



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 12:14 PM UTC

PDB ID : 6U2P / pdb_00006u2p
Title : PCSK9 in complex with compound 5
Authors : Lu, J.; Soisson, S.
Deposited on : 2019-08-20
Resolution : 2.04 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

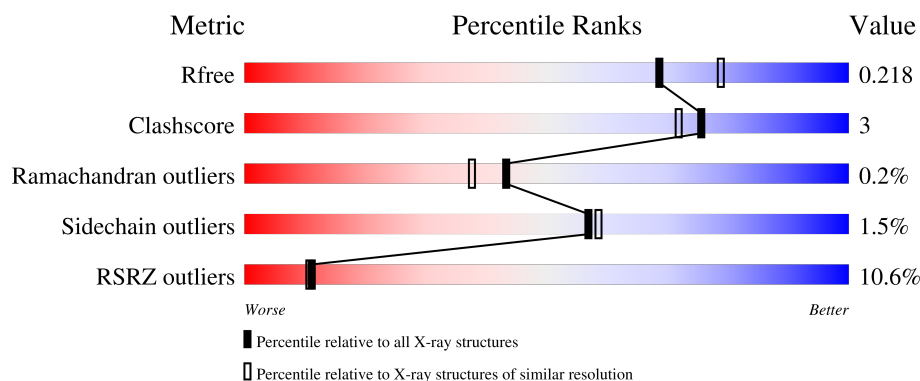
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.04 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	2260 (2.04-2.04)
Clashscore	190562	2333 (2.04-2.04)
Ramachandran outliers	187476	2318 (2.04-2.04)
Sidechain outliers	187428	2318 (2.04-2.04)
RSRZ outliers	180081	2260 (2.04-2.04)

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	
1	B	707	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 4547 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	2	0
			756	486	136	132	2			
1	B	481	Total	C	N	O	S	0	0	0
			3555	2194	657	672	32			

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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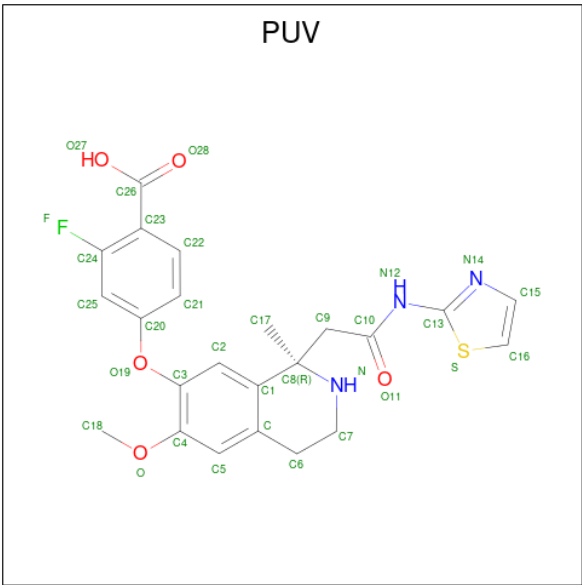
Chain	Residue	Modelled	Actual	Comment	Reference
B	711	PRO	-	expression tag	UNP Q8NBP7
B	712	ARG	-	expression tag	UNP Q8NBP7
B	713	PHE	-	expression tag	UNP Q8NBP7
B	714	GLU	-	expression tag	UNP Q8NBP7
B	715	GLY	-	expression tag	UNP Q8NBP7
B	716	LYS	-	expression tag	UNP Q8NBP7
B	717	PRO	-	expression tag	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 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			4	2	2		
2	A	1	Total	C	O	0	0
			4	2	2		
2	B	1	Total	C	O	0	0
			4	2	2		
2	B	1	Total	C	O	0	0
			4	2	2		
2	B	1	Total	C	O	0	0
			4	2	2		

- Molecule 3 is 2-fluoro-4-{[(1R)-6-methoxy-1-methyl-1-{2-oxo-2-[(1,3-thiazol-2-yl)amino]ethyl}-1,2,3,4-tetrahydroisoquinolin-7-yl]oxy}benzoic acid (CCD ID: PUV) (formula: C₂₃H₂₂FN₃O₅S) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
			Total	C	F	N	O	S		
3	B	1	33	23	1	3	5	1	0	0

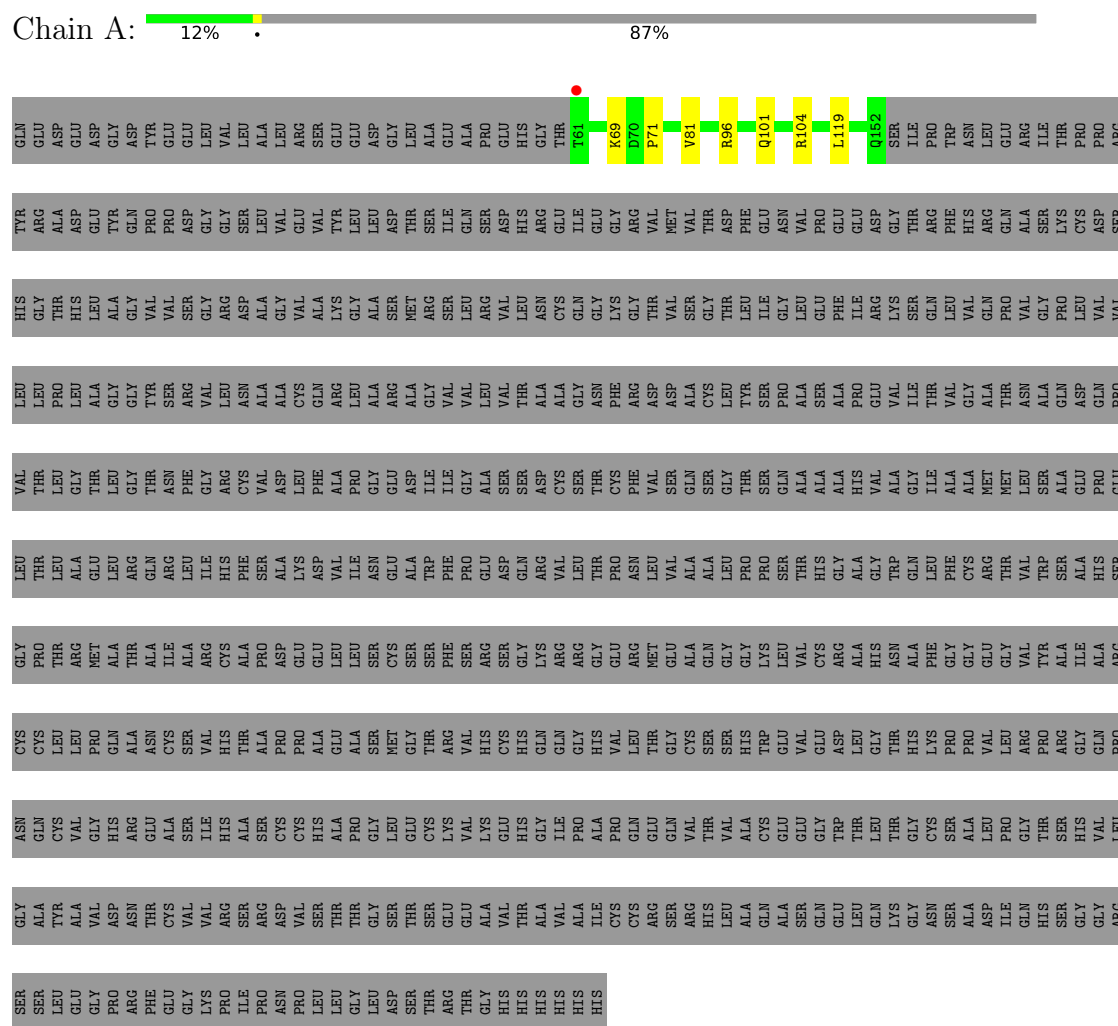
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	43	Total	O	0	0
			43	43		
4	B	140	Total	O	0	0
			140	140		

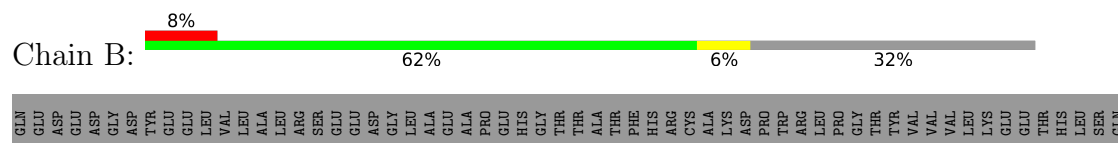
3 Residue-property plots

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: Proprotein convertase subtilisin/kexin type 9



- Molecule 1: Proprotein convertase subtilisin/kexin type 9





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	62.85Å 70.65Å 149.34Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.42 – 2.04 20.42 – 2.04	Depositor EDS
% Data completeness (in resolution range)	100.0 (20.42-2.04) 99.9 (20.42-2.04)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.61 (at 2.04Å)	Xtriage
Refinement program	BUSTER 2.11.7	Depositor
R, R_{free}	0.183 , 0.216 0.186 , 0.218	Depositor DCC
R_{free} test set	2168 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	30.1	Xtriage
Anisotropy	0.128	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 50.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	4547	wwPDB-VP
Average B, all atoms (Å ²)	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.03% 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: PUV, EDO

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	0.84	0/773	1.13	0/1046
1	B	0.85	0/3616	1.19	10/4907 (0.2%)
All	All	0.85	0/4389	1.18	10/5953 (0.2%)

There are no bond length outliers.

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	205	PHE	N-CA-C	-8.60	97.06	109.96
1	B	224	ASP	CA-CB-CG	7.52	120.12	112.60
1	B	480	ASP	CA-CB-CG	6.43	119.03	112.60
1	B	203	THR	CA-C-N	6.09	131.01	122.36
1	B	203	THR	C-N-CA	6.09	131.01	122.36
1	B	407	THR	N-CA-C	-6.04	102.74	110.53
1	B	479	PRO	CA-C-N	5.64	132.10	123.47
1	B	479	PRO	C-N-CA	5.64	132.10	123.47
1	B	463	ALA	N-CA-C	-5.58	102.23	110.48
1	B	336	VAL	N-CA-C	5.28	115.50	108.11

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	756	0	773	3	0
1	B	3555	0	3464	22	0
2	A	8	0	12	0	0
2	B	12	0	18	0	0
3	B	33	0	0	1	0
4	A	43	0	0	0	0
4	B	140	0	0	0	0
All	All	4547	0	4267	26	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 (26) 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:185:LEU:HD11	1:B:271:ILE:HD11	1.65	0.79
1:B:344:GLN:NE2	1:B:425:ASN:HB3	2.00	0.77
1:B:193:HIS:HD2	1:B:195:GLU:H	1.38	0.68
1:B:344:GLN:HE22	1:B:425:ASN:HB3	1.58	0.68
1:B:398:MET:HE3	1:B:444:LEU:HD21	1.77	0.66
1:B:344:GLN:HE22	1:B:425:ASN:H	1.49	0.59
1:A:101:GLN:HG2	1:A:104:ARG:HH21	1.71	0.56
1:B:513:ASN:HD21	1:B:517:GLY:HA2	1.70	0.55
1:B:495:ARG:HH11	1:B:644:VAL:HG23	1.74	0.53
1:A:69[B]:LYS:HG3	1:A:71:PRO:HD2	1.91	0.52
1:B:200:VAL:HG22	1:B:247:MET:HB2	1.92	0.52
1:B:490:SER:HB2	1:B:520:VAL:HG12	1.90	0.52
1:B:205:PHE:CZ	1:B:266:ILE:HG22	2.45	0.51
1:B:186:ASP:OD1	1:B:288:PRO:HG2	2.11	0.50
1:B:205:PHE:CE1	1:B:266:ILE:HG22	2.46	0.49
1:B:638:LEU:HB2	1:B:673:THR:HB	1.94	0.49
1:B:410:GLU:HA	1:B:528:LEU:HD11	1.98	0.46
1:B:468:THR:HB	1:B:471:ALA:HB2	1.97	0.45
1:B:529:LEU:HG	1:B:532:ALA:HB3	1.98	0.45
1:B:344:GLN:HE22	1:B:425:ASN:N	2.16	0.43
1:B:367:ASP:HA	1:B:381:SER:OG	2.19	0.43
1:B:183:TYR:CZ	1:B:248:ARG:HD2	2.54	0.42
1:B:193:HIS:CD2	1:B:195:GLU:H	2.27	0.42
3:B:804:PUV:O11	3:B:804:PUV:S	2.78	0.42
1:B:156:TRP:CH2	1:B:364:PRO:HB3	2.54	0.42
1:A:81:VAL:HG13	1:A:119[B]:LEU:HD13	2.03	0.41

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	92/707 (13%)	89 (97%)	3 (3%)	0	100	100
1	B	461/707 (65%)	450 (98%)	10 (2%)	1 (0%)	43	37
All	All	553/1414 (39%)	539 (98%)	13 (2%)	1 (0%)	43	37

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	280	VAL

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	81/571 (14%)	80 (99%)	1 (1%)	63	65
1	B	381/571 (67%)	375 (98%)	6 (2%)	55	56
All	All	462/1142 (40%)	455 (98%)	7 (2%)	57	58

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	96	ARG
1	B	189	ILE

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Mol	Chain	Res	Type
1	B	224	ASP
1	B	375	CYS
1	B	468	THR
1	B	546	MET
1	B	606	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	99	GLN
1	A	113	HIS
1	A	116	HIS
1	B	193	HIS
1	B	207	ASN
1	B	342	GLN
1	B	344	GLN
1	B	464	HIS
1	B	513	ASN
1	B	537	HIS
1	B	621	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](#)

6 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	EDO	B	801	-	3,3,3	0.47	0	2,2,2	0.42	0
3	PUV	B	804	-	35,36,36	0.80	1 (2%)	41,52,52	1.09	2 (4%)
2	EDO	A	801	-	3,3,3	0.34	0	2,2,2	0.57	0
2	EDO	A	802	-	3,3,3	0.60	0	2,2,2	0.22	0
2	EDO	B	803	-	3,3,3	0.38	0	2,2,2	0.46	0
2	EDO	B	802	-	3,3,3	0.50	0	2,2,2	0.36	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	EDO	B	801	-	-	0/1/1/1	-
3	PUV	B	804	-	-	2/19/32/32	0/4/4/4
2	EDO	A	801	-	-	0/1/1/1	-
2	EDO	A	802	-	-	0/1/1/1	-
2	EDO	B	803	-	-	0/1/1/1	-
2	EDO	B	802	-	-	0/1/1/1	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	804	PUV	C7-N	2.67	1.50	1.47

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	804	PUV	C6-C-C5	-2.21	115.56	119.91
3	B	804	PUV	O28-C26-C23	-2.03	117.12	121.97

There are no chirality outliers.

All (2) torsion outliers are listed below:

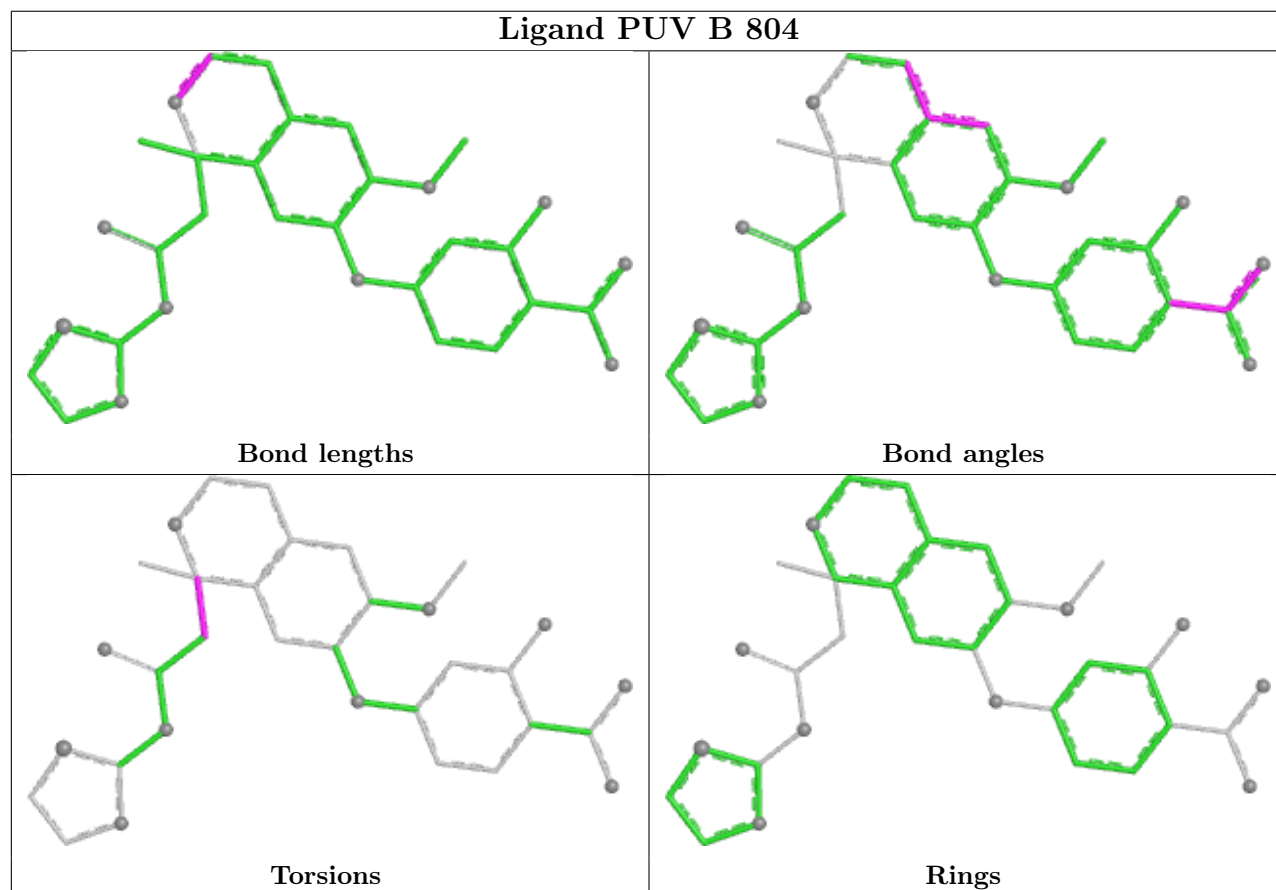
Mol	Chain	Res	Type	Atoms
3	B	804	PUV	N-C8-C9-C10
3	B	804	PUV	C17-C8-C9-C10

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	804	PUV	1	0

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



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	92/707 (13%)	-0.27	1 (1%) 78 80	15, 28, 50, 60	2 (2%)
1	B	481/707 (68%)	0.29	60 (12%) 8 7	17, 32, 71, 121	1 (0%)
All	All	573/1414 (40%)	0.20	61 (10%) 11 11	15, 32, 69, 121	3 (0%)

All (61) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	571	LEU	7.0
1	B	542	ALA	5.9
1	B	616	PRO	5.7
1	B	557	HIS	5.6
1	B	205	PHE	5.1
1	B	448	THR	4.8
1	B	517	GLY	4.8
1	B	204	ASP	4.7
1	B	568	VAL	4.6
1	B	220	ALA	4.6
1	B	469	ARG	4.5
1	B	544	ALA	4.5
1	B	467	PRO	4.4
1	B	449	HIS	4.1
1	B	221	SER	4.0
1	B	208	VAL	3.9
1	B	671	ALA	3.5
1	B	468	THR	3.5
1	B	470	MET	3.4
1	B	207	ASN	3.3
1	B	546	MET	3.3
1	B	547	GLY	3.2
1	B	453	TRP	3.2
1	B	532	ALA	3.2

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Mol	Chain	Res	Type	RSRZ
1	B	515	PHE	3.1
1	B	553	HIS	3.1
1	B	569	GLU	2.9
1	B	545	SER	2.9
1	B	206	GLU	2.8
1	B	350	THR	2.8
1	B	585	PRO	2.8
1	B	428	TRP	2.8
1	B	471	ALA	2.6
1	B	447	SER	2.6
1	B	659	ARG	2.6
1	B	530	PRO	2.6
1	B	223	CYS	2.5
1	B	452	GLY	2.5
1	B	534	CYS	2.5
1	B	514	ALA	2.5
1	B	167	ARG	2.4
1	B	584	GLN	2.4
1	B	639	PRO	2.4
1	B	203	THR	2.3
1	B	478	ALA	2.3
1	B	466	GLY	2.3
1	A	61	THR	2.3
1	B	348	LEU	2.3
1	B	472	THR	2.2
1	B	502	ALA	2.2
1	B	615	ILE	2.2
1	B	516	GLY	2.2
1	B	602	HIS	2.1
1	B	210	GLU	2.1
1	B	349	GLY	2.1
1	B	643	HIS	2.1
1	B	153	SER	2.1
1	B	556	GLY	2.1
1	B	586	ASN	2.1
1	B	479	PRO	2.0
1	B	179	LEU	2.0

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

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

6.3 Carbohydrates [i](#)

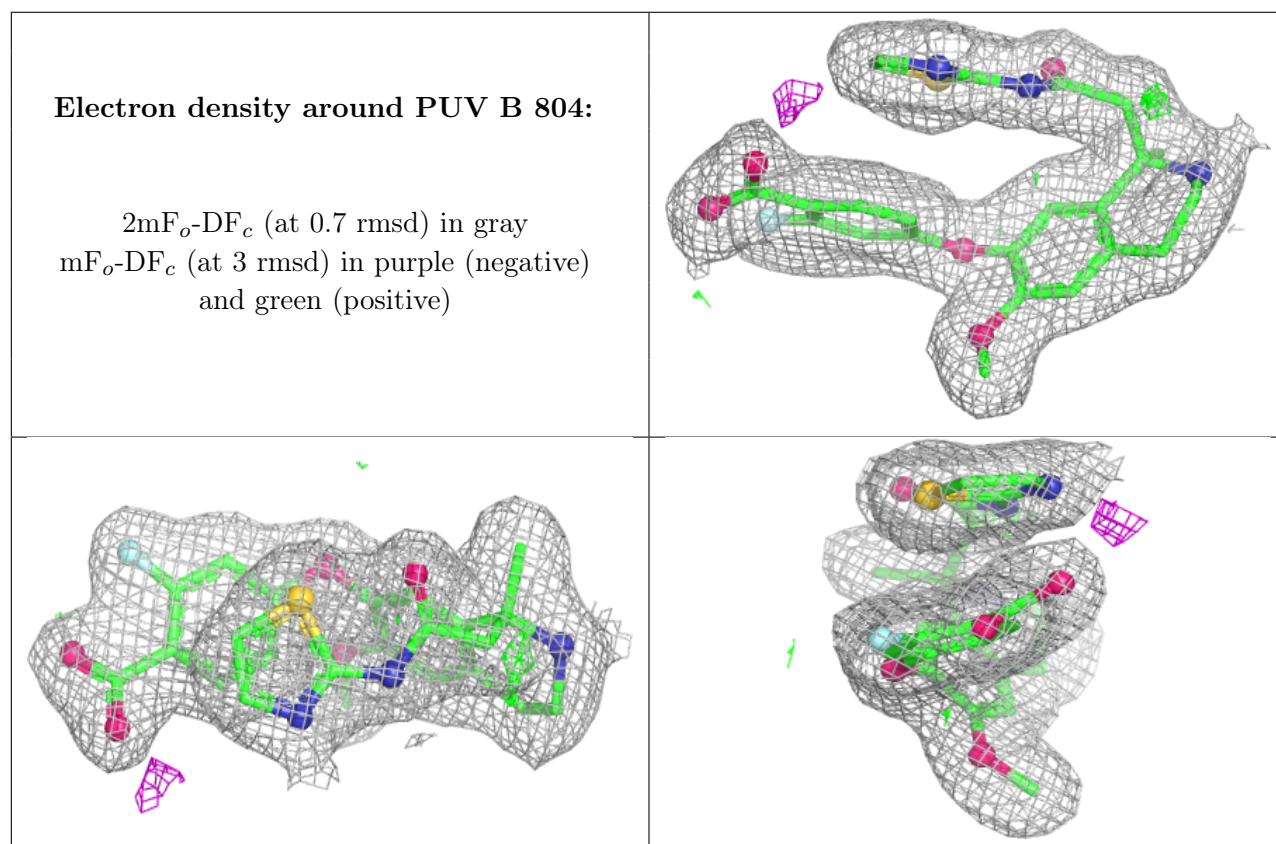
There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	EDO	A	802	4/4	0.72	0.18	44,50,54,56	0
2	EDO	A	801	4/4	0.92	0.10	39,40,43,44	0
2	EDO	B	801	4/4	0.92	0.12	31,34,36,38	0
2	EDO	B	803	4/4	0.95	0.08	33,33,35,36	0
3	PUV	B	804	33/33	0.96	0.06	17,23,30,32	0
2	EDO	B	802	4/4	0.97	0.06	33,33,34,37	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.