



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 04:58 PM UTC

PDB ID : 2Y3A / pdb_00002y3a
Title : Crystal structure of p110beta in complex with icSH2 of p85beta and the drug GDC-0941
Authors : Zhang, X.; Vadas, O.; Perisic, O.; Williams, R.L.
Deposited on : 2010-12-20
Resolution : 3.30 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

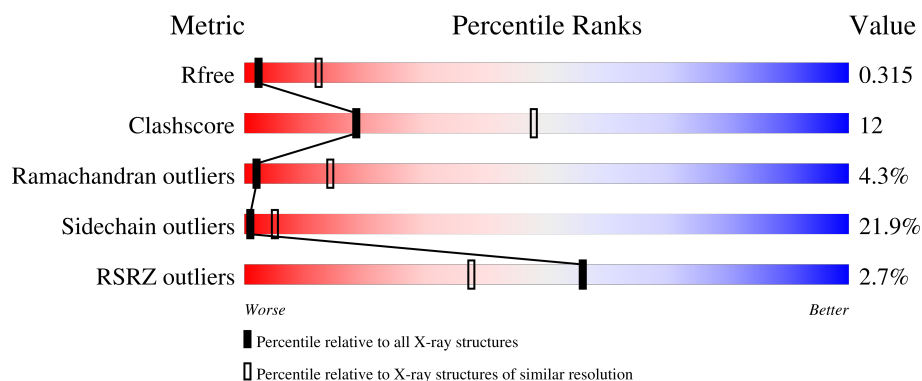
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.30 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	1169 (3.32-3.28)
Clashscore	190562	1209 (3.32-3.28)
Ramachandran outliers	187476	1188 (3.32-3.28)
Sidechain outliers	187428	1187 (3.32-3.28)
RSRZ outliers	180081	1169 (3.32-3.28)

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	1092	2% 48% 31% 9% 11%
2	B	302	4% 45% 25% 8% 22%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 9848 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 BETA ISOFORM.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	976	Total	C	N	O	S	0	0	0
			7862	5047	1323	1443	49			

There are 29 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-27	MET	-	expression tag	UNP Q8BTI9
A	-26	SER	-	expression tag	UNP Q8BTI9
A	-25	TYR	-	expression tag	UNP Q8BTI9
A	-24	TYR	-	expression tag	UNP Q8BTI9
A	-23	HIS	-	expression tag	UNP Q8BTI9
A	-22	HIS	-	expression tag	UNP Q8BTI9
A	-21	HIS	-	expression tag	UNP Q8BTI9
A	-20	HIS	-	expression tag	UNP Q8BTI9
A	-19	HIS	-	expression tag	UNP Q8BTI9
A	-18	HIS	-	expression tag	UNP Q8BTI9
A	-17	ASP	-	expression tag	UNP Q8BTI9
A	-16	TYR	-	expression tag	UNP Q8BTI9
A	-15	ASP	-	expression tag	UNP Q8BTI9
A	-14	ILE	-	expression tag	UNP Q8BTI9
A	-13	PRO	-	expression tag	UNP Q8BTI9
A	-12	THR	-	expression tag	UNP Q8BTI9
A	-11	THR	-	expression tag	UNP Q8BTI9
A	-10	GLU	-	expression tag	UNP Q8BTI9
A	-9	ASN	-	expression tag	UNP Q8BTI9
A	-8	LEU	-	expression tag	UNP Q8BTI9
A	-7	TYR	-	expression tag	UNP Q8BTI9
A	-6	PHE	-	expression tag	UNP Q8BTI9
A	-5	GLN	-	expression tag	UNP Q8BTI9
A	-4	GLY	-	expression tag	UNP Q8BTI9
A	-3	ALA	-	expression tag	UNP Q8BTI9
A	-2	MET	-	expression tag	UNP Q8BTI9

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLY	-	expression tag	UNP Q8BTI9
A	0	SER	-	expression tag	UNP Q8BTI9
A	123	LEU	ARG	conflict	UNP Q8BTI9

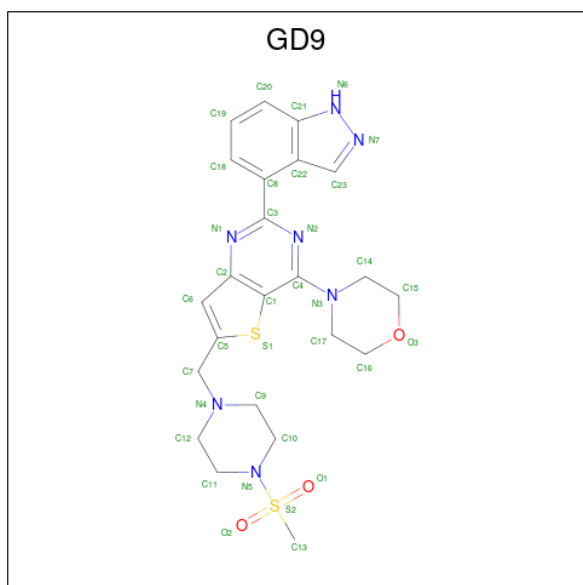
- Molecule 2 is a protein called PHOSPHATIDYLINOSITOL 3-KINASE REGULATORY SUBUNIT BETA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	236	Total	C	N	O	S	0	0	0
			1951	1214	355	373	9			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	421	MET	-	expression tag	UNP O08908
B	422	SER	-	expression tag	UNP O08908

- Molecule 3 is 2-(1H-indazol-4-yl)-6-{[4-(methylsulfonyl)piperazin-1-yl]methyl}-4-morpholin-4-yl-thieno[3,2-d]pyrimidine (CCD ID: GD9) (formula: C₂₃H₂₇N₇O₃S₂).

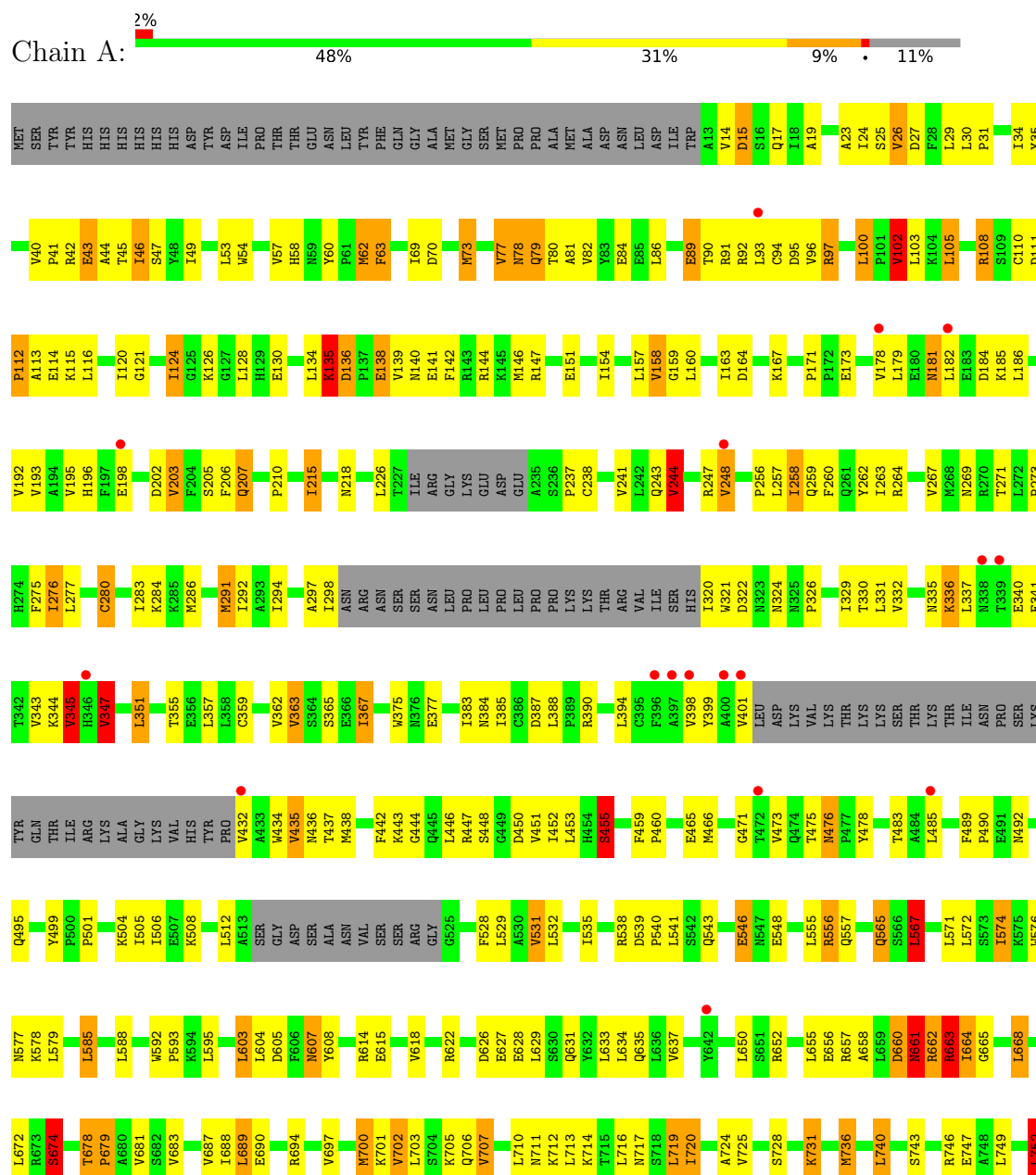


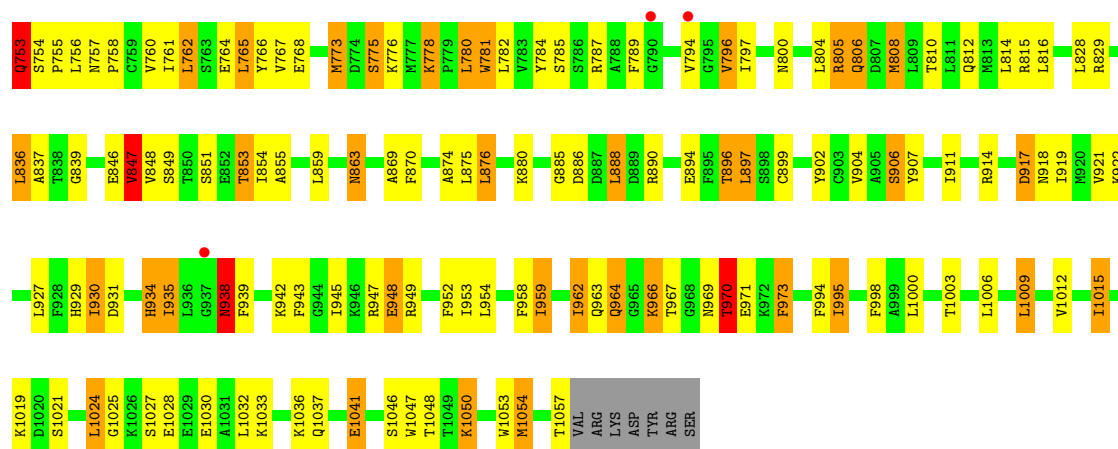
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	S	0	0
			35	23	7	3	2		

3 Residue-property plots

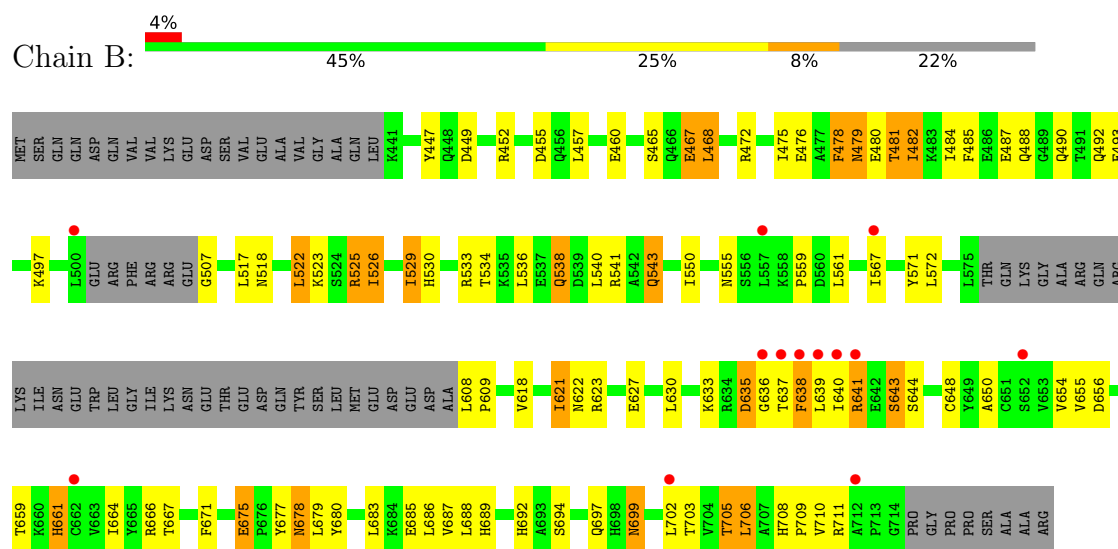
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: PHOSPHATIDYLINOSITOL-4,5-BISPHOSPHATE 3-KINASE CATALYTIC SUBUNIT BETA ISOFORM





● Molecule 2: PHOSPHATIDYLINOSITOL 3-KINASE REGULATORY SUBUNIT BETA



4 Data and refinement statistics

Property	Value	Source
Space group	P 65 2 2	Depositor
Cell constants a, b, c, α , β , γ	134.31Å 134.31Å 428.06Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	44.68 – 3.30 44.68 – 3.30	Depositor EDS
% Data completeness (in resolution range)	(Not available) (44.68-3.30) 96.5 (44.68-3.30)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.53 (at 3.32Å)	Xtriage
Refinement program	BUSTER 2.8.0	Depositor
R, R_{free}	0.234 , 0.296 0.252 , 0.315	Depositor DCC
R_{free} test set	1764 reflections (5.15%)	wwPDB-VP
Wilson B-factor (Å ²)	99.7	Xtriage
Anisotropy	0.669	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 129.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	9848	wwPDB-VP
Average B, all atoms (Å ²)	127.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.80% 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: GD9

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	0.88	2/8028 (0.0%)	1.56	106/10858 (1.0%)
2	B	0.88	0/1984	1.59	22/2665 (0.8%)
All	All	0.88	2/10012 (0.0%)	1.57	128/13523 (0.9%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	672	LEU	C-N	5.41	1.40	1.33
1	A	124	ILE	CG1-CD1	-5.21	1.31	1.51

All (128) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	661	ASN	CA-CB-CG	9.62	122.22	112.60
1	A	102	VAL	N-CA-C	8.21	120.06	109.30
1	A	938	ASN	CA-CB-CG	7.93	120.53	112.60
1	A	662	ARG	N-CA-C	-7.89	103.78	113.41
1	A	752	LEU	CA-C-N	7.58	136.02	121.54
1	A	752	LEU	C-N-CA	7.58	136.02	121.54
1	A	244	VAL	N-CA-CB	7.58	119.23	110.82
1	A	115	LYS	N-CA-C	-7.49	102.79	112.23
1	A	158	VAL	N-CA-C	7.43	118.23	110.72
1	A	124	ILE	N-CA-C	7.30	117.43	110.42
2	B	678	ASN	CA-CB-CG	7.29	119.89	112.60
1	A	847	VAL	N-CA-CB	7.07	118.43	110.72
1	A	930	ILE	N-CA-C	7.07	124.04	109.34
1	A	874	ALA	CA-C-N	7.06	131.03	120.31
1	A	874	ALA	C-N-CA	7.06	131.03	120.31
1	A	345	VAL	N-CA-C	6.93	118.04	110.21
2	B	643	SER	CA-C-N	6.92	129.55	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	643	SER	C-N-CA	6.92	129.55	120.28
1	A	248	VAL	N-CA-CB	6.88	119.16	112.28
1	A	114	GLU	N-CA-C	-6.85	103.07	113.89
1	A	848	VAL	CA-C-N	6.66	130.21	120.82
1	A	848	VAL	C-N-CA	6.66	130.21	120.82
1	A	678	THR	CB-CA-C	6.63	117.41	109.85
1	A	531	VAL	N-CA-CB	6.63	118.14	110.65
1	A	121	GLY	CA-C-N	6.54	128.88	120.70
1	A	121	GLY	C-N-CA	6.54	128.88	120.70
1	A	206	PHE	CA-C-N	6.52	131.31	122.84
1	A	206	PHE	C-N-CA	6.52	131.31	122.84
1	A	853	THR	CB-CA-C	6.38	120.10	109.89
2	B	517	LEU	CA-C-N	6.33	129.94	120.31
2	B	517	LEU	C-N-CA	6.33	129.94	120.31
1	A	237	PRO	CA-C-N	6.26	129.82	120.31
1	A	237	PRO	C-N-CA	6.26	129.82	120.31
1	A	267	VAL	CA-C-N	6.20	128.87	120.38
1	A	267	VAL	C-N-CA	6.20	128.87	120.38
1	A	958	PHE	CA-CB-CG	6.13	119.93	113.80
1	A	438	MET	CA-C-N	6.12	130.15	120.47
1	A	438	MET	C-N-CA	6.12	130.15	120.47
1	A	663	ARG	CA-C-N	6.04	128.69	120.77
1	A	663	ARG	C-N-CA	6.04	128.69	120.77
1	A	475	THR	CA-C-N	6.02	129.43	120.83
1	A	475	THR	C-N-CA	6.02	129.43	120.83
1	A	662	ARG	CA-C-N	6.00	132.99	121.54
1	A	662	ARG	C-N-CA	6.00	132.99	121.54
1	A	1025	GLY	CA-C-N	5.99	129.62	120.82
1	A	1025	GLY	C-N-CA	5.99	129.62	120.82
1	A	113	ALA	CA-C-N	5.99	131.33	121.99
1	A	113	ALA	C-N-CA	5.99	131.33	121.99
1	A	672	LEU	CA-C-O	-5.97	114.75	120.90
2	B	640	ILE	N-CA-C	5.92	117.30	108.23
1	A	185	LYS	N-CA-C	-5.91	104.68	112.72
1	A	966	LYS	CA-C-N	5.78	132.57	121.54
1	A	966	LYS	C-N-CA	5.78	132.57	121.54
1	A	789	PHE	N-CA-C	5.76	118.42	111.40
1	A	668	LEU	CA-C-N	5.71	127.86	120.44
1	A	668	LEU	C-N-CA	5.71	127.86	120.44
1	A	455	SER	N-CA-C	5.69	117.41	110.41
1	A	335	ASN	N-CA-C	5.66	118.61	109.83
1	A	1024	LEU	N-CA-C	5.62	119.40	112.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	79	GLN	CA-C-N	5.58	131.03	123.11
1	A	79	GLN	C-N-CA	5.58	131.03	123.11
1	A	135	LYS	CA-C-N	5.48	128.10	120.65
1	A	135	LYS	C-N-CA	5.48	128.10	120.65
1	A	707	VAL	N-CA-CB	5.48	116.96	110.55
1	A	1041	GLU	CB-CG-CD	5.46	121.88	112.60
2	B	675	GLU	N-CA-C	5.45	121.86	109.81
1	A	907	TYR	CA-C-N	5.45	127.43	120.56
1	A	907	TYR	C-N-CA	5.45	127.43	120.56
1	A	297	ALA	CA-C-N	5.44	131.49	121.70
1	A	297	ALA	C-N-CA	5.44	131.49	121.70
1	A	753	GLN	N-CA-C	5.43	122.37	110.80
1	A	337	LEU	CA-C-N	5.41	128.53	120.90
1	A	337	LEU	C-N-CA	5.41	128.53	120.90
2	B	540	LEU	N-CA-C	-5.40	105.31	111.14
1	A	855	ALA	N-CA-C	-5.39	105.31	111.14
2	B	685	GLU	CA-C-N	5.38	127.95	120.63
2	B	685	GLU	C-N-CA	5.38	127.95	120.63
1	A	438	MET	N-CA-C	5.37	118.22	110.28
1	A	962	ILE	CA-C-N	5.33	127.37	120.44
1	A	962	ILE	C-N-CA	5.33	127.37	120.44
1	A	375	TRP	N-CA-C	5.33	114.87	107.73
1	A	351	LEU	N-CA-C	5.30	118.10	109.24
1	A	917	ASP	CA-CB-CG	5.29	117.89	112.60
1	A	775	SER	CA-C-N	5.29	129.06	120.60
1	A	775	SER	C-N-CA	5.29	129.06	120.60
1	A	576	TRP	CA-C-N	5.25	127.84	120.28
1	A	576	TRP	C-N-CA	5.25	127.84	120.28
1	A	660	ASP	CA-C-N	5.25	131.57	121.54
1	A	660	ASP	C-N-CA	5.25	131.57	121.54
1	A	664	ILE	CA-C-N	5.24	125.92	119.99
1	A	664	ILE	C-N-CA	5.24	125.92	119.99
1	A	15	ASP	CA-CB-CG	5.23	117.83	112.60
2	B	699	ASN	CA-C-N	5.20	127.25	120.28
2	B	699	ASN	C-N-CA	5.20	127.25	120.28
2	B	507	GLY	CA-C-N	5.20	128.92	120.60
2	B	507	GLY	C-N-CA	5.20	128.92	120.60
1	A	607	ASN	CA-CB-CG	5.19	117.79	112.60
1	A	62	MET	CA-C-N	5.19	131.45	121.54
1	A	62	MET	C-N-CA	5.19	131.45	121.54
1	A	262	TYR	CA-C-N	5.17	127.28	120.60
1	A	262	TYR	C-N-CA	5.17	127.28	120.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	181	ASN	CA-CB-CG	5.17	117.77	112.60
1	A	136	ASP	CA-CB-CG	5.15	117.75	112.60
2	B	479	ASN	CA-CB-CG	5.13	117.73	112.60
2	B	465	SER	CA-C-N	5.12	127.15	120.28
2	B	465	SER	C-N-CA	5.12	127.15	120.28
1	A	702	VAL	N-CA-C	5.12	115.84	110.62
1	A	904	VAL	CA-C-N	5.09	127.81	120.38
1	A	904	VAL	C-N-CA	5.09	127.81	120.38
1	A	355	THR	CA-C-N	5.09	127.99	120.82
1	A	355	THR	C-N-CA	5.09	127.99	120.82
1	A	501	PRO	CA-C-N	5.08	128.73	120.60
1	A	501	PRO	C-N-CA	5.08	128.73	120.60
1	A	159	GLY	CA-C-N	5.08	131.24	121.54
1	A	159	GLY	C-N-CA	5.08	131.24	121.54
2	B	686	LEU	CA-C-N	5.08	127.15	120.60
2	B	686	LEU	C-N-CA	5.08	127.15	120.60
1	A	567	LEU	CD1-CG-CD2	-5.06	99.66	110.80
1	A	906	SER	CA-C-N	5.06	127.01	120.44
1	A	906	SER	C-N-CA	5.06	127.01	120.44
1	A	284	LYS	CA-C-N	5.04	127.34	120.54
1	A	284	LYS	C-N-CA	5.04	127.34	120.54
1	A	773	MET	CA-C-N	5.04	127.54	120.28
1	A	773	MET	C-N-CA	5.04	127.54	120.28
1	A	764	GLU	N-CA-C	5.03	117.59	110.10
2	B	635	ASP	CA-CB-CG	5.03	117.63	112.60
2	B	627	GLU	CA-C-N	5.01	127.75	120.79
2	B	627	GLU	C-N-CA	5.01	127.75	120.79

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	7862	0	7903	198	0
2	B	1951	0	1916	49	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	35	0	27	6	0
All	All	9848	0	9846	237	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 12.

All (237) 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:661:ASN:HB2	1:A:665:GLY:H	1.35	0.91
2:B:475:ILE:HG23	2:B:536:LEU:HD23	1.54	0.89
1:A:448:SER:HA	1:A:489:PHE:HB2	1.57	0.87
1:A:969:ASN:HD21	1:A:971:GLU:HG3	1.40	0.87
1:A:1019:LYS:HA	1:A:1024:LEU:HD12	1.58	0.85
1:A:359:CYS:HB2	1:A:383:ILE:HD11	1.60	0.82
1:A:784:TYR:HB2	1:A:794:VAL:HG23	1.64	0.80
1:A:896:THR:HG23	1:A:962:ILE:HG12	1.71	0.73
1:A:797:ILE:HD11	1:A:847:VAL:HG23	1.71	0.72
1:A:54:TRP:HA	1:A:57:VAL:HG13	1.72	0.72
1:A:938:ASN:HB3	1:A:948:GLU:HB3	1.70	0.72
1:A:754:SER:HB2	1:A:762:LEU:HD13	1.71	0.71
1:A:171:PRO:HD2	1:A:662:ARG:HA	1.71	0.71
1:A:94:CYS:O	1:A:97:ARG:HG3	1.90	0.70
1:A:345:VAL:HG11	1:A:367:ILE:H	1.57	0.70
1:A:41:PRO:HG2	1:A:44:ALA:HB2	1.74	0.69
2:B:475:ILE:CG2	2:B:536:LEU:HD23	2.22	0.69
1:A:40:VAL:HG11	1:A:49:ILE:HG12	1.74	0.69
1:A:91:ARG:HD2	1:A:96:VAL:HB	1.75	0.68
1:A:147:ARG:HG3	1:A:694:ARG:HD3	1.77	0.66
1:A:713:LEU:HD21	1:A:782:LEU:HD11	1.78	0.66
1:A:808:MET:HE2	1:A:836:LEU:HD23	1.78	0.65
1:A:906:SER:HB3	1:A:914:ARG:NH1	2.12	0.65
1:A:110:CYS:C	1:A:112:PRO:HD2	2.22	0.65
1:A:154:ILE:HD11	1:A:694:ARG:O	1.96	0.65
1:A:969:ASN:HB3	1:A:973:PHE:CZ	2.32	0.64
1:A:73:MET:HG2	1:A:108:ARG:HA	1.79	0.64
2:B:482:ILE:HD13	2:B:533:ARG:HH11	1.64	0.63
1:A:80:THR:O	1:A:82:VAL:N	2.29	0.63
1:A:77:VAL:HG21	2:B:481:THR:HG23	1.82	0.62
1:A:998:PHE:HD1	1:A:1009:LEU:HD11	1.64	0.62
2:B:694:SER:HA	2:B:705:THR:HG22	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:643:SER:OG	2:B:648:CYS:HB3	2.00	0.62
1:A:35:TYR:HB2	2:B:522:LEU:HD23	1.83	0.61
2:B:635:ASP:HB2	2:B:656:ASP:HA	1.81	0.60
1:A:674:SER:HA	1:A:839:GLY:HA2	1.84	0.60
1:A:906:SER:HA	1:A:911:ILE:HD12	1.84	0.59
1:A:210:PRO:O	1:A:258:ILE:HG13	2.02	0.59
1:A:703:LEU:O	1:A:707:VAL:HG23	2.01	0.59
2:B:467:GLU:HB3	2:B:543:GLN:HE22	1.67	0.59
1:A:434:TRP:HD1	1:A:460:PRO:HG3	1.68	0.59
1:A:629:LEU:HD22	1:A:657:ARG:HD3	1.85	0.59
1:A:46:ILE:HG22	1:A:89:GLU:HA	1.84	0.58
1:A:193:VAL:HG23	1:A:273:PRO:HB2	1.84	0.58
1:A:256:PRO:HG2	1:A:259:GLN:HB2	1.85	0.58
1:A:435:VAL:HG13	1:A:455:SER:HA	1.86	0.58
1:A:635:GLN:HE22	1:A:812:GLN:HE22	1.50	0.57
1:A:863:ASN:CB	1:A:870:PHE:HA	2.35	0.57
2:B:478:PHE:HB3	2:B:533:ARG:HD2	1.85	0.57
1:A:142:PHE:HE2	1:A:442:PHE:HD2	1.50	0.57
1:A:215:ILE:HA	1:A:218:ASN:HD22	1.69	0.57
1:A:1012:VAL:HA	1:A:1015:ILE:HD12	1.87	0.57
1:A:40:VAL:CG1	1:A:49:ILE:HG12	2.34	0.56
1:A:43:GLU:HB2	1:A:92:ARG:HE	1.69	0.56
1:A:173:GLU:O	1:A:260:PHE:HA	2.06	0.56
1:A:347:VAL:HA	1:A:398:VAL:HG12	1.88	0.56
1:A:146:MET:HE2	1:A:655:LEU:HD13	1.88	0.56
1:A:476:ASN:HD22	1:A:478:TYR:H	1.52	0.56
1:A:720:ILE:HD11	1:A:736:MET:HB2	1.89	0.55
1:A:1047:TRP:CE3	2:B:697:GLN:HB3	2.41	0.55
1:A:711:ASN:HA	1:A:714:LYS:HD2	1.87	0.55
1:A:574:ILE:HD11	1:A:585:LEU:HG	1.87	0.55
1:A:959:ILE:HG21	2:B:677:TYR:HE1	1.71	0.55
2:B:623:ARG:HG3	2:B:641:ARG:NH1	2.21	0.55
2:B:608:LEU:N	2:B:609:PRO:HD3	2.21	0.55
1:A:58:HIS:HA	1:A:63:PHE:HB3	1.89	0.55
1:A:195:VAL:HG12	1:A:275:PHE:HB2	1.89	0.55
2:B:638:PHE:CD1	2:B:706:LEU:HB3	2.41	0.55
1:A:259:GLN:HA	1:A:264:ARG:HH21	1.73	0.54
3:A:2058:GD9:S1	3:A:2058:GD9:H17	2.48	0.54
1:A:687:VAL:O	1:A:690:GLU:HG3	2.07	0.54
2:B:526:ILE:HD12	2:B:530:HIS:CD2	2.43	0.53
1:A:387:ASP:HB3	1:A:578:LYS:HA	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:628:GLU:O	1:A:631:GLN:HB2	2.09	0.53
1:A:329:ILE:HD12	1:A:489:PHE:HD1	1.73	0.53
1:A:35:TYR:H	2:B:518:ASN:HD21	1.55	0.53
1:A:773:MET:HE2	3:A:2058:GD9:H12A	1.91	0.53
2:B:699:ASN:HB3	2:B:702:LEU:HG	1.90	0.53
1:A:963:GLN:HG3	1:A:973:PHE:HE2	1.73	0.52
1:A:124:ILE:HG23	1:A:689:LEU:HD13	1.90	0.52
1:A:806:GLN:HG3	1:A:1006:LEU:HD12	1.92	0.52
1:A:683:VAL:O	1:A:687:VAL:HG23	2.10	0.52
1:A:130:GLU:O	1:A:134:LEU:HG	2.10	0.52
1:A:528:PHE:HA	1:A:531:VAL:HG22	1.91	0.51
1:A:943:PHE:HA	2:B:455:ASP:CG	2.36	0.51
1:A:781:TRP:CZ2	1:A:847:VAL:HG21	2.45	0.51
1:A:806:GLN:O	1:A:810:THR:HG23	2.11	0.51
1:A:54:TRP:O	1:A:57:VAL:HG22	2.10	0.51
1:A:80:THR:C	1:A:82:VAL:H	2.18	0.51
2:B:641:ARG:HG3	2:B:650:ALA:HB3	1.93	0.51
1:A:138:GLU:HG3	1:A:442:PHE:CZ	2.46	0.50
1:A:766:TYR:HD2	1:A:785:SER:HB2	1.76	0.50
1:A:23:ALA:HA	1:A:41:PRO:HA	1.93	0.50
1:A:447:ARG:HH21	1:A:451:VAL:HG11	1.75	0.50
1:A:567:LEU:HD23	1:A:592:TRP:CG	2.47	0.50
1:A:120:ILE:HG22	1:A:128:LEU:HD21	1.94	0.50
1:A:387:ASP:HA	1:A:579:LEU:HG	1.93	0.50
1:A:914:ARG:HA	1:A:918:ASN:HD21	1.76	0.50
1:A:959:ILE:HG21	2:B:677:TYR:CE1	2.47	0.50
1:A:652:ARG:O	1:A:656:GLU:HB2	2.12	0.49
1:A:706:GLN:HE22	1:A:755:PRO:HA	1.77	0.49
1:A:963:GLN:HG3	1:A:973:PHE:CE2	2.48	0.49
1:A:280:CYS:O	1:A:283:ILE:HG13	2.12	0.49
1:A:614:ARG:O	1:A:618:VAL:HG22	2.11	0.49
1:A:655:LEU:HD11	1:A:688:ILE:HG23	1.95	0.49
1:A:702:VAL:HA	1:A:705:LYS:HD2	1.93	0.49
1:A:706:GLN:NE2	1:A:755:PRO:HA	2.27	0.49
1:A:876:LEU:HD22	1:A:880:LYS:HE3	1.94	0.49
1:A:1050:LYS:HE2	1:A:1054:MET:HE1	1.92	0.49
1:A:244:VAL:HG22	1:A:247:ARG:HB2	1.95	0.49
2:B:482:ILE:HG13	2:B:529:ILE:HD11	1.95	0.48
1:A:504:LYS:O	1:A:508:LYS:HG3	2.13	0.48
1:A:782:LEU:HB2	1:A:796:VAL:HG12	1.95	0.48
1:A:810:THR:CG2	1:A:935:ILE:HG21	2.44	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:663:ARG:HH22	1:A:757:ASN:HD21	1.62	0.48
1:A:714:LYS:HG2	1:A:800:ASN:ND2	2.28	0.48
1:A:24:ILE:HD13	1:A:42:ARG:HE	1.79	0.48
1:A:540:PRO:HG2	1:A:995:ILE:HG13	1.96	0.48
1:A:728:SER:HB3	1:A:731:LYS:HB2	1.96	0.48
2:B:468:LEU:HD22	2:B:543:GLN:HE21	1.78	0.48
1:A:138:GLU:OE2	1:A:139:VAL:HG23	2.13	0.48
1:A:952:PHE:HE1	1:A:954:LEU:HG	1.77	0.48
1:A:658:ALA:HB1	1:A:665:GLY:HA2	1.96	0.47
2:B:630:LEU:HD22	2:B:654:VAL:HG23	1.96	0.47
1:A:78:ASN:ND2	1:A:79:GLN:H	2.12	0.47
3:A:2058:GD9:S1	3:A:2058:GD9:C17	3.03	0.47
2:B:637:THR:HG22	2:B:708:HIS:HB2	1.96	0.47
1:A:138:GLU:HG3	1:A:442:PHE:CE1	2.49	0.47
1:A:963:GLN:O	1:A:964:GLN:HB2	2.13	0.47
1:A:30:LEU:HD22	1:A:105:LEU:HD22	1.96	0.47
1:A:77:VAL:CG2	2:B:481:THR:HG23	2.44	0.47
1:A:436:ASN:O	1:A:473:VAL:HA	2.15	0.47
1:A:29:LEU:HD22	2:B:488:GLN:HG3	1.97	0.47
1:A:810:THR:HG21	1:A:935:ILE:HG21	1.97	0.46
1:A:54:TRP:HA	1:A:57:VAL:CG1	2.43	0.46
1:A:164:ASP:HA	1:A:167:LYS:HD2	1.97	0.46
1:A:207:GLN:CD	1:A:207:GLN:H	2.23	0.46
1:A:478:TYR:OH	2:B:472:ARG:HB2	2.16	0.46
1:A:934:HIS:HB2	1:A:939:PHE:HB2	1.97	0.46
1:A:283:ILE:HA	1:A:286:MET:HE2	1.97	0.46
1:A:902:TYR:CD2	1:A:929:HIS:HD2	2.33	0.46
2:B:638:PHE:CE2	2:B:706:LEU:HD22	2.51	0.46
1:A:535:ILE:HG23	1:A:548:GLU:OE1	2.16	0.46
1:A:603:LEU:HA	1:A:608:TYR:CD2	2.51	0.46
1:A:60:TYR:O	1:A:63:PHE:HD2	1.99	0.46
1:A:27:ASP:HB2	1:A:102:VAL:HB	1.97	0.46
1:A:572:LEU:HD11	1:A:607:ASN:HB3	1.98	0.46
1:A:626:ASP:HB3	1:A:664:ILE:HD11	1.98	0.46
1:A:784:TYR:HB2	1:A:794:VAL:CG2	2.40	0.45
1:A:714:LYS:HG2	1:A:800:ASN:HD22	1.81	0.45
1:A:716:LEU:HA	1:A:719:LEU:HD23	1.98	0.45
1:A:26:VAL:HG21	1:A:103:LEU:HD12	1.99	0.45
1:A:716:LEU:HD11	1:A:740:LEU:HD22	1.97	0.45
2:B:475:ILE:HG23	2:B:536:LEU:CD2	2.38	0.45
1:A:134:LEU:C	1:A:136:ASP:H	2.25	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:142:PHE:HE2	1:A:442:PHE:CD2	2.32	0.45
1:A:459:PHE:N	1:A:460:PRO:CD	2.80	0.45
2:B:485:PHE:O	2:B:488:GLN:HB2	2.17	0.45
1:A:728:SER:HB3	1:A:731:LYS:HD2	1.98	0.44
1:A:432:VAL:HB	2:B:555:ASN:HB3	1.99	0.44
1:A:635:GLN:H	1:A:635:GLN:NE2	2.14	0.44
1:A:863:ASN:HB2	1:A:870:PHE:HA	2.00	0.44
1:A:243:GLN:HB3	1:A:276:ILE:HG22	2.00	0.44
1:A:899:CYS:HA	1:A:927:LEU:HD22	2.00	0.44
2:B:487:GLU:HA	2:B:490:GLN:CD	2.42	0.44
1:A:158:VAL:HA	1:A:291:MET:SD	2.58	0.44
2:B:623:ARG:HG2	2:B:661:HIS:ND1	2.33	0.44
2:B:618:VAL:HB	2:B:621:ILE:HD12	1.99	0.44
1:A:749:LEU:O	1:A:765:LEU:HD11	2.18	0.43
2:B:480:GLU:O	2:B:484:ILE:HD12	2.18	0.43
1:A:437:THR:HA	1:A:473:VAL:HG23	1.99	0.43
2:B:623:ARG:HE	2:B:661:HIS:HB2	1.82	0.43
1:A:911:ILE:O	1:A:914:ARG:NH1	2.51	0.43
2:B:630:LEU:HA	2:B:633:LYS:HD2	1.99	0.43
1:A:151:GLU:HA	1:A:154:ILE:HD12	2.01	0.43
1:A:401:VAL:HA	2:B:559:PRO:HG3	2.00	0.43
1:A:592:TRP:CD1	1:A:593:PRO:HD2	2.54	0.43
1:A:31:PRO:HD3	1:A:105:LEU:HD23	2.01	0.43
1:A:434:TRP:CD1	1:A:460:PRO:HG3	2.52	0.43
1:A:567:LEU:O	1:A:571:LEU:HG	2.19	0.43
1:A:851:SER:HA	1:A:922:LYS:HA	2.01	0.43
1:A:952:PHE:CE1	1:A:954:LEU:HG	2.54	0.43
1:A:192:VAL:O	1:A:273:PRO:HD2	2.18	0.43
1:A:196:HIS:HB3	1:A:203:VAL:HG23	2.00	0.43
2:B:525:ARG:O	2:B:529:ILE:HG23	2.18	0.43
1:A:97:ARG:HH22	1:A:711:ASN:HB3	1.84	0.42
1:A:196:HIS:HB3	1:A:203:VAL:HA	2.00	0.42
1:A:717:ASN:HB2	1:A:780:LEU:HD21	2.00	0.42
1:A:805:ARG:H	1:A:805:ARG:HG2	1.68	0.42
1:A:398:VAL:HG23	1:A:432:VAL:HA	2.00	0.42
1:A:604:LEU:HD23	1:A:614:ARG:HD3	2.01	0.42
1:A:829:ARG:HG3	1:A:894:GLU:HG2	2.01	0.42
1:A:880:LYS:HG2	1:A:888:LEU:HD11	2.00	0.42
2:B:630:LEU:HB3	2:B:654:VAL:CG2	2.50	0.42
1:A:914:ARG:HH21	1:A:953:ILE:HD12	1.84	0.42
1:A:816:LEU:HD23	1:A:994:PHE:CE1	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:828:LEU:HA	1:A:897:LEU:HB2	2.01	0.42
1:A:154:ILE:HA	1:A:157:LEU:HD12	2.02	0.42
1:A:343:VAL:HG11	1:A:399:TYR:CE2	2.54	0.42
1:A:435:VAL:HG11	1:A:453:LEU:HB3	2.02	0.42
1:A:627:GLU:OE2	1:A:662:ARG:NH1	2.52	0.42
1:A:678:THR:HA	1:A:679:PRO:HD2	1.77	0.42
1:A:705:LYS:HD3	1:A:752:LEU:HB3	2.02	0.42
1:A:92:ARG:HB2	1:A:95:ASP:CG	2.45	0.41
1:A:321:TRP:HE1	1:A:579:LEU:HD12	1.85	0.41
1:A:565:GLN:H	1:A:565:GLN:HG3	1.51	0.41
1:A:808:MET:CE	1:A:837:ALA:H	2.33	0.41
2:B:472:ARG:HA	2:B:475:ILE:HG12	2.01	0.41
3:A:2058:GD9:N2	3:A:2058:GD9:H23	2.35	0.41
1:A:336:LYS:HE3	1:A:483:THR:HB	2.01	0.41
1:A:340:GLU:HB3	1:A:343:VAL:O	2.20	0.41
1:A:556:ARG:HD2	1:A:588:LEU:HD11	2.03	0.41
1:A:326:PRO:HA	1:A:384:ASN:HA	2.01	0.41
1:A:343:VAL:HG11	1:A:399:TYR:HE2	1.85	0.41
1:A:605:ASP:HB3	1:A:1000:LEU:HD23	2.03	0.41
2:B:671:PHE:O	2:B:680:TYR:HB2	2.20	0.41
1:A:27:ASP:OD1	2:B:525:ARG:HD3	2.21	0.41
1:A:663:ARG:HB2	1:A:758:PRO:HG2	2.01	0.41
3:A:2058:GD9:H23	3:A:2058:GD9:H14	2.01	0.41
1:A:34:ILE:HD11	1:A:62:MET:HB2	2.02	0.41
1:A:100:LEU:HD12	1:A:100:LEU:HA	1.81	0.41
1:A:478:TYR:CZ	2:B:472:ARG:HD2	2.56	0.41
1:A:663:ARG:HH22	1:A:757:ASN:ND2	2.18	0.41
1:A:756:LEU:HD23	1:A:836:LEU:HB2	2.03	0.41
1:A:808:MET:HE3	1:A:837:ALA:H	1.85	0.41
2:B:522:LEU:O	2:B:526:ILE:HG23	2.21	0.41
1:A:144:ARG:HG2	1:A:147:ARG:HH12	1.86	0.40
1:A:969:ASN:O	2:B:675:GLU:CG	2.69	0.40
2:B:538:GLN:HE21	2:B:541:ARG:HH22	1.69	0.40
1:A:444:GLY:HA3	1:A:499:TYR:CD1	2.56	0.40
1:A:757:ASN:HD22	1:A:760:VAL:H	1.69	0.40
3:A:2058:GD9:C6	3:A:2058:GD9:C12	2.99	0.40
1:A:804:LEU:O	1:A:808:MET:HB2	2.22	0.40
1:A:969:ASN:CG	1:A:970:THR:H	2.30	0.40
1:A:567:LEU:HD13	1:A:571:LEU:HD11	2.03	0.40
1:A:775:SER:O	1:A:778:LYS:HD3	2.22	0.40
2:B:687:VAL:HG13	2:B:706:LEU:HD11	2.04	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	966/1092 (88%)	818 (85%)	105 (11%)	43 (4%)	2	13
2	B	230/302 (76%)	202 (88%)	20 (9%)	8 (4%)	3	18
All	All	1196/1394 (86%)	1020 (85%)	125 (10%)	51 (4%)	2	14

All (51) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	19	ALA
1	A	63	PHE
1	A	81	ALA
1	A	492	ASN
1	A	546	GLU
1	A	661	ASN
1	A	967	THR
2	B	709	PRO
2	B	711	ARG
1	A	135	LYS
1	A	198	GLU
1	A	322	ASP
1	A	324	ASN
1	A	663	ARG
1	A	746	ARG
1	A	753	GLN
1	A	787	ARG
1	A	863	ASN
1	A	869	ALA
1	A	885	GLY
1	A	966	LYS
2	B	447	TYR

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Mol	Chain	Res	Type
2	B	705	THR
1	A	184	ASP
1	A	344	LYS
1	A	466	MET
1	A	942	LYS
1	A	970	THR
1	A	1009	LEU
2	B	636	GLY
2	B	703	THR
1	A	160	LEU
1	A	367	ILE
1	A	674	SER
1	A	700	MET
1	A	724	ALA
2	B	571	TYR
1	A	70	ASP
1	A	111	ASP
1	A	112	PRO
1	A	347	VAL
1	A	603	LEU
1	A	332	VAL
1	A	539	ASP
1	A	679	PRO
2	B	641	ARG
1	A	471	GLY
1	A	490	PRO
1	A	767	VAL
1	A	725	VAL
1	A	363	VAL

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	871/976 (89%)	679 (78%)	192 (22%)	1 5
2	B	212/268 (79%)	167 (79%)	45 (21%)	1 5

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	1083/1244 (87%)	846 (78%)	237 (22%)	1 5

All (237) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	14	VAL
1	A	15	ASP
1	A	17	GLN
1	A	25	SER
1	A	26	VAL
1	A	43	GLU
1	A	45	THR
1	A	46	ILE
1	A	47	SER
1	A	53	LEU
1	A	69	ILE
1	A	73	MET
1	A	77	VAL
1	A	78	ASN
1	A	84	GLU
1	A	86	LEU
1	A	89	GLU
1	A	90	THR
1	A	93	LEU
1	A	97	ARG
1	A	100	LEU
1	A	102	VAL
1	A	105	LEU
1	A	108	ARG
1	A	116	LEU
1	A	126	LYS
1	A	135	LYS
1	A	138	GLU
1	A	140	ASN
1	A	141	GLU
1	A	163	ILE
1	A	178	VAL
1	A	179	LEU
1	A	181	ASN
1	A	182	LEU
1	A	186	LEU
1	A	202	ASP

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Mol	Chain	Res	Type
1	A	203	VAL
1	A	205	SER
1	A	207	GLN
1	A	215	ILE
1	A	226	LEU
1	A	238	CYS
1	A	241	VAL
1	A	244	VAL
1	A	248	VAL
1	A	257	LEU
1	A	258	ILE
1	A	263	ILE
1	A	269	ASN
1	A	271	THR
1	A	276	ILE
1	A	277	LEU
1	A	280	CYS
1	A	291	MET
1	A	292	ILE
1	A	294	ILE
1	A	298	ILE
1	A	320	ILE
1	A	330	THR
1	A	331	LEU
1	A	336	LYS
1	A	341	GLU
1	A	345	VAL
1	A	347	VAL
1	A	351	LEU
1	A	357	LEU
1	A	362	VAL
1	A	363	VAL
1	A	365	SER
1	A	377	GLU
1	A	385	ILE
1	A	388	LEU
1	A	390	ARG
1	A	394	LEU
1	A	435	VAL
1	A	443	LYS
1	A	446	LEU
1	A	450	ASP

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Mol	Chain	Res	Type
1	A	452	ILE
1	A	455	SER
1	A	465	GLU
1	A	476	ASN
1	A	485	LEU
1	A	495	GLN
1	A	505	ILE
1	A	506	ILE
1	A	512	LEU
1	A	529	LEU
1	A	532	LEU
1	A	538	ARG
1	A	541	LEU
1	A	543	GLN
1	A	546	GLU
1	A	555	LEU
1	A	556	ARG
1	A	557	GLN
1	A	565	GLN
1	A	567	LEU
1	A	574	ILE
1	A	577	ASN
1	A	585	LEU
1	A	595	LEU
1	A	615	GLU
1	A	622	ARG
1	A	633	LEU
1	A	634	LEU
1	A	637	VAL
1	A	650	LEU
1	A	660	ASP
1	A	661	ASN
1	A	663	ARG
1	A	668	LEU
1	A	674	SER
1	A	681	VAL
1	A	689	LEU
1	A	697	VAL
1	A	700	MET
1	A	701	LYS
1	A	710	LEU
1	A	712	LYS

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Mol	Chain	Res	Type
1	A	719	LEU
1	A	720	ILE
1	A	731	LYS
1	A	736	MET
1	A	740	LEU
1	A	743	SER
1	A	747	GLU
1	A	752	LEU
1	A	753	GLN
1	A	761	ILE
1	A	762	LEU
1	A	765	LEU
1	A	768	GLU
1	A	776	LYS
1	A	778	LYS
1	A	780	LEU
1	A	781	TRP
1	A	796	VAL
1	A	805	ARG
1	A	806	GLN
1	A	808	MET
1	A	814	LEU
1	A	815	ARG
1	A	836	LEU
1	A	846	GLU
1	A	847	VAL
1	A	849	SER
1	A	853	THR
1	A	854	ILE
1	A	859	LEU
1	A	875	LEU
1	A	876	LEU
1	A	886	ASP
1	A	888	LEU
1	A	890	ARG
1	A	896	THR
1	A	897	LEU
1	A	917	ASP
1	A	919	ILE
1	A	921	VAL
1	A	930	ILE
1	A	931	ASP

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Mol	Chain	Res	Type
1	A	934	HIS
1	A	935	ILE
1	A	938	ASN
1	A	945	ILE
1	A	947	ARG
1	A	948	GLU
1	A	949	ARG
1	A	959	ILE
1	A	964	GLN
1	A	970	THR
1	A	973	PHE
1	A	995	ILE
1	A	1003	THR
1	A	1015	ILE
1	A	1021	SER
1	A	1027	SER
1	A	1028	GLU
1	A	1030	GLU
1	A	1032	LEU
1	A	1033	LYS
1	A	1036	LYS
1	A	1037	GLN
1	A	1041	GLU
1	A	1046	SER
1	A	1048	THR
1	A	1050	LYS
1	A	1053	TRP
1	A	1054	MET
1	A	1057	THR
2	B	449	ASP
2	B	452	ARG
2	B	457	LEU
2	B	460	GLU
2	B	467	GLU
2	B	468	LEU
2	B	476	GLU
2	B	478	PHE
2	B	479	ASN
2	B	481	THR
2	B	482	ILE
2	B	492	GLN
2	B	493	GLU

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Mol	Chain	Res	Type
2	B	497	LYS
2	B	522	LEU
2	B	523	LYS
2	B	525	ARG
2	B	526	ILE
2	B	529	ILE
2	B	534	THR
2	B	538	GLN
2	B	543	GLN
2	B	550	ILE
2	B	561	LEU
2	B	567	ILE
2	B	572	LEU
2	B	621	ILE
2	B	622	ASN
2	B	638	PHE
2	B	639	LEU
2	B	644	SER
2	B	655	VAL
2	B	659	THR
2	B	661	HIS
2	B	664	ILE
2	B	666	ARG
2	B	667	THR
2	B	678	ASN
2	B	679	LEU
2	B	683	LEU
2	B	688	LEU
2	B	689	HIS
2	B	692	HIS
2	B	706	LEU
2	B	710	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (32) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	37	GLN
1	A	78	ASN
1	A	174	HIS
1	A	261	GLN
1	A	274	HIS
1	A	325	ASN

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Mol	Chain	Res	Type
1	A	445	GLN
1	A	474	GLN
1	A	476	ASN
1	A	495	GLN
1	A	547	ASN
1	A	577	ASN
1	A	623	GLN
1	A	638	GLN
1	A	666	GLN
1	A	717	ASN
1	A	737	HIS
1	A	742	GLN
1	A	800	ASN
1	A	812	GLN
1	A	871	ASN
1	A	929	HIS
1	A	960	HIS
1	A	1016	GLN
1	A	1037	GLN
2	B	518	ASN
2	B	530	HIS
2	B	538	GLN
2	B	543	GLN
2	B	622	ASN
2	B	625	GLN
2	B	697	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

1 ligand is 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	GD9	A	2058	-	39,40,40	1.98	10 (25%)	51,59,59	3.44	26 (50%)

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	GD9	A	2058	-	-	5/18/36/36	0/6/6/6

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	2058	GD9	C23-N7	-5.62	1.28	1.32
3	A	2058	GD9	C2-C1	4.26	1.44	1.40
3	A	2058	GD9	C17-N3	3.75	1.53	1.46
3	A	2058	GD9	C13-S2	3.31	1.83	1.75
3	A	2058	GD9	C12-N4	2.97	1.54	1.46
3	A	2058	GD9	N6-N7	2.71	1.38	1.36
3	A	2058	GD9	C14-N3	2.27	1.50	1.46
3	A	2058	GD9	C19-C18	2.27	1.42	1.38
3	A	2058	GD9	C6-C5	-2.16	1.31	1.36
3	A	2058	GD9	C3-N1	-2.08	1.29	1.34

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	2058	GD9	C23-N7-N6	11.49	112.02	106.02
3	A	2058	GD9	C21-N6-N7	-9.63	106.80	111.52
3	A	2058	GD9	C22-C23-N7	-7.21	108.33	111.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	2058	GD9	O2-S2-N5	-6.89	101.26	107.02
3	A	2058	GD9	C1-C4-N2	-6.68	114.36	122.33
3	A	2058	GD9	C11-C12-N4	4.21	119.13	110.65
3	A	2058	GD9	C12-N4-C9	4.20	117.90	108.84
3	A	2058	GD9	C4-N2-C3	4.08	125.48	115.92
3	A	2058	GD9	O1-S2-O2	3.58	123.82	118.46
3	A	2058	GD9	C16-C17-N3	3.54	116.64	109.93
3	A	2058	GD9	C20-C21-C22	-3.45	119.93	122.66
3	A	2058	GD9	C13-S2-N5	3.24	111.08	107.27
3	A	2058	GD9	C17-N3-C14	3.15	118.66	111.57
3	A	2058	GD9	O1-S2-N5	-2.98	104.53	107.02
3	A	2058	GD9	C7-N4-C12	2.97	115.77	111.14
3	A	2058	GD9	C7-C5-S1	2.96	127.03	121.42
3	A	2058	GD9	C2-N1-C3	2.89	118.88	116.24
3	A	2058	GD9	C21-C22-C23	2.89	106.14	104.41
3	A	2058	GD9	C5-C7-N4	-2.67	107.01	112.46
3	A	2058	GD9	C1-S1-C5	-2.51	90.54	91.92
3	A	2058	GD9	C11-N5-C10	2.50	114.99	112.12
3	A	2058	GD9	C15-C14-N3	2.38	114.44	109.93
3	A	2058	GD9	O1-S2-C13	-2.38	105.03	108.30
3	A	2058	GD9	N2-C3-N1	-2.35	121.27	125.13
3	A	2058	GD9	C7-C5-C6	-2.30	120.19	127.51
3	A	2058	GD9	C10-C9-N4	2.03	114.74	110.65

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	2058	GD9	C10-N5-S2-C13
3	A	2058	GD9	C10-N5-S2-O2
3	A	2058	GD9	C11-N5-S2-O2
3	A	2058	GD9	C10-N5-S2-O1
3	A	2058	GD9	C11-N5-S2-C13

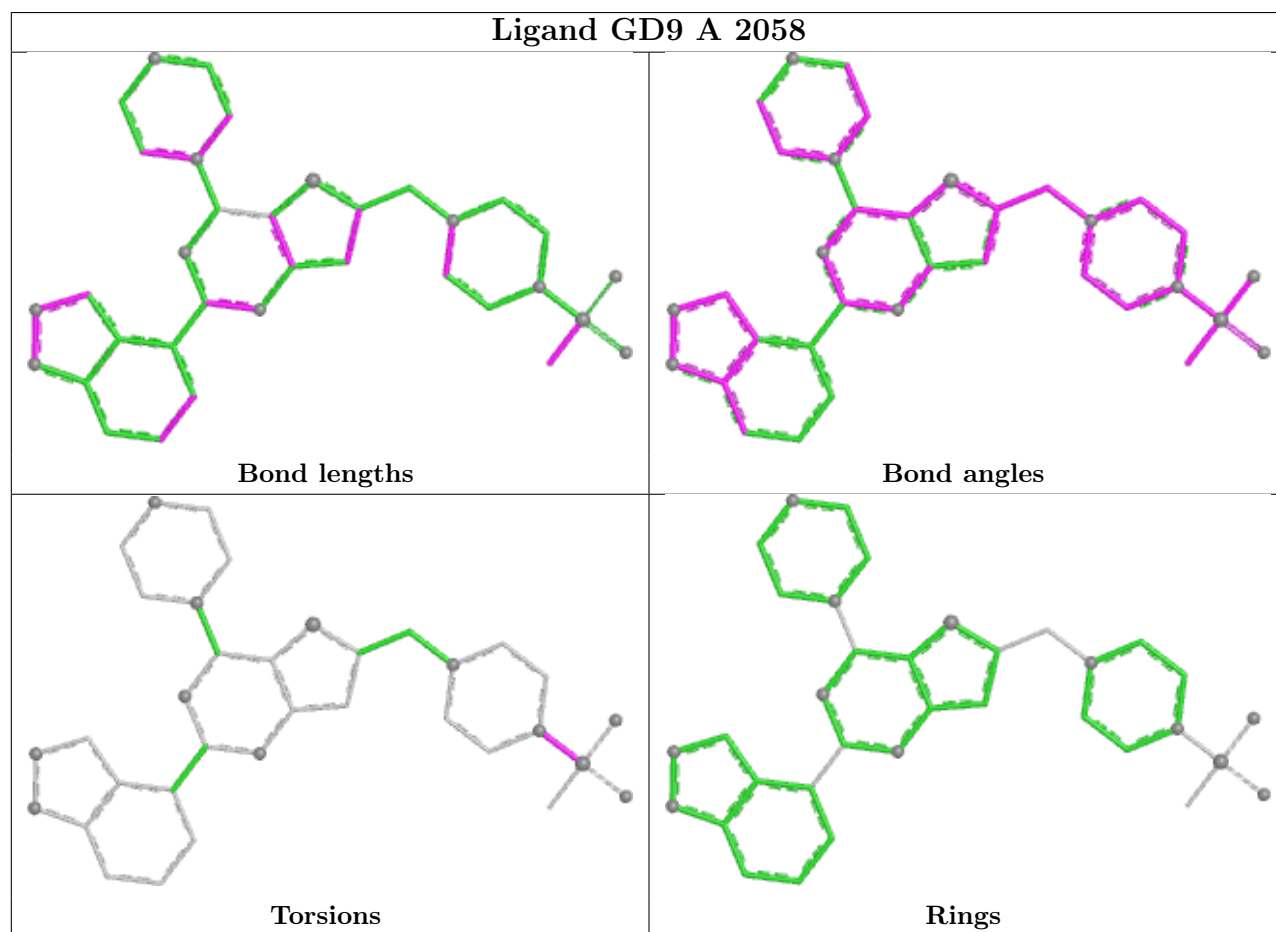
There are no ring outliers.

1 monomer is involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	2058	GD9	6	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	976/1092 (89%)	0.02	20 (2%)	65 46	65, 116, 192, 219	0
2	B	236/302 (78%)	0.18	13 (5%)	30 21	80, 138, 215, 231	0
All	All	1212/1394 (86%)	0.05	33 (2%)	56 37	65, 119, 195, 231	0

All (33) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	432	VAL	3.9
2	B	638	PHE	3.7
1	A	794	VAL	3.7
2	B	639	LEU	3.7
2	B	662	CYS	3.6
2	B	637	THR	3.2
1	A	396	PHE	3.2
1	A	346	HIS	2.9
1	A	937	GLY	2.8
1	A	178	VAL	2.7
1	A	397	ALA	2.7
2	B	567	ILE	2.7
2	B	640	ILE	2.6
1	A	485	LEU	2.6
1	A	400	ALA	2.6
1	A	642	TYR	2.5
1	A	472	THR	2.5
2	B	500	LEU	2.5
1	A	93	LEU	2.4
1	A	401	VAL	2.4
1	A	198	GLU	2.3
2	B	702	LEU	2.3
1	A	248	VAL	2.3
1	A	182	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
2	B	557	LEU	2.3
1	A	338	ASN	2.3
2	B	641	ARG	2.3
1	A	339	THR	2.2
2	B	652	SER	2.2
2	B	712	ALA	2.1
1	A	398	VAL	2.1
1	A	790	GLY	2.0
2	B	636	GLY	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](#)

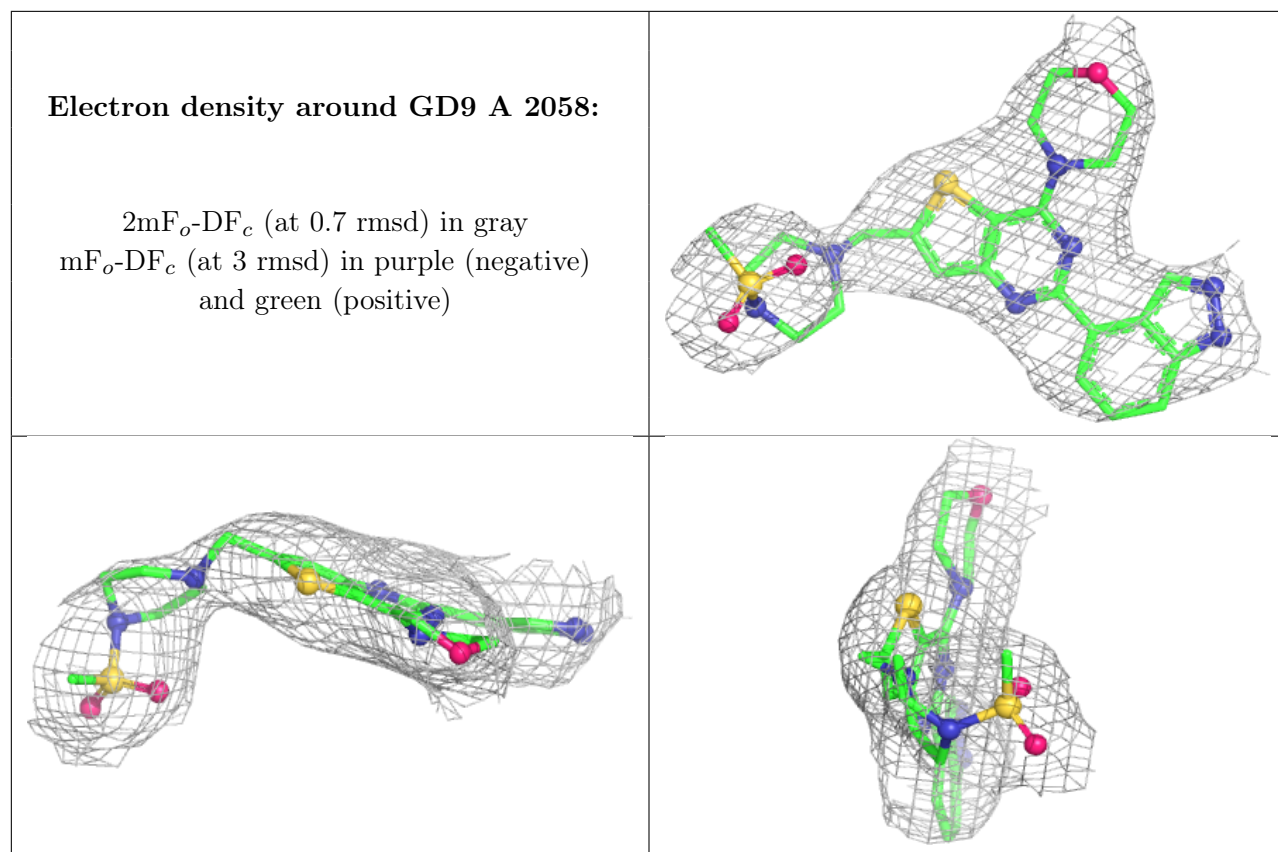
There are no oligosaccharides in this entry.

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
3	GD9	A	2058	35/35	0.94	0.09	67,97,129,130	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.