



Full wwPDB X-ray Structure Validation Report ⓘ

May 15, 2020 – 02:16 am BST

PDB ID : 3APF
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 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

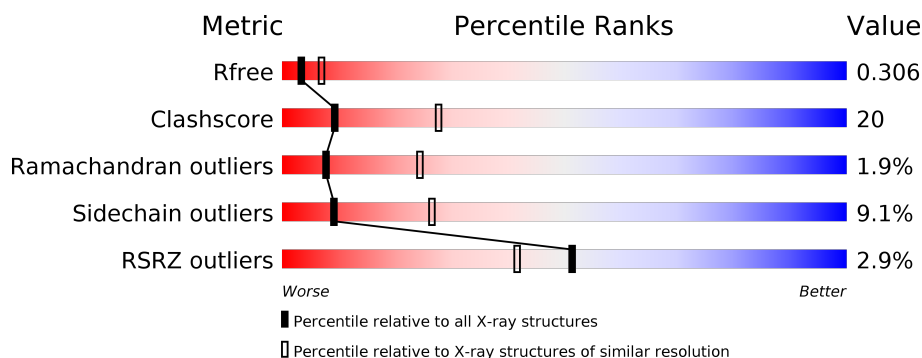
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.82 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}	130704	3617 (2.84-2.80)
Clashscore	141614	4060 (2.84-2.80)
Ramachandran outliers	138981	3978 (2.84-2.80)
Sidechain outliers	138945	3980 (2.84-2.80)
RSRZ outliers	127900	3552 (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 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	966	<div> <div>2%</div> <div> <div></div> <div>53%</div> <div>29%</div> <div>5%</div> <div>13%</div> </div> </div>

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
			Total	C	N	O	S			
1	A	840	6567	4211	1116	1206	34	0	0	0

There are 7 discrepancies between the modelled and reference sequences:

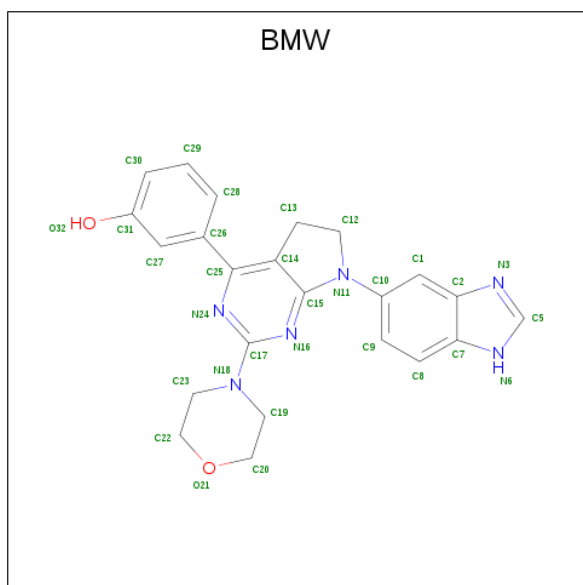
Chain	Residue	Modelled	Actual	Comment	Reference
A	137	GLY	-	EXPRESSION TAG	UNP P48736
A	138	PRO	-	EXPRESSION TAG	UNP P48736
A	139	LEU	-	EXPRESSION TAG	UNP P48736
A	140	HIS	-	EXPRESSION TAG	UNP P48736
A	141	MET	-	EXPRESSION TAG	UNP P48736
A	142	GLY	-	EXPRESSION TAG	UNP P48736
A	143	SER	-	EXPRESSION TAG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

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



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

- 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 (three-letter code: BMW) (formula: C₂₃H₂₂N₆O₂).



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

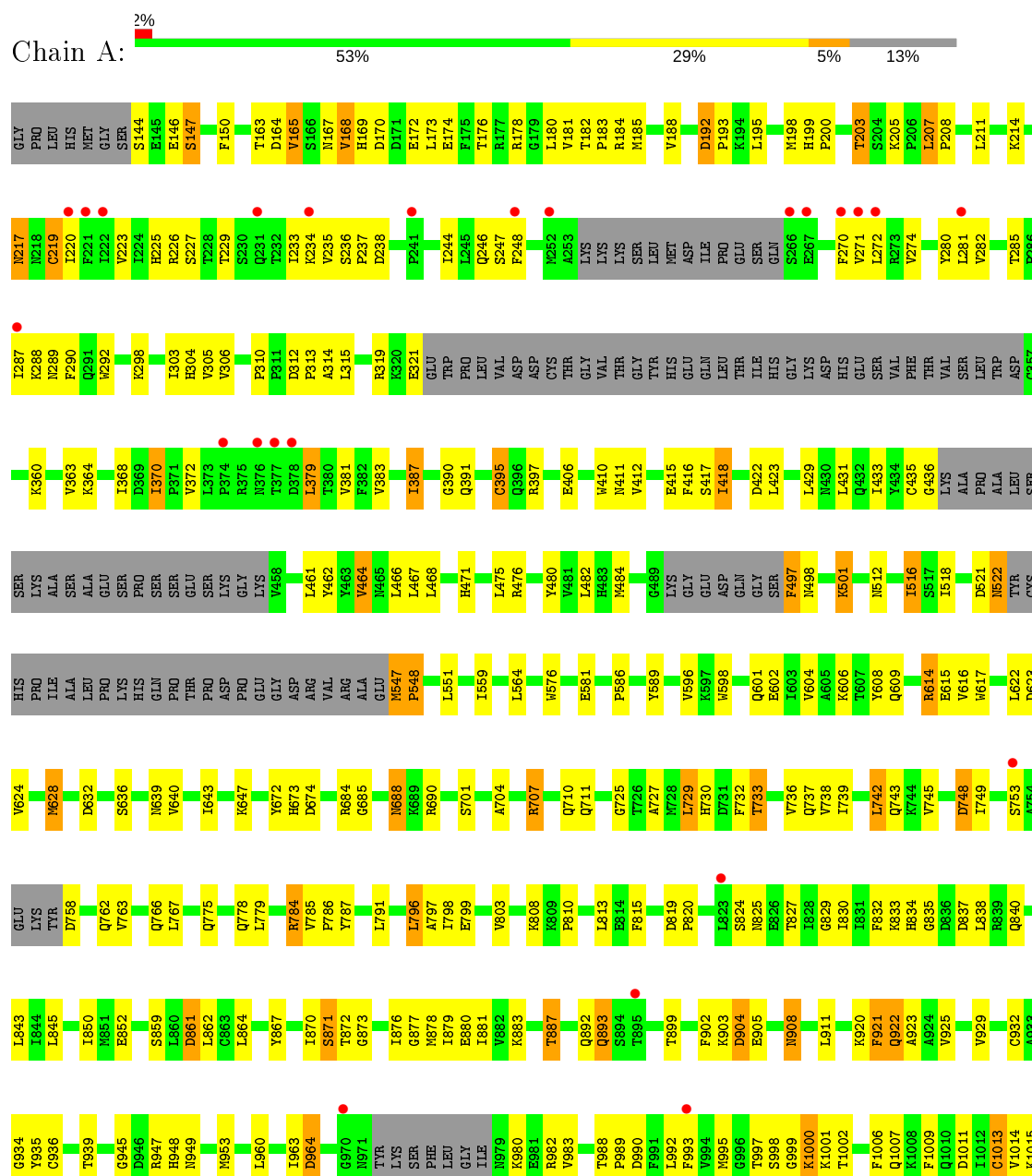
- Molecule 4 is water.

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

3 Residue-property plots [i](#)

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: Phosphatidylinositol-4,5-bisphosphate 3-kinase catalytic subunit gamma isoform



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 57.03 – 2.82	Depositor EDS
% Data completeness (in resolution range)	100.0 (62.23-2.82) 99.4 (57.03-2.82)	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 , 0.306	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)	0.30 , 60.2	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

5.1 Standard geometry

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

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	0.60	0/6707	0.72	0/9111

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	6567	0	6378	257	0
2	A	10	0	0	1	0
3	A	31	0	22	3	0
4	A	3	0	0	0	0
All	All	6611	0	6400	258	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 (258) 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:429:LEU:HB2	1:A:468:LEU:HD21	1.49	0.94
1:A:861:ASP:C	1:A:862:LEU:HD23	1.89	0.94
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:922:GLN:HA	1:A:922:GLN:HE21	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:829:GLY:C	1:A:881:ILE:HD12	2.06	0.75
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:840:GLN:HG2	1:A:1039:MET:HE2	1.69	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:207:LEU:HD13	1:A:288:LYS:HB2	1.78	0.63
1:A:1013:CYS:O	1:A:1016:ALA:N	2.31	0.63
1:A:564:LEU:CD1	1:A:1048:ILE:HG22	2.26	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:1032:SER:O	1:A:1036:MET:HE2	2.01	0.60
1:A:219:CYS:HA	1:A:235:VAL:O	2.01	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:272:LEU:N	1:A:272:LEU:HD23	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: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
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:922:GLN:HE21	1:A:922:GLN:CA	2.18	0.57
1:A:893:GLN:HE21	1:A:893:GLN:C	2.10	0.56
1:A:192:ASP:OD1	1:A:192:ASP:C	2.44	0.56
1:A:997:THR:HG23	1:A:1001:LYS:CB	2.36	0.55
3:A:1103:BMW:H13A	3:A:1103:BMW:H28	1.87	0.55
1:A:471:HIS:H	1:A:471:HIS:CD2	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:1006:PHE:O	1:A:1007:GLN:C	2.46	0.54
1:A:435:CYS:O	1:A:435:CYS:SG	2.66	0.54
1:A:1006:PHE:O	1:A:1009:PHE:N	2.41	0.53
1:A:887:THR:HG22	1:A:953:MET:CE	2.39	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:876:ILE:O	1:A:876:ILE:HG23	2.08	0.53
1:A:867:TYR:CE2	1:A:963:ILE:HG22	2.44	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:861:ASP:C	1:A:861:ASP:OD1	2.47	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:808:LYS:O	1:A:810:PRO:HD3	2.10	0.51
1:A:1040:PRO:O	1:A:1041:GLN:CB	2.58	0.51
1:A:168:VAL:CG1	1:A:169:HIS:N	2.73	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:739:ILE:HG21	1:A:878:MET:HE1	1.92	0.51
1:A:862:LEU:N	1:A:862:LEU:HD23	2.19	0.51
1:A:862:LEU:HD12	1:A:934:GLY:HA2	1.93	0.51
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: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: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: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:1007:GLN:O	1:A:1011:ASP:N	2.45	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:949:ASN:HB3	1:A:1083:GLN:HE22	1.76	0.49
1:A:632:ASP:C	1:A:632:ASP:OD1	2.51	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: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: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:N	1:A:602:GLU:OE1	2.41	0.48
1:A:983:VAL:HG13	1:A:983:VAL:O	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:1089:HIS:HA	1:A:1092:LEU:HB2	1.95	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
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:725:GLY:C	1:A:729:LEU:HD12	2.33	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:948:HIS:N	2:A:2:SO4:O1	2.44	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:997:THR:CG2	1:A:998:SER:N	2.78	0.47
1:A:990:ASP:OD1	1:A:990:ASP:N	2.48	0.47
1:A:180:LEU:C	1:A:183:PRO:HD2	2.35	0.47
1:A:1074:VAL:O	1:A:1078:LYS:CG	2.60	0.46
1:A:622:LEU:HD12	1:A:623:ASP:N	2.29	0.46
1:A:165:VAL:O	1:A:165:VAL:HG12	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: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:908:ASN:C	1:A:908:ASN:HD22	2.18	0.46
1:A:368:ILE:HG21	1:A:433:ILE:HD11	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:964:ASP:C	1:A:964:ASP:OD1	2.54	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
1:A:193:PRO:HB2	1:A:313:PRO:HB3	1.99	0.45
1:A:614:ARG:CG	1:A:614:ARG:O	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:684:ARG:O	1:A:685:GLY:C	2.52	0.45
1:A:704:ALA:CB	1:A:873:GLY:HA2	2.46	0.45
1:A:1013:CYS:O	1:A:1015:LYS:N	2.50	0.45
1:A:614:ARG:HG3	1:A:614:ARG:O	2.17	0.45
1:A:1073:GLU:O	1:A:1074:VAL:C	2.54	0.44
1:A:303:ILE:O	1:A:304:HIS:CG	2.70	0.44
1:A:1089:HIS:C	1:A:1091:VAL:N	2.71	0.44
1:A:164:ASP:C	1:A:164:ASP:OD1	2.54	0.44
1:A:410:TRP:HB3	1:A:412:VAL:HG22	2.00	0.44
1:A:893:GLN:NE2	1:A:893:GLN:C	2.71	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:879:ILE:HD12	1:A:879:ILE:N	2.33	0.43
1:A:983:VAL:CG2	1:A:1075:CYS:SG	3.06	0.43
1:A:778:GLN:N	1:A:778:GLN:OE1	2.52	0.43
1:A:1060:ASN:HD21	1:A:1063:ASP:HB2	1.84	0.43
1:A:236:SER:C	1:A:238:ASP:H	2.22	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:198:MET:O	1:A:199:HIS:C	2.57	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1050:TYR:C	1:A:1050:TYR:CD1	2.92	0.43
1:A:497:PHE:HB3	1:A:498:ASN:H	1.67	0.43
1:A:737:GLN:O	1:A:738:VAL:C	2.56	0.43
1:A:953:MET:HE3	3:A:1103:BMW:N16	2.34	0.42
1:A:606:LYS:O	1:A:609:GLN:HG2	2.18	0.42
1:A:688:ASN:C	1:A:688:ASN:OD1	2.56	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:1069:LEU:O	1:A:1072:ILE:HG12	2.18	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: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:199:HIS:O	1:A:200:PRO:C	2.56	0.42
1:A:830:ILE:N	1:A:881:ILE:HD12	2.34	0.42
1:A:1086:TRP:HA	1:A:1086:TRP:CE3	2.55	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: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: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:1029:ILE:HA	1:A:1029:ILE:HD13	1.79	0.41
1:A:920:LYS:O	1:A:922:GLN:N	2.54	0.41
1:A:423:LEU:HA	1:A:423:LEU:HD23	1.72	0.41
1:A:602:GLU:N	1:A:602:GLU:CD	2.73	0.41
1:A:185:MET:CE	1:A:321:GLU:HG3	2.50	0.41
1:A:395:CYS:HB3	1:A:418:ILE:HD11	1.99	0.41
1:A:887:THR:HG22	1:A:953:MET:HE2	2.02	0.41
1:A:903:LYS:O	1:A:905:GLU:N	2.54	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:1076:ARG:C	1:A:1078:LYS:H	2.24	0.41
1:A:462:TYR:HB3	1:A:484:MET:HE2	2.03	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:287:ILE:HA	1:A:287:ILE:HD12	1.91	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:497:PHE:HE1	1:A:501:LYS:HE3	1.87	0.40
1:A:932:CYS:O	1:A:936:CYS:SG	2.66	0.40
1:A:904:ASP:O	1:A:993:PHE:HB3	2.21	0.40
1:A:819:ASP:HA	1:A:820:PRO:HD3	1.88	0.40
1:A:185:MET:HE2	1:A:321:GLU:HG3	2.02	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:845:LEU:HD23	1:A:845:LEU:HA	1.96	0.40
1:A:704:ALA:HB1	1:A:873:GLY:HA2	2.03	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%)	8	24

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

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Mol	Chain	Res	Type
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%)	631 (91%)	63 (9%)	9 26

All (63) 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	208	PRO
1	A	214	LYS
1	A	217	ASN
1	A	219	CYS
1	A	246	GLN
1	A	319	ARG
1	A	370	ILE
1	A	372	VAL
1	A	379	LEU
1	A	387	ILE
1	A	395	CYS
1	A	417	SER
1	A	418	ILE

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Mol	Chain	Res	Type
1	A	464	VAL
1	A	475	LEU
1	A	497	PHE
1	A	501	LYS
1	A	512	ASN
1	A	516	ILE
1	A	522	ASN
1	A	547	MET
1	A	614	ARG
1	A	615	GLU
1	A	616	VAL
1	A	628	MET
1	A	636	SER
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	753	SER
1	A	758	ASP
1	A	763	VAL
1	A	775	GLN
1	A	779	LEU
1	A	784	ARG
1	A	796	LEU
1	A	799	GLU
1	A	832	PHE
1	A	861	ASP
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	1045	LYS
1	A	1051	ILE
1	A	1061	GLU
1	A	1072	ILE

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Mol	Chain	Res	Type
1	A	1091	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	167	ASN
1	A	169	HIS
1	A	391	GLN
1	A	471	HIS
1	A	512	ASN
1	A	554	GLN
1	A	585	HIS
1	A	601	GLN
1	A	705	GLN
1	A	734	GLN
1	A	775	GLN
1	A	840	GLN
1	A	893	GLN
1	A	922	GLN
1	A	1007	GLN
1	A	1023	HIS
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 carbohydrates 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	-	33,36,36	1.66	2 (6%)	40,52,52	1.90	9 (22%)
2	SO4	A	2	-	4,4,4	0.15	0	6,6,6	0.18	0
2	SO4	A	1	-	4,4,4	0.15	0	6,6,6	0.17	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	-	-	1/12/29/29	0/6/6/6

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1103	BMW	C26-C25	-7.48	1.40	1.49
3	A	1103	BMW	C10-N11	-3.57	1.33	1.42

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1103	BMW	C12-N11-C15	4.45	112.32	109.55
3	A	1103	BMW	N16-C17-N18	4.42	122.56	117.11
3	A	1103	BMW	N16-C15-N11	4.30	133.10	125.62
3	A	1103	BMW	O21-C22-C23	-3.75	103.55	111.80
3	A	1103	BMW	C17-N16-C15	3.19	120.88	114.97
3	A	1103	BMW	N24-C17-N16	-3.15	121.11	126.31
3	A	1103	BMW	C23-N18-C19	3.00	118.15	111.52
3	A	1103	BMW	C14-C25-N24	-2.94	117.93	122.78
3	A	1103	BMW	C26-C25-N24	2.83	118.85	115.09

There are no chirality outliers.

All (1) torsion outliers are listed below:

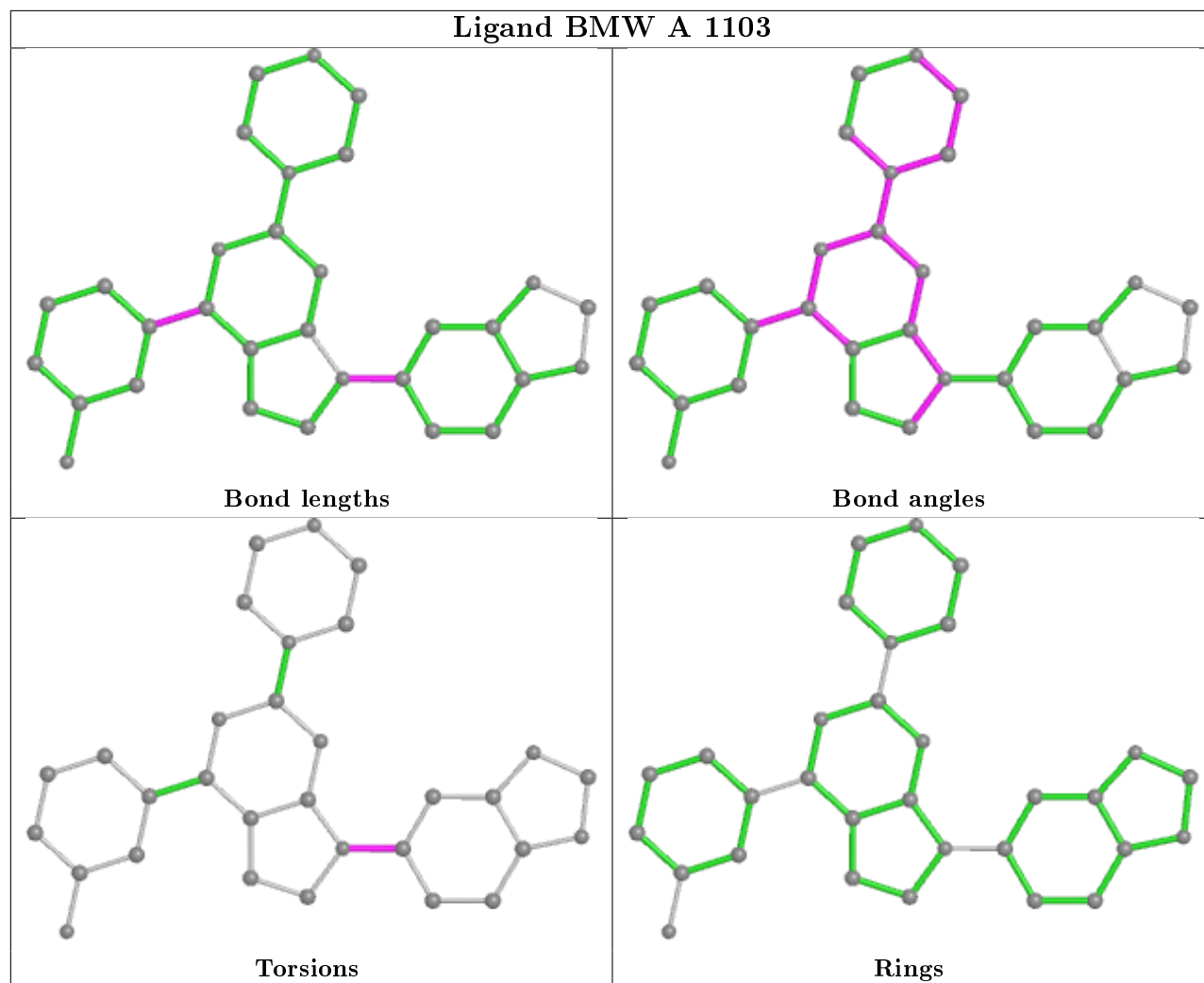
Mol	Chain	Res	Type	Atoms
3	A	1103	BMW	C1-C10-N11-C15

There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1103	BMW	3	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%)	0.05	24 (2%)	51 41	24, 64, 109, 126	0

All (24) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	266	SER	5.6
1	A	222	ILE	5.0
1	A	221	PHE	4.9
1	A	376	ASN	4.3
1	A	220	ILE	4.0
1	A	374	PRO	3.9
1	A	241	PRO	3.6
1	A	267	GLU	3.4
1	A	970	GLY	3.4
1	A	377	THR	3.1
1	A	287	ILE	2.9
1	A	252	MET	2.9
1	A	271	VAL	2.8
1	A	231	GLN	2.7
1	A	281	LEU	2.7
1	A	895	THR	2.6
1	A	823	LEU	2.5
1	A	234	LYS	2.4
1	A	272	LEU	2.4
1	A	248	PHE	2.3
1	A	270	PHE	2.2
1	A	753	SER	2.2
1	A	993	PHE	2.1
1	A	378	ASP	2.1

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](#)

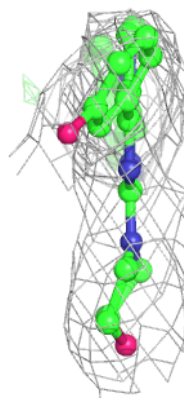
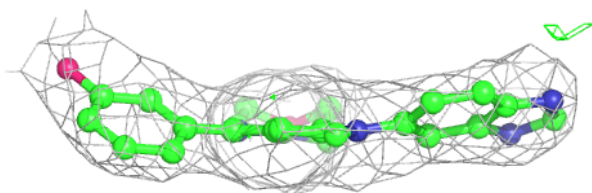
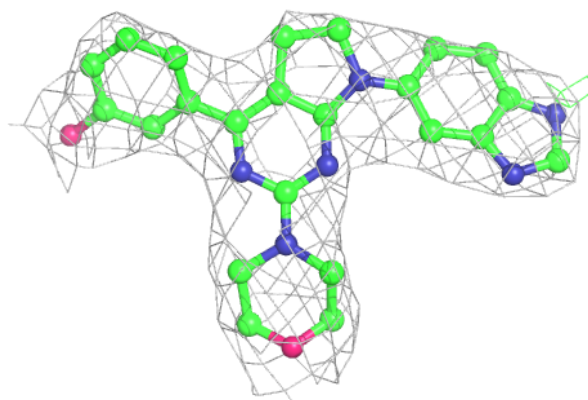
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	SO4	A	2	5/5	0.89	0.17	94,103,106,106	0
2	SO4	A	1	5/5	0.90	0.15	98,101,104,108	0
3	BMW	A	1103	31/31	0.94	0.18	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.

Electron density around BMW A 1103:

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



6.5 Other polymers ⓘ

There are no such residues in this entry.