	0.75
1:A:395:CYS:CB	1:A:418:ILE:HD11	2.16	0.75
1:A:892:GLN:OE1	1:A:902:PHE:CB	2.33	0.75
1:A:729:LEU:O	1:A:733:THR:CG2	2.34	0.74
1:A:180:LEU:O	1:A:183:PRO:HD2	1.86	0.74
1:A:271:VAL:HG22	1:A:310:PRO:HG3	1.68	0.74
1:A:167:ASN:HD22	1:A:711:GLN:NE2	1.86	0.73
1:A:1074:VAL:O	1:A:1078:LYS:HG2	1.88	0.73
1:A:312:ASP:OD2	1:A:314:ALA:HB3	1.88	0.73
1:A:1088:LEU:O	1:A:1092:LEU:HB2	1.88	0.72
1:A:244:ILE:HG23	1:A:247:SER:HB2	1.71	0.72
1:A:622:LEU:HD13	1:A:647:LYS:HB3	1.73	0.71
1:A:203:THR:OG1	1:A:205:LYS:HG3	1.92	0.69
1:A:379:LEU:HB3	1:A:436:GLY:O	1.93	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:767:LEU:CD2	1:A:803:VAL:HG23	2.22	0.69
1:A:935:TYR:O	1:A:939:THR:HG23	1.92	0.69
1:A:233:ILE:HG22	1:A:234:LYS:O	1.95	0.67
1:A:285:THR:HG22	1:A:289:ASN:HB2	1.76	0.67
1:A:834:HIS:HB2	1:A:876:ILE:HD12	1.77	0.67
1:A:732:PHE:O	1:A:736:VAL:HG23	1.96	0.66
1:A:762:GLN:O	1:A:766:GLN:N	2.22	0.66
1:A:464:VAL:CG1	1:A:516:ILE:HD11	2.26	0.65
1:A:707:ARG:HA	1:A:710:GLN:OE1	1.96	0.65
1:A:482:LEU:HB2	1:A:516:ILE:CD1	2.27	0.65
1:A:368:ILE:HG22	1:A:516:ILE:HG23	1.79	0.64
1:A:274:VAL:HG21	1:A:292:TRP:CD1	2.33	0.63
1:A:207:LEU:HD13	1:A:288:LYS:HB2	1.78	0.63
1:A:564:LEU:CD1	1:A:1048:ILE:HG22	2.26	0.63
1:A:1013:CYS:O	1:A:1016:ALA:N	2.31	0.63
1:A:223:VAL:O	1:A:225:HIS:CD2	2.52	0.63
1:A:908:ASN:HD21	1:A:921:PHE:HZ	1.47	0.62
1:A:397:ARG:HD2	1:A:415:GLU:O	1.98	0.62
1:A:305:VAL:HG23	1:A:306:VAL:N	2.13	0.62
1:A:749:ILE:HD13	1:A:749:ILE:N	2.15	0.62
1:A:226:ARG:HB3	1:A:229:THR:OG1	2.00	0.61
1:A:997:THR:HG23	1:A:1001:LYS:HB2	1.81	0.61
1:A:548:PRO:HG2	1:A:551:LEU:HD12	1.83	0.61
1:A:725:GLY:O	1:A:729:LEU:HD12	2.00	0.61
1:A:893:GLN:HE21	1:A:893:GLN:C	2.10	0.60
1:A:192:ASP:C	1:A:192:ASP:OD1	2.44	0.60
1:A:219:CYS:HA	1:A:235:VAL:O	2.01	0.60
1:A:739:ILE:HG21	1:A:878:MET:HE1	1.83	0.60
1:A:1020:LEU:HD22	1:A:1027:LEU:HD11	1.83	0.60
1:A:559:ILE:O	1:A:559:ILE:HG22	2.00	0.60
1:A:608:TYR:CE2	1:A:639:ASN:ND2	2.69	0.59
1:A:953:MET:HE3	1:A:963:ILE:HD13	1.84	0.59
1:A:272:LEU:HD23	1:A:272:LEU:N	2.17	0.59
1:A:564:LEU:HD11	1:A:1048:ILE:CG2	2.33	0.59
1:A:998:SER:O	1:A:1000:LYS:N	2.35	0.59
1:A:1006:PHE:O	1:A:1007:GLN:C	2.46	0.58
1:A:887:THR:CG2	1:A:953:MET:HE2	2.28	0.58
1:A:608:TYR:CZ	1:A:639:ASN:ND2	2.71	0.58
1:A:168:VAL:HG13	1:A:170:ASP:N	2.17	0.58
1:A:547:MET:CE	1:A:581:GLU:HG3	2.33	0.57
1:A:467:LEU:HD13	1:A:672:TYR:CE1	2.39	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:920:LYS:O	1:A:923:ALA:N	2.36	0.57
1:A:223:VAL:O	1:A:225:HIS:HD2	1.87	0.57
1:A:861:ASP:C	1:A:861:ASP:OD1	2.47	0.57
1:A:922:GLN:HE21	1:A:922:GLN:CA	2.18	0.57
1:A:997:THR:HG23	1:A:1001:LYS:CB	2.36	0.55
3:A:1103:BMW:H28	3:A:1103:BMW:H13A	1.87	0.55
1:A:471:HIS:CD2	1:A:471:HIS:H	2.23	0.55
1:A:1002:THR:HG22	1:A:1007:GLN:HE21	1.71	0.55
1:A:182:THR:HB	1:A:183:PRO:HD3	1.89	0.54
1:A:838:LEU:HD12	1:A:877:GLY:HA3	1.89	0.54
1:A:745:VAL:O	1:A:749:ILE:HG12	2.06	0.54
1:A:870:ILE:HG22	1:A:871:SER:O	2.07	0.54
1:A:435:CYS:O	1:A:435:CYS:SG	2.66	0.54
1:A:632:ASP:C	1:A:632:ASP:OD1	2.51	0.54
1:A:1006:PHE:O	1:A:1009:PHE:N	2.41	0.53
1:A:1032:SER:O	1:A:1036:MET:HE2	2.08	0.53
1:A:198:MET:HG2	1:A:280:TYR:CG	2.44	0.53
1:A:370:ILE:HD12	1:A:370:ILE:H	1.73	0.53
1:A:416:PHE:HB3	1:A:418:ILE:HD12	1.91	0.53
1:A:867:TYR:CE2	1:A:963:ILE:HG22	2.44	0.53
1:A:876:ILE:O	1:A:876:ILE:HG23	2.08	0.53
1:A:725:GLY:C	1:A:729:LEU:HD12	2.33	0.53
1:A:837:ASP:HB3	1:A:840:GLN:HE21	1.74	0.53
1:A:370:ILE:CD1	1:A:406:GLU:HA	2.39	0.52
1:A:176:THR:HG23	1:A:674:ASP:HB2	1.91	0.52
1:A:872:THR:OG1	1:A:877:GLY:HA2	2.10	0.52
1:A:829:GLY:O	1:A:881:ILE:HB	2.09	0.52
1:A:905:GLU:HA	1:A:993:PHE:CD2	2.44	0.52
1:A:312:ASP:HB3	1:A:315:LEU:HG	1.91	0.52
1:A:387:ILE:HD13	1:A:468:LEU:HD11	1.92	0.52
1:A:163:THR:O	1:A:165:VAL:HG23	2.09	0.52
1:A:785:VAL:HG23	1:A:791:LEU:O	2.09	0.52
1:A:988:THR:HG22	1:A:1079:GLY:O	2.10	0.52
1:A:180:LEU:C	1:A:183:PRO:HD2	2.35	0.51
1:A:808:LYS:O	1:A:810:PRO:HD3	2.10	0.51
1:A:168:VAL:CG1	1:A:169:HIS:N	2.73	0.51
1:A:1040:PRO:O	1:A:1041:GLN:CB	2.58	0.51
1:A:360:LYS:HB3	1:A:416:PHE:O	2.11	0.51
1:A:925:VAL:O	1:A:929:VAL:HG23	2.11	0.51
1:A:862:LEU:HD23	1:A:862:LEU:N	2.19	0.51
1:A:862:LEU:HD12	1:A:934:GLY:HA2	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:640:VAL:O	1:A:643:ILE:HG12	2.11	0.51
1:A:738:VAL:HG12	1:A:742:LEU:HD12	1.93	0.51
1:A:908:ASN:C	1:A:908:ASN:HD22	2.18	0.51
1:A:211:LEU:HD21	1:A:298:LYS:HA	1.93	0.51
1:A:989:PRO:HA	1:A:992:LEU:HD12	1.93	0.51
1:A:992:LEU:O	1:A:995:MET:N	2.44	0.50
1:A:431:LEU:HD13	1:A:516:ILE:HD13	1.92	0.50
1:A:185:MET:HE2	1:A:321:GLU:HG3	1.91	0.50
1:A:964:ASP:OD1	1:A:964:ASP:C	2.54	0.50
1:A:181:VAL:CG1	1:A:185:MET:SD	3.00	0.50
1:A:939:THR:HB	1:A:945:GLY:HA2	1.93	0.50
1:A:173:LEU:HD23	1:A:673:HIS:CD2	2.47	0.49
1:A:684:ARG:O	1:A:685:GLY:C	2.52	0.49
1:A:852:GLU:HG2	1:A:864:LEU:HD12	1.93	0.49
1:A:787:TYR:CE1	1:A:880:GLU:HB2	2.48	0.49
1:A:368:ILE:CG2	1:A:516:ILE:HG23	2.43	0.49
1:A:429:LEU:HB2	1:A:468:LEU:CD2	2.31	0.49
1:A:742:LEU:HD22	1:A:813:LEU:HD11	1.92	0.49
1:A:980:LYS:O	1:A:982:ARG:HG2	2.13	0.49
1:A:1007:GLN:O	1:A:1011:ASP:N	2.45	0.49
1:A:949:ASN:HB3	1:A:1083:GLN:HE22	1.76	0.49
1:A:1073:GLU:O	1:A:1074:VAL:C	2.54	0.49
1:A:164:ASP:OD1	1:A:164:ASP:C	2.54	0.49
1:A:233:ILE:HD11	1:A:248:PHE:HD1	1.77	0.49
1:A:624:VAL:O	1:A:628:MET:HB2	2.13	0.49
1:A:843:LEU:HD13	1:A:1034:MET:HG3	1.95	0.49
1:A:893:GLN:C	1:A:893:GLN:NE2	2.71	0.49
1:A:908:ASN:HA	1:A:911:LEU:HD12	1.95	0.49
1:A:963:ILE:HD12	3:A:1103:BMW:C14	2.43	0.49
1:A:953:MET:HE3	1:A:963:ILE:CD1	2.43	0.48
1:A:236:SER:O	1:A:238:ASP:N	2.45	0.48
1:A:521:ASP:OD1	1:A:522:ASN:N	2.46	0.48
1:A:602:GLU:OE1	1:A:602:GLU:N	2.41	0.48
1:A:983:VAL:O	1:A:983:VAL:HG13	2.13	0.48
1:A:144:SER:HA	1:A:147:SER:HB3	1.95	0.48
1:A:1035:LEU:HD12	1:A:1048:ILE:HG12	1.94	0.48
1:A:236:SER:C	1:A:238:ASP:H	2.22	0.48
1:A:1089:HIS:HA	1:A:1092:LEU:HB2	1.95	0.48
1:A:198:MET:O	1:A:199:HIS:C	2.57	0.48
1:A:305:VAL:CG2	1:A:306:VAL:N	2.77	0.48
1:A:838:LEU:HD12	1:A:877:GLY:CA	2.43	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:840:GLN:HG2	1:A:1039:MET:HE2	1.96	0.48
1:A:1050:TYR:CD1	1:A:1050:TYR:C	2.92	0.48
1:A:1089:HIS:C	1:A:1091:VAL:N	2.71	0.48
1:A:737:GLN:O	1:A:738:VAL:C	2.56	0.47
1:A:303:ILE:CG2	1:A:304:HIS:N	2.77	0.47
1:A:383:VAL:HG22	1:A:433:ILE:HD13	1.97	0.47
1:A:480:TYR:HB2	1:A:518:ILE:HG13	1.96	0.47
1:A:997:THR:HG22	1:A:998:SER:N	2.28	0.47
1:A:688:ASN:OD1	1:A:688:ASN:C	2.56	0.47
1:A:281:LEU:HA	1:A:290:PHE:CE2	2.49	0.47
1:A:784:ARG:O	1:A:786:PRO:HD3	2.15	0.47
1:A:270:PHE:HA	1:A:310:PRO:HD3	1.96	0.47
1:A:303:ILE:HG22	1:A:304:HIS:N	2.30	0.47
1:A:948:HIS:N	2:A:2:SO4:O1	2.44	0.47
1:A:997:THR:CG2	1:A:998:SER:N	2.78	0.47
1:A:990:ASP:N	1:A:990:ASP:OD1	2.48	0.47
1:A:622:LEU:HD12	1:A:623:ASP:N	2.29	0.46
1:A:1074:VAL:O	1:A:1078:LYS:CG	2.60	0.46
1:A:165:VAL:HG12	1:A:165:VAL:O	2.15	0.46
1:A:282:VAL:O	1:A:290:PHE:HZ	1.97	0.46
1:A:381:VAL:HG12	1:A:435:CYS:HB2	1.96	0.46
1:A:739:ILE:CG2	1:A:878:MET:HE1	2.45	0.46
1:A:220:ILE:N	1:A:235:VAL:O	2.46	0.46
1:A:303:ILE:O	1:A:304:HIS:CD2	2.69	0.46
1:A:285:THR:HG22	1:A:289:ASN:CB	2.44	0.46
1:A:422:ASP:HA	1:A:601:GLN:HB2	1.96	0.46
1:A:748:ASP:HB2	1:A:749:ILE:HD13	1.97	0.46
1:A:368:ILE:HG21	1:A:433:ILE:HD11	1.98	0.46
1:A:602:GLU:N	1:A:602:GLU:CD	2.73	0.46
1:A:181:VAL:HG12	1:A:185:MET:SD	2.56	0.46
1:A:466:LEU:HD11	1:A:476:ARG:HD3	1.98	0.46
1:A:381:VAL:HG12	1:A:435:CYS:CB	2.46	0.46
1:A:576:TRP:CZ3	1:A:596:VAL:HG22	2.51	0.46
1:A:172:GLU:HG3	1:A:471:HIS:CG	2.51	0.46
1:A:1038:GLY:C	1:A:1039:MET:HE2	2.41	0.46
1:A:199:HIS:O	1:A:200:PRO:C	2.56	0.45
1:A:824:SER:OG	1:A:825:ASN:N	2.49	0.45
1:A:850:ILE:HD13	1:A:1030:LEU:CD1	2.46	0.45
1:A:1076:ARG:C	1:A:1078:LYS:H	2.24	0.45
1:A:364:LYS:HE2	1:A:411:ASN:OD1	2.16	0.45
1:A:168:VAL:HG13	1:A:169:HIS:N	2.31	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:193:PRO:HB2	1:A:313:PRO:HB3	1.99	0.45
1:A:614:ARG:O	1:A:614:ARG:CG	2.65	0.45
1:A:935:TYR:O	1:A:939:THR:CG2	2.64	0.45
1:A:168:VAL:HG13	1:A:170:ASP:O	2.17	0.45
1:A:207:LEU:CD1	1:A:288:LYS:HB2	2.44	0.45
1:A:390:GLY:O	1:A:391:GLN:HB2	2.17	0.45
1:A:704:ALA:CB	1:A:873:GLY:HA2	2.46	0.45
1:A:614:ARG:O	1:A:614:ARG:HG3	2.17	0.45
1:A:1013:CYS:O	1:A:1015:LYS:N	2.50	0.45
1:A:926:GLU:O	1:A:927:ARG:C	2.60	0.44
1:A:1013:CYS:O	1:A:1014:VAL:C	2.61	0.44
1:A:303:ILE:O	1:A:304:HIS:CG	2.70	0.44
1:A:1006:PHE:CD1	1:A:1006:PHE:C	2.94	0.44
1:A:410:TRP:HB3	1:A:412:VAL:HG22	2.00	0.44
1:A:623:ASP:OD1	1:A:623:ASP:C	2.60	0.44
1:A:233:ILE:HD11	1:A:248:PHE:CD1	2.52	0.44
1:A:947:ARG:NH2	1:A:963:ILE:O	2.50	0.44
1:A:748:ASP:OD1	1:A:748:ASP:N	2.51	0.44
1:A:840:GLN:HG2	1:A:1039:MET:CE	2.49	0.43
1:A:879:ILE:HD12	1:A:879:ILE:N	2.33	0.43
1:A:778:GLN:N	1:A:778:GLN:OE1	2.52	0.43
1:A:983:VAL:CG2	1:A:1075:CYS:SG	3.06	0.43
1:A:1023:HIS:O	1:A:1024:THR:C	2.60	0.43
1:A:271:VAL:CG2	1:A:310:PRO:HG3	2.45	0.43
1:A:767:LEU:HD22	1:A:803:VAL:HG22	1.98	0.43
1:A:796:LEU:HG	1:A:815:PHE:CE1	2.53	0.43
1:A:1060:ASN:HD21	1:A:1063:ASP:HB2	1.84	0.43
1:A:211:LEU:HD11	1:A:298:LYS:HB2	2.01	0.43
1:A:586:PRO:HA	1:A:589:TYR:CD1	2.53	0.43
1:A:397:ARG:HH21	1:A:416:PHE:HA	1.82	0.43
1:A:903:LYS:C	1:A:905:GLU:N	2.77	0.43
1:A:497:PHE:HB3	1:A:498:ASN:H	1.67	0.43
1:A:271:VAL:C	1:A:272:LEU:HD23	2.44	0.42
1:A:606:LYS:O	1:A:609:GLN:HG2	2.18	0.42
1:A:150:PHE:CD2	1:A:150:PHE:C	2.94	0.42
1:A:509:ASP:OD1	1:A:509:ASP:C	2.62	0.42
1:A:833:LYS:O	1:A:876:ILE:HA	2.18	0.42
1:A:1052:ARG:O	1:A:1056:THR:N	2.52	0.42
1:A:727:ALA:O	1:A:730:HIS:HB3	2.19	0.42
1:A:738:VAL:CG1	1:A:742:LEU:HD12	2.50	0.42
1:A:846:GLN:O	1:A:847:ILE:C	2.59	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1069:LEU:O	1:A:1072:ILE:HG12	2.18	0.42
1:A:220:ILE:HD12	1:A:237:PRO:HB3	2.01	0.42
1:A:879:ILE:HG22	1:A:880:GLU:N	2.34	0.42
1:A:405:THR:C	1:A:407:GLU:N	2.77	0.42
1:A:297:LEU:O	1:A:298:LYS:C	2.62	0.42
1:A:690:ARG:O	1:A:691:ILE:C	2.63	0.42
1:A:173:LEU:CD2	1:A:673:HIS:CD2	3.02	0.42
1:A:850:ILE:HD13	1:A:1030:LEU:HD13	2.02	0.42
1:A:1086:TRP:CE3	1:A:1086:TRP:HA	2.55	0.42
1:A:303:ILE:HD12	1:A:303:ILE:N	2.35	0.42
1:A:808:LYS:HG2	1:A:835:GLY:HA3	2.02	0.42
1:A:852:GLU:CD	1:A:864:LEU:HD12	2.45	0.42
1:A:903:LYS:C	1:A:905:GLU:H	2.28	0.41
1:A:796:LEU:O	1:A:798:ILE:N	2.53	0.41
1:A:168:VAL:CG1	1:A:170:ASP:O	2.69	0.41
1:A:363:VAL:O	1:A:363:VAL:HG13	2.19	0.41
1:A:482:LEU:HD12	1:A:516:ILE:CD1	2.50	0.41
1:A:695:LEU:O	1:A:696:PHE:C	2.64	0.41
1:A:920:LYS:O	1:A:922:GLN:N	2.54	0.41
1:A:1029:ILE:HD13	1:A:1029:ILE:HA	1.79	0.41
1:A:423:LEU:HD23	1:A:423:LEU:HA	1.72	0.41
1:A:395:CYS:HB3	1:A:418:ILE:HD11	1.99	0.41
1:A:903:LYS:O	1:A:905:GLU:N	2.54	0.41
1:A:172:GLU:O	1:A:176:THR:OG1	2.29	0.41
1:A:192:ASP:OD2	1:A:195:LEU:HD12	2.21	0.41
1:A:244:ILE:O	1:A:244:ILE:HG22	2.21	0.41
1:A:908:ASN:HA	1:A:911:LEU:HB2	2.03	0.41
1:A:939:THR:O	1:A:940:PHE:C	2.64	0.41
1:A:184:ARG:O	1:A:188:VAL:HG23	2.21	0.41
1:A:614:ARG:HB2	1:A:617:TRP:HB3	2.03	0.41
1:A:688:ASN:OD1	1:A:690:ARG:N	2.54	0.41
1:A:170:ASP:OD1	1:A:170:ASP:C	2.64	0.40
1:A:287:ILE:HD12	1:A:287:ILE:HA	1.91	0.40
1:A:497:PHE:HE1	1:A:501:LYS:HE3	1.87	0.40
1:A:904:ASP:O	1:A:993:PHE:HB3	2.21	0.40
1:A:932:CYS:O	1:A:936:CYS:SG	2.66	0.40
1:A:819:ASP:HA	1:A:820:PRO:HD3	1.88	0.40
1:A:1032:SER:C	1:A:1036:MET:HE2	2.46	0.40
1:A:435:CYS:SG	1:A:461:LEU:HD11	2.61	0.40
1:A:598:TRP:CE3	1:A:604:VAL:HG22	2.57	0.40
1:A:704:ALA:HB1	1:A:873:GLY:HA2	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:845:LEU:HD23	1:A:845:LEU:HA	1.96	0.40
1:A:707:ARG:NH1	1:A:707:ARG:H	2.20	0.40
1:A:827:THR:OG1	1:A:883:LYS:NZ	2.54	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	824/966 (85%)	713 (86%)	95 (12%)	16 (2%)	6	20

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	227	SER
1	A	859	SER
1	A	921	PHE
1	A	1000	LYS
1	A	1014	VAL
1	A	797	ALA
1	A	904	ASP
1	A	964	ASP
1	A	999	GLY
1	A	1013	CYS
1	A	1077	ASP
1	A	1061	GLU
1	A	165	VAL
1	A	217	ASN
1	A	1079	GLY
1	A	548	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	694/862 (80%)	621 (90%)	73 (10%)	6 21

All (73) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	146	GLU
1	A	147	SER
1	A	150	PHE
1	A	168	VAL
1	A	192	ASP
1	A	203	THR
1	A	207	LEU
1	A	214	LYS
1	A	217	ASN
1	A	219	CYS
1	A	246	GLN
1	A	272	LEU
1	A	282	VAL
1	A	302	GLU
1	A	305	VAL
1	A	306	VAL
1	A	319	ARG
1	A	370	ILE
1	A	372	VAL
1	A	379	LEU
1	A	383	VAL
1	A	387	ILE
1	A	395	CYS
1	A	397	ARG
1	A	417	SER
1	A	418	ILE
1	A	420	ILE
1	A	464	VAL
1	A	475	LEU
1	A	501	LYS

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Mol	Chain	Res	Type
1	A	512	ASN
1	A	516	ILE
1	A	518	ILE
1	A	522	ASN
1	A	547	MET
1	A	615	GLU
1	A	616	VAL
1	A	636	SER
1	A	662	GLN
1	A	682	LEU
1	A	688	ASN
1	A	701	SER
1	A	707	ARG
1	A	729	LEU
1	A	733	THR
1	A	742	LEU
1	A	743	GLN
1	A	748	ASP
1	A	749	ILE
1	A	753	SER
1	A	763	VAL
1	A	772	GLU
1	A	775	GLN
1	A	779	LEU
1	A	796	LEU
1	A	799	GLU
1	A	801	CYS
1	A	850	ILE
1	A	854	ILE
1	A	861	ASP
1	A	862	LEU
1	A	871	SER
1	A	887	THR
1	A	893	GLN
1	A	899	THR
1	A	908	ASN
1	A	922	GLN
1	A	960	LEU
1	A	1039	MET
1	A	1051	ILE
1	A	1061	GLU
1	A	1072	ILE

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Mol	Chain	Res	Type
1	A	1091	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	167	ASN
1	A	169	HIS
1	A	386	ASN
1	A	471	HIS
1	A	512	ASN
1	A	554	GLN
1	A	601	GLN
1	A	734	GLN
1	A	743	GLN
1	A	775	GLN
1	A	840	GLN
1	A	893	GLN
1	A	908	ASN
1	A	922	GLN
1	A	971	ASN
1	A	1007	GLN
1	A	1023	HIS
1	A	1071	GLN
1	A	1083	GLN

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

3 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	BMW	A	1103	-	35,36,36	1.77	5 (14%)	49,52,52	1.96	12 (24%)
2	SO4	A	2	-	4,4,4	0.27	0	6,6,6	0.21	0
2	SO4	A	1	-	4,4,4	0.25	0	6,6,6	0.16	0

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	BMW	A	1103	-	-	0/12/29/29	0/6/6/6

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1103	BMW	C26-C25	-7.76	1.40	1.49
3	A	1103	BMW	C10-N11	-3.46	1.33	1.41
3	A	1103	BMW	C2-N3	-3.33	1.33	1.39
3	A	1103	BMW	C7-N6	-2.86	1.33	1.37
3	A	1103	BMW	C15-N11	-2.74	1.34	1.38

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1103	BMW	C25-N24-C17	5.69	121.81	116.27
3	A	1103	BMW	N16-C15-N11	4.23	133.10	125.27
3	A	1103	BMW	C12-N11-C15	4.14	112.32	109.46
3	A	1103	BMW	N16-C17-N18	3.82	122.56	117.12
3	A	1103	BMW	O21-C22-C23	-3.82	103.55	111.77
3	A	1103	BMW	N6-C5-N3	-3.30	108.84	113.87
3	A	1103	BMW	C14-C25-N24	-3.07	117.93	122.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1103	BMW	C17-N16-C15	2.96	120.88	114.97
3	A	1103	BMW	C23-N18-C19	2.93	118.15	111.57
3	A	1103	BMW	N24-C17-N16	-2.90	121.11	126.27
3	A	1103	BMW	C26-C25-N24	2.75	118.85	115.10
3	A	1103	BMW	C8-C7-C2	-2.08	119.82	122.10

There are no chirality outliers.

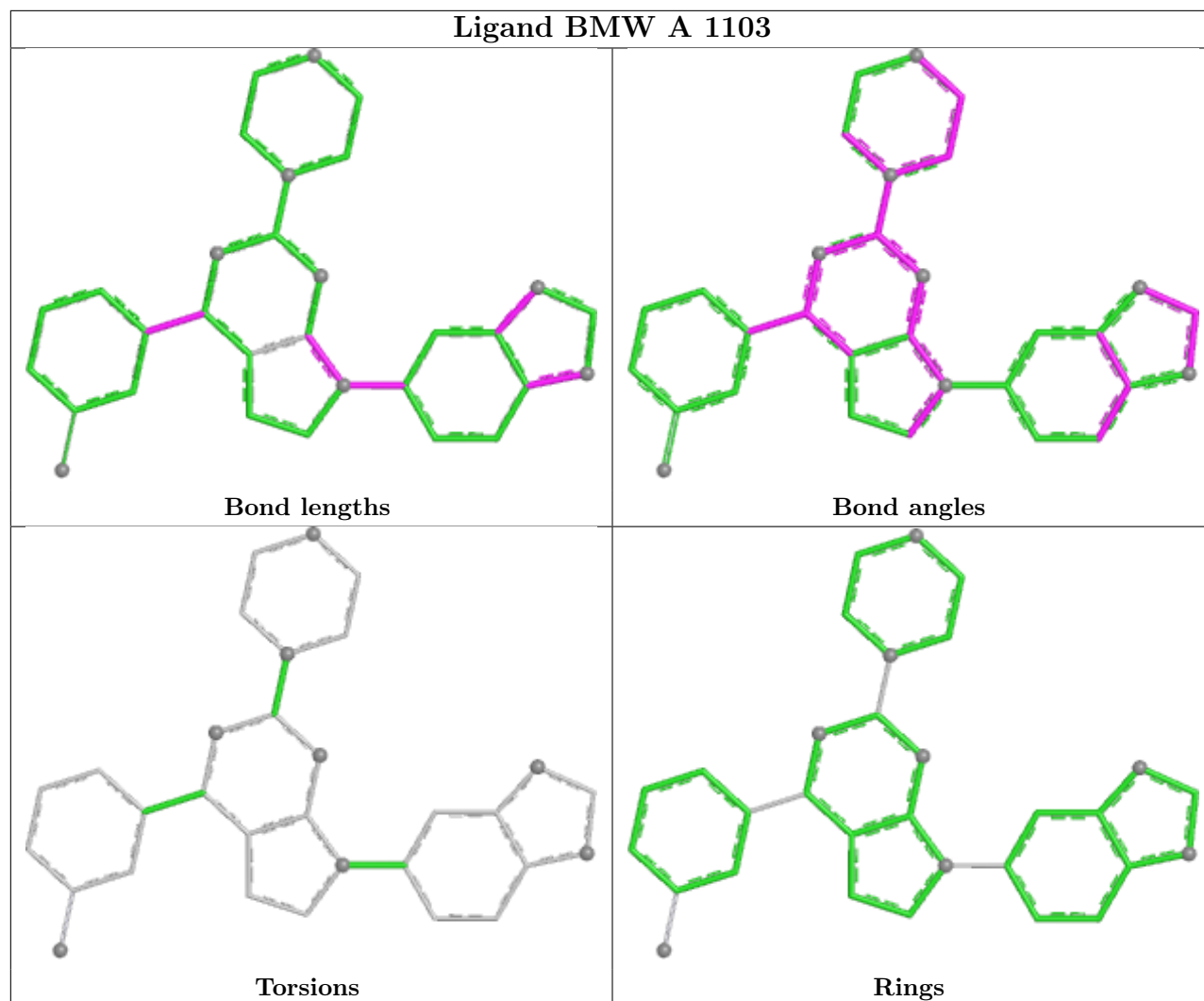
There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1103	BMW	2	0
2	A	2	SO4	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 ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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	840/966 (86%)	0.02	18 (2%) 63 54	24, 64, 109, 126	0

All (18) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	754	ALA	3.7
1	A	272	LEU	2.7
1	A	1092	LEU	2.5
1	A	926	GLU	2.5
1	A	993	PHE	2.5
1	A	271	VAL	2.5
1	A	248	PHE	2.4
1	A	1004	PRO	2.4
1	A	253	ALA	2.4
1	A	981	GLU	2.4
1	A	245	LEU	2.2
1	A	1090	LEU	2.2
1	A	1084	PHE	2.1
1	A	376	ASN	2.1
1	A	1091	VAL	2.1
1	A	989	PRO	2.1
1	A	237	PRO	2.0
1	A	759	VAL	2.0

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

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

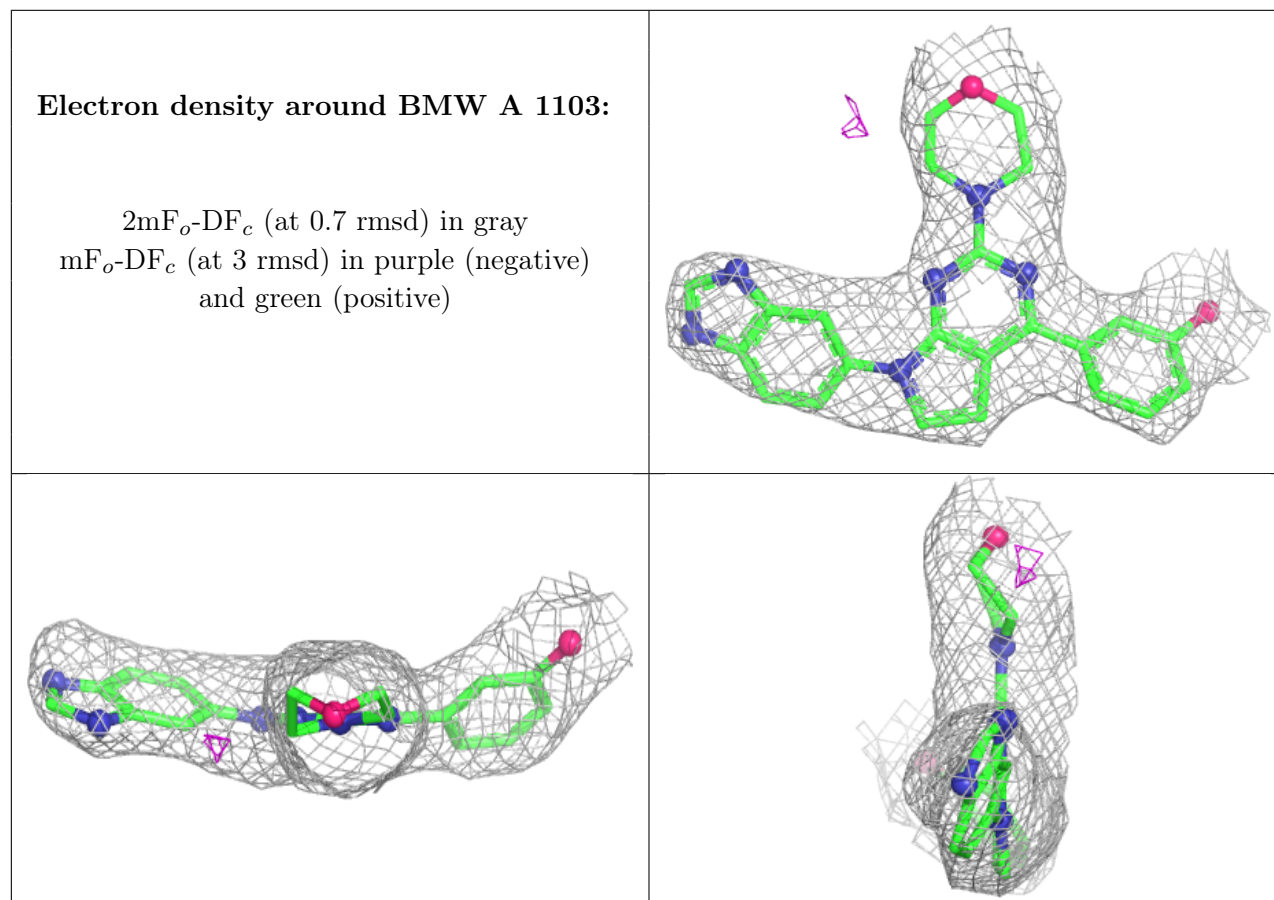
There are no oligosaccharides in this entry.

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	1	5/5	0.84	0.14	98,101,104,108	0
2	SO4	A	2	5/5	0.85	0.10	94,103,106,106	0
3	BMW	A	1103	31/31	0.92	0.10	53,70,87,90	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.



6.5 Other polymers [i](#)

There are no such residues in this entry.