



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 02:05 PM UTC

PDB ID : 3WQH / pdb_00003wqh
Title : Crystal Structure of human DPP-IV in complex with Anagliptin
Authors : Watanabe, Y.S.; Okada, S.; Motoyama, T.; Takahashi, R.; Adachi, H.; Oka, M.
Deposited on : 2014-01-27
Resolution : 2.85 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

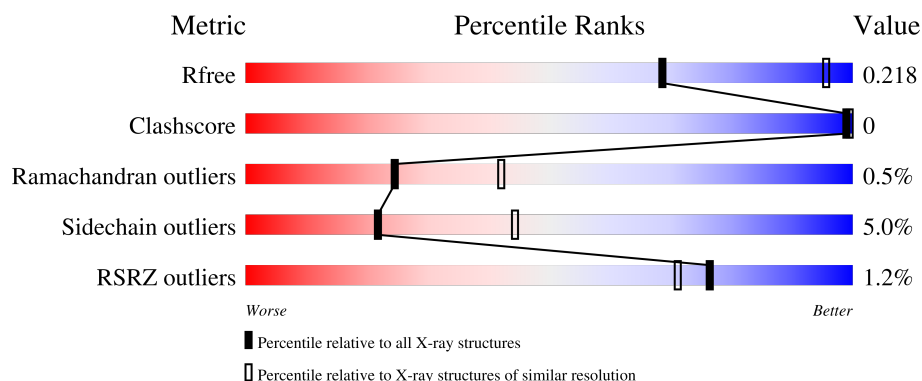
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.85 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	1407 (2.88-2.84)
Clashscore	190562	1446 (2.88-2.84)
Ramachandran outliers	187476	1406 (2.88-2.84)
Sidechain outliers	187428	1407 (2.88-2.84)
RSRZ outliers	180081	1408 (2.88-2.84)

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	730	% 91% 8%
1	B	730	2% 89% 10%

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 12269 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.

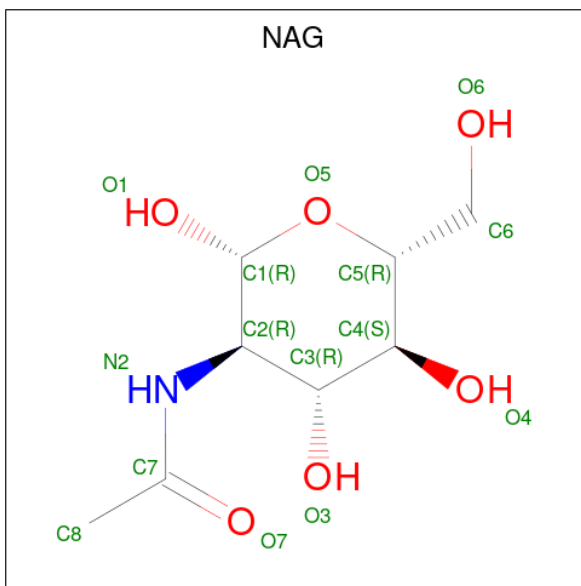
- Molecule 1 is a protein called Dipeptidyl peptidase 4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	728	Total	C	N	O	S	0	0	0
			5963	3827	982	1128	26			
1	B	728	Total	C	N	O	S	0	0	0
			5963	3827	982	1128	26			

There are 4 discrepancies between the modelled and reference sequences:

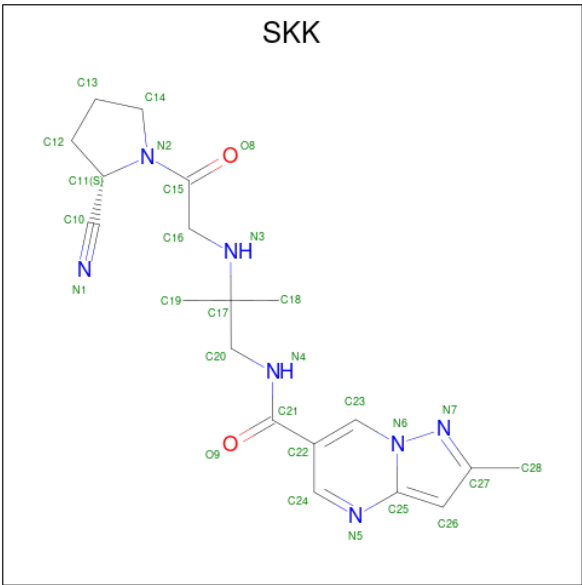
Chain	Residue	Modelled	Actual	Comment	Reference
A	37	GLY	-	expression tag	UNP P27487
A	38	PRO	-	expression tag	UNP P27487
B	37	GLY	-	expression tag	UNP P27487
B	38	PRO	-	expression tag	UNP P27487

- Molecule 2 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	A	1	Total	C	N	O	0	0
			15	8	1	6		
2	B	1	Total	C	N	O	0	0
			14	8	1	5		
2	B	1	Total	C	N	O	0	0
			14	8	1	5		
2	B	1	Total	C	N	O	0	0
			14	8	1	5		
2	B	1	Total	C	N	O	0	0
			14	8	1	5		
2	B	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 3 is N-[2-({2-[(2S)-2-cyanopyrrolidin-1-yl]-2-oxoethyl}amino)-2-methylpropyl]-2-methylpyrazolo[1,5-a]pyrimidine-6-carboxamide (CCD ID: SKK) (formula: C₁₉H₂₅N₇O₂).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			28	19	7	2		
3	B	1	Total	C	N	O	0	0
			28	19	7	2		

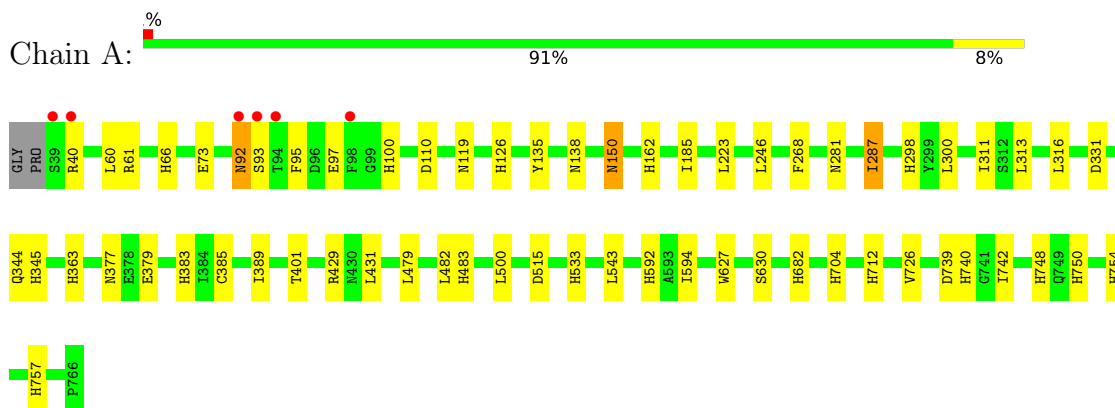
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	54	Total	O	0	0
			54	54		
4	B	50	Total	O	0	0
			50	50		

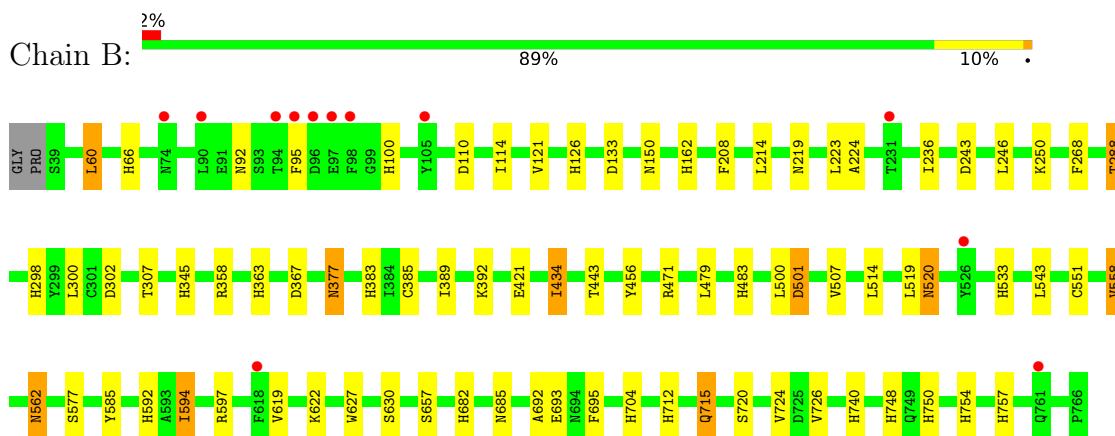
3 Residue-property plots

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: Dipeptidyl peptidase 4



• Molecule 1: Dipeptidyl peptidase 4



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	65.16Å 68.99Å 419.60Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.67 – 2.85 47.67 – 2.85	Depositor EDS
% Data completeness (in resolution range)	100.0 (47.67-2.85) 99.9 (47.67-2.85)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.71 (at 2.86Å)	Xtriage
Refinement program	PRIME-X 2.2	Depositor
R, R_{free}	0.227 , 0.288 0.220 , 0.218	Depositor DCC
R_{free} test set	2276 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	49.1	Xtriage
Anisotropy	1.165	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 45.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	12269	wwPDB-VP
Average B, all atoms (Å ²)	53.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.73% 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: SKK, NAG

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	0.67	0/6135	1.21	28/8344 (0.3%)
1	B	0.68	0/6135	1.22	39/8344 (0.5%)
All	All	0.68	0/12270	1.22	67/16688 (0.4%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	3

There are no bond length outliers.

All (67) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	150	ASN	CA-CB-CG	10.91	123.51	112.60
1	B	377	ASN	CA-CB-CG	8.18	120.78	112.60
1	B	501	ASP	CA-CB-CG	7.46	120.06	112.60
1	A	389	ILE	N-CA-C	7.06	118.67	110.62
1	B	389	ILE	N-CA-C	6.80	117.30	110.23
1	B	692	ALA	N-CA-C	6.78	119.54	111.33
1	B	562	ASN	CA-CB-CG	6.58	119.18	112.60
1	A	110	ASP	CA-CB-CG	6.52	119.12	112.60
1	A	739	ASP	CA-CB-CG	6.48	119.08	112.60
1	B	520	ASN	CA-CB-CG	6.38	118.97	112.60
1	A	363	HIS	ND1-CE1-NE2	6.08	114.48	108.40
1	A	331	ASP	CB-CA-C	6.08	119.49	110.62
1	A	748	HIS	ND1-CE1-NE2	6.01	114.41	108.40
1	A	750	HIS	ND1-CE1-NE2	6.01	114.41	108.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	748	HIS	ND1-CE1-NE2	5.99	114.39	108.40
1	B	383	HIS	ND1-CE1-NE2	5.98	114.38	108.40
1	B	483	HIS	ND1-CE1-NE2	5.98	114.38	108.40
1	B	434	ILE	CB-CA-C	5.97	117.84	110.73
1	B	592	HIS	ND1-CE1-NE2	5.97	114.37	108.40
1	A	126	HIS	ND1-CE1-NE2	5.96	114.36	108.40
1	A	483	HIS	ND1-CE1-NE2	5.96	114.36	108.40
1	A	754	HIS	ND1-CE1-NE2	5.96	114.36	108.40
1	B	363	HIS	ND1-CE1-NE2	5.95	114.35	108.40
1	B	757	HIS	ND1-CE1-NE2	5.93	114.33	108.40
1	B	712	HIS	ND1-CE1-NE2	5.93	114.33	108.40
1	B	754	HIS	ND1-CE1-NE2	5.90	114.30	108.40
1	A	757	HIS	ND1-CE1-NE2	5.90	114.30	108.40
1	A	383	HIS	ND1-CE1-NE2	5.89	114.30	108.40
1	B	682	HIS	ND1-CE1-NE2	5.89	114.29	108.40
1	A	66	HIS	ND1-CE1-NE2	5.88	114.28	108.40
1	B	533	HIS	ND1-CE1-NE2	5.88	114.28	108.40
1	A	345	HIS	ND1-CE1-NE2	5.86	114.26	108.40
1	B	298	HIS	ND1-CE1-NE2	5.86	114.26	108.40
1	B	345	HIS	ND1-CE1-NE2	5.85	114.25	108.40
1	B	126	HIS	ND1-CE1-NE2	5.85	114.25	108.40
1	B	367	ASP	CA-CB-CG	5.85	118.45	112.60
1	A	377	ASN	CA-CB-CG	5.85	118.45	112.60
1	A	533	HIS	ND1-CE1-NE2	5.84	114.24	108.40
1	A	100	HIS	ND1-CE1-NE2	5.84	114.24	108.40
1	B	100	HIS	ND1-CE1-NE2	5.84	114.24	108.40
1	B	740	HIS	ND1-CE1-NE2	5.83	114.23	108.40
1	A	162	HIS	ND1-CE1-NE2	5.83	114.23	108.40
1	A	740	HIS	ND1-CE1-NE2	5.83	114.23	108.40
1	A	682	HIS	ND1-CE1-NE2	5.80	114.20	108.40
1	B	162	HIS	ND1-CE1-NE2	5.80	114.20	108.40
1	B	750	HIS	ND1-CE1-NE2	5.80	114.20	108.40
1	B	66	HIS	ND1-CE1-NE2	5.79	114.19	108.40
1	B	219	ASN	CA-CB-CG	5.79	118.39	112.60
1	A	712	HIS	ND1-CE1-NE2	5.78	114.18	108.40
1	B	471	ARG	CB-CA-C	5.78	120.33	111.95
1	A	592	HIS	ND1-CE1-NE2	5.76	114.16	108.40
1	A	298	HIS	ND1-CE1-NE2	5.75	114.15	108.40
1	B	704	HIS	ND1-CE1-NE2	5.73	114.13	108.40
1	B	208	PHE	CA-CB-CG	5.67	119.47	113.80
1	B	685	ASN	CA-CB-CG	5.66	118.26	112.60
1	B	92	ASN	CA-CB-CG	5.63	118.23	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	704	HIS	ND1-CE1-NE2	5.62	114.02	108.40
1	B	288	THR	CA-CB-CG2	5.62	120.05	110.50
1	B	695	PHE	CA-CB-CG	5.50	119.30	113.80
1	A	150	ASN	N-CA-CB	5.46	118.04	110.17
1	B	121	VAL	CB-CA-C	5.30	116.45	110.41
1	B	110	ASP	CA-CB-CG	5.29	117.89	112.60
1	B	421	GLU	N-CA-C	5.20	117.34	111.11
1	A	138	ASN	CA-CB-CG	5.14	117.74	112.60
1	B	585	TYR	CB-CA-C	5.07	117.36	110.06
1	B	594	ILE	CA-CB-CG2	5.05	119.08	110.50
1	A	119	ASN	CA-CB-CG	5.01	117.61	112.60

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	742	ILE	Peptide
1	A	92	ASN	Peptide
1	A	95	PHE	Peptide

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	5963	0	5679	2	0
1	B	5963	0	5679	7	0
2	A	99	0	93	0	0
2	B	84	0	78	1	0
3	A	28	0	25	0	0
3	B	28	0	25	0	0
4	A	54	0	0	0	0
4	B	50	0	0	0	0
All	All	12269	0	11579	9	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 0.

All (9) 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:657:SER:H	1:B:715:GLN:NE2	2.03	0.56
1:A:268:PHE:CE2	1:A:313:LEU:HD21	2.48	0.48
1:B:224:ALA:HB1	1:B:268:PHE:CZ	2.48	0.47
1:B:60:LEU:HD23	1:B:60:LEU:C	2.42	0.44
1:B:456:TYR:CD2	1:B:558:VAL:HG12	2.53	0.42
1:B:720:SER:O	1:B:724:VAL:HG23	2.19	0.42
1:A:287:ILE:HD13	1:A:287:ILE:C	2.45	0.41
1:B:392:LYS:HD2	1:B:392:LYS:H	1.85	0.41
1:B:133:ASP:OD1	2:B:802:NAG:H83	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	726/730 (100%)	663 (91%)	59 (8%)	4 (1%)	21	38
1	B	726/730 (100%)	674 (93%)	49 (7%)	3 (0%)	30	48
All	All	1452/1460 (100%)	1337 (92%)	108 (7%)	7 (0%)	24	42

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	93	SER
1	A	630	SER
1	B	630	SER
1	A	73	GLU
1	A	92	ASN
1	B	95	PHE
1	B	551	CYS

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	653/654 (100%)	625 (96%)	28 (4%)	26	50
1	B	653/654 (100%)	616 (94%)	37 (6%)	18	39
All	All	1306/1308 (100%)	1241 (95%)	65 (5%)	22	44

All (65) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	40	ARG
1	A	60	LEU
1	A	61	ARG
1	A	97	GLU
1	A	135	TYR
1	A	150	ASN
1	A	185	ILE
1	A	223	LEU
1	A	246	LEU
1	A	281	ASN
1	A	287	ILE
1	A	300	LEU
1	A	311	ILE
1	A	316	LEU
1	A	344	GLN
1	A	379	GLU
1	A	385	CYS
1	A	401	THR
1	A	429	ARG
1	A	431	LEU
1	A	479	LEU
1	A	482	LEU
1	A	500	LEU
1	A	515	ASP
1	A	543	LEU
1	A	594	ILE
1	A	627	TRP

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Mol	Chain	Res	Type
1	A	726	VAL
1	B	60	LEU
1	B	114	ILE
1	B	150	ASN
1	B	214	LEU
1	B	223	LEU
1	B	236	ILE
1	B	243	ASP
1	B	246	LEU
1	B	250	LYS
1	B	288	THR
1	B	300	LEU
1	B	302	ASP
1	B	307	THR
1	B	358	ARG
1	B	377	ASN
1	B	385	CYS
1	B	434	ILE
1	B	443	THR
1	B	479	LEU
1	B	500	LEU
1	B	501	ASP
1	B	507	VAL
1	B	514	LEU
1	B	519	LEU
1	B	520	ASN
1	B	543	LEU
1	B	558	VAL
1	B	562	ASN
1	B	577	SER
1	B	594	ILE
1	B	597	ARG
1	B	619	VAL
1	B	622	LYS
1	B	627	TRP
1	B	693	GLU
1	B	715	GLN
1	B	726	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (40) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	80	ASN
1	A	119	ASN
1	A	123	GLN
1	A	138	ASN
1	A	169	ASN
1	A	227	GLN
1	A	247	GLN
1	A	263	ASN
1	A	363	HIS
1	A	369	ASN
1	A	420	ASN
1	A	435	GLN
1	A	508	GLN
1	A	533	HIS
1	A	572	ASN
1	A	679	ASN
1	A	731	GLN
1	A	748	HIS
1	B	80	ASN
1	B	103	ASN
1	B	138	ASN
1	B	141	GLN
1	B	179	ASN
1	B	227	GLN
1	B	263	ASN
1	B	338	ASN
1	B	345	HIS
1	B	363	HIS
1	B	369	ASN
1	B	430	ASN
1	B	435	GLN
1	B	450	ASN
1	B	483	HIS
1	B	505	GLN
1	B	520	ASN
1	B	572	ASN
1	B	586	GLN
1	B	697	GLN
1	B	715	GLN
1	B	731	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

15 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	NAG	A	803	1	14,14,15	1.22	2 (14%)	17,19,21	1.05	1 (5%)
2	NAG	B	803	1	14,14,15	1.27	2 (14%)	17,19,21	1.00	1 (5%)
2	NAG	A	801	1	14,14,15	1.11	2 (14%)	17,19,21	1.23	1 (5%)
2	NAG	B	804	1	14,14,15	1.00	1 (7%)	17,19,21	1.00	1 (5%)
3	SKK	B	807	-	30,30,30	0.92	1 (3%)	32,43,43	0.95	1 (3%)
2	NAG	A	802	1	14,14,15	1.45	2 (14%)	17,19,21	0.89	0
2	NAG	A	807	-	15,15,15	1.14	1 (6%)	21,21,21	1.37	3 (14%)
2	NAG	B	801	1	14,14,15	0.97	1 (7%)	17,19,21	1.32	1 (5%)
2	NAG	B	805	1	14,14,15	1.40	3 (21%)	17,19,21	1.73	5 (29%)
2	NAG	B	806	1	14,14,15	1.21	2 (14%)	17,19,21	1.68	3 (17%)
3	SKK	A	808	-	30,30,30	0.89	1 (3%)	32,43,43	0.80	0
2	NAG	A	805	1	14,14,15	1.03	2 (14%)	17,19,21	0.97	1 (5%)
2	NAG	A	806	1	14,14,15	1.23	1 (7%)	17,19,21	1.03	1 (5%)
2	NAG	B	802	1	14,14,15	1.03	2 (14%)	17,19,21	0.87	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	NAG	A	804	1	14,14,15	1.07	2 (14%)	17,19,21	0.95	1 (5%)

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	NAG	A	803	1	-	1/6/23/26	0/1/1/1
2	NAG	B	803	1	-	0/6/23/26	0/1/1/1
2	NAG	A	801	1	-	2/6/23/26	0/1/1/1
2	NAG	B	804	1	-	0/6/23/26	0/1/1/1
3	SKK	B	807	-	-	3/20/32/32	0/3/3/3
2	NAG	A	802	1	-	4/6/23/26	0/1/1/1
2	NAG	A	807	-	-	0/6/26/26	0/1/1/1
2	NAG	B	801	1	-	0/6/23/26	0/1/1/1
2	NAG	B	805	1	-	2/6/23/26	0/1/1/1
2	NAG	B	806	1	-	0/6/23/26	0/1/1/1
3	SKK	A	808	-	-	4/20/32/32	0/3/3/3
2	NAG	A	805	1	-	0/6/23/26	0/1/1/1
2	NAG	A	806	1	-	2/6/23/26	0/1/1/1
2	NAG	B	802	1	-	0/6/23/26	0/1/1/1
2	NAG	A	804	1	-	0/6/23/26	0/1/1/1

All (25) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	802	NAG	C1-C2	3.74	1.57	1.52
2	B	805	NAG	C1-C2	3.27	1.56	1.52
2	A	807	NAG	C1-C2	3.12	1.56	1.52
2	A	806	NAG	O5-C1	-2.96	1.38	1.43
2	B	803	NAG	C1-C2	2.93	1.56	1.52
2	A	803	NAG	C1-C2	2.82	1.56	1.52
2	B	806	NAG	C1-C2	2.71	1.56	1.52
2	B	805	NAG	O5-C1	-2.65	1.39	1.43
2	A	802	NAG	O5-C1	-2.51	1.39	1.43
2	B	803	NAG	O5-C1	-2.44	1.39	1.43
2	A	801	NAG	O5-C1	-2.42	1.39	1.43
2	A	804	NAG	O5-C1	-2.37	1.39	1.43
2	B	806	NAG	O5-C1	-2.32	1.39	1.43
2	B	804	NAG	O5-C1	-2.30	1.39	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	801	NAG	C1-C2	2.27	1.55	1.52
2	A	805	NAG	O5-C1	-2.23	1.40	1.43
2	B	805	NAG	C3-C2	2.20	1.57	1.52
3	A	808	SKK	C25-N6	2.19	1.42	1.38
2	B	802	NAG	C1-C2	2.10	1.55	1.52
3	B	807	SKK	C25-N6	2.07	1.42	1.38
2	B	801	NAG	C1-C2	2.07	1.55	1.52
2	A	804	NAG	C1-C2	2.07	1.55	1.52
2	B	802	NAG	O5-C1	-2.06	1.40	1.43
2	A	805	NAG	C1-C2	2.02	1.55	1.52
2	A	803	NAG	O5-C1	-2.01	1.40	1.43

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	801	NAG	C1-O5-C5	4.38	118.05	112.19
2	B	805	NAG	C1-C2-N2	-4.17	103.86	110.43
2	B	806	NAG	C1-O5-C5	3.68	117.11	112.19
2	B	806	NAG	C1-C2-N2	-3.62	104.72	110.43
2	A	801	NAG	C1-O5-C5	3.60	117.01	112.19
2	B	805	NAG	O3-C3-C4	-2.90	103.53	110.38
2	A	807	NAG	C1-C2-N2	-2.72	107.58	110.73
2	B	806	NAG	C4-C3-C2	2.65	114.90	111.02
2	B	804	NAG	C1-O5-C5	2.63	115.70	112.19
2	A	804	NAG	C1-O5-C5	2.47	115.50	112.19
2	B	805	NAG	C4-C3-C2	2.44	114.60	111.02
2	A	806	NAG	C1-O5-C5	2.43	115.44	112.19
2	B	805	NAG	C1-O5-C5	2.38	115.38	112.19
2	A	807	NAG	C3-C4-C5	-2.37	105.94	110.23
2	A	807	NAG	C6-C5-C4	2.33	118.75	113.02
2	B	805	NAG	O5-C5-C6	-2.17	103.44	107.66
2	A	805	NAG	C1-O5-C5	2.17	115.09	112.19
3	B	807	SKK	C22-C21-N4	-2.11	114.58	116.75
2	B	803	NAG	O3-C3-C4	-2.03	105.60	110.38
2	A	803	NAG	C1-C2-N2	-2.01	107.26	110.43

There are no chirality outliers.

All (18) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	808	SKK	C15-C16-N3-C17
3	A	808	SKK	N4-C21-C22-C23

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Mol	Chain	Res	Type	Atoms
3	A	808	SKK	O9-C21-C22-C23
3	B	807	SKK	N4-C21-C22-C23
3	B	807	SKK	O9-C21-C22-C23
2	B	805	NAG	C1-C2-N2-C7
2	A	802	NAG	C4-C5-C6-O6
2	A	802	NAG	O5-C5-C6-O6
3	B	807	SKK	C15-C16-N3-C17
2	A	806	NAG	C3-C2-N2-C7
3	A	808	SKK	C18-C17-N3-C16
2	A	801	NAG	C1-C2-N2-C7
2	A	802	NAG	C1-C2-N2-C7
2	A	803	NAG	C1-C2-N2-C7
2	A	806	NAG	C1-C2-N2-C7
2	A	801	NAG	C4-C5-C6-O6
2	A	802	NAG	C3-C2-N2-C7
2	B	805	NAG	C3-C2-N2-C7

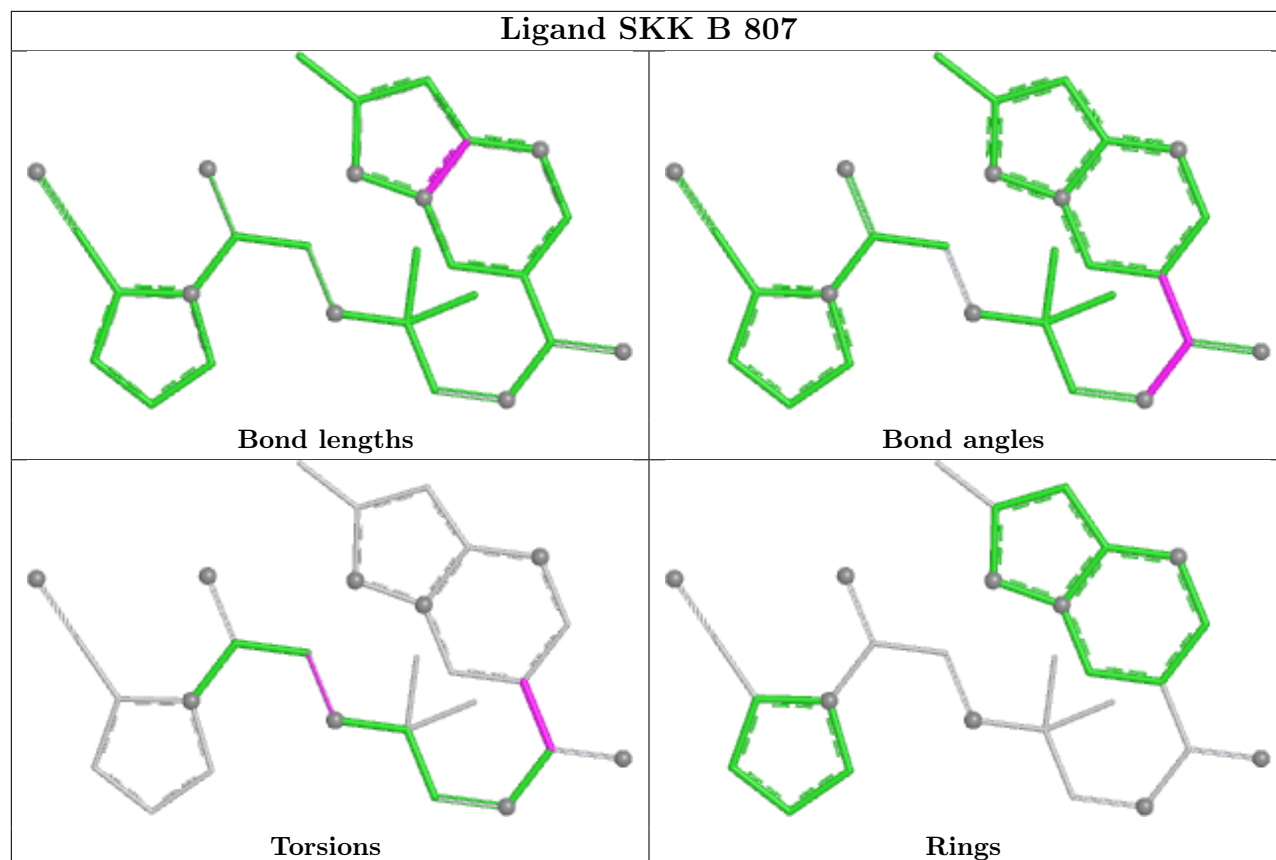
There are no ring outliers.

1 monomer is involved in 1 short contact:

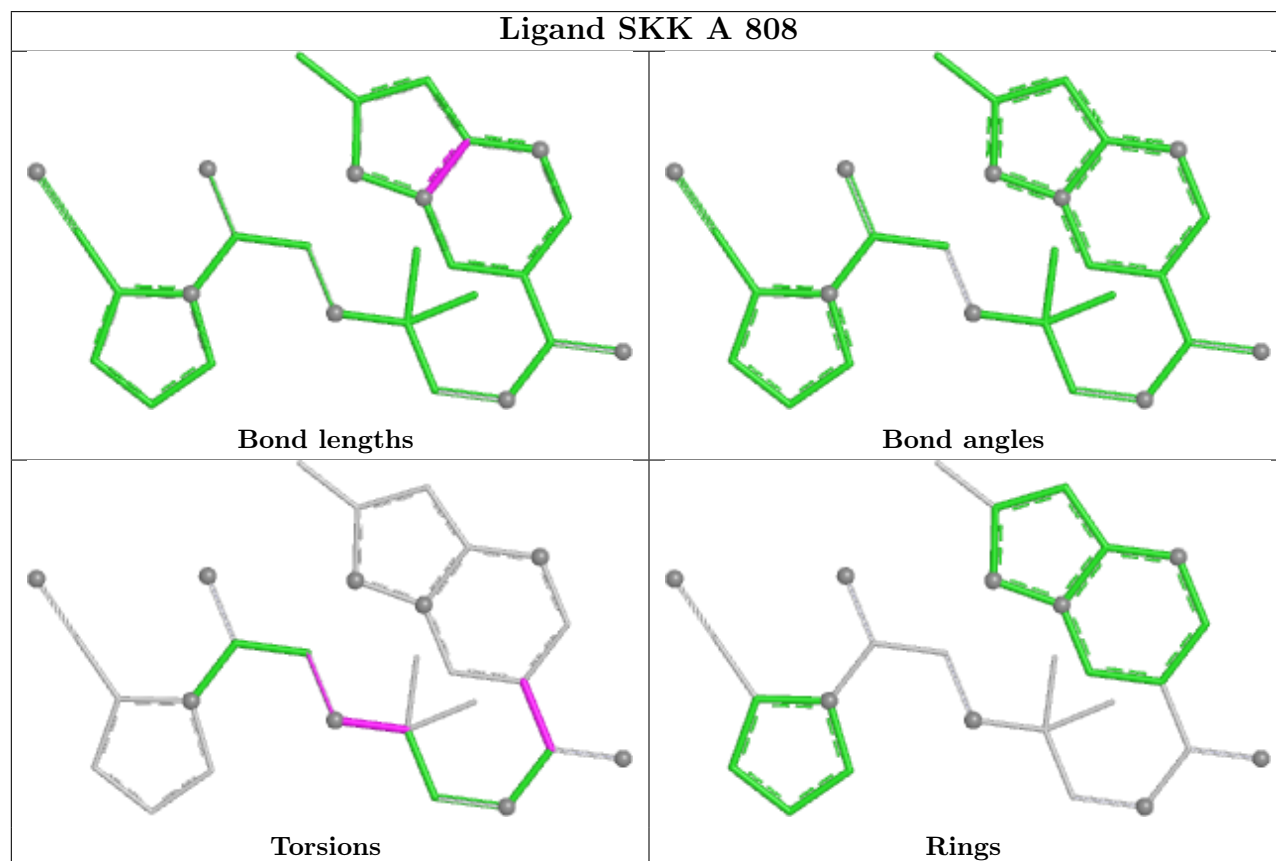
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	802	NAG	1	0

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.

Ligand SKK B 807



Ligand SKK A 808



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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	728/730 (99%)	0.05	6 (0%) 82 78	30, 53, 81, 99	0
1	B	728/730 (99%)	-0.06	12 (1%) 70 64	29, 47, 77, 100	0
All	All	1456/1460 (99%)	-0.00	18 (1%) 76 71	29, 51, 79, 100	0

All (18) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	94	THR	4.4
1	B	90	LEU	3.9
1	B	105	TYR	3.4
1	B	95	PHE	3.0
1	A	92	ASN	2.8
1	B	526	TYR	2.7
1	B	74	ASN	2.6
1	A	39	SER	2.5
1	B	231	THR	2.4
1	A	93	SER	2.4
1	A	98	PHE	2.4
1	B	761	GLN	2.4
1	B	96	ASP	2.2
1	A	94	THR	2.2
1	B	618	PHE	2.1
1	B	98	PHE	2.1
1	A	40	ARG	2.1
1	B	97	GLU	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](#)

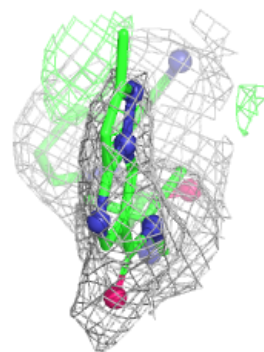
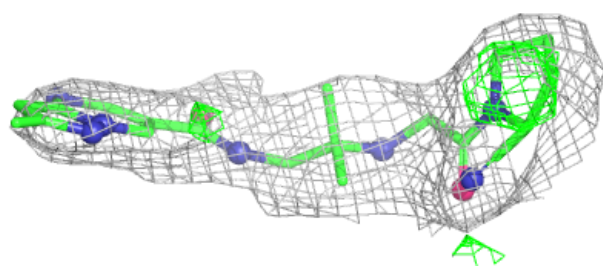
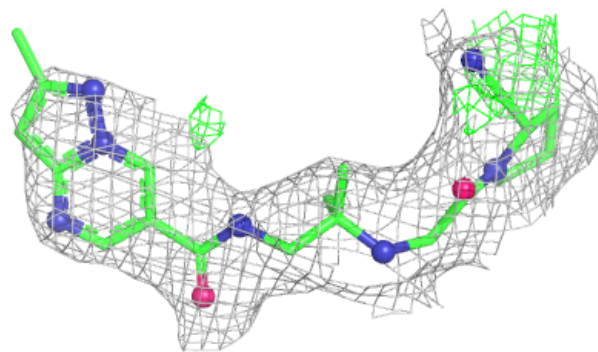
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

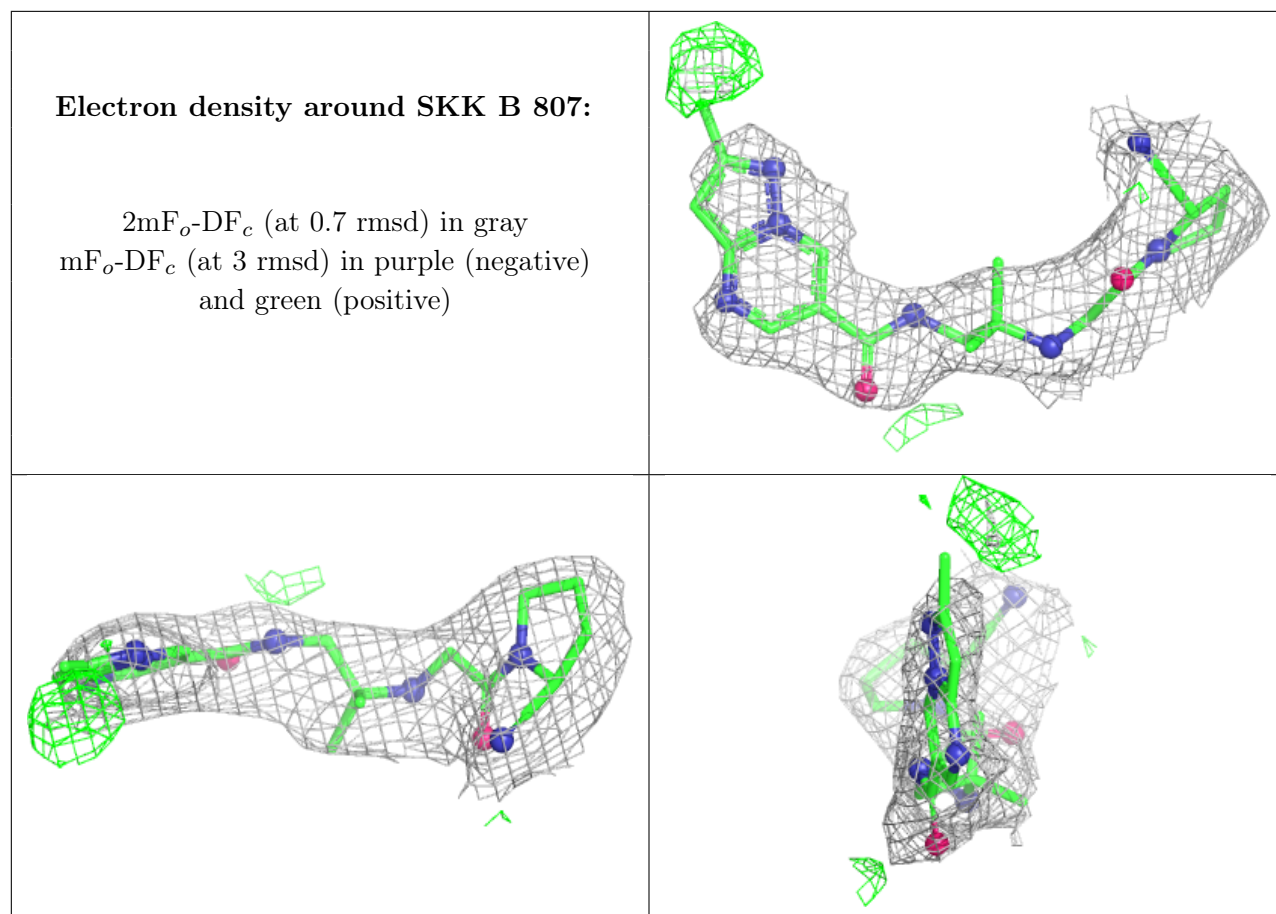
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	NAG	A	807	15/15	0.39	0.21	71,78,82,84	0
2	NAG	A	802	14/15	0.51	0.17	88,92,94,94	0
2	NAG	B	802	14/15	0.55	0.14	94,98,99,99	0
2	NAG	A	805	14/15	0.75	0.13	81,83,84,84	0
2	NAG	A	803	14/15	0.80	0.12	62,65,71,71	0
2	NAG	B	804	14/15	0.81	0.12	55,57,58,60	0
2	NAG	B	806	14/15	0.81	0.12	63,66,74,77	0
2	NAG	B	805	14/15	0.83	0.12	82,84,86,86	0
2	NAG	A	806	14/15	0.83	0.12	63,66,67,70	0
2	NAG	B	803	14/15	0.84	0.10	54,58,64,64	0
2	NAG	A	801	14/15	0.85	0.09	54,58,62,65	0
2	NAG	B	801	14/15	0.86	0.10	43,46,50,50	0
3	SKK	A	808	28/28	0.87	0.15	52,60,80,80	0
2	NAG	A	804	14/15	0.89	0.09	34,49,55,59	0
3	SKK	B	807	28/28	0.89	0.16	59,71,86,87	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 SKK A 808:

$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)





6.5 Other polymers [i](#)

There are no such residues in this entry.