



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 09:53 PM UTC

PDB ID : 4QIN / pdb_00004qin
Title : Structure of the human smoothened receptor in complex with SAG1.5
Authors : Wang, C.; Wu, H.; Evron, T.; Vardy, E.; Han, G.W.; Huang, X.-P.; Hufeisen, S.J.; Mangano, T.J.; Urban, D.J.; Katritch, V.; Cherezov, V.; Caron, M.G.; Roth, B.L.; Stevens, R.C.; GPCR Network (GPCR)
Deposited on : 2014-05-31
Resolution : 2.60 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

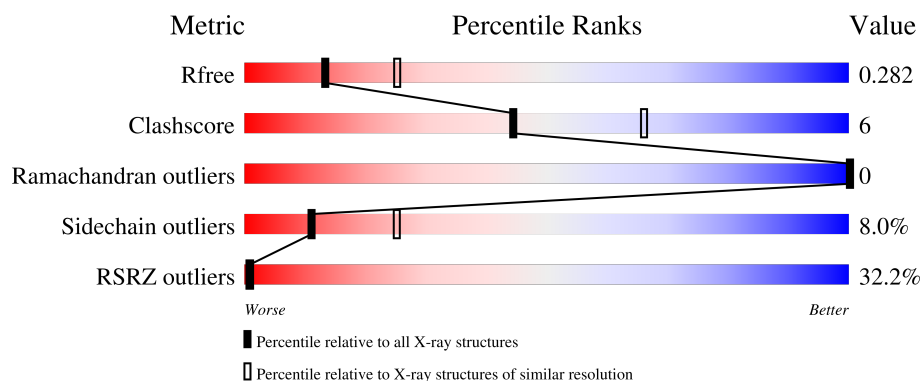
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (2.60-2.60)

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	468	

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 3454 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.

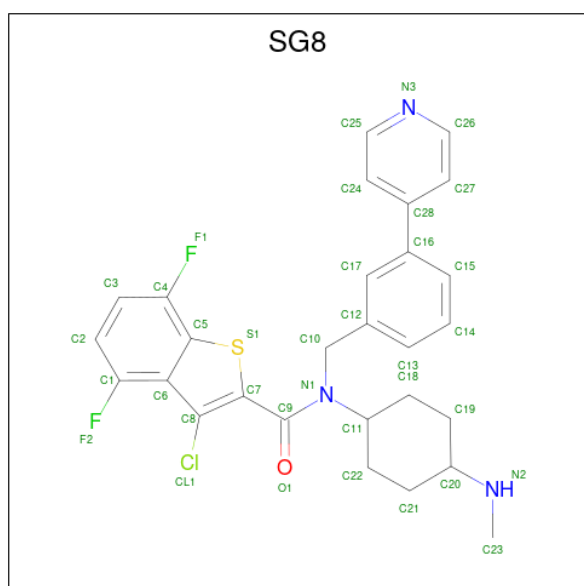
- Molecule 1 is a protein called Smoothened homolog/Soluble cytochrome b562 chimeric protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	447	Total	C	N	O	S	0	0	0
			3411	2215	556	619	21			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	187	GLY	-	expression tag	UNP Q99835
A	188	GLY	-	expression tag	UNP Q99835
A	189	THR	-	expression tag	UNP Q99835
A	1007	TRP	MET	engineered mutation	UNP P0ABE7
A	1102	ILE	HIS	engineered mutation	UNP P0ABE7
A	1106	LEU	ARG	engineered mutation	UNP P0ABE7

- Molecule 2 is 3-chloro-4,7-difluoro-N-[trans-4-(methylamino)cyclohexyl]-N-[3-(pyridin-4-yl)benzyl]-1-benzothiophene-2-carboxamide (CCD ID: SG8) (formula: $C_{28}H_{26}ClF_2N_3OS$).



Mol	Chain	Residues	Atoms							ZeroOcc	AltConf
2	A	1	Total	C	Cl	F	N	O	S	0	0
			36	28	1	2	3	1	1		

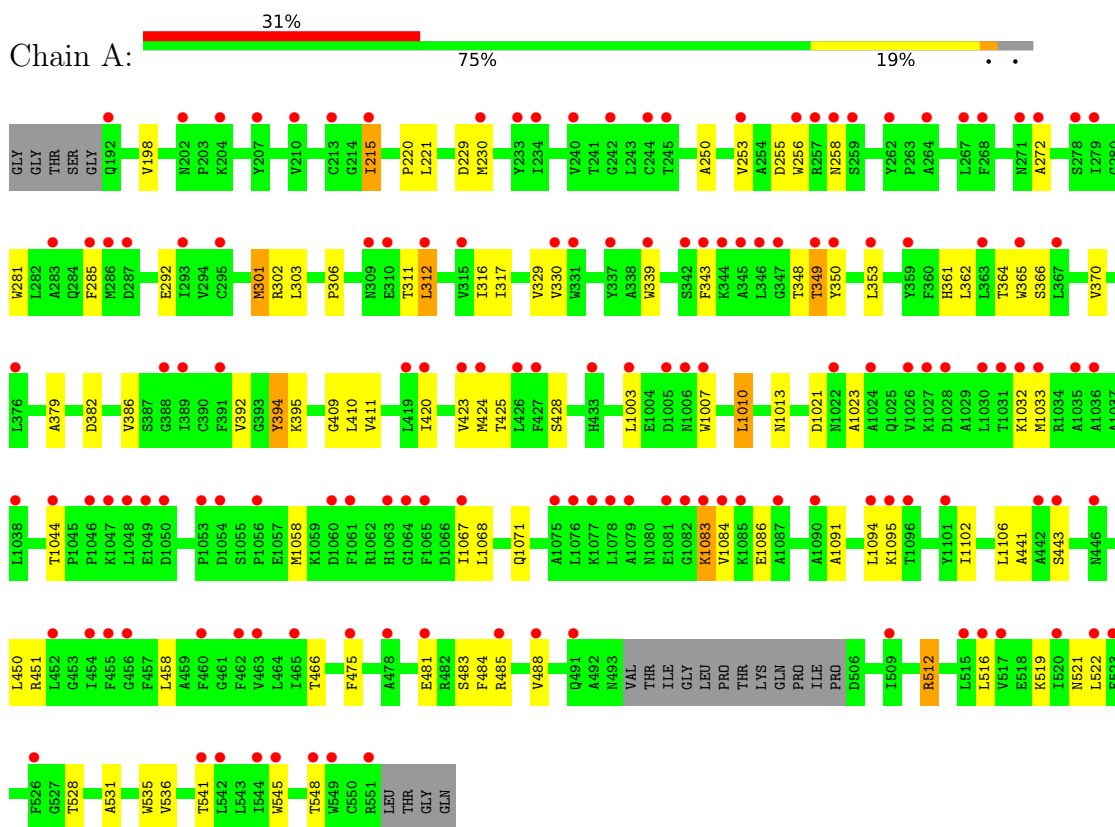
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	7	Total	O	0	0
			7	7		

3 Residue-property plots [i](#)

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: Smoothened homolog/Soluble cytochrome b562 chimeric protein



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	72.22Å 158.93Å 60.02Å 90.00° 90.26° 90.00°	Depositor
Resolution (Å)	44.42 – 2.60 44.42 – 2.60	Depositor EDS
% Data completeness (in resolution range)	72.1 (44.42-2.60) 72.8 (44.42-2.60)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.99 (at 2.58Å)	Xtriage
Refinement program	BUSTER 2.10.0	Depositor
R, R_{free}	0.225 , 0.260 0.244 , 0.282	Depositor DCC
R_{free} test set	755 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å ²)	53.1	Xtriage
Anisotropy	0.049	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 52.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.55$, $\langle L^2 \rangle = 0.39$	Xtriage
Estimated twinning fraction	0.006 for -h,-k,l	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	3454	wwPDB-VP
Average B, all atoms (Å ²)	61.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.03% 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: SG8

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	0/3498	1.41	26/4772 (0.5%)

There are no bond length outliers.

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	428	SER	CA-C-N	6.62	128.97	120.70
1	A	428	SER	C-N-CA	6.62	128.97	120.70
1	A	311	THR	CA-C-N	6.59	131.73	120.72
1	A	311	THR	C-N-CA	6.59	131.73	120.72
1	A	255	ASP	CA-CB-CG	5.87	118.47	112.60
1	A	353	LEU	CA-C-N	5.85	128.93	120.38
1	A	353	LEU	C-N-CA	5.85	128.93	120.38
1	A	349	THR	CA-C-N	5.74	132.50	121.54
1	A	349	THR	C-N-CA	5.74	132.50	121.54
1	A	1021	ASP	CA-CB-CG	5.60	118.20	112.60
1	A	349	THR	N-CA-C	-5.58	106.45	113.20
1	A	1083	LYS	CA-C-N	5.55	127.76	120.60
1	A	1083	LYS	C-N-CA	5.55	127.76	120.60
1	A	409	GLY	CA-C-N	5.43	127.50	120.44
1	A	409	GLY	C-N-CA	5.43	127.50	120.44
1	A	443	SER	CA-C-N	5.36	129.78	121.26
1	A	443	SER	C-N-CA	5.36	129.78	121.26
1	A	285	PHE	CA-CB-CG	-5.11	108.69	113.80
1	A	258	ASN	CA-CB-CG	5.09	117.69	112.60
1	A	512	ARG	N-CA-CB	-5.06	105.78	111.10
1	A	441	ALA	CA-C-N	5.05	131.18	121.54
1	A	441	ALA	C-N-CA	5.05	131.18	121.54
1	A	272	ALA	CA-C-N	5.03	127.28	120.44
1	A	272	ALA	C-N-CA	5.03	127.28	120.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1003	LEU	CA-C-N	5.01	127.26	120.44
1	A	1003	LEU	C-N-CA	5.01	127.26	120.44

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	3411	0	3220	40	0
2	A	36	0	26	4	0
3	A	7	0	0	0	0
All	All	3454	0	3246	40	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 6.

All (40) 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:382:ASP:HB2	1:A:394:TYR:HB2	1.60	0.82
1:A:215:ILE:HD11	1:A:220:PRO:HG2	1.62	0.80
1:A:301:MET:HE3	2:A:1201:SG8:H8	1.66	0.78
1:A:312:LEU:H	1:A:312:LEU:HD13	1.55	0.72
1:A:329:VAL:HB	1:A:411:VAL:HG21	1.71	0.71
1:A:306:PRO:HD2	1:A:379:ALA:HA	1.75	0.69
1:A:215:ILE:HD11	1:A:220:PRO:CG	2.28	0.64
1:A:221:LEU:O	1:A:512:ARG:HD2	1.96	0.64
1:A:343:PHE:HB3	1:A:425:THR:HG21	1.85	0.58
1:A:215:ILE:CD1	1:A:220:PRO:HG2	2.33	0.57
1:A:215:ILE:HD13	1:A:484:PHE:HZ	1.71	0.56
1:A:1044:THR:HA	1:A:1058:MET:HE1	1.86	0.56
1:A:420:ILE:O	1:A:424:MET:HG3	2.08	0.54
1:A:330:VAL:HG21	1:A:364:THR:HA	1.91	0.53
1:A:281:TRP:CH2	1:A:522:LEU:HD21	2.44	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:312:LEU:O	1:A:316:ILE:HG12	2.09	0.52
1:A:366:SER:O	1:A:370:VAL:HG23	2.10	0.52
1:A:536:VAL:HB	1:A:541:THR:HG21	1.92	0.52
1:A:451:ARG:NH1	1:A:535:TRP:O	2.45	0.50
1:A:1023:ALA:HB2	1:A:1084:VAL:HG22	1.94	0.50
1:A:301:MET:CE	2:A:1201:SG8:H8	2.39	0.50
1:A:303:LEU:HD13	1:A:395:LYS:HD2	1.94	0.50
1:A:250:ALA:HA	1:A:253:VAL:HG12	1.95	0.48
1:A:330:VAL:CG2	1:A:364:THR:HA	2.42	0.48
1:A:1010:LEU:HD11	1:A:1068:LEU:HD21	1.95	0.48
1:A:458:LEU:HD23	1:A:531:ALA:HB1	1.94	0.48
1:A:481:GLU:HG2	2:A:1201:SG8:H25	1.94	0.48
1:A:1068:LEU:HD22	1:A:1102:ILE:HD11	1.96	0.47
1:A:339:TRP:HH2	1:A:423:VAL:HG13	1.79	0.47
1:A:1013:ASN:HD22	1:A:1033:MET:HG3	1.80	0.47
1:A:1091:ALA:O	1:A:1094:LEU:HB2	2.14	0.47
1:A:1083:LYS:HB3	1:A:1086:GLU:HB2	1.97	0.45
1:A:230:MET:HE1	1:A:519:LYS:HG3	1.97	0.45
1:A:466:THR:HG23	1:A:521:ASN:HD21	1.81	0.45
1:A:215:ILE:HD13	1:A:484:PHE:CZ	2.50	0.45
1:A:348:THR:C	1:A:350:TYR:H	2.25	0.45
1:A:1067:ILE:O	1:A:1071:GLN:HG2	2.18	0.43
1:A:361:HIS:O	1:A:365:TRP:HD1	2.01	0.43
1:A:301:MET:HE3	2:A:1201:SG8:C15	2.42	0.42
1:A:545:TRP:HA	1:A:548:THR:HG22	2.03	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	443/468 (95%)	420 (95%)	23 (5%)	0	100	100

There are no Ramachandran outliers to report.

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	338/390 (87%)	311 (92%)	27 (8%)	11	25

All (27) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	198	VAL
1	A	215	ILE
1	A	229	ASP
1	A	256	TRP
1	A	292	GLU
1	A	301	MET
1	A	302	ARG
1	A	312	LEU
1	A	317	ILE
1	A	349	THR
1	A	362	LEU
1	A	386	VAL
1	A	392	VAL
1	A	394	TYR
1	A	410	LEU
1	A	1007	TRP
1	A	1010	LEU
1	A	1032	LYS
1	A	1095	LYS
1	A	1106	LEU
1	A	450	LEU
1	A	475	PHE
1	A	483	SER
1	A	485	ARG
1	A	488	VAL
1	A	516	LEU
1	A	528	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	192	GLN
1	A	231	HIS
1	A	396	ASN
1	A	433	HIS
1	A	1013	ASN
1	A	1080	ASN
1	A	1093	GLN
1	A	491	GLN
1	A	521	ASN

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	$\# Z > 2$
2	SG8	A	1201	-	40,40,40	3.22	12 (30%)	51,57,57	1.76	15 (29%)

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	SG8	A	1201	-	-	4/22/32/32	0/5/5/5

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1201	SG8	C9-N1	10.40	1.49	1.34
2	A	1201	SG8	C17-C12	7.77	1.52	1.39
2	A	1201	SG8	C14-C13	7.40	1.51	1.38
2	A	1201	SG8	C15-C16	6.69	1.52	1.39
2	A	1201	SG8	C27-C26	5.97	1.50	1.38
2	A	1201	SG8	C25-N3	5.64	1.49	1.33
2	A	1201	SG8	C24-C28	4.77	1.48	1.39
2	A	1201	SG8	C10-C12	3.77	1.58	1.51
2	A	1201	SG8	C9-C7	2.85	1.53	1.49
2	A	1201	SG8	C18-C11	2.45	1.58	1.52
2	A	1201	SG8	C11-N1	2.27	1.52	1.47
2	A	1201	SG8	C8-C7	2.05	1.40	1.36

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1201	SG8	C3-C4-C5	-4.10	119.59	122.87
2	A	1201	SG8	C22-C11-N1	3.61	116.84	111.83
2	A	1201	SG8	O1-C9-C7	-3.48	114.58	119.66
2	A	1201	SG8	C10-N1-C11	-3.31	115.08	118.34
2	A	1201	SG8	C18-C19-C20	3.27	115.08	111.49
2	A	1201	SG8	C19-C18-C11	2.94	115.66	109.98
2	A	1201	SG8	C7-C9-N1	2.91	124.32	119.32
2	A	1201	SG8	C23-N2-C20	-2.84	111.09	114.33
2	A	1201	SG8	C22-C11-C18	2.80	117.51	111.17
2	A	1201	SG8	C10-N1-C9	2.72	124.53	116.97
2	A	1201	SG8	F1-C4-C5	2.69	119.96	118.03
2	A	1201	SG8	C24-C25-N3	-2.47	119.38	123.60
2	A	1201	SG8	C27-C26-N3	-2.41	119.49	123.60
2	A	1201	SG8	C21-C22-C11	2.24	114.30	109.98
2	A	1201	SG8	C21-C20-N2	2.01	120.34	110.53

There are no chirality outliers.

All (4) torsion outliers are listed below:

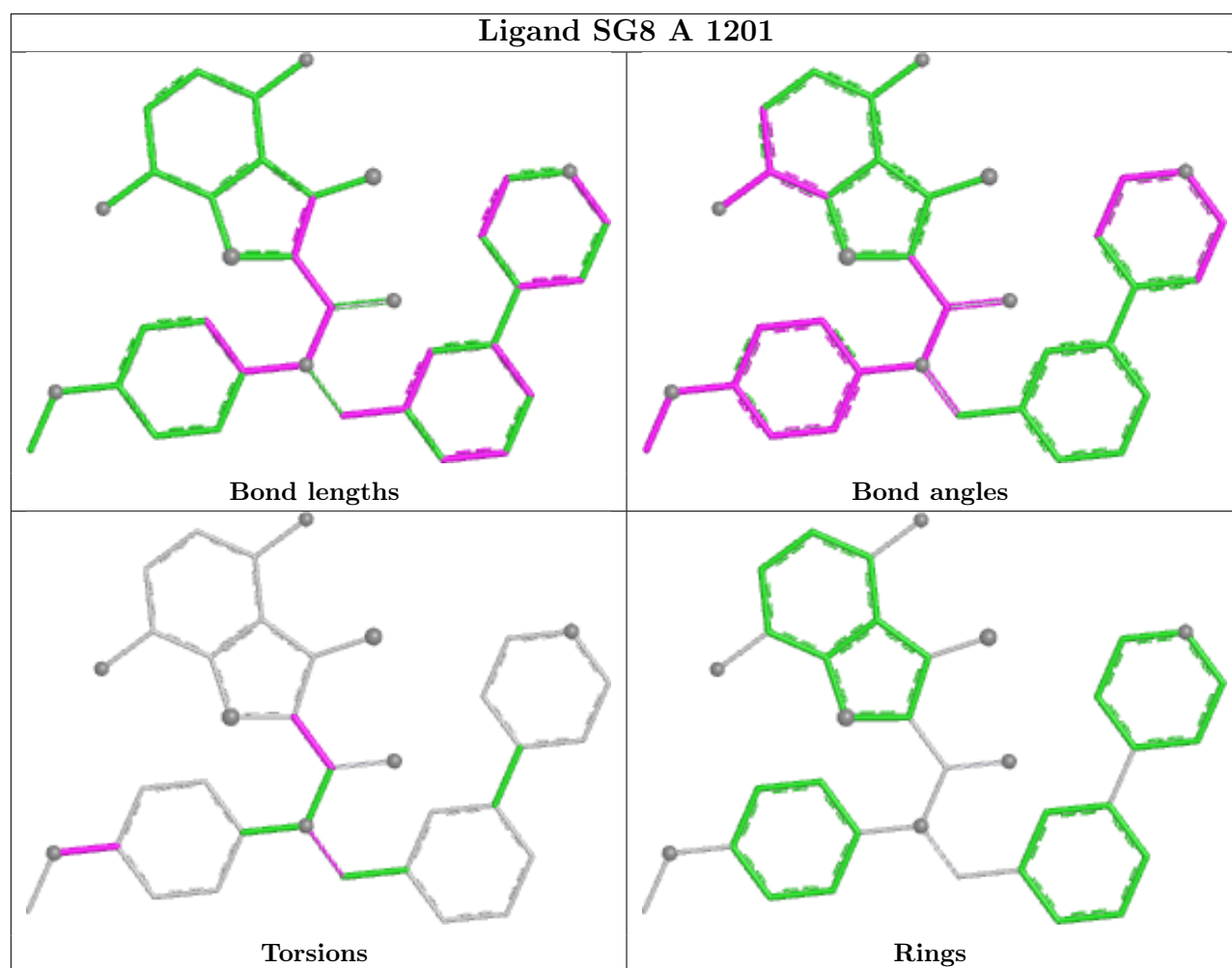
Mol	Chain	Res	Type	Atoms
2	A	1201	SG8	C19-C20-N2-C23
2	A	1201	SG8	C21-C20-N2-C23
2	A	1201	SG8	C12-C10-N1-C9
2	A	1201	SG8	S1-C7-C9-O1

There are no ring outliers.

1 monomer is involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1201	SG8	4	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	447/468 (95%)	1.63	144 (32%) 1 1	23, 56, 107, 120	0

All (144) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	262	TYR	5.1
1	A	353	LEU	4.6
1	A	343	PHE	4.2
1	A	446	ASN	4.2
1	A	1084	VAL	4.0
1	A	443	SER	4.0
1	A	359	TYR	4.0
1	A	452	LEU	3.9
1	A	1082	GLY	3.8
1	A	549	TRP	3.8
1	A	342	SER	3.8
1	A	1075	ALA	3.7
1	A	462	PHE	3.7
1	A	1056	PRO	3.7
1	A	1065	PHE	3.7
1	A	1049	GLU	3.7
1	A	312	LEU	3.6
1	A	256	TRP	3.3
1	A	442	ALA	3.3
1	A	1076	LEU	3.3
1	A	346	LEU	3.3
1	A	427	PHE	3.3
1	A	545	TRP	3.3
1	A	426	LEU	3.3
1	A	244	CYS	3.2
1	A	1054	ASP	3.2
1	A	339	TRP	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	1024	ALA	3.1
1	A	1087	ALA	3.1
1	A	551	ARG	3.1
1	A	349	THR	3.1
1	A	389	ILE	3.1
1	A	1081	GLU	3.1
1	A	516	LEU	3.0
1	A	1077	LYS	3.0
1	A	344	LYS	3.0
1	A	542	LEU	2.9
1	A	257	ARG	2.9
1	A	345	ALA	2.9
1	A	485	ARG	2.9
1	A	350	TYR	2.9
1	A	1027	LYS	2.9
1	A	1047	LYS	2.9
1	A	1033	MET	2.8
1	A	245	THR	2.8
1	A	1079	ALA	2.8
1	A	1090	ALA	2.8
1	A	523	PHE	2.8
1	A	259	SER	2.7
1	A	1064	GLY	2.7
1	A	285	PHE	2.7
1	A	1094	LEU	2.7
1	A	481	GLU	2.7
1	A	1053	PRO	2.7
1	A	1046	PRO	2.7
1	A	1085	LYS	2.7
1	A	1048	LEU	2.6
1	A	455	PHE	2.6
1	A	509	ILE	2.6
1	A	475	PHE	2.6
1	A	1050	ASP	2.6
1	A	1060	ASP	2.6
1	A	1038	LEU	2.5
1	A	463	VAL	2.5
1	A	363	LEU	2.5
1	A	207	TYR	2.5
1	A	1061	PHE	2.5
1	A	1083	LYS	2.5
1	A	215	ILE	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	544	ILE	2.5
1	A	1031	THR	2.4
1	A	278	SER	2.4
1	A	526	PHE	2.4
1	A	1067	ILE	2.4
1	A	347	GLY	2.4
1	A	1026	VAL	2.4
1	A	1101	TYR	2.4
1	A	376	LEU	2.4
1	A	1006	ASN	2.4
1	A	192	GLN	2.4
1	A	388	GLY	2.4
1	A	420	ILE	2.3
1	A	253	VAL	2.3
1	A	315	VAL	2.3
1	A	460	PHE	2.3
1	A	478	ALA	2.3
1	A	520	ILE	2.3
1	A	1095	LYS	2.3
1	A	210	VAL	2.3
1	A	488	VAL	2.3
1	A	268	PHE	2.3
1	A	1078	LEU	2.3
1	A	242	GLY	2.3
1	A	454	ILE	2.3
1	A	309	ASN	2.3
1	A	287	ASP	2.3
1	A	548	THR	2.2
1	A	202	ASN	2.2
1	A	258	ASN	2.2
1	A	271	ASN	2.2
1	A	1005	ASP	2.2
1	A	1028	ASP	2.2
1	A	456	GLY	2.2
1	A	267	LEU	2.2
1	A	1003	LEU	2.2
1	A	234	ILE	2.2
1	A	295	CYS	2.2
1	A	515	LEU	2.2
1	A	423	VAL	2.2
1	A	283	ALA	2.2
1	A	204	LYS	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	230	MET	2.2
1	A	240	VAL	2.2
1	A	517	VAL	2.2
1	A	331	TRP	2.2
1	A	365	TRP	2.2
1	A	433	HIS	2.2
1	A	337	TYR	2.2
1	A	1032	LYS	2.2
1	A	1030	LEU	2.2
1	A	1063	HIS	2.2
1	A	391	PHE	2.2
1	A	272	ALA	2.1
1	A	1007	TRP	2.1
1	A	1036	ALA	2.1
1	A	424	MET	2.1
1	A	465	ILE	2.1
1	A	1035	ALA	2.1
1	A	330	VAL	2.1
1	A	310	GLU	2.1
1	A	1044	THR	2.1
1	A	286	MET	2.1
1	A	293	ILE	2.1
1	A	264	ALA	2.0
1	A	367	LEU	2.0
1	A	491	GLN	2.0
1	A	279	ILE	2.0
1	A	213	CYS	2.0
1	A	233	TYR	2.0
1	A	1096	THR	2.0
1	A	541	THR	2.0
1	A	419	LEU	2.0
1	A	522	LEU	2.0
1	A	1022	ASN	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 ⓘ

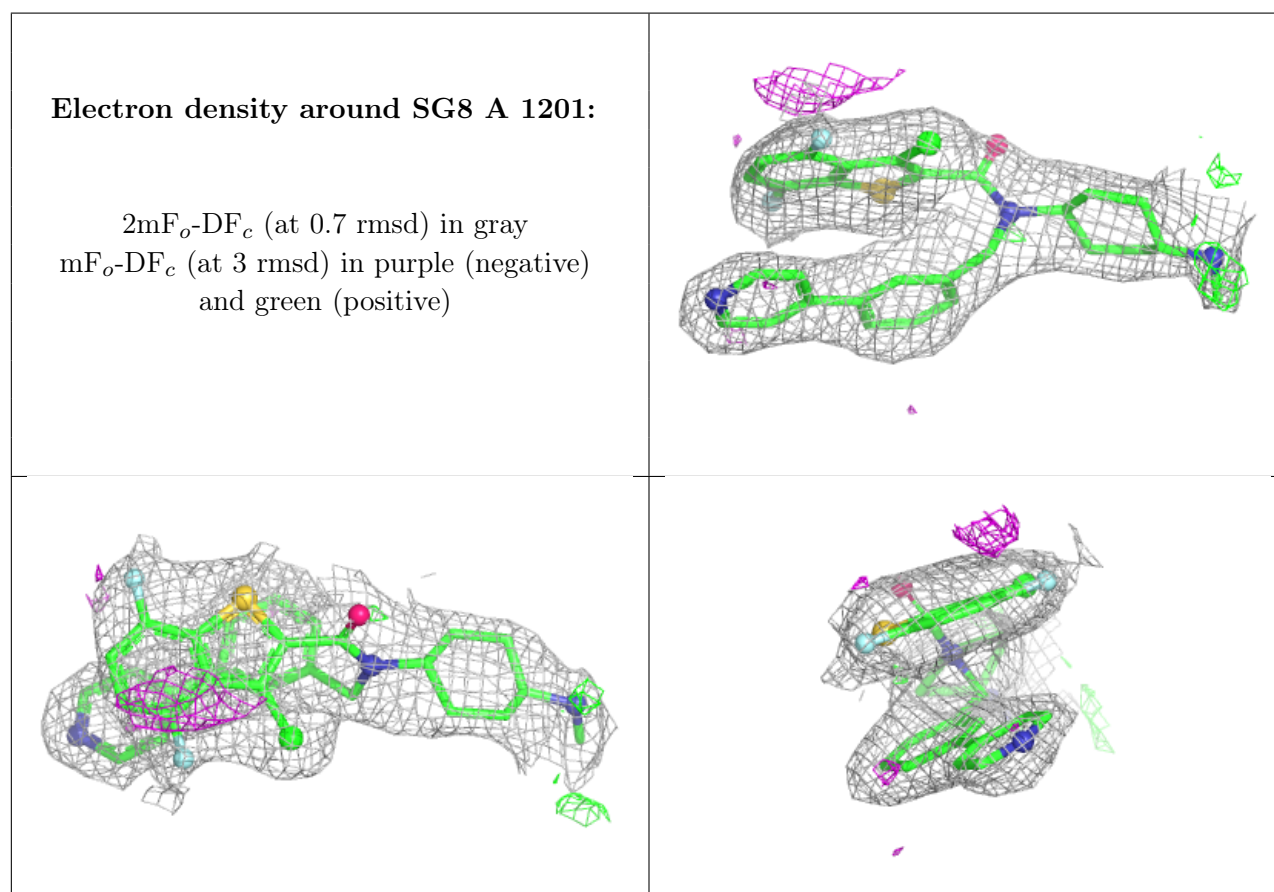
There are no oligosaccharides in this entry.

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	SG8	A	1201	36/36	0.89	0.13	20,46,52,54	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.