Full wwPDB X-ray Structure Validation Report ⓘ

Aug 17, 2022 – 01:49 PM EDT

PDB ID	:	3WQH
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)

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	:	2.29
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)	:	2.29

1 Overall quality at a glance ⓘ

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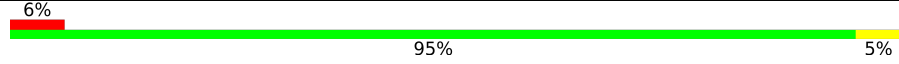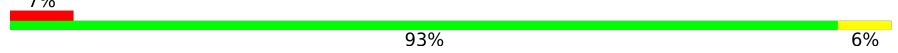*X-RAY DIFFRACTION*

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.
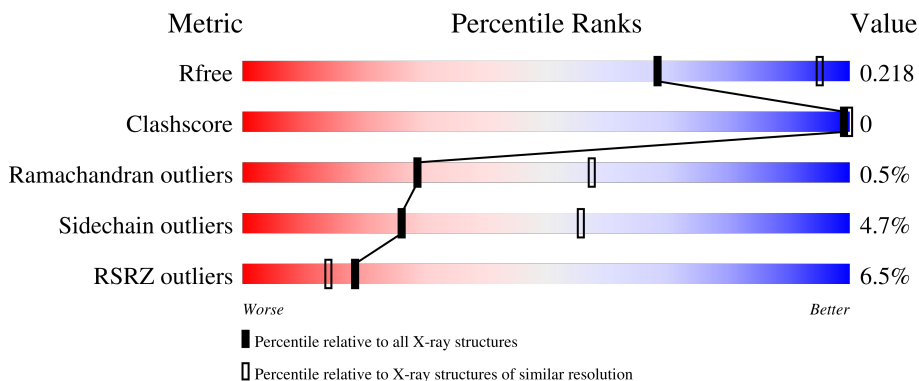
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	3168 (2.90-2.82)
Clashscore	141614	3438 (2.90-2.82)
Ramachandran outliers	138981	3348 (2.90-2.82)
Sidechain outliers	138945	3351 (2.90-2.82)
RSRZ outliers	127900	3103 (2.90-2.82)

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 <=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	6% — 95% — 5%
1	B	730	7% — 93% — 6%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	NAG	B	802	-	-	-	X

2 Entry composition ⓘ

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 (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).
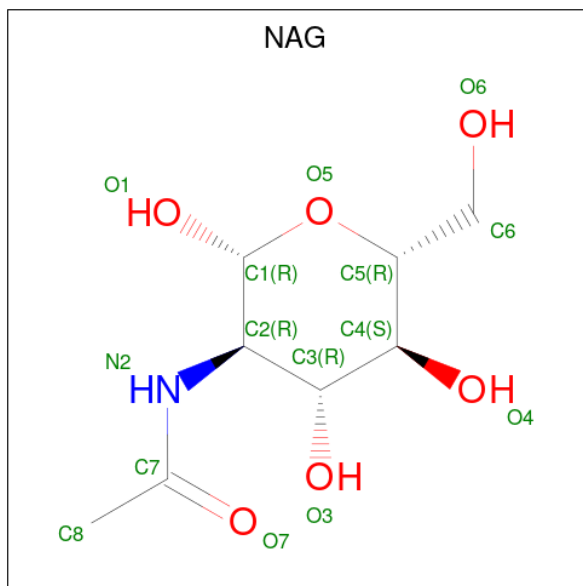
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total 14	C 8	N 1	O 5	0	0
2	A	1	Total 14	C 8	N 1	O 5	0	0
2	A	1	Total 14	C 8	N 1	O 5	0	0
2	A	1	Total 14	C 8	N 1	O 5	0	0
2	A	1	Total 14	C 8	N 1	O 5	0	0
2	A	1	Total 14	C 8	N 1	O 5	0	0
2	A	1	Total 15	C 8	N 1	O 6	0	0
2	B	1	Total 14	C 8	N 1	O 5	0	0
2	B	1	Total 14	C 8	N 1	O 5	0	0
2	B	1	Total 14	C 8	N 1	O 5	0	0
2	B	1	Total 14	C 8	N 1	O 5	0	0
2	B	1	Total 14	C 8	N 1	O 5	0	0
2	B	1	Total 14	C 8	N 1	O 5	0	0

- Molecule 3 is N-[2-({2-[(2S)-2-cyanopyrrolidin-1-yl]-2-oxoethyl}amino)-2-methylpropyl]-2-methylpyrazolo[1,5-a]pyrimidine-6-carboxamide (three-letter code: SKK) (formula: $C_{19}H_{25}N_7O_2$).
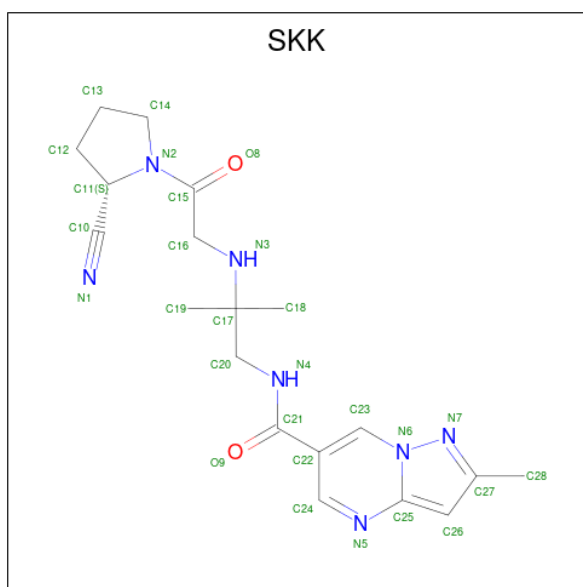
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			28	19	7	2		
3	B	1	Total	C	N	O	0	0
			28	19	7	2		

• 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
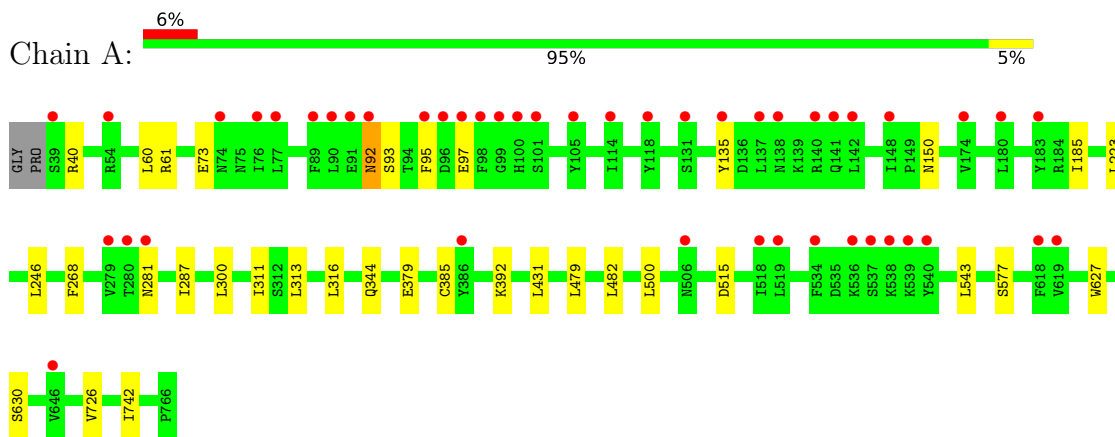
- Molecule 1: Dipeptidyl peptidase 4
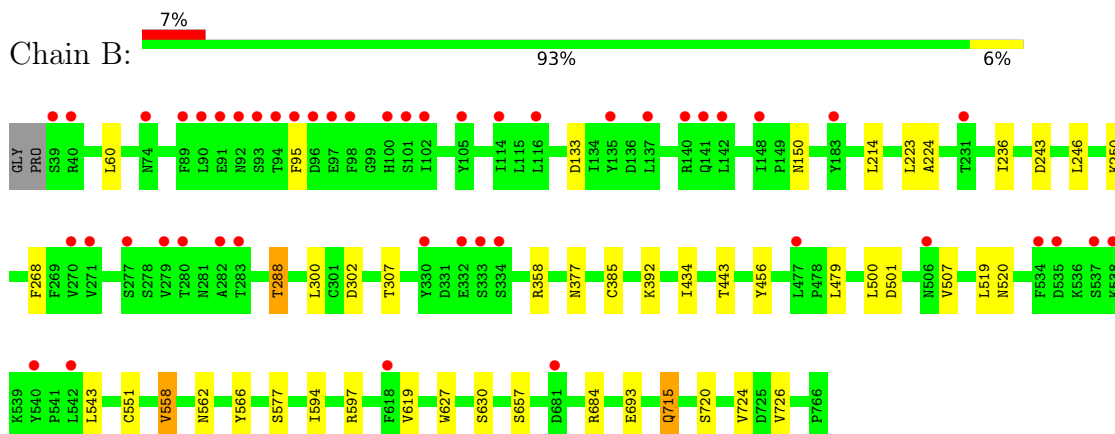
4 Data and refinement statistics ⓘ

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 49.11 – 2.85	Depositor EDS
% Data completeness (in resolution range)	100.0 (47.67-2.85) 100.0 (49.11-2.85)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [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)	0.35 , 53.7	EDS
L-test for twinning[2]	$< |L| > = 0.46, < L^2 > = 0.29$	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.*

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[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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: NAG, SKK

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	0.69	0/6135	1.00	0/8344
1	B	0.69	0/6135	1.00	2/8344 (0.0%)
All	All	0.69	0/12270	1.00	2/16688 (0.0%)

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 (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	288	THR	CA-CB-CG2	5.47	120.05	112.40
1	B	558	VAL	CA-CB-CG2	5.14	118.61	110.90

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 (i)

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	1	0
1	B	5963	0	5679	6	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	7	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 (7) 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: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: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 (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	726/730 (100%)	663 (91%)	59 (8%)	4 (1%)	25	53
1	B	726/730 (100%)	674 (93%)	49 (7%)	3 (0%)	34	62
All	All	1452/1460 (100%)	1337 (92%)	108 (7%)	7 (0%)	29	57

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%)	626 (96%)	27 (4%)	30	61
1	B	653/654 (100%)	618 (95%)	35 (5%)	22	49
All	All	1306/1308 (100%)	1244 (95%)	62 (5%)	26	56

All (62) 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

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Mol	Chain	Res	Type
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	392	LYS
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	577	SER
1	A	627	TRP
1	A	726	VAL
1	B	60	LEU
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	519	LEU

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Mol	Chain	Res	Type
1	B	520	ASN
1	B	543	LEU
1	B	562	ASN
1	B	566	TYR
1	B	577	SER
1	B	594	ILE
1	B	597	ARG
1	B	619	VAL
1	B	627	TRP
1	B	684	ARG
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 (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	123	GLN
1	A	247	GLN
1	A	263	ASN
1	A	344	GLN
1	A	420	ASN
1	A	508	GLN
1	A	679	ASN
1	A	731	GLN
1	B	141	GLN
1	B	263	ASN
1	B	377	ASN
1	B	520	ASN
1	B	562	ASN
1	B	715	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 monosaccharides 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	#$|Z| > 2$
3	SKK	A	808	-	26,30,30	0.87	1 (3%)	29,43,43	0.75	0
2	NAG	B	804	1	14,14,15	1.02	1 (7%)	17,19,21	0.98	1 (5%)
2	NAG	A	802	1	14,14,15	1.40	2 (14%)	17,19,21	0.87	0
2	NAG	B	806	1	14,14,15	1.19	2 (14%)	17,19,21	1.65	3 (17%)
3	SKK	B	807	-	26,30,30	0.96	0	29,43,43	0.90	0
2	NAG	B	805	1	14,14,15	1.37	3 (21%)	17,19,21	1.71	5 (29%)
2	NAG	A	804	1	14,14,15	1.06	1 (7%)	17,19,21	0.94	1 (5%)
2	NAG	B	802	1	14,14,15	1.02	1 (7%)	17,19,21	0.86	0
2	NAG	A	803	1	14,14,15	1.19	2 (14%)	17,19,21	1.12	1 (5%)
2	NAG	B	801	1	14,14,15	0.96	0	17,19,21	1.31	1 (5%)
2	NAG	A	807	-	15,15,15	1.13	1 (6%)	21,21,21	1.38	3 (14%)
2	NAG	A	801	1	14,14,15	1.11	2 (14%)	17,19,21	1.22	1 (5%)
2	NAG	B	803	1	14,14,15	1.25	2 (14%)	17,19,21	1.01	1 (5%)
2	NAG	A	806	1	14,14,15	1.24	1 (7%)	17,19,21	1.01	1 (5%)
2	NAG	A	805	1	14,14,15	1.03	1 (7%)	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
3	SKK	A	808	-	-	2/20/32/32	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	B	804	1	-	0/6/23/26	0/1/1/1
2	NAG	A	802	1	-	3/6/23/26	0/1/1/1
2	NAG	B	806	1	-	0/6/23/26	0/1/1/1
3	SKK	B	807	-	-	1/20/32/32	0/3/3/3
2	NAG	B	805	1	-	2/6/23/26	0/1/1/1
2	NAG	A	804	1	-	0/6/23/26	0/1/1/1
2	NAG	B	802	1	-	0/6/23/26	0/1/1/1
2	NAG	A	803	1	-	0/6/23/26	0/1/1/1
2	NAG	B	801	1	-	0/6/23/26	0/1/1/1
2	NAG	A	807	-	-	0/6/26/26	0/1/1/1
2	NAG	A	801	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	806	1	-	1/6/23/26	0/1/1/1
2	NAG	A	805	1	-	0/6/23/26	0/1/1/1

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	802	NAG	C1-C2	3.42	1.57	1.52
2	A	806	NAG	O5-C1	-3.13	1.38	1.43
2	A	807	NAG	C1-C2	3.12	1.56	1.52
2	B	805	NAG	C1-C2	2.99	1.56	1.52
2	B	805	NAG	O5-C1	-2.80	1.39	1.43
2	B	803	NAG	C1-C2	2.68	1.56	1.52
2	A	802	NAG	O5-C1	-2.65	1.39	1.43
2	B	803	NAG	O5-C1	-2.57	1.39	1.43
2	A	803	NAG	C1-C2	2.57	1.56	1.52
2	A	801	NAG	O5-C1	-2.56	1.39	1.43
2	A	804	NAG	O5-C1	-2.50	1.39	1.43
2	B	806	NAG	C1-C2	2.48	1.56	1.52
2	B	806	NAG	O5-C1	-2.46	1.39	1.43
2	B	804	NAG	O5-C1	-2.43	1.39	1.43
2	A	805	NAG	O5-C1	-2.36	1.40	1.43
3	A	808	SKK	C24-C22	2.27	1.42	1.39
2	B	802	NAG	O5-C1	-2.18	1.40	1.43
2	B	805	NAG	C3-C2	2.17	1.57	1.52
2	A	803	NAG	O5-C1	-2.12	1.40	1.43
2	A	801	NAG	C1-C2	2.07	1.55	1.52

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	801	NAG	C1-O5-C5	4.33	118.05	112.19
2	B	805	NAG	C1-C2-N2	-3.88	103.86	110.49
2	B	806	NAG	C1-O5-C5	3.63	117.11	112.19
2	A	801	NAG	C1-O5-C5	3.56	117.01	112.19
2	B	806	NAG	C1-C2-N2	-3.38	104.72	110.49
2	B	805	NAG	O3-C3-C4	-2.95	103.53	110.35
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	2.59	115.70	112.19
2	A	803	NAG	O5-C5-C6	2.46	111.06	107.20
2	A	807	NAG	C6-C5-C4	2.45	118.75	113.00
2	B	805	NAG	C4-C3-C2	2.44	114.60	111.02
2	A	804	NAG	C1-O5-C5	2.44	115.50	112.19
2	A	807	NAG	C3-C4-C5	-2.41	105.94	110.24
2	B	805	NAG	O5-C5-C6	-2.40	103.44	107.20
2	A	806	NAG	C1-O5-C5	2.40	115.44	112.19
2	B	805	NAG	C1-O5-C5	2.35	115.38	112.19
2	A	805	NAG	C1-O5-C5	2.14	115.09	112.19
2	B	803	NAG	O3-C3-C4	-2.05	105.60	110.35

There are no chirality outliers.

All (10) torsion outliers are listed below:

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

Bond lengths

Bond angles

Torsions

Rings

Ligand SKK B 807
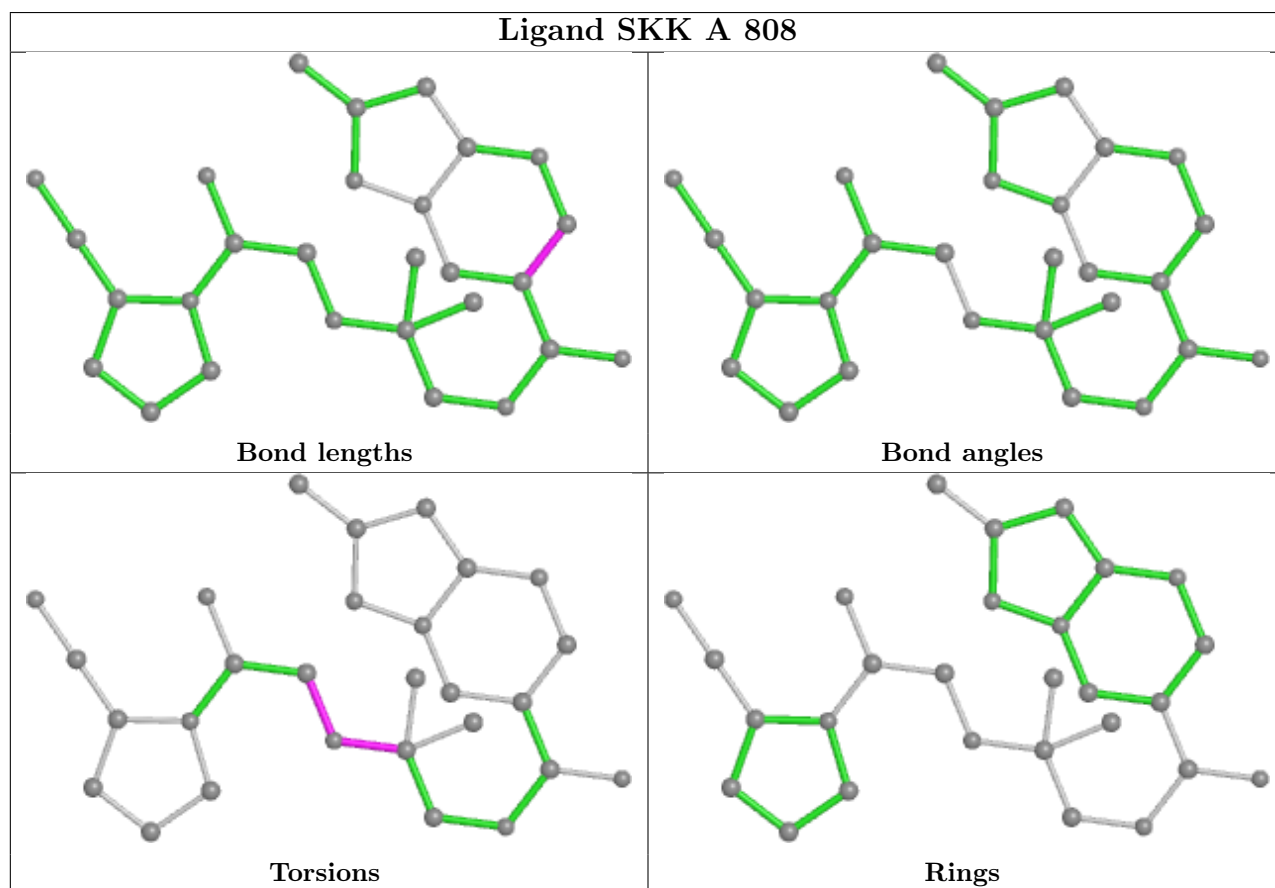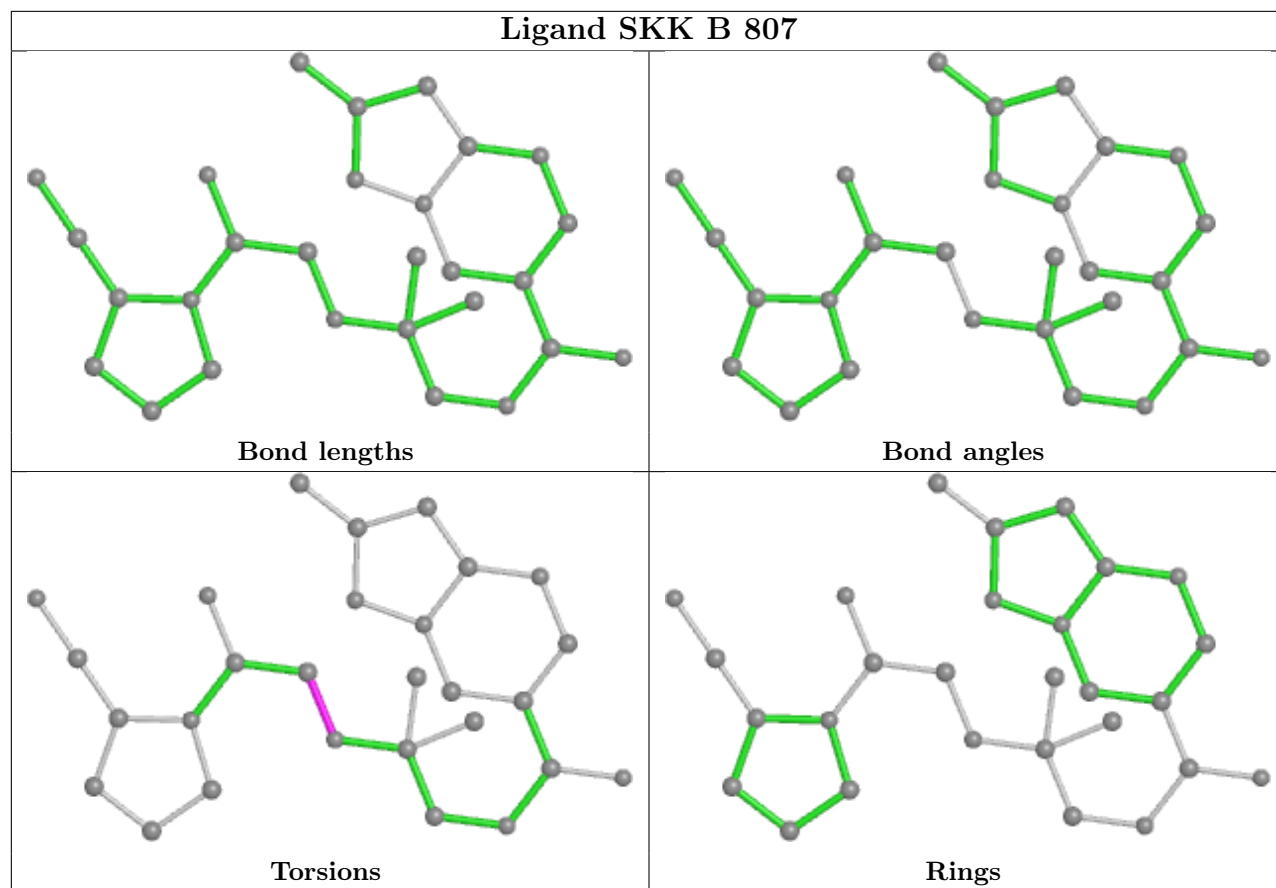
5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	728/730 (99%)	0.45	46 (6%)	20	15	30, 53, 81, 99	0
1	B	728/730 (99%)	0.38	48 (6%)	18	14	29, 47, 77, 100	0
All	All	1456/1460 (99%)	0.42	94 (6%)	18	14	29, 51, 79, 100	0

All (94) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	92	ASN	7.7
1	A	98	PHE	7.6
1	A	97	GLU	6.5
1	B	96	ASP	6.3
1	B	95	PHE	6.3
1	B	105	TYR	5.9
1	B	94	THR	5.7
1	A	96	ASP	5.4
1	B	90	LEU	5.3
1	B	100	HIS	4.6
1	B	97	GLU	4.5
1	B	101	SER	4.5
1	A	142	LEU	4.4
1	B	116	LEU	4.4
1	B	98	PHE	4.2
1	A	105	TYR	4.0
1	A	135	TYR	3.9
1	B	114	ILE	3.7
1	A	279	VAL	3.7
1	A	131	SER	3.7
1	B	140	ARG	3.7
1	B	137	LEU	3.6
1	B	506	ASN	3.6
1	B	332	GLU	3.4

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Mol	Chain	Res	Type	RSRZ
1	A	618	PHE	3.2
1	A	89	PHE	3.2
1	A	280	THR	3.2
1	B	135	TYR	3.1
1	B	618	PHE	3.1
1	A	101	SER	3.1
1	B	89	PHE	3.1
1	A	140	ARG	3.1
1	A	519	LEU	3.1
1	B	535	ASP	3.0
1	B	39	SER	3.0
1	B	333	SER	3.0
1	A	91	GLU	2.9
1	A	619	VAL	2.9
1	B	538	LYS	2.9
1	A	141	GLN	2.8
1	A	90	LEU	2.8
1	A	174	VAL	2.8
1	B	540	TYR	2.8
1	B	93	SER	2.8
1	B	142	LEU	2.7
1	A	183	TYR	2.7
1	A	95	PHE	2.7
1	B	330	TYR	2.7
1	B	534	PHE	2.6
1	A	538	LYS	2.6
1	B	681	ASP	2.6
1	A	54	ARG	2.5
1	B	280	THR	2.5
1	A	100	HIS	2.4
1	A	39	SER	2.4
1	B	148	ILE	2.4
1	B	542	LEU	2.4
1	A	138	ASN	2.4
1	A	77	LEU	2.4
1	B	270	VAL	2.4
1	B	74	ASN	2.4
1	B	141	GLN	2.4
1	A	536	LYS	2.4
1	A	99	GLY	2.3
1	B	91	GLU	2.3
1	B	279	VAL	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	281	ASN	2.3
1	B	277	SER	2.3
1	A	76	ILE	2.3
1	B	102	ILE	2.2
1	A	118	TYR	2.2
1	A	540	TYR	2.2
1	A	114	ILE	2.2
1	B	282	ALA	2.2
1	A	180	LEU	2.2
1	A	386	TYR	2.2
1	A	148	ILE	2.2
1	A	506	ASN	2.1
1	B	271	VAL	2.1
1	B	283	THR	2.1
1	A	74	ASN	2.1
1	A	537	SER	2.1
1	B	231	THR	2.1
1	B	40	ARG	2.1
1	A	518	ILE	2.1
1	A	539	LYS	2.1
1	B	92	ASN	2.1
1	B	477	LEU	2.1
1	B	183	TYR	2.1
1	A	646	VAL	2.1
1	B	334	SER	2.1
1	A	137	LEU	2.1
1	A	534	PHE	2.1
1	B	537	SER	2.1

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 monosaccharides in this entry.

6.4 Ligands ⓘ

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	802	14/15	0.68	0.33	88,92,94,94	0
2	NAG	A	807	15/15	0.70	0.25	71,78,82,84	0
2	NAG	B	802	14/15	0.76	0.53	94,98,99,99	0
2	NAG	A	805	14/15	0.78	0.30	81,83,84,84	0
2	NAG	A	803	14/15	0.84	0.18	62,65,71,71	0
2	NAG	B	804	14/15	0.86	0.29	55,57,58,60	0
2	NAG	A	801	14/15	0.88	0.26	54,58,62,65	0
2	NAG	B	805	14/15	0.88	0.32	82,84,86,86	0
3	SKK	A	808	28/28	0.88	0.34	52,60,80,80	0
2	NAG	A	806	14/15	0.89	0.16	63,66,67,70	0
2	NAG	B	806	14/15	0.89	0.20	63,66,74,77	0
2	NAG	B	801	14/15	0.89	0.21	43,46,50,50	0
2	NAG	B	803	14/15	0.90	0.17	54,58,64,64	0
3	SKK	B	807	28/28	0.90	0.35	59,71,86,87	0
2	NAG	A	804	14/15	0.93	0.18	34,49,55,59	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)
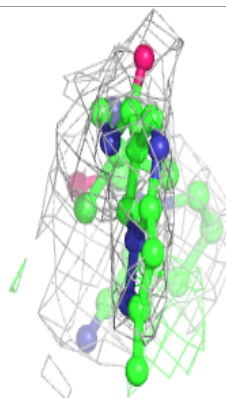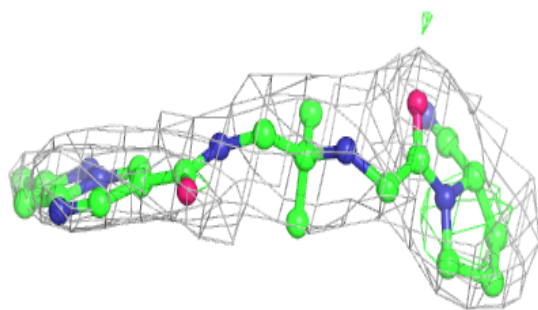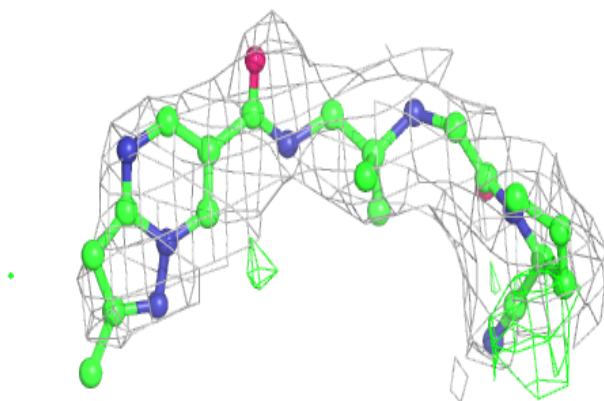
Electron density around SKK B 807:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)
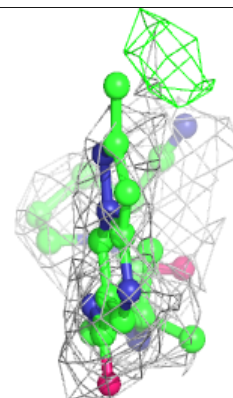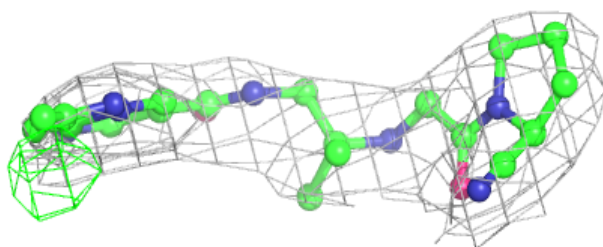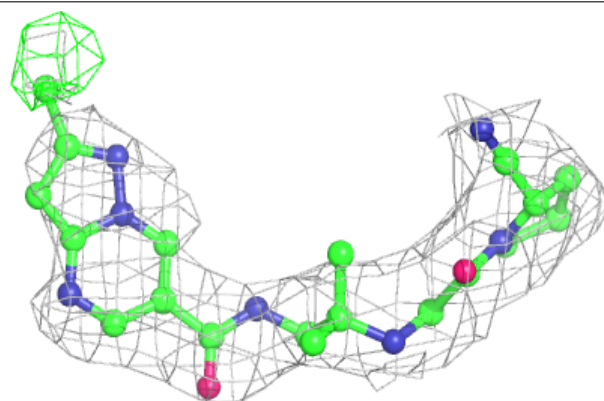
6.5 Other polymers (i)

There are no such residues in this entry.