



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 06:47 PM UTC

PDB ID : 6U36 / pdb_00006u36
Title : PCSK9 in complex with a Fab and compound 14
Authors : Lu, J.; Soisson, S.
Deposited on : 2019-08-21
Resolution : 2.70 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

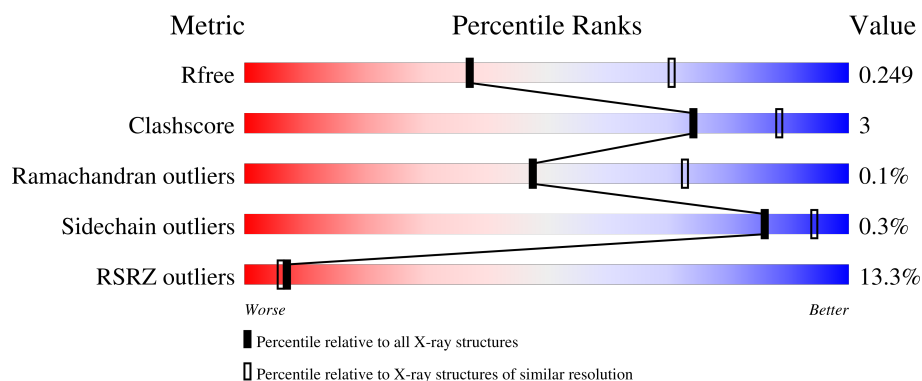
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

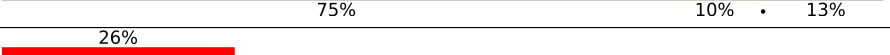
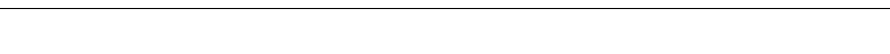
The reported resolution of this entry is 2.70 Å.

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	3538 (2.70-2.70)
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (2.70-2.70)

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	707	 13% 87%
1	B	707	 7% 62% 6% 32%
2	H	246	 10% 75% 10% 13%
3	L	215	 26% 91% 7%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 7361 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 Proprotein convertase subtilisin/kexin type 9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	92	Total	C	N	O	S	0	0	0
			712	460	122	128	2			
1	B	481	Total	C	N	O	S	0	0	0
			3463	2141	630	662	30			

There are 94 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	474	ILE	VAL	engineered mutation	UNP Q8NBP7
A	670	GLU	GLY	engineered mutation	UNP Q8NBP7
A	693	LYS	-	expression tag	UNP Q8NBP7
A	694	GLY	-	expression tag	UNP Q8NBP7
A	695	ASN	-	expression tag	UNP Q8NBP7
A	696	SER	-	expression tag	UNP Q8NBP7
A	697	ALA	-	expression tag	UNP Q8NBP7
A	698	ASP	-	expression tag	UNP Q8NBP7
A	699	ILE	-	expression tag	UNP Q8NBP7
A	700	GLN	-	expression tag	UNP Q8NBP7
A	701	HIS	-	expression tag	UNP Q8NBP7
A	702	SER	-	expression tag	UNP Q8NBP7
A	703	GLY	-	expression tag	UNP Q8NBP7
A	704	GLY	-	expression tag	UNP Q8NBP7
A	705	ARG	-	expression tag	UNP Q8NBP7
A	706	SER	-	expression tag	UNP Q8NBP7
A	707	SER	-	expression tag	UNP Q8NBP7
A	708	LEU	-	expression tag	UNP Q8NBP7
A	709	GLU	-	expression tag	UNP Q8NBP7
A	710	GLY	-	expression tag	UNP Q8NBP7
A	711	PRO	-	expression tag	UNP Q8NBP7
A	712	ARG	-	expression tag	UNP Q8NBP7
A	713	PHE	-	expression tag	UNP Q8NBP7
A	714	GLU	-	expression tag	UNP Q8NBP7
A	715	GLY	-	expression tag	UNP Q8NBP7

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Chain	Residue	Modelled	Actual	Comment	Reference
A	716	LYS	-	expression tag	UNP Q8NBP7
A	717	PRO	-	expression tag	UNP Q8NBP7
A	718	ILE	-	expression tag	UNP Q8NBP7
A	719	PRO	-	expression tag	UNP Q8NBP7
A	720	ASN	-	expression tag	UNP Q8NBP7
A	721	PRO	-	expression tag	UNP Q8NBP7
A	722	LEU	-	expression tag	UNP Q8NBP7
A	723	LEU	-	expression tag	UNP Q8NBP7
A	724	GLY	-	expression tag	UNP Q8NBP7
A	725	LEU	-	expression tag	UNP Q8NBP7
A	726	ASP	-	expression tag	UNP Q8NBP7
A	727	SER	-	expression tag	UNP Q8NBP7
A	728	THR	-	expression tag	UNP Q8NBP7
A	729	ARG	-	expression tag	UNP Q8NBP7
A	730	THR	-	expression tag	UNP Q8NBP7
A	731	GLY	-	expression tag	UNP Q8NBP7
A	732	HIS	-	expression tag	UNP Q8NBP7
A	733	HIS	-	expression tag	UNP Q8NBP7
A	734	HIS	-	expression tag	UNP Q8NBP7
A	735	HIS	-	expression tag	UNP Q8NBP7
A	736	HIS	-	expression tag	UNP Q8NBP7
A	737	HIS	-	expression tag	UNP Q8NBP7
B	474	ILE	VAL	engineered mutation	UNP Q8NBP7
B	670	GLU	GLY	engineered mutation	UNP Q8NBP7
B	693	LYS	-	expression tag	UNP Q8NBP7
B	694	GLY	-	expression tag	UNP Q8NBP7
B	695	ASN	-	expression tag	UNP Q8NBP7
B	696	SER	-	expression tag	UNP Q8NBP7
B	697	ALA	-	expression tag	UNP Q8NBP7
B	698	ASP	-	expression tag	UNP Q8NBP7
B	699	ILE	-	expression tag	UNP Q8NBP7
B	700	GLN	-	expression tag	UNP Q8NBP7
B	701	HIS	-	expression tag	UNP Q8NBP7
B	702	SER	-	expression tag	UNP Q8NBP7
B	703	GLY	-	expression tag	UNP Q8NBP7
B	704	GLY	-	expression tag	UNP Q8NBP7
B	705	ARG	-	expression tag	UNP Q8NBP7
B	706	SER	-	expression tag	UNP Q8NBP7
B	707	SER	-	expression tag	UNP Q8NBP7
B	708	LEU	-	expression tag	UNP Q8NBP7
B	709	GLU	-	expression tag	UNP Q8NBP7
B	710	GLY	-	expression tag	UNP Q8NBP7

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Chain	Residue	Modelled	Actual	Comment	Reference
B	711	PRO	-	expression tag	UNP Q8NBP7
B	712	ARG	-	expression tag	UNP Q8NBP7
B	713	PHE	-	expression tag	UNP Q8NBP7
B	714	GLU	-	expression tag	UNP Q8NBP7
B	715	GLY	-	expression tag	UNP Q8NBP7
B	716	LYS	-	expression tag	UNP Q8NBP7
B	717	PRO	-	expression tag	UNP Q8NBP7
B	718	ILE	-	expression tag	UNP Q8NBP7
B	719	PRO	-	expression tag	UNP Q8NBP7
B	720	ASN	-	expression tag	UNP Q8NBP7
B	721	PRO	-	expression tag	UNP Q8NBP7
B	722	LEU	-	expression tag	UNP Q8NBP7
B	723	LEU	-	expression tag	UNP Q8NBP7
B	724	GLY	-	expression tag	UNP Q8NBP7
B	725	LEU	-	expression tag	UNP Q8NBP7
B	726	ASP	-	expression tag	UNP Q8NBP7
B	727	SER	-	expression tag	UNP Q8NBP7
B	728	THR	-	expression tag	UNP Q8NBP7
B	729	ARG	-	expression tag	UNP Q8NBP7
B	730	THR	-	expression tag	UNP Q8NBP7
B	731	GLY	-	expression tag	UNP Q8NBP7
B	732	HIS	-	expression tag	UNP Q8NBP7
B	733	HIS	-	expression tag	UNP Q8NBP7
B	734	HIS	-	expression tag	UNP Q8NBP7
B	735	HIS	-	expression tag	UNP Q8NBP7
B	736	HIS	-	expression tag	UNP Q8NBP7
B	737	HIS	-	expression tag	UNP Q8NBP7

- Molecule 2 is a protein called Fab Heavy Chain.

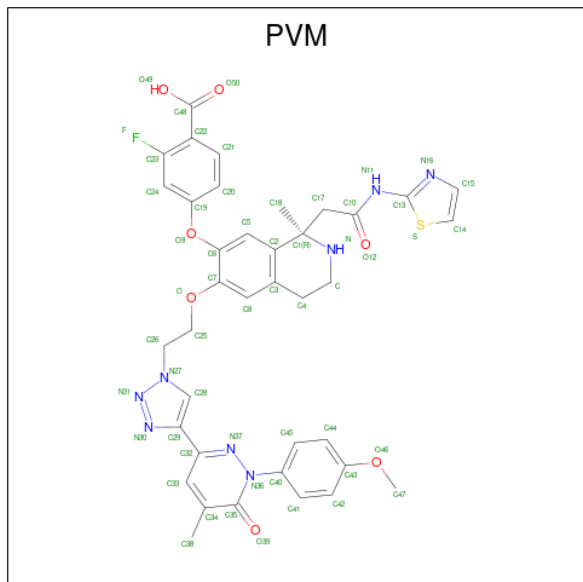
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	213	Total	C	N	O	S	0	0	0
			1583	1005	263	309	6			

- Molecule 3 is a protein called Fab Light Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	L	210	Total	C	N	O	S	0	0	0
			1520	955	249	312	4			

- Molecule 4 is 2-fluoro-4-([(1R)-6-(2-{4-[1-(4-methoxyphenyl)-5-methyl-6-oxo-1,6-dihydro pyridazin-3-yl]-1H-1,2,3-triazol-1-yl}ethoxy)-1-methyl-1-{2-oxo-2-[(1,3-thiazol-2-yl)ami

no[ethyl]-1,2,3,4-tetrahydroisoquinolin-7-yl]oxy}benzoic acid (CCD ID: PVM) (formula: $C_{38}H_{35}FN_8O_7S$) (labeled as "Ligand of Interest" by depositor).



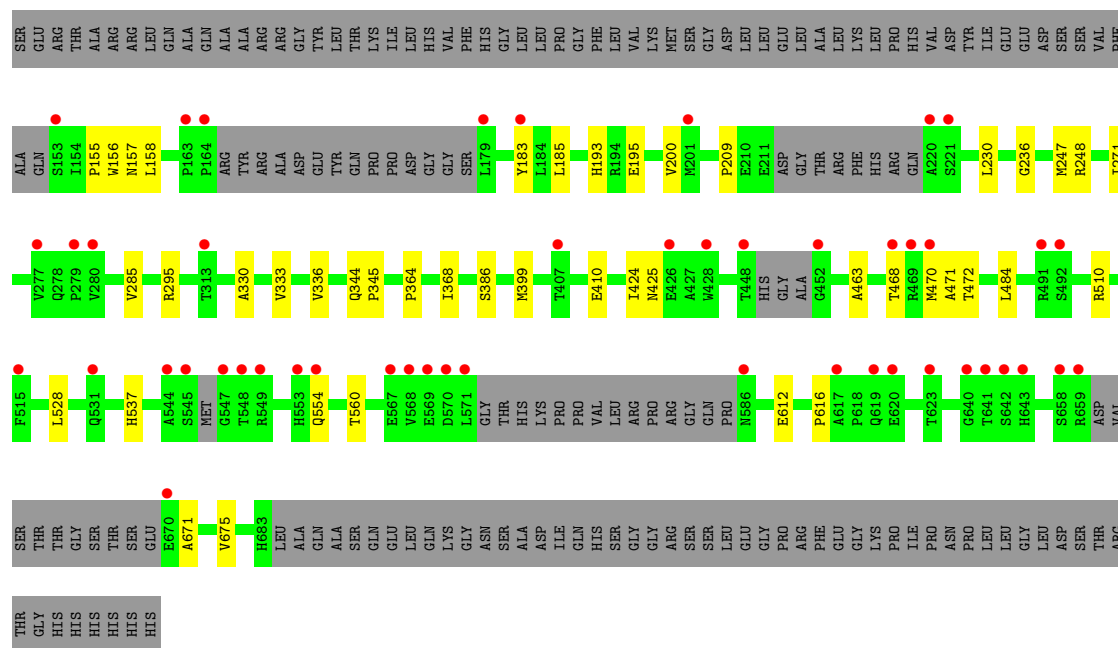
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
4	B	1	Total	C	F	N	O	S	0	0
			55	38	1	8	7	1		

- Molecule 5 is water.

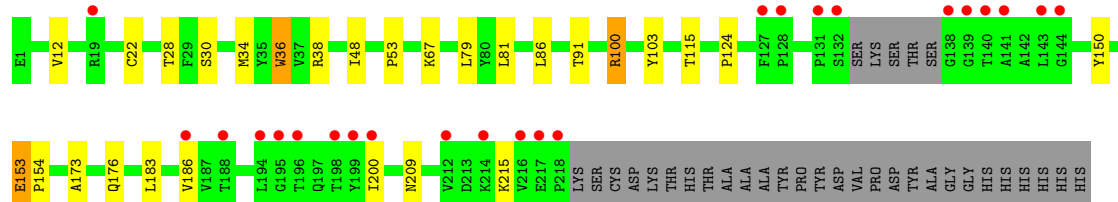
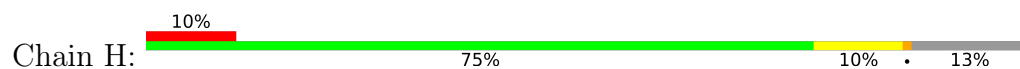
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	O	0	0
			1	1		
5	B	19	Total	O	0	0
			19	19		
5	H	7	Total	O	0	0
			7	7		
5	L	1	Total	O	0	0
			1	1		

- Molecule 1: Proprotein convertase subtilisin/kexin type 9

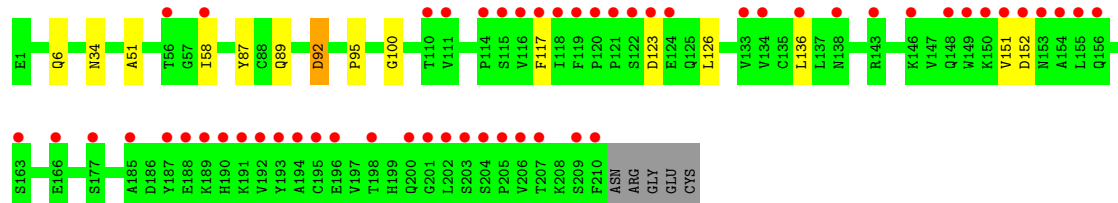
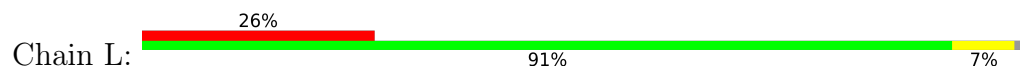




• Molecule 2: Fab Heavy Chain



• Molecule 3: Fab Light Chain



4 Data and refinement statistics

Property	Value	Source
Space group	P 65	Depositor
Cell constants a, b, c, α , β , γ	155.60Å 155.60Å 152.45Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	36.67 – 2.70 36.67 – 2.70	Depositor EDS
% Data completeness (in resolution range)	99.9 (36.67-2.70) 100.0 (36.67-2.70)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.39 (at 2.68Å)	Xtriage
Refinement program	BUSTER 2.11.7	Depositor
R, R_{free}	0.240 , 0.251 0.233 , 0.249	Depositor DCC
R_{free} test set	2925 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å ²)	69.7	Xtriage
Anisotropy	0.127	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 32.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.029 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	7361	wwPDB-VP
Average B, all atoms (Å ²)	73.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.66% 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: PVM

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	0.68	0/728	1.20	1/989 (0.1%)
1	B	0.70	1/3525 (0.0%)	1.24	4/4803 (0.1%)
2	H	0.63	0/1625	1.16	8/2217 (0.4%)
3	L	0.64	0/1558	1.11	4/2140 (0.2%)
All	All	0.67	1/7436 (0.0%)	1.19	17/10149 (0.2%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	399	MET	SD-CE	-5.24	1.66	1.79

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L	152	ASP	CA-CB-CG	7.90	120.50	112.60
1	A	117	GLY	N-CA-C	6.59	121.21	112.77
3	L	151	VAL	CA-C-N	5.71	130.93	122.82
3	L	151	VAL	C-N-CA	5.71	130.93	122.82
1	B	463	ALA	N-CA-C	-5.60	102.99	110.55
2	H	36	TRP	N-CA-C	-5.55	99.23	108.34
2	H	100	ARG	N-CA-C	-5.39	98.50	107.99
2	H	176	GLN	CA-C-N	5.32	127.67	120.38
2	H	176	GLN	C-N-CA	5.32	127.67	120.38
1	B	209	PRO	CA-C-N	5.32	131.69	121.54
1	B	209	PRO	C-N-CA	5.32	131.69	121.54
2	H	67	LYS	N-CA-C	5.22	117.05	111.36
1	B	336	VAL	N-CA-C	5.20	115.34	107.75
3	L	92	ASP	CA-CB-CG	5.16	117.76	112.60
2	H	153	GLU	N-CA-C	-5.14	102.73	110.24
2	H	28	THR	CA-C-N	5.05	127.36	120.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	28	THR	C-N-CA	5.05	127.36	120.54

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	712	0	708	1	0
1	B	3463	0	3299	24	0
2	H	1583	0	1500	13	0
3	L	1520	0	1363	8	0
4	B	55	0	0	0	0
5	A	1	0	0	0	0
5	B	19	0	0	0	0
5	H	7	0	0	0	0
5	L	1	0	0	0	0
All	All	7361	0	6870	44	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 3.

All (44) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:344:GLN:HE22	1:B:425:ASN:H	1.38	0.69
1:B:185:LEU:HD11	1:B:271:ILE:HD11	1.77	0.67
3:L:6:GLN:HE22	3:L:87:TYR:HA	1.64	0.63
1:B:468:THR:HB	1:B:471:ALA:HB2	1.80	0.62
1:B:200:VAL:HG22	1:B:247:MET:HB2	1.83	0.60
3:L:6:GLN:HE21	3:L:100:GLY:HA3	1.68	0.59
1:B:183:TYR:HE1	1:B:248:ARG:HD3	1.69	0.58
3:L:34:ASN:HD22	3:L:89:GLN:NE2	2.04	0.56
2:H:12:VAL:HG11	2:H:86:LEU:HD12	1.88	0.55
3:L:34:ASN:HD22	3:L:89:GLN:HE22	1.52	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:193:HIS:HD2	1:B:195:GLU:H	1.56	0.54
2:H:38:ARG:HB3	2:H:48:ILE:HD11	1.90	0.53
1:B:157:ASN:ND2	1:B:368:ILE:HG23	2.24	0.53
2:H:124:PRO:HB3	2:H:150:TYR:HB3	1.91	0.53
1:B:156:TRP:CH2	1:B:364:PRO:HB3	2.45	0.51
2:H:30:SER:HA	2:H:53:PRO:HB2	1.91	0.51
2:H:22:CYS:HB3	2:H:79:LEU:HB3	1.93	0.50
1:B:157:ASN:HD22	1:B:368:ILE:HG23	1.76	0.49
1:B:155:PRO:HB2	1:B:157:ASN:OD1	2.13	0.49
2:H:186:VAL:HG11	3:L:136:LEU:HD22	1.96	0.47
1:A:65:HIS:CE1	1:B:295:ARG:HH11	2.33	0.47
1:B:484:LEU:HB3	1:B:560:THR:HB	1.97	0.47
1:B:472:THR:HG21	1:B:510:ARG:NH1	2.29	0.46
1:B:537:HIS:CE1	1:B:554:GLN:HE22	2.33	0.46
1:B:612:GLU:HG2	1:B:675:VAL:HG22	1.98	0.46
1:B:616:PRO:HA	1:B:671:ALA:HA	1.98	0.46
2:H:200:ILE:HG22	2:H:215:LYS:HA	1.98	0.46
2:H:173:ALA:HB2	2:H:183:LEU:HD12	1.99	0.44
1:B:345:PRO:HD3	1:B:424:ILE:HG23	2.00	0.43
3:L:123:ASP:HA	3:L:126:LEU:HD12	2.01	0.43
2:H:36:TRP:CE2	2:H:81:LEU:HB2	2.54	0.42
2:H:34:MET:HB3	2:H:79:LEU:HD22	2.02	0.42
1:B:230:LEU:HD11	1:B:386:SER:HB3	2.02	0.42
1:B:410:GLU:HA	1:B:528:LEU:HD11	2.01	0.41
1:B:155:PRO:HD2	1:B:158:LEU:HD12	2.01	0.41
2:H:100:ARG:HD2	2:H:103:TYR:HB2	2.01	0.41
1:B:468:THR:HG22	1:B:470:MET:H	1.85	0.41
3:L:92:ASP:HB3	3:L:95:PRO:O	2.21	0.41
3:L:117:PHE:HD2	3:L:136:LEU:HD23	1.86	0.41
1:B:195:GLU:HG3	1:B:236:GLY:HA2	2.03	0.40
2:H:91:THR:HG23	2:H:115:THR:HA	2.03	0.40
2:H:153:GLU:HG2	2:H:154:PRO:HA	2.02	0.40
1:B:183:TYR:HB2	1:B:285:VAL:HG22	2.04	0.40
1:B:330:ALA:O	1:B:333:VAL:HG22	2.21	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	90/707 (13%)	88 (98%)	2 (2%)	0	100	100
1	B	467/707 (66%)	452 (97%)	15 (3%)	0	100	100
2	H	209/246 (85%)	204 (98%)	5 (2%)	0	100	100
3	L	208/215 (97%)	197 (95%)	10 (5%)	1 (0%)	24	48
All	All	974/1875 (52%)	941 (97%)	32 (3%)	1 (0%)	48	73

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	L	51	ALA

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	74/571 (13%)	74 (100%)	0	100	100
1	B	358/571 (63%)	358 (100%)	0	100	100
2	H	168/203 (83%)	167 (99%)	1 (1%)	78	91
3	L	157/186 (84%)	156 (99%)	1 (1%)	78	91
All	All	757/1531 (49%)	755 (100%)	2 (0%)	86	94

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	H	209	ASN
3	L	58	ILE

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

Mol	Chain	Res	Type
1	A	65	HIS
1	A	99	GLN
1	A	113	HIS
1	B	193	HIS
1	B	278	GLN
1	B	344	GLN
1	B	417	HIS
1	B	464	HIS
1	B	503	GLN
1	B	554	GLN
2	H	82	GLN
2	H	197	GLN
2	H	209	ASN
3	L	6	GLN
3	L	89	GLN
3	L	125	GLN
3	L	161	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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	$\# Z > 2$
4	PVM	B	801	-	60,61,61	1.00	5 (8%)	70,88,88	1.34	9 (12%)

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
4	PVM	B	801	-	-	6/29/46/46	0/7/7/7

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	801	PVM	C18-C1	-2.27	1.51	1.53
4	B	801	PVM	C35-C34	2.27	1.49	1.44
4	B	801	PVM	C33-C32	2.18	1.47	1.42
4	B	801	PVM	C-N	2.08	1.49	1.47
4	B	801	PVM	C17-C10	-2.02	1.49	1.51

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	801	PVM	C47-O46-C43	-4.52	107.80	117.50
4	B	801	PVM	O12-C10-N11	2.54	127.26	122.44
4	B	801	PVM	C4-C3-C8	-2.42	115.13	119.91
4	B	801	PVM	C29-C28-N27	-2.40	102.56	104.95
4	B	801	PVM	C32-C33-C34	-2.38	116.78	121.34
4	B	801	PVM	C21-C22-C23	2.28	119.23	116.70
4	B	801	PVM	C-C4-C3	2.24	114.63	110.66
4	B	801	PVM	O50-C48-C22	-2.22	116.67	121.97
4	B	801	PVM	C28-N27-N31	2.18	112.88	110.75

There are no chirality outliers.

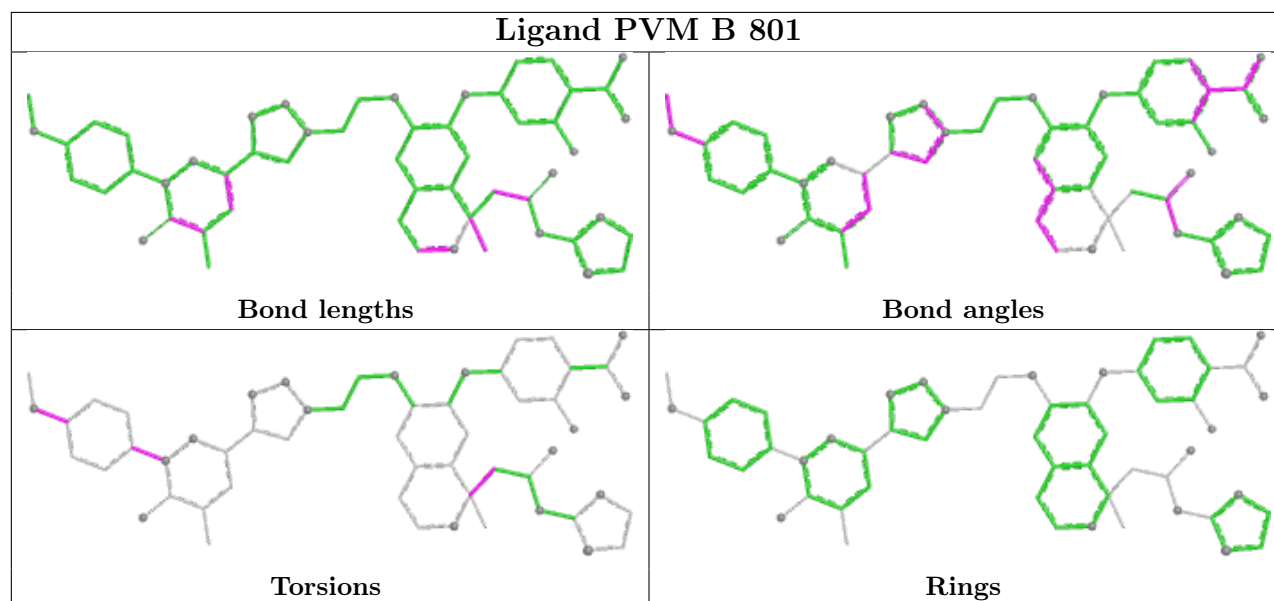
All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	801	PVM	C44-C43-O46-C47
4	B	801	PVM	C42-C43-O46-C47
4	B	801	PVM	C45-C40-N36-N37
4	B	801	PVM	C41-C40-N36-N37
4	B	801	PVM	N-C1-C17-C10
4	B	801	PVM	C18-C1-C17-C10

There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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	92/707 (13%)	0.48	5 (5%) 31 27	49, 69, 91, 97	0
1	B	481/707 (68%)	0.67	48 (9%) 12 10	48, 63, 85, 97	0
2	H	213/246 (86%)	0.90	24 (11%) 10 8	58, 72, 111, 130	0
3	L	210/215 (97%)	1.44	55 (26%) 1 1	61, 91, 122, 127	0
All	All	996/1875 (53%)	0.87	132 (13%) 7 6	48, 69, 114, 130	0

All (132) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	586	ASN	6.2
3	L	202	LEU	6.0
2	H	138	GLY	5.6
3	L	118	ILE	5.4
1	B	571	LEU	5.4
1	B	220	ALA	5.4
3	L	123	ASP	4.9
1	B	548	THR	4.9
3	L	124	GLU	4.8
3	L	153	ASN	4.8
2	H	140	THR	4.7
2	H	194	LEU	4.7
3	L	191	LYS	4.6
1	B	619	GLN	4.5
1	B	547	GLY	4.5
1	B	448	THR	4.4
1	B	544	ALA	4.4
2	H	144	GLY	4.3
3	L	210	PHE	4.2
3	L	192	VAL	4.2
3	L	195	CYS	4.2

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Mol	Chain	Res	Type	RSRZ
1	B	642	SER	4.2
3	L	188	GLU	4.0
3	L	205	PRO	4.0
3	L	110	THR	4.0
3	L	203	SER	3.9
2	H	218	PRO	3.9
3	L	117	PHE	3.9
1	B	221	SER	3.9
1	B	545	SER	3.9
1	B	570	ASP	3.9
2	H	217	GLU	3.8
3	L	206	VAL	3.8
2	H	131	PRO	3.6
1	B	568	VAL	3.6
3	L	201	GLY	3.6
3	L	155	LEU	3.5
3	L	198	THR	3.5
1	B	643	HIS	3.5
1	B	183	TYR	3.4
3	L	149	TRP	3.4
1	B	515	PHE	3.4
3	L	116	VAL	3.4
3	L	143	ARG	3.3
1	B	641	THR	3.3
2	H	132	SER	3.3
1	B	179	LEU	3.3
3	L	114	PRO	3.3
1	B	279	PRO	3.3
2	H	143	LEU	3.3
1	B	659	ARG	3.2
1	B	620	GLU	3.2
1	B	531	GLN	3.1
1	B	164	PRO	3.1
1	B	617	ALA	3.1
3	L	193	TYR	3.1
1	B	407	THR	3.1
3	L	133	VAL	3.1
3	L	177	SER	3.1
1	B	468	THR	3.1
3	L	154	ALA	3.0
3	L	194	ALA	3.0
3	L	200	GLN	3.0

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Mol	Chain	Res	Type	RSRZ
2	H	214	LYS	3.0
2	H	127	PHE	3.0
2	H	128	PRO	2.9
3	L	156	GLN	2.9
2	H	200	ILE	2.8
3	L	119	PHE	2.8
3	L	134	VAL	2.8
1	B	163	PRO	2.8
3	L	189	LYS	2.8
1	B	554	GLN	2.8
2	H	196	THR	2.8
2	H	198	THR	2.8
1	B	452	GLY	2.7
2	H	188	THR	2.7
3	L	148	GLN	2.7
1	B	658	SER	2.7
1	B	280	VAL	2.7
1	B	313	THR	2.7
1	B	469	ARG	2.7
1	B	549	ARG	2.7
3	L	196	GLU	2.7
3	L	146	LYS	2.7
3	L	185	ALA	2.6
3	L	58	ILE	2.6
3	L	120	PRO	2.6
1	A	108	LEU	2.6
3	L	150	LYS	2.6
1	B	491	ARG	2.5
3	L	207	THR	2.5
3	L	187	TYR	2.5
3	L	122	SER	2.5
1	A	61	THR	2.5
3	L	56	THR	2.5
1	B	553	HIS	2.5
3	L	111	VAL	2.5
3	L	151	VAL	2.5
3	L	152	ASP	2.4
1	B	470	MET	2.4
2	H	199	TYR	2.4
3	L	115	SER	2.4
3	L	190	HIS	2.3
1	B	623	THR	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	492	SER	2.3
1	B	428	TRP	2.3
2	H	186	VAL	2.3
2	H	212	VAL	2.3
1	B	640	GLY	2.3
1	B	569	GLU	2.3
2	H	139	GLY	2.3
2	H	216	VAL	2.3
1	A	85	GLU	2.2
3	L	138	ASN	2.2
2	H	19	ARG	2.2
3	L	163	SER	2.2
3	L	136	LEU	2.2
3	L	121	PRO	2.2
2	H	141	ALA	2.2
1	A	116	HIS	2.2
1	A	87	HIS	2.1
1	B	153	SER	2.1
3	L	166	GLU	2.1
2	H	195	GLY	2.1
1	B	201	MET	2.1
1	B	277	VAL	2.1
1	B	426	GLU	2.0
1	B	567	GLU	2.0
3	L	209	SER	2.0
1	B	670	GLU	2.0
3	L	204	SER	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.

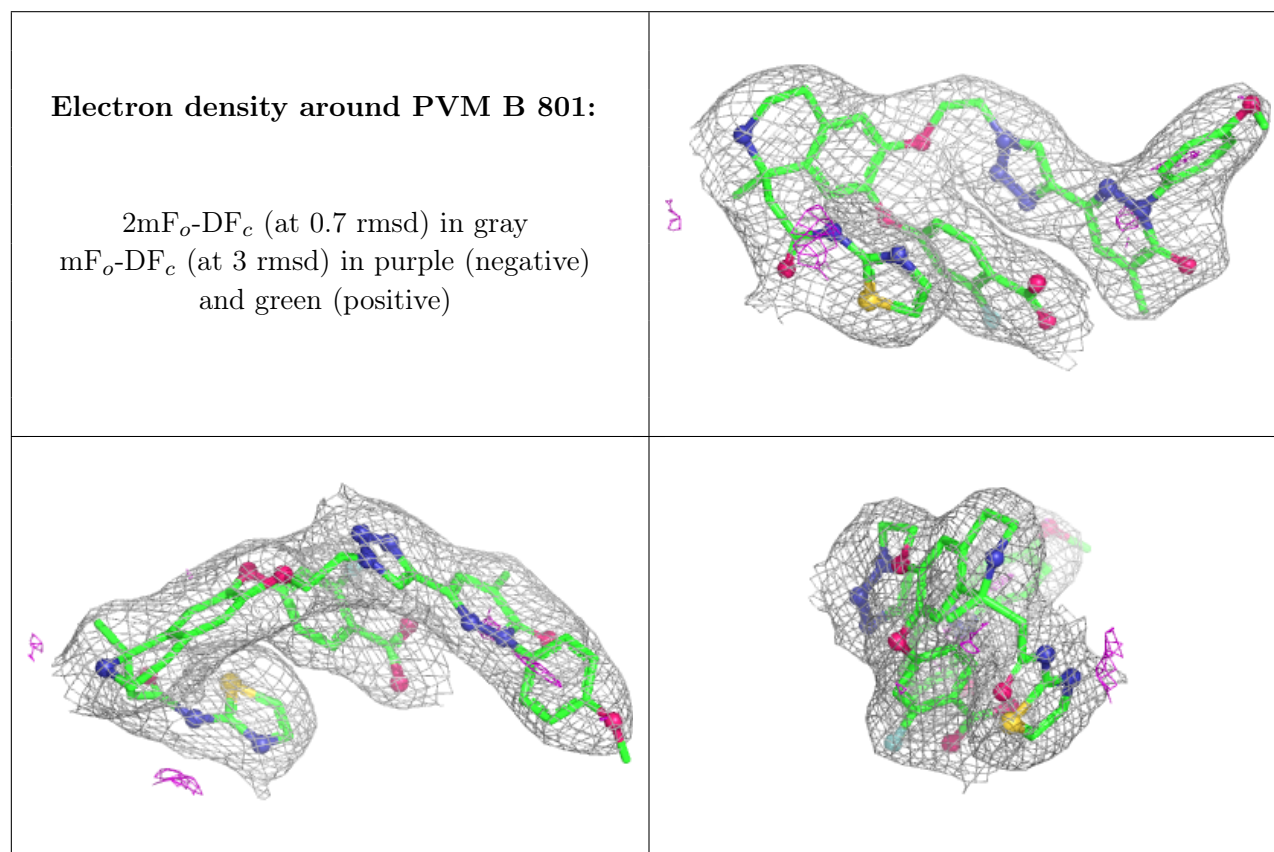
6.4 Ligands [i](#)

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(Å ²)	Q<0.9
4	PVM	B	801	55/55	0.95	0.09	49,55,70,75	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 ⓘ

There are no such residues in this entry.