



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 19, 2026 – 03:09 AM UTC

PDB ID : 6HP8 / pdb_00006hp8
Title : Crystal structure of DPP8 in complex with Val-BoroPro
Authors : Ross, B.H.; Huber, R.
Deposited on : 2018-09-19
Resolution : 2.50 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

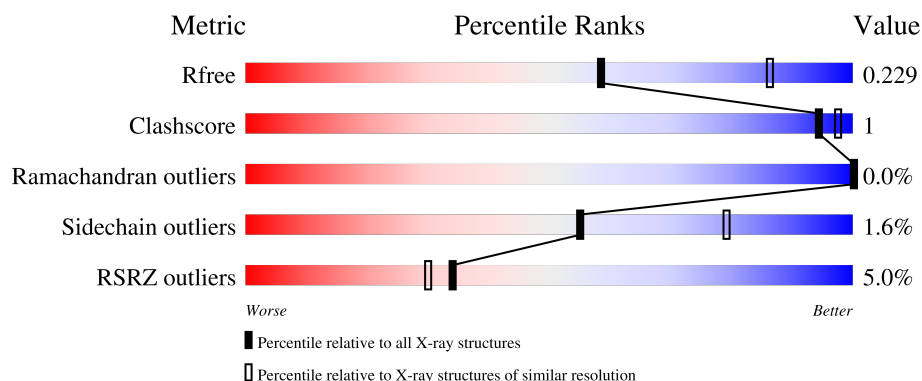
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

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	898	5% 89% • 7%
1	B	898	5% 88% • 7%
1	C	898	4% 89% • 7%

2 Entry composition [i](#)

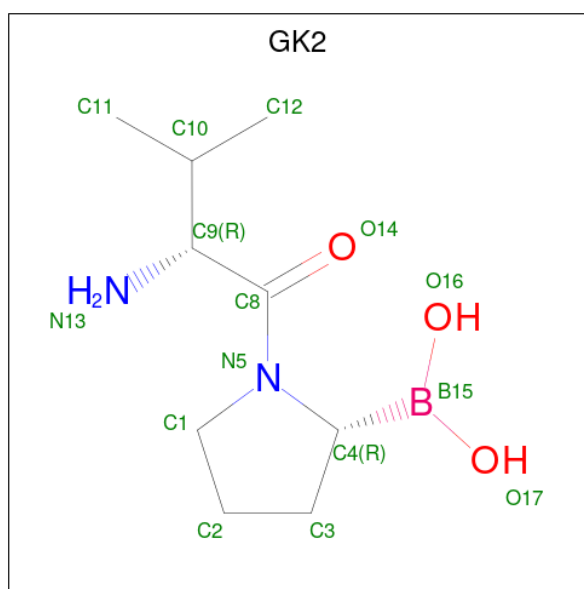
There are 5 unique types of molecules in this entry. The entry contains 21265 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 8.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	836	Total	C	N	O	S	0	1	0
			6803	4368	1144	1265	26			
1	B	835	Total	C	N	O	S	0	1	0
			6795	4362	1143	1264	26			
1	C	837	Total	C	N	O	S	0	1	0
			6814	4377	1145	1266	26			

- Molecule 2 is [(2 {R})-1-[(2 {R})-2-azanyl-3-methyl-butanoyl]pyrrolidin-2-yl]boronic acid (CCD ID: GK2) (formula: C₉H₁₉BN₂O₃) (labeled as "Ligand of Interest" by depositor).

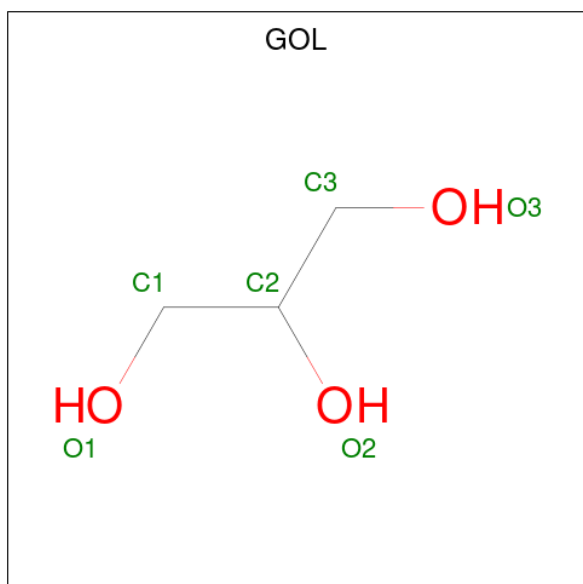


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	B	C	N	O	0	0
			15	1	9	2	3		
2	B	1	Total	B	C	N	O	0	0
			15	1	9	2	3		
2	C	1	Total	B	C	N	O	0	0
			15	1	9	2	3		

- Molecule 3 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Na	0	0
			1	1		
3	B	1	Total	Na	0	0
			1	1		
3	C	1	Total	Na	0	0
			1	1		

- Molecule 4 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			6	3	3		
4	A	1	Total	C	O	0	0
			6	3	3		
4	A	1	Total	C	O	0	0
			6	3	3		
4	A	1	Total	C	O	1	0
			6	3	3		
4	A	1	Total	C	O	0	0
			6	3	3		
4	B	1	Total	C	O	0	0
			6	3	3		
4	B	1	Total	C	O	0	0
			6	3	3		
4	B	1	Total	C	O	0	0
			6	3	3		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	C	O	0	0
			6	3	3		
4	B	1	Total	C	O	0	0
			6	3	3		
4	C	1	Total	C	O	0	0
			6	3	3		
4	C	1	Total	C	O	0	0
			6	3	3		
4	C	1	Total	C	O	0	0
			6	3	3		
4	C	1	Total	C	O	0	0
			6	3	3		
4	C	1	Total	C	O	0	0
			6	3	3		

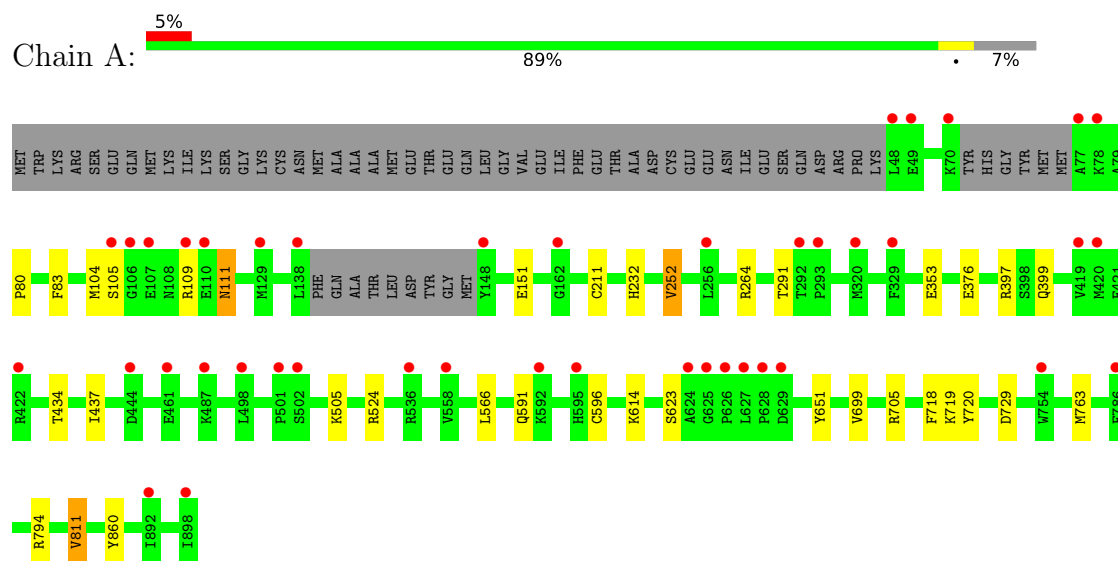
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	258	Total	O	0	0
			258	258		
5	B	210	Total	O	0	0
			210	210		
5	C	247	Total	O	0	0
			247	247		

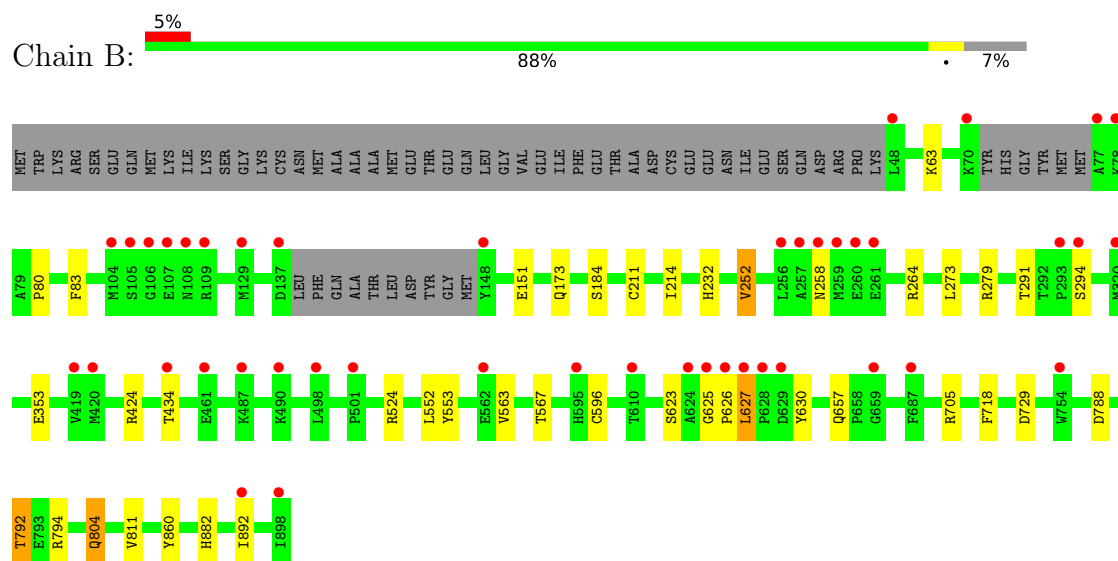
3 Residue-property plots [i](#)

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.

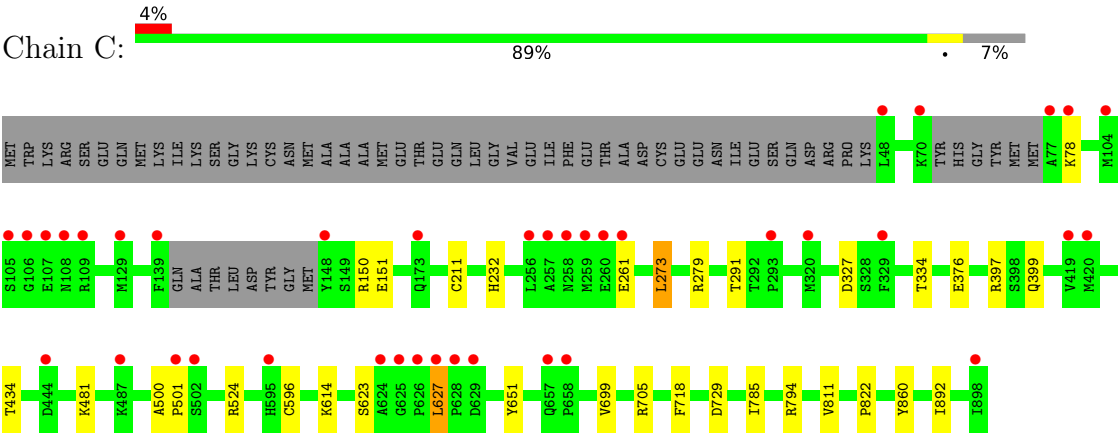
- Molecule 1: Dipeptidyl peptidase 8



- Molecule 1: Dipeptidyl peptidase 8



- Molecule 1: Dipeptidyl peptidase 8



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	163.16Å 245.32Å 261.59Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	44.62 – 2.50 44.62 – 2.50	Depositor EDS
% Data completeness (in resolution range)	99.9 (44.62-2.50) 99.9 (44.62-2.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.59 (at 2.51Å)	Xtriage
Refinement program	REFMAC 7.0	Depositor
R, R_{free}	0.203 , 0.228 0.206 , 0.229	Depositor DCC
R_{free} test set	8992 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	50.7	Xtriage
Anisotropy	0.175	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 23.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	21265	wwPDB-VP
Average B, all atoms (Å ²)	52.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.47% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: NA, GOL, GK2

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	1.01	0/6989	1.04	1/9479 (0.0%)
1	B	1.01	0/6981	1.04	1/9468 (0.0%)
1	C	1.00	0/7001	1.04	1/9495 (0.0%)
All	All	1.01	0/20971	1.04	3/28442 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	860	TYR	CB-CA-C	5.35	116.22	110.65
1	B	860	TYR	CB-CA-C	5.13	115.98	110.65
1	A	860	TYR	CB-CA-C	5.06	115.91	110.65

There are no chirality outliers.

There are no planarity outliers.

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	6803	0	6630	17	0
1	B	6795	0	6618	19	0
1	C	6814	0	6639	16	0
2	A	15	0	0	0	0
2	B	15	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	15	0	0	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
4	A	30	0	40	0	0
4	B	30	0	40	0	0
4	C	30	0	40	0	0
5	A	258	0	0	2	0
5	B	210	0	0	2	0
5	C	247	0	0	2	0
All	All	21265	0	20007	51	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 1.

All (51) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:804:GLN:HE21	1:B:804:GLN:HA	1.54	0.72
1:C:705:ARG:HD3	1:C:729:ASP:OD2	1.98	0.64
1:B:705:ARG:HD3	1:B:729:ASP:OD2	1.99	0.63
1:B:252:VAL:HG13	1:B:264:ARG:HB3	1.82	0.60
1:C:627:LEU:HD12	1:C:627:LEU:N	2.16	0.60
1:A:252:VAL:HG13	1:A:264:ARG:HB3	1.82	0.60
1:A:524:ARG:NH2	5:A:1001:HOH:O	2.36	0.59
1:C:500:ALA:HB1	1:C:501:PRO:HD2	1.88	0.55
1:B:524:ARG:NH2	5:B:1001:HOH:O	2.36	0.54
1:B:627:LEU:HB3	1:B:630:TYR:HB3	1.91	0.52
1:A:651:TYR:HB2	1:A:699:VAL:HB	1.92	0.51
1:A:376:GLU:HG3	1:A:397:ARG:HB2	1.92	0.51
1:B:596:CYS:SG	1:B:623:SER:HB2	2.50	0.51
1:C:524:ARG:NH1	5:C:1004:HOH:O	2.44	0.51
1:B:788:ASP:O	1:B:792:THR:HG22	2.10	0.51
1:A:596:CYS:SG	1:A:623:SER:HB2	2.51	0.50
1:B:788:ASP:O	1:B:792:THR:CG2	2.59	0.50
1:C:596:CYS:SG	1:C:623:SER:HB2	2.53	0.49
1:A:566:LEU:O	1:A:614:LYS:HD3	2.12	0.49
1:C:892:ILE:HD12	1:C:892:ILE:N	2.27	0.49
1:C:376:GLU:HG3	1:C:397:ARG:HB2	1.93	0.49
1:B:804:GLN:HA	1:B:804:GLN:NE2	2.25	0.48
1:C:211:CYS:HB3	1:C:232:HIS:CD2	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:794:ARG:NH2	5:A:1002:HOH:O	2.39	0.48
1:B:553:TYR:HB3	1:B:563:VAL:CG1	2.44	0.47
1:A:399:GLN:OE1	1:A:794:ARG:HD3	2.15	0.47
1:B:892:ILE:HD12	1:B:892:ILE:N	2.29	0.46
1:A:763:MET:SD	1:A:811:VAL:HG12	2.56	0.46
1:C:399:GLN:OE1	1:C:794:ARG:HD3	2.16	0.46
1:C:794:ARG:NH2	5:C:1002:HOH:O	2.38	0.46
1:C:273:LEU:HD22	1:C:279:ARG:NH2	2.31	0.46
1:A:719:LYS:HG2	1:A:720:TYR:CD2	2.51	0.46
1:B:273:LEU:HD13	1:B:279:ARG:NH2	2.31	0.45
1:B:211:CYS:HB3	1:B:232:HIS:CD2	2.52	0.45
1:C:651:TYR:HB2	1:C:699:VAL:HB	1.99	0.45
1:A:211:CYS:HB3	1:A:232:HIS:CD2	2.52	0.45
1:A:705:ARG:HD3	1:A:729:ASP:OD2	2.17	0.44
1:A:596:CYS:SG	1:A:623:SER:CB	3.06	0.44
1:B:552:LEU:HB3	1:B:567:THR:HG23	2.01	0.43
1:B:625:GLY:O	1:B:626:PRO:C	2.62	0.43
1:B:882:HIS:CE1	1:C:822:PRO:HG3	2.54	0.42
1:C:596:CYS:SG	1:C:623:SER:CB	3.07	0.42
1:C:334:THR:CG2	1:C:785:ILE:HA	2.50	0.42
1:B:184:SER:HA	1:B:214:ILE:CD1	2.51	0.41
1:B:794:ARG:NH2	5:B:1004:HOH:O	2.47	0.41
1:A:437:ILE:HB	1:A:505:LYS:HA	2.02	0.41
1:B:80:PRO:HB2	1:B:83:PHE:CZ	2.56	0.41
1:C:150:ARG:NH1	1:C:327:ASP:OD2	2.51	0.41
1:A:80:PRO:HB2	1:A:83:PHE:CZ	2.56	0.40
1:A:104:MET:HE2	1:A:111:ASN:ND2	2.37	0.40
1:A:105:SER:HB2	1:A:109:ARG:NH2	2.35	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	831/898 (92%)	805 (97%)	26 (3%)	0	100	100
1	B	830/898 (92%)	808 (97%)	21 (2%)	1 (0%)	48	68
1	C	832/898 (93%)	810 (97%)	22 (3%)	0	100	100
All	All	2493/2694 (92%)	2423 (97%)	69 (3%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	294	SER

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	743/795 (94%)	734 (99%)	9 (1%)	63	83
1	B	742/795 (93%)	727 (98%)	15 (2%)	48	75
1	C	744/795 (94%)	733 (98%)	11 (2%)	57	80
All	All	2229/2385 (94%)	2194 (98%)	35 (2%)	55	79

All (35) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	111	ASN
1	A	151	GLU
1	A	252	VAL
1	A	291	THR
1	A	353	GLU
1	A	434	THR
1	A	591	GLN
1	A	718	PHE
1	A	811	VAL
1	B	63	LYS
1	B	151	GLU
1	B	173	GLN

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Mol	Chain	Res	Type
1	B	252	VAL
1	B	258	ASN
1	B	291	THR
1	B	353	GLU
1	B	424	ARG
1	B	434	THR
1	B	627	LEU
1	B	657	GLN
1	B	718	PHE
1	B	792	THR
1	B	804	GLN
1	B	811	VAL
1	C	78	LYS
1	C	151	GLU
1	C	261	GLU
1	C	273	LEU
1	C	291	THR
1	C	434	THR
1	C	481	LYS
1	C	614	LYS
1	C	627	LEU
1	C	718	PHE
1	C	811	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	81	HIS
1	A	111	ASN
1	A	123	ASN
1	A	181	GLN
1	A	199	GLN
1	A	200	GLN
1	A	253	HIS
1	A	423	GLN
1	A	458	GLN
1	A	460	HIS
1	A	580	HIS
1	A	801	GLN
1	A	882	HIS
1	B	200	GLN
1	B	205	ASN

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Mol	Chain	Res	Type
1	B	253	HIS
1	B	366	GLN
1	B	423	GLN
1	B	448	ASN
1	B	550	HIS
1	B	559	ASN
1	B	654	HIS
1	B	690	ASN
1	B	801	GLN
1	B	804	GLN
1	B	858	GLN
1	B	882	HIS
1	C	60	GLN
1	C	173	GLN
1	C	199	GLN
1	C	213	ASN
1	C	258	ASN
1	C	423	GLN
1	C	525	HIS
1	C	550	HIS
1	C	559	ASN
1	C	580	HIS
1	C	840	HIS
1	C	858	GLN
1	C	882	HIS

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

Of 21 ligands modelled in this entry, 3 are monoatomic - leaving 18 for Mogul analysis.

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	GK2	B	901	1	10,15,15	0.78	0	13,21,21	1.17	1 (7%)
4	GOL	A	905	-	5,5,5	0.11	0	5,5,5	0.33	0
4	GOL	A	903	-	5,5,5	0.08	0	5,5,5	0.25	0
4	GOL	C	904	-	5,5,5	0.09	0	5,5,5	0.27	0
4	GOL	A	904	-	5,5,5	0.10	0	5,5,5	0.29	0
4	GOL	B	903	-	5,5,5	0.10	0	5,5,5	0.27	0
4	GOL	C	906	-	5,5,5	0.10	0	5,5,5	0.29	0
4	GOL	B	904	-	5,5,5	0.09	0	5,5,5	0.30	0
4	GOL	C	905	-	5,5,5	0.09	0	5,5,5	0.27	0
4	GOL	A	906	-	5,5,5	2.18	1 (20%)	5,5,5	2.91	2 (40%)
4	GOL	B	905	-	5,5,5	0.09	0	5,5,5	0.26	0
4	GOL	B	906	-	5,5,5	0.09	0	5,5,5	0.28	0
2	GK2	A	901	1	10,15,15	0.73	0	13,21,21	1.09	1 (7%)
4	GOL	B	907	-	5,5,5	0.09	0	5,5,5	0.30	0
4	GOL	C	907	-	5,5,5	0.10	0	5,5,5	0.27	0
2	GK2	C	901	1	10,15,15	0.75	0	13,21,21	1.06	0
4	GOL	C	903	-	5,5,5	0.09	0	5,5,5	0.24	0
4	GOL	A	907	-	5,5,5	0.09	0	5,5,5	0.25	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	GK2	B	901	1	-	3/12/26/26	0/1/1/1
4	GOL	A	905	-	-	4/4/4/4	-
4	GOL	A	903	-	-	2/4/4/4	-
4	GOL	C	904	-	-	2/4/4/4	-
4	GOL	A	904	-	-	0/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	GOL	B	903	-	-	2/4/4/4	-
4	GOL	C	906	-	-	2/4/4/4	-
4	GOL	B	904	-	-	2/4/4/4	-
4	GOL	C	905	-	-	0/4/4/4	-
4	GOL	A	906	-	-	0/4/4/4	-
4	GOL	B	905	-	-	2/4/4/4	-
4	GOL	B	906	-	-	0/4/4/4	-
2	GK2	A	901	1	-	2/12/26/26	0/1/1/1
4	GOL	B	907	-	-	4/4/4/4	-
4	GOL	C	907	-	-	4/4/4/4	-
2	GK2	C	901	1	-	2/12/26/26	0/1/1/1
4	GOL	C	903	-	-	2/4/4/4	-
4	GOL	A	907	-	-	2/4/4/4	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	906	GOL	O1-C1	4.81	1.62	1.42

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	906	GOL	O1-C1-C2	5.77	136.34	110.38
4	A	906	GOL	O2-C2-C1	-2.41	99.22	109.18
2	A	901	GK2	C2-C3-C4	2.06	107.51	104.11
2	B	901	GK2	C2-C3-C4	2.05	107.51	104.11

There are no chirality outliers.

All (35) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	905	GOL	O1-C1-C2-C3
4	A	905	GOL	C1-C2-C3-O3
4	B	904	GOL	O1-C1-C2-C3
4	B	905	GOL	C1-C2-C3-O3
4	B	907	GOL	O1-C1-C2-C3
4	B	907	GOL	C1-C2-C3-O3
4	C	904	GOL	O1-C1-C2-C3
4	C	907	GOL	C1-C2-C3-O3

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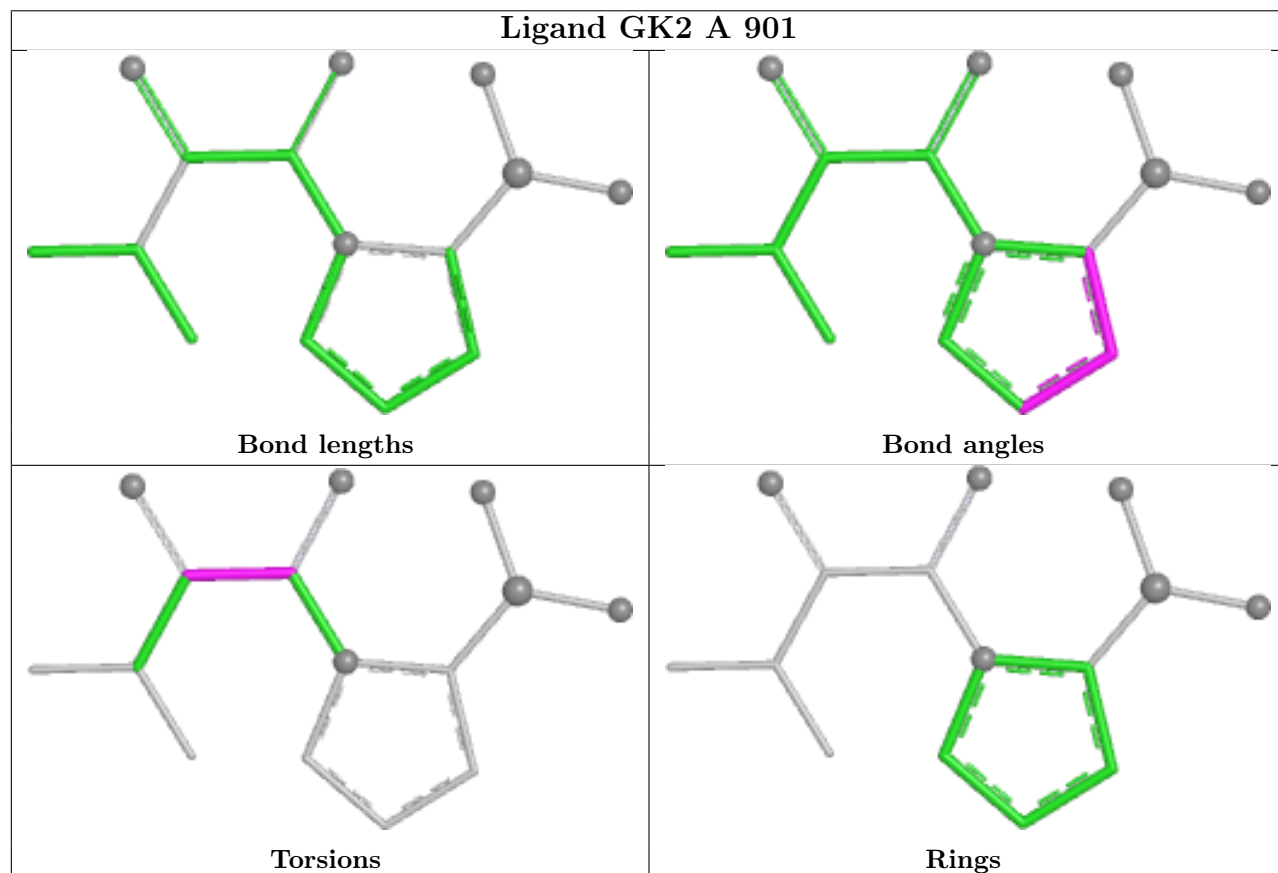
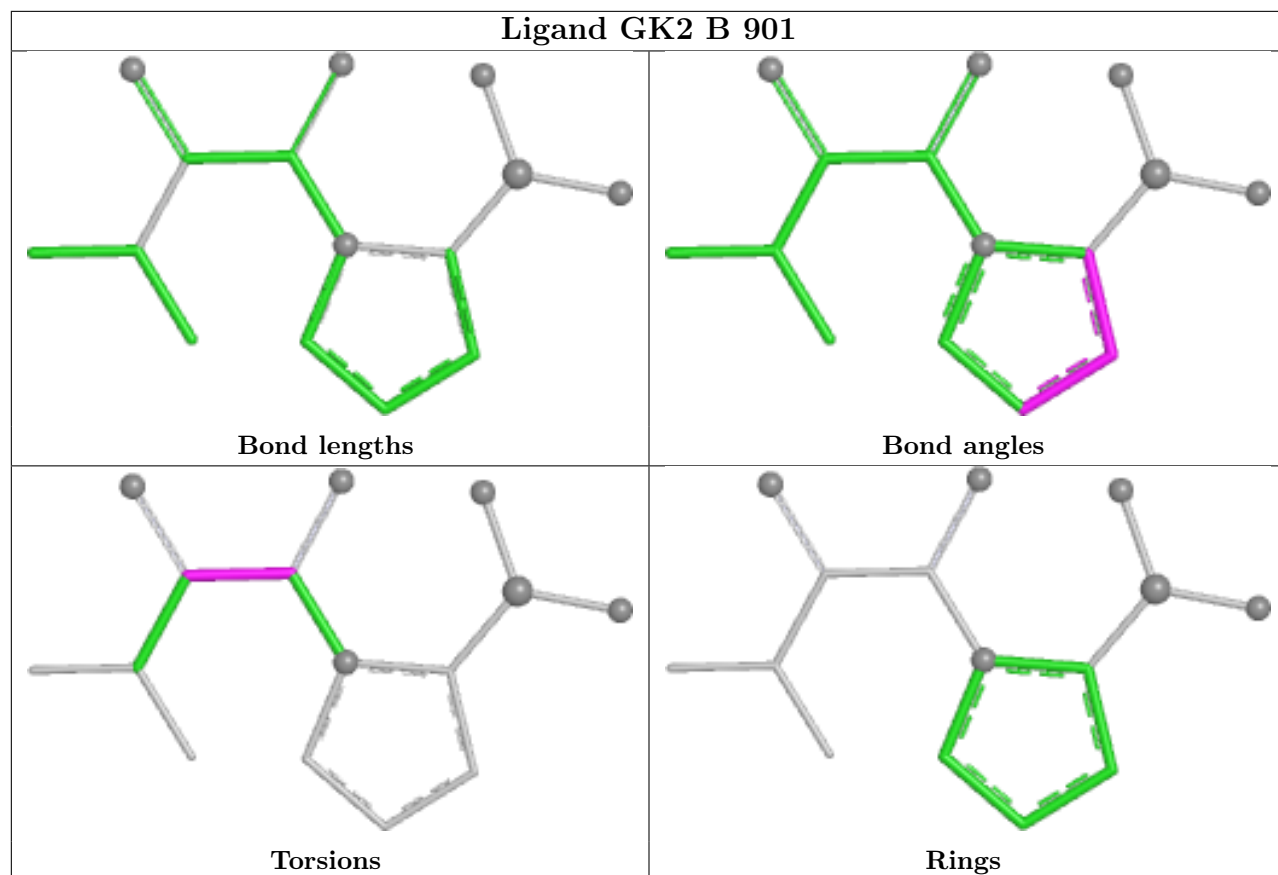
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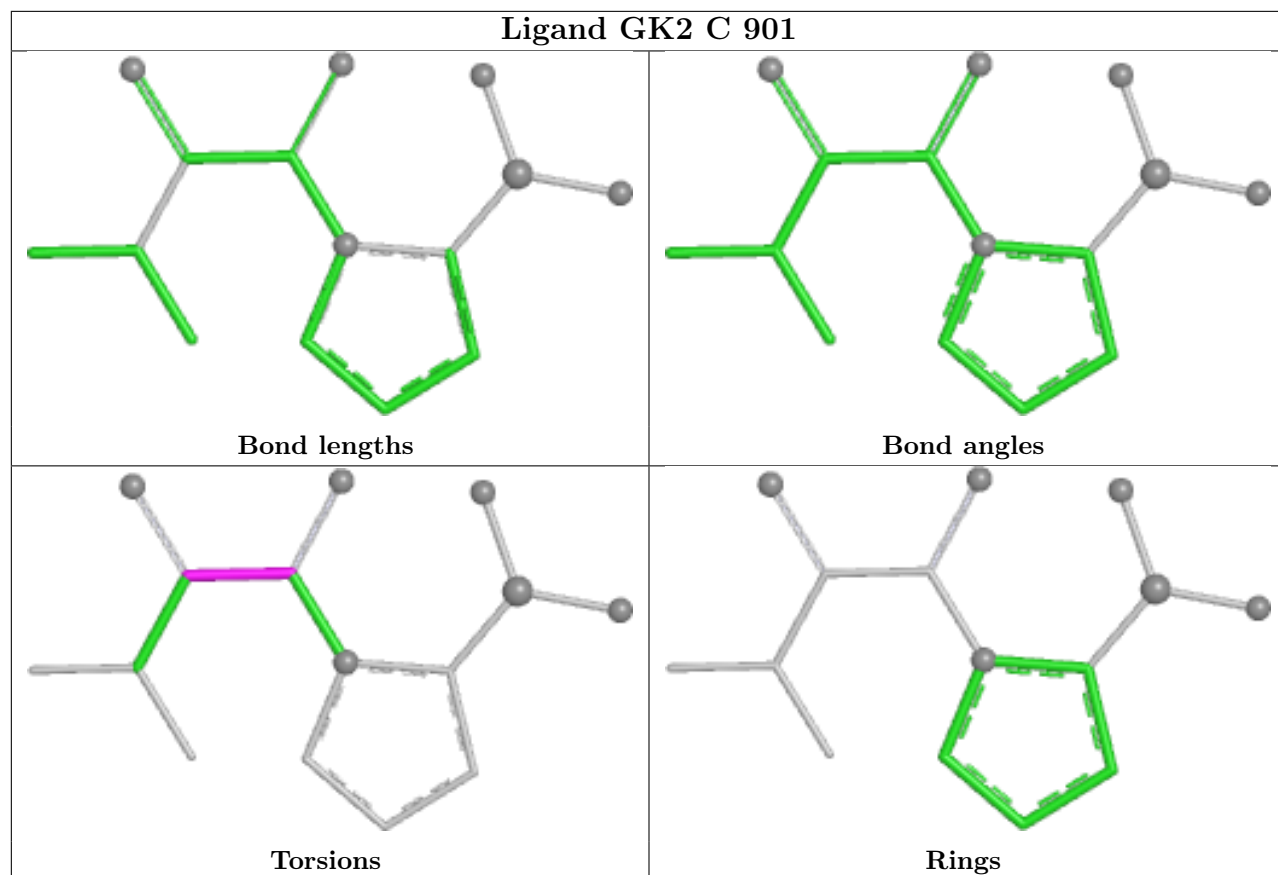
Mol	Chain	Res	Type	Atoms
4	A	903	GOL	O1-C1-C2-O2
4	A	907	GOL	O2-C2-C3-O3
4	B	907	GOL	O1-C1-C2-O2
2	A	901	GK2	O14-C8-C9-C10
2	B	901	GK2	O14-C8-C9-C10
2	C	901	GK2	O14-C8-C9-C10
2	B	901	GK2	N5-C8-C9-C10
4	A	903	GOL	O1-C1-C2-C3
4	A	907	GOL	C1-C2-C3-O3
4	B	903	GOL	O1-C1-C2-C3
4	C	903	GOL	O1-C1-C2-C3
4	C	906	GOL	C1-C2-C3-O3
4	C	907	GOL	O1-C1-C2-C3
4	A	905	GOL	O1-C1-C2-O2
4	A	905	GOL	O2-C2-C3-O3
4	B	904	GOL	O1-C1-C2-O2
4	B	905	GOL	O2-C2-C3-O3
4	C	904	GOL	O1-C1-C2-O2
4	C	907	GOL	O2-C2-C3-O3
4	B	907	GOL	O2-C2-C3-O3
4	C	907	GOL	O1-C1-C2-O2
2	A	901	GK2	N5-C8-C9-C10
2	C	901	GK2	N5-C8-C9-C10
4	C	906	GOL	O2-C2-C3-O3
2	B	901	GK2	O14-C8-C9-N13
4	B	903	GOL	O1-C1-C2-O2
4	C	903	GOL	O1-C1-C2-O2

There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less 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	836/898 (93%)	0.27	42 (5%) 34 30	21, 49, 77, 120	1 (0%)
1	B	835/898 (92%)	0.32	44 (5%) 32 28	22, 51, 79, 112	1 (0%)
1	C	837/898 (93%)	0.22	39 (4%) 36 32	22, 48, 78, 116	1 (0%)
All	All	2508/2694 (93%)	0.27	125 (4%) 34 30	21, 49, 78, 120	3 (0%)

All (125) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	139	PHE	8.2
1	C	106	GLY	7.2
1	A	106	GLY	6.6
1	A	138	LEU	5.7
1	B	106	GLY	5.4
1	C	70	LYS	5.3
1	B	77	ALA	5.1
1	A	77	ALA	5.0
1	C	105	SER	5.0
1	A	105	SER	4.9
1	C	148	TYR	4.9
1	B	898	ILE	4.8
1	C	624	ALA	4.7
1	C	420	MET	4.5
1	B	70	LYS	4.4
1	B	420	MET	4.4
1	C	625	GLY	4.4
1	C	107	GLU	4.3
1	C	419	VAL	4.1
1	C	628	PRO	4.1
1	B	78	LYS	4.1
1	C	627	LEU	4.0
1	A	898	ILE	3.9

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Mol	Chain	Res	Type	RSRZ
1	B	628	PRO	3.9
1	A	78	LYS	3.8
1	B	627	LEU	3.8
1	B	626	PRO	3.8
1	B	624	ALA	3.7
1	A	628	PRO	3.6
1	A	148	TYR	3.6
1	B	104	MET	3.6
1	C	256	LEU	3.6
1	A	70	LYS	3.5
1	C	109	ARG	3.5
1	A	624	ALA	3.5
1	C	898	ILE	3.4
1	A	422	ARG	3.4
1	A	420	MET	3.3
1	C	104	MET	3.3
1	A	107	GLU	3.3
1	B	419	VAL	3.2
1	A	595	HIS	3.2
1	C	108	ASN	3.2
1	B	105	SER	3.1
1	B	48	LEU	3.1
1	A	419	VAL	3.1
1	A	502	SER	3.1
1	B	109	ARG	3.1
1	A	627	LEU	3.0
1	A	109	ARG	3.0
1	B	610	THR	3.0
1	C	78	LYS	3.0
1	B	107	GLU	3.0
1	A	48	LEU	2.9
1	C	77	ALA	2.9
1	B	595	HIS	2.9
1	B	293	PRO	2.9
1	C	626	PRO	2.9
1	B	108	ASN	2.8
1	B	256	LEU	2.8
1	B	148	TYR	2.8
1	C	293	PRO	2.8
1	B	257	ALA	2.7
1	C	129	MET	2.7
1	C	501	PRO	2.7

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Mol	Chain	Res	Type	RSRZ
1	C	48	LEU	2.7
1	B	501	PRO	2.7
1	B	258	ASN	2.7
1	C	320	MET	2.7
1	B	490	LYS	2.6
1	A	129	MET	2.6
1	C	657	GLN	2.6
1	A	501	PRO	2.6
1	B	261	GLU	2.5
1	B	461	GLU	2.5
1	A	444	ASP	2.5
1	A	754	TRP	2.5
1	B	687	PHE	2.5
1	A	320	MET	2.5
1	B	562	GLU	2.4
1	B	629	ASP	2.4
1	A	329[A]	PHE	2.4
1	A	592	LYS	2.4
1	B	320	MET	2.4
1	A	629	ASP	2.4
1	C	658	PRO	2.4
1	A	625	GLY	2.4
1	A	461	GLU	2.4
1	A	536	ARG	2.3
1	A	487	LYS	2.3
1	B	892	ILE	2.3
1	B	625	GLY	2.2
1	B	129	MET	2.2
1	C	329[A]	PHE	2.2
1	A	293	PRO	2.2
1	C	261	GLU	2.2
1	C	258	ASN	2.2
1	B	487	LYS	2.2
1	C	173	GLN	2.2
1	B	259	MET	2.2
1	A	256	LEU	2.2
1	C	487	LYS	2.2
1	B	294	SER	2.1
1	C	444	ASP	2.1
1	A	626	PRO	2.1
1	B	754	TRP	2.1
1	A	162	GLY	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	434	THR	2.1
1	B	498	LEU	2.1
1	A	558	VAL	2.1
1	A	292	THR	2.1
1	A	110	GLU	2.1
1	C	260	GLU	2.1
1	C	259	MET	2.1
1	C	257	ALA	2.1
1	B	659	GLY	2.1
1	A	49	GLU	2.1
1	B	260	GLU	2.1
1	B	137	ASP	2.1
1	C	629	ASP	2.1
1	C	595	HIS	2.1
1	A	892	ILE	2.0
1	C	502	SER	2.0
1	A	786	PHE	2.0
1	A	498	LEU	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
4	GOL	C	907	6/6	0.74	0.33	69,71,72,72	0
4	GOL	B	905	6/6	0.83	0.22	71,73,73,74	0
4	GOL	C	904	6/6	0.84	0.22	70,72,73,73	0
4	GOL	A	907	6/6	0.86	0.19	69,71,72,72	0
4	GOL	A	903	6/6	0.88	0.21	72,74,75,76	0

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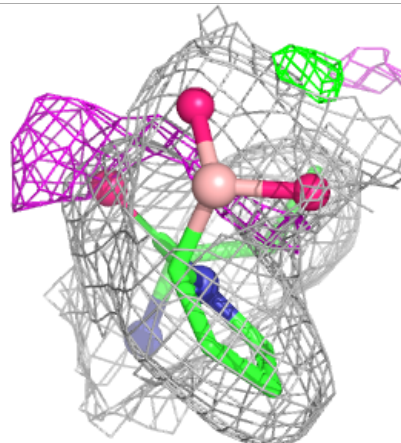
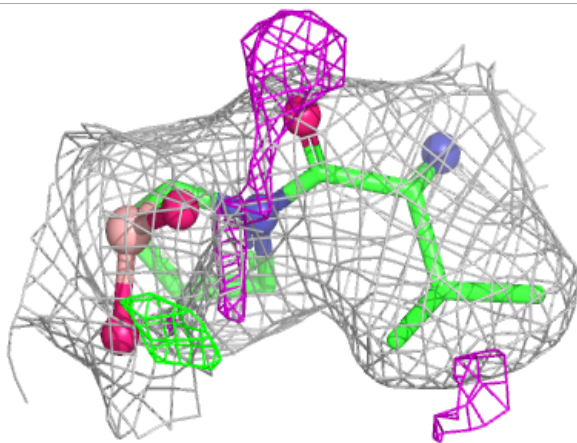
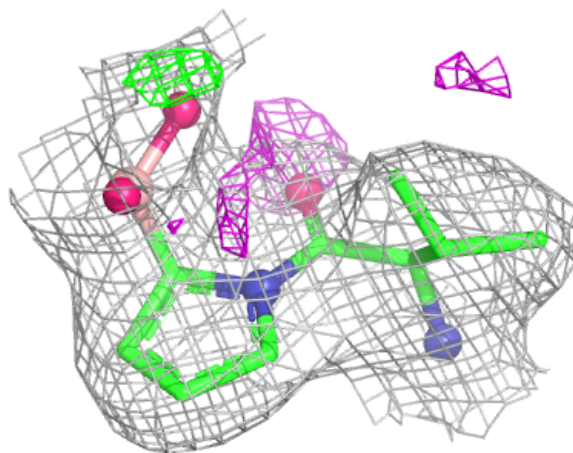
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	GOL	A	906	6/6	0.88	0.24	58,62,69,78	1
4	GOL	A	905	6/6	0.91	0.15	62,63,64,64	0
4	GOL	C	906	6/6	0.91	0.17	77,79,80,80	0
3	NA	A	902	1/1	0.91	0.11	51,51,51,51	0
4	GOL	C	903	6/6	0.92	0.18	73,76,77,78	0
3	NA	B	902	1/1	0.92	0.06	42,42,42,42	0
4	GOL	B	903	6/6	0.92	0.17	69,70,71,71	0
2	GK2	C	901	15/15	0.92	0.12	39,39,40,41	0
2	GK2	B	901	15/15	0.93	0.12	41,41,42,42	0
4	GOL	B	904	6/6	0.93	0.12	53,54,54,55	0
2	GK2	A	901	15/15	0.93	0.12	42,43,44,45	0
4	GOL	B	906	6/6	0.93	0.16	64,65,66,66	0
4	GOL	C	905	6/6	0.94	0.16	68,70,72,74	0
4	GOL	A	904	6/6	0.94	0.10	49,51,51,51	0
4	GOL	B	907	6/6	0.94	0.13	68,70,71,71	0
3	NA	C	902	1/1	0.97	0.05	39,39,39,39	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.

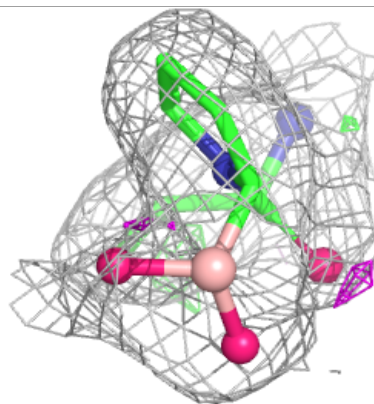
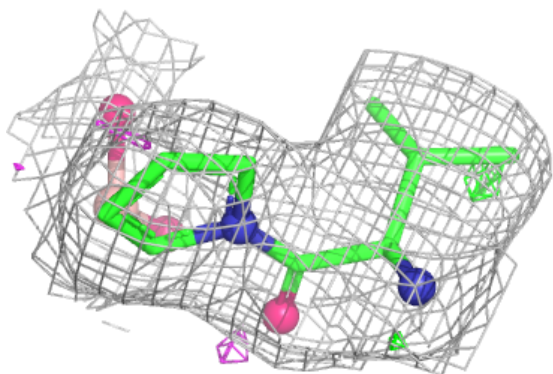
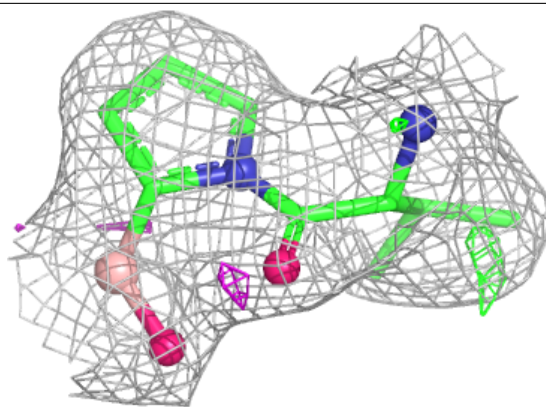
Electron density around GK2 C 901:

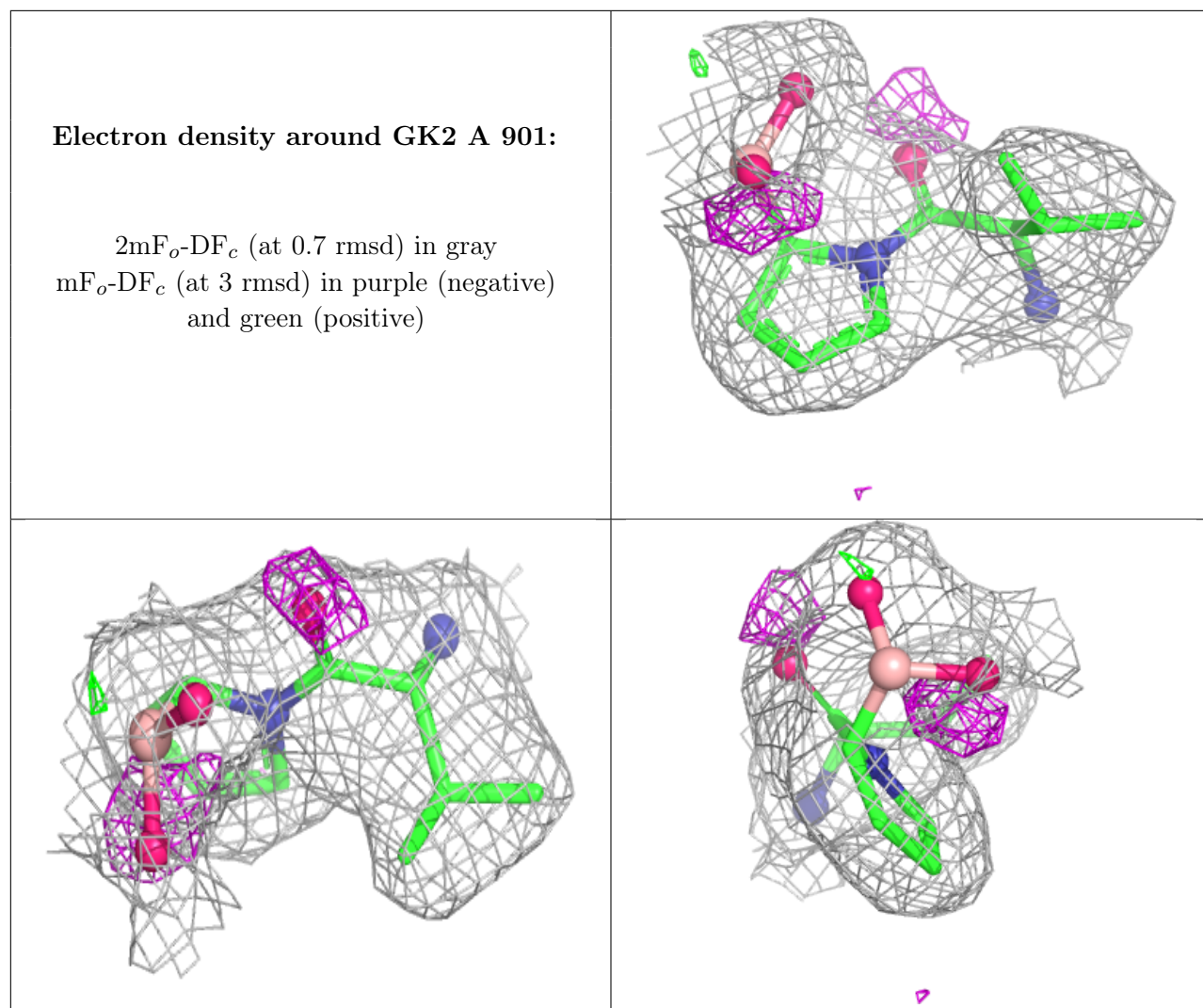
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around GK2 B 901:

$2mF_o-DF_c$ (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.