Full wwPDB X-ray Structure Validation Report ⓘ

May 13, 2020 – 09:14 pm BST

PDB ID	:	6U38
Title	:	PCSK9 in complex with a Fab and compound 8
Authors	:	Lu, J.; Soisson, S.
Deposited on	:	2019-08-21
Resolution	:	2.73 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:

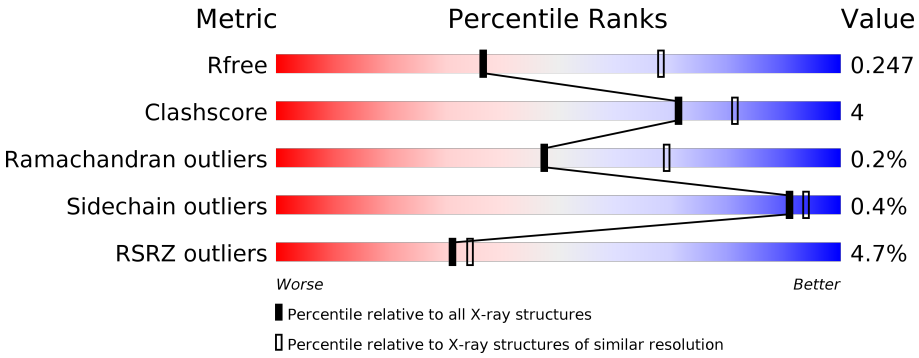
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.73 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	1271 (2.76-2.72)
Clashscore	141614	1322 (2.76-2.72)
Ramachandran outliers	138981	1297 (2.76-2.72)
Sidechain outliers	138945	1298 (2.76-2.72)
RSRZ outliers	127900	1243 (2.76-2.72)

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 <=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	2% 62% 7% 32%
2	H	246	4% 79% 8% 12%
3	L	215	9% 87% 11%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 7473 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
			730	468	130	130	2			
1	B	482	Total	C	N	O	S	0	0	0
			3486	2151	640	665	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.

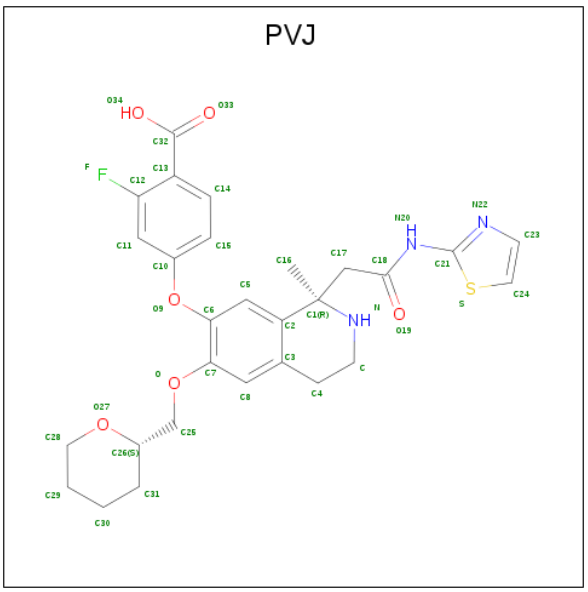
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	216	Total	C	N	O	S	0	0	0
			1612	1023	267	316	6			

- 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
			1548	978	254	312	4			

- Molecule 4 is 2-fluoro-4-{[(1R)-1-methyl-6-{[(2S)-oxan-2-yl]methoxy}-1-{2-oxo-2-[(1,3-thiazol-2-yl)amino]ethyl}-1,2,3,4-tetrahydroisoquinolin-7-yl]oxy}benzoic acid (three-letter code:

PVJ) (formula: $C_{28}H_{30}FN_3O_6S$) (labeled as "Ligand of Interest" by author).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	1	Total C F N O S 39 28 1 3 6 1	0	0

- Molecule 5 is water.

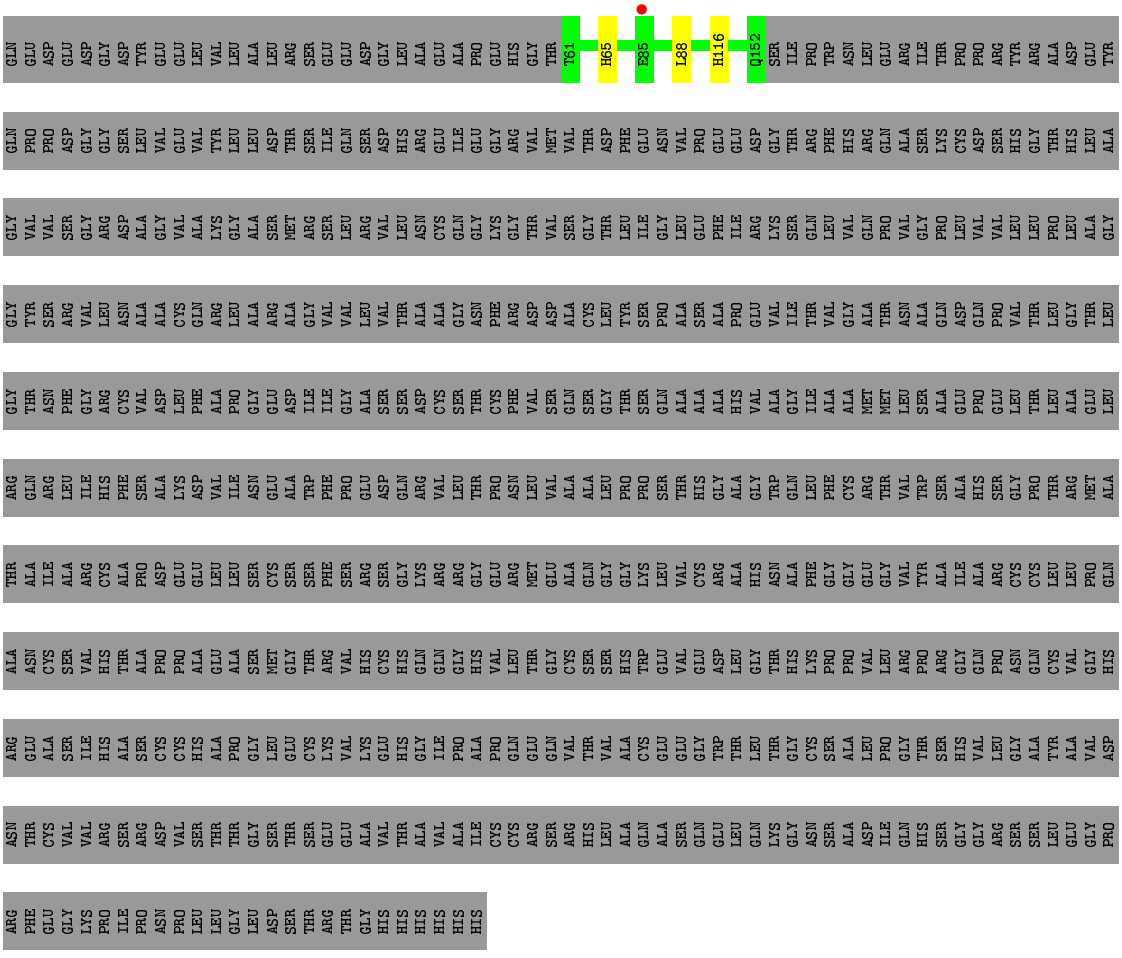
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	7	Total O 7 7	0	0
5	B	29	Total O 29 29	0	0
5	H	20	Total O 20 20	0	0
5	L	2	Total O 2 2	0	0

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.

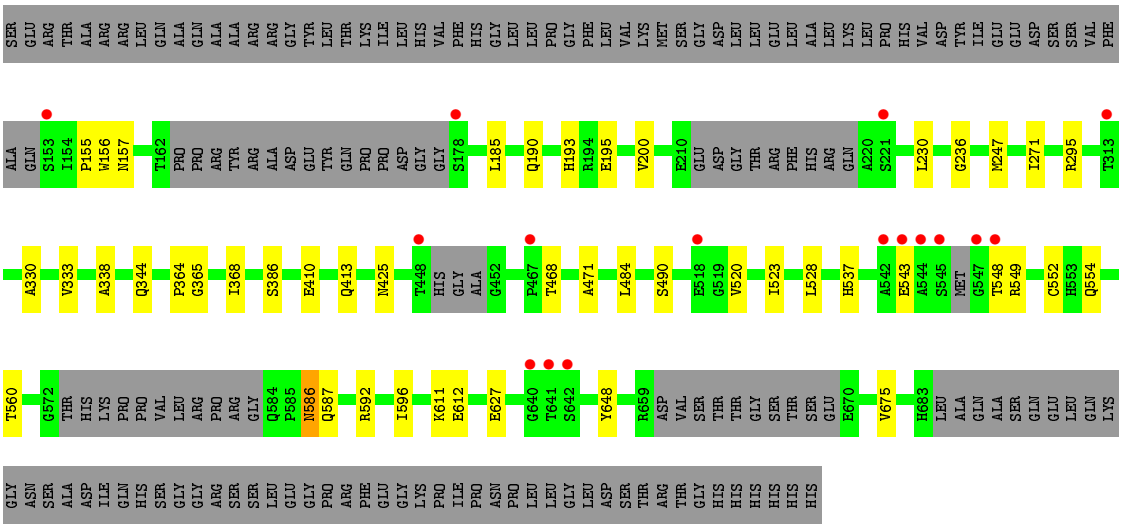
- Molecule 1: Proprotein convertase subtilisin/kexin type 9

Chain A:



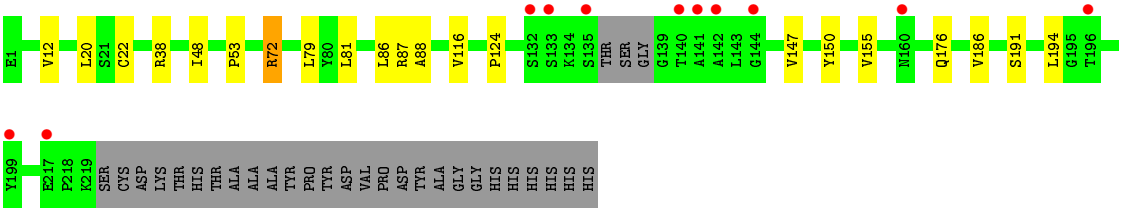
- Molecule 1: Proprotein convertase subtilisin/kexin type 9

Chain B:



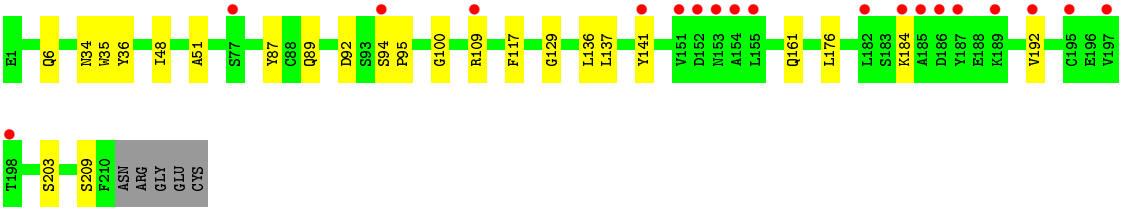
- Molecule 2: Fab Heavy Chain

Chain H:



- Molecule 3: Fab Light Chain

Chain L:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 65	Depositor
Cell constants a, b, c, α, β, γ	155.03Å 155.03Å 151.92Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	38.76 – 2.73 38.76 – 2.73	Depositor EDS
% Data completeness (in resolution range)	100.0 (38.76-2.73) 100.0 (38.76-2.73)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.62 (at 2.73Å)	Xtriage
Refinement program	BUSTER 2.11.7	Depositor
R, R_{free}	0.227 , 0.243 0.231 , 0.247	Depositor DCC
R_{free} test set	2780 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å^2)	54.3	Xtriage
Anisotropy	0.017	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 38.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	0.036 for h,-h-k,-l	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	7473	wwPDB-VP
Average B, all atoms (Å^2)	57.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.78% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: PVJ

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	0.38	0/747	0.63	0/1012
1	B	0.40	0/3547	0.67	0/4827
2	H	0.37	0/1654	0.70	0/2255
3	L	0.39	0/1586	0.71	1/2175 (0.0%)
All	All	0.39	0/7534	0.68	1/10269 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	L	94	SER	CB-CA-C	5.25	120.06	110.10

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	730	0	730	2	0
1	B	3486	0	3351	25	0
2	H	1612	0	1535	12	0
3	L	1548	0	1442	15	0
4	B	39	0	0	0	0
5	A	7	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	B	29	0	0	0	0
5	H	20	0	0	0	0
5	L	2	0	0	0	0
All	All	7473	0	7058	51	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 4.

All (51) 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)
2:H:53:PRO:HA	2:H:72:ARG:HD2	1.75	0.69
3:L:109:ARG:HG2	3:L:141:TYR:CD1	2.36	0.61
3:L:6:GLN:HE21	3:L:100:GLY:HA3	1.65	0.60
2:H:22:CYS:HB3	2:H:79:LEU:HB3	1.84	0.59
3:L:109:ARG:HD3	3:L:141:TYR:HB2	1.84	0.59
1:B:185:LEU:HD11	1:B:271:ILE:HD11	1.85	0.58
1:B:200:VAL:HG22	1:B:247:MET:HB2	1.86	0.57
3:L:92:ASP:OD2	3:L:95:PRO:HD2	2.05	0.56
3:L:117:PHE:HB2	3:L:136:LEU:HB3	1.88	0.55
3:L:6:GLN:HE22	3:L:87:TYR:HA	1.70	0.55
1:B:468:THR:HB	1:B:471:ALA:HB2	1.89	0.54
3:L:34:ASN:HD22	3:L:89:GLN:HE22	1.56	0.54
2:H:12:VAL:HG11	2:H:86:LEU:HD12	1.90	0.53
2:H:186:VAL:HG11	3:L:136:LEU:HD22	1.90	0.53
1:B:549:ARG:HB3	1:B:587:GLN:HE21	1.74	0.52
1:B:611:LYS:HE3	1:B:627:GLU:HG3	1.90	0.51
1:B:230:LEU:HD11	1:B:386:SER:HB3	1.94	0.50
2:H:147:VAL:HG11	2:H:155:VAL:HG11	1.94	0.50
2:H:38:ARG:HB3	2:H:48:ILE:HD11	1.94	0.50
1:B:338:ALA:HB1	1:B:365:GLY:HA3	1.95	0.49
3:L:192:VAL:HG12	3:L:209:SER:HB3	1.96	0.48
1:B:523:ILE:HD13	1:B:648:TYR:HB3	1.95	0.48
3:L:34:ASN:HD22	3:L:89:GLN:NE2	2.12	0.47
2:H:20:LEU:HD12	2:H:81:LEU:HD23	1.96	0.47
1:A:88:LEU:HD13	1:A:116:HIS:HB3	1.97	0.46
2:H:87:ARG:O	2:H:116:VAL:HG21	2.14	0.46
3:L:36:TYR:HE2	3:L:89:GLN:HE21	1.63	0.46
1:B:612:GLU:HG2	1:B:675:VAL:HG22	1.98	0.46
1:B:537:HIS:CE1	1:B:554:GLN:HE22	2.33	0.46
2:H:176:GLN:HA	3:L:161:GLN:HE22	1.81	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:484:LEU:HB3	1:B:560:THR:HB	1.97	0.46
1:B:156:TRP:CH2	1:B:364:PRO:HB3	2.52	0.45
1:B:330:ALA:O	1:B:333:VAL:HG22	2.17	0.44
1:B:490:SER:HB2	1:B:520:VAL:HG12	1.99	0.44
3:L:129:GLY:HA2	3:L:184:LYS:HD3	2.00	0.44
2:H:191:SER:HA	2:H:194:LEU:HD23	2.00	0.43
1:B:548:THR:HG22	1:B:596:ILE:HG22	2.00	0.43
2:H:124:PRO:HB3	2:H:150:TYR:HB3	1.99	0.43
1:B:193:HIS:HD2	1:B:195:GLU:H	1.66	0.42
1:B:157:ASN:HD22	1:B:368:ILE:HG23	1.84	0.42
1:B:543:GLU:HA	1:B:592:ARG:HB2	2.02	0.42
1:B:413:GLN:HG3	1:B:528:LEU:HG	2.02	0.42
2:H:88:ALA:HA	2:H:116:VAL:HG23	2.02	0.42
1:B:344:GLN:HE22	1:B:425:ASN:H	1.66	0.42
1:B:410:GLU:HA	1:B:528:LEU:HD11	2.01	0.41
1:B:552:CYS:HB2	1:B:586:ASN:HD21	1.85	0.41
1:A:65:HIS:CE1	1:B:295:ARG:HH11	2.39	0.41
3:L:35:TRP:HB2	3:L:48:ILE:HB	2.03	0.41
1:B:155:PRO:HB2	1:B:157:ASN:OD1	2.21	0.40
3:L:137:LEU:HB2	3:L:176:LEU:HB3	2.02	0.40
1:B:195:GLU:HG3	1:B:236:GLY:HA2	2.03	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	90/707 (13%)	88 (98%)	2 (2%)	0	100	100
1	B	468/707 (66%)	450 (96%)	18 (4%)	0	100	100
2	H	212/246 (86%)	204 (96%)	8 (4%)	0	100	100
3	L	208/215 (97%)	188 (90%)	18 (9%)	2 (1%)	15	28

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	978/1875 (52%)	930 (95%)	46 (5%)	2 (0%)	47 69

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	L	203	SER
3	L	51	ALA

5.3.2 Protein sidechains (i)

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	77/571 (14%)	77 (100%)	0	100 100
1	B	365/571 (64%)	363 (100%)	2 (0%)	88 92
2	H	173/203 (85%)	172 (99%)	1 (1%)	86 91
3	L	166/186 (89%)	166 (100%)	0	100 100
All	All	781/1531 (51%)	778 (100%)	3 (0%)	91 94

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	190	GLN
1	B	586	ASN
2	H	72	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	65	HIS
1	A	113	HIS
1	B	190	GLN
1	B	193	HIS
1	B	344	GLN

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Mol	Chain	Res	Type
1	B	464	HIS
1	B	554	GLN
1	B	586	ASN
1	B	587	GLN
2	H	77	ASN
3	L	6	GLN
3	L	89	GLN
3	L	161	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

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	PVJ	B	801	-	38,43,43	1.04	3 (7%)	39,61,61	1.45	5 (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	PVJ	B	801	-	-	3/16/43/43	0/5/5/5

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	801	PVJ	C1-C2	-3.42	1.49	1.52
4	B	801	PVJ	C16-C1	-2.24	1.52	1.53
4	B	801	PVJ	C-N	2.13	1.49	1.47

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	B	801	PVJ	O-C25-C26	-4.45	97.29	107.94
4	B	801	PVJ	C14-C13-C12	2.73	120.03	116.10
4	B	801	PVJ	C25-O-C7	-2.40	112.93	118.27
4	B	801	PVJ	O9-C6-C7	2.34	124.23	116.87
4	B	801	PVJ	O19-C18-N20	2.12	127.50	123.63

There are no chirality outliers.

All (3) torsion outliers are listed below:

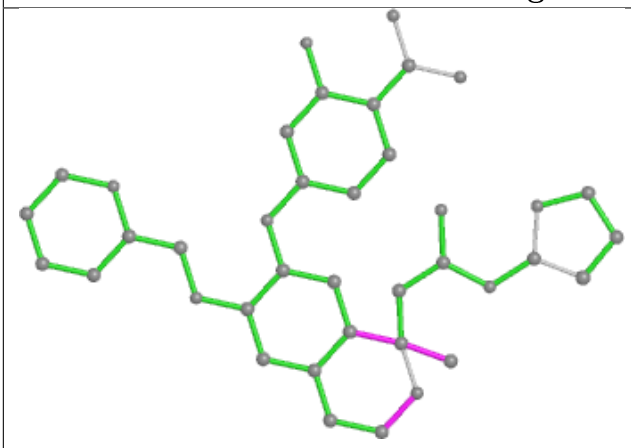
Mol	Chain	Res	Type	Atoms
4	B	801	PVJ	N-C1-C17-C18
4	B	801	PVJ	C6-C7-O-C25
4	B	801	PVJ	C26-C25-O-C7

There are no ring outliers.

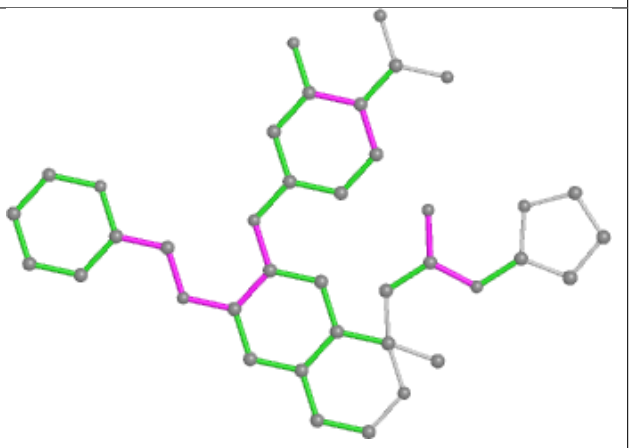
No monomer is involved in short contacts.

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 then 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.

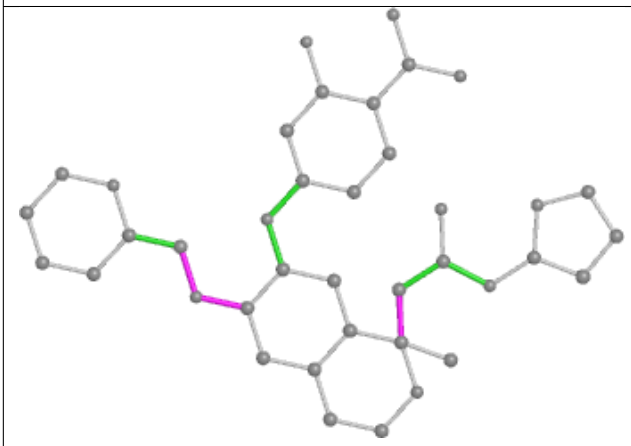
Ligand PVJ B 801



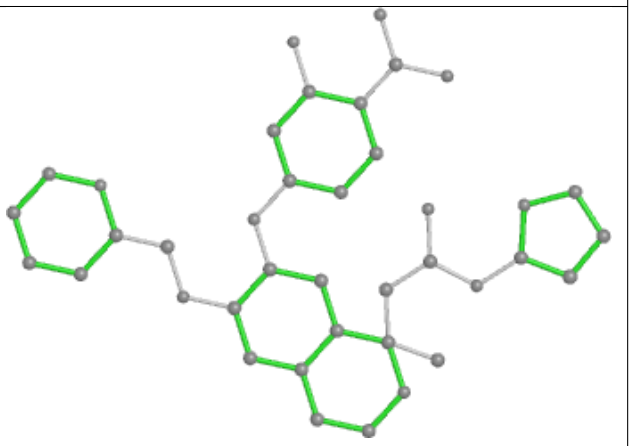
Bond lengths



Bond angles



Torsions



Rings

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, 95^{th} 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%)	0.13	1 (1%) 80 85	34, 53, 77, 79	0
1	B	482/707 (68%)	0.32	16 (3%) 46 52	31, 47, 72, 91	0
2	H	216/246 (87%)	0.29	11 (5%) 28 31	40, 54, 95, 104	0
3	L	210/215 (97%)	0.55	19 (9%) 9 10	40, 73, 105, 110	0
All	All	1000/1875 (53%)	0.34	47 (4%) 31 34	31, 53, 97, 110	0

All (47) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	178	SER	6.3
2	H	196	THR	4.8
3	L	184	LYS	4.0
1	B	547	GLY	3.9
3	L	141	TYR	3.8
3	L	182	LEU	3.7
3	L	94	SER	3.6
1	B	640	GLY	3.4
3	L	185	ALA	3.4
2	H	133	SER	3.3
1	B	548	THR	3.2
2	H	135	SER	3.1
3	L	153	ASN	3.0
3	L	198	THR	3.0
3	L	154	ALA	3.0
1	B	543	GLU	3.0
1	B	448	THR	3.0
3	L	151	VAL	3.0
1	B	542	ALA	3.0
1	B	221	SER	2.9
2	H	140	THR	2.9

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Mol	Chain	Res	Type	RSRZ
1	B	642	SER	2.8
1	B	545	SER	2.8
3	L	109	ARG	2.7
3	L	187	TYR	2.7
1	A	85	GLU	2.7
3	L	186	ASP	2.5
2	H	144	GLY	2.5
1	B	544	ALA	2.5
2	H	217	GLU	2.5
3	L	189	LYS	2.5
2	H	141	ALA	2.4
3	L	77	SER	2.4
3	L	192	VAL	2.4
2	H	199	TYR	2.3
3	L	152	ASP	2.3
2	H	160	ASN	2.3
3	L	195	CYS	2.3
1	B	467	PRO	2.3
1	B	153	SER	2.2
1	B	518	GLU	2.2
3	L	197	VAL	2.1
3	L	155	LEU	2.1
2	H	142	ALA	2.1
1	B	313	THR	2.1
1	B	641	THR	2.0
2	H	132	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 carbohydrates in this entry.

6.4 Ligands (i)

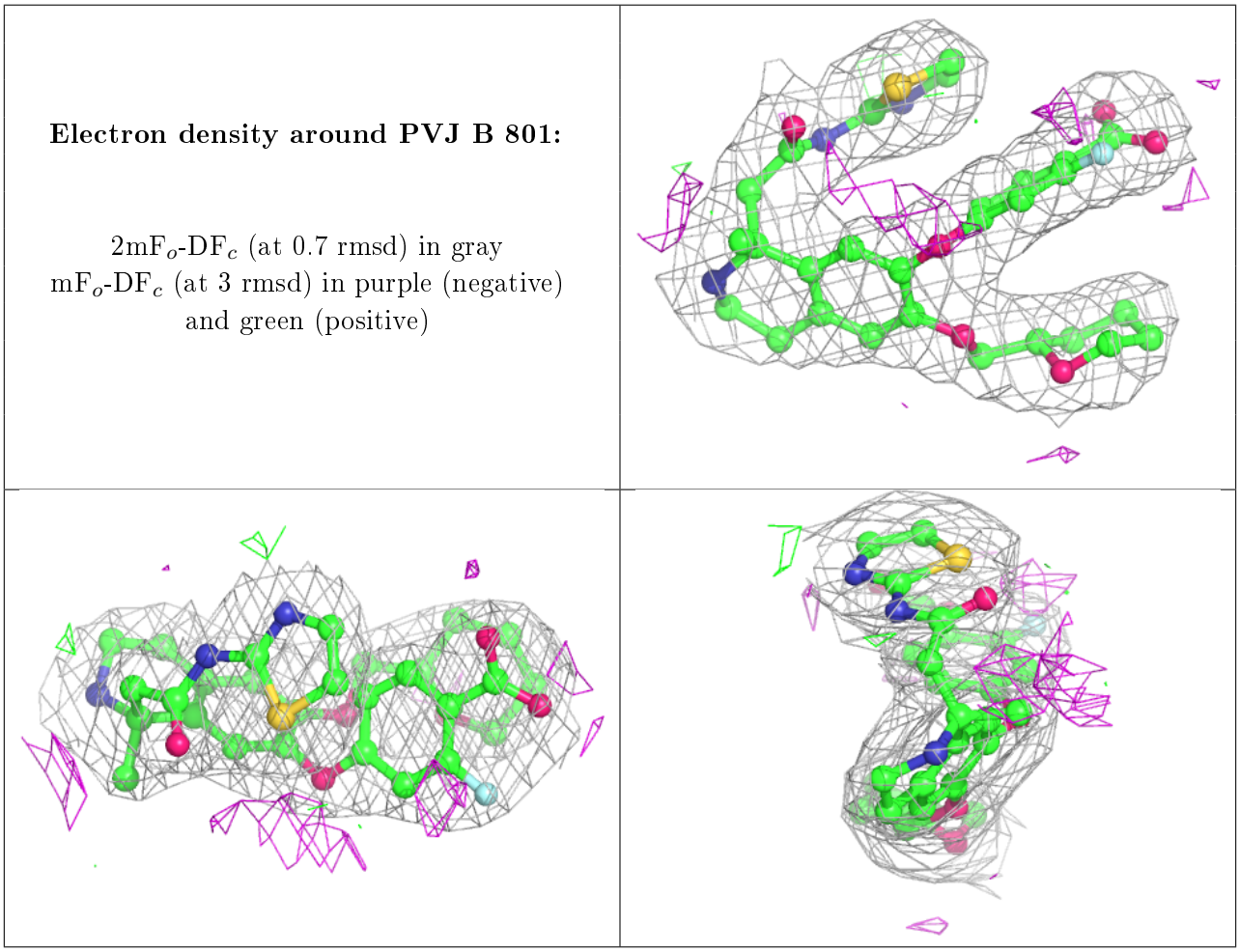
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' 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	PVJ	B	801	39/39	0.97	0.19	31,36,41,44	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 PVJ B 801:

$2mF_o$-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.