



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 06:05 PM UTC

PDB ID : 6VKK / pdb_00006vkk
Title : Crystal Structure of human PARP-1 CAT domain bound to inhibitor rucaparib
Authors : Steffen, J.D.; Pascal, J.M.
Deposited on : 2020-01-21
Resolution : 2.10 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

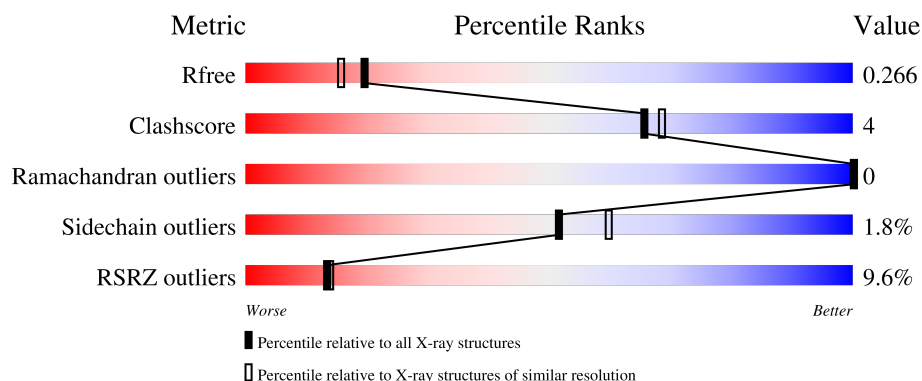
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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	6658 (2.10-2.10)
Clashscore	190562	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)
RSRZ outliers	180081	6662 (2.10-2.10)

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	372	8% 84% 9% 7%
1	B	372	6% 84% 9% 7%
1	C	372	8% 83% 8% 9%
1	D	372	13% 79% 12% 9%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 11126 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 Poly [ADP-ribose] polymerase 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	345	Total	C	N	O	S	0	0	0
			2719	1734	460	514	11			
1	D	339	Total	C	N	O	S	0	0	0
			2670	1702	452	506	10			
1	C	340	Total	C	N	O	S	0	1	0
			2685	1711	455	509	10			
1	B	345	Total	C	N	O	S	0	1	0
			2724	1737	461	515	11			

There are 88 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	640	MET	-	initiating methionine	UNP P09874
A	641	GLY	-	expression tag	UNP P09874
A	642	SER	-	expression tag	UNP P09874
A	643	SER	-	expression tag	UNP P09874
A	644	HIS	-	expression tag	UNP P09874
A	645	HIS	-	expression tag	UNP P09874
A	646	HIS	-	expression tag	UNP P09874
A	647	HIS	-	expression tag	UNP P09874
A	648	HIS	-	expression tag	UNP P09874
A	649	HIS	-	expression tag	UNP P09874
A	650	SER	-	expression tag	UNP P09874
A	651	SER	-	expression tag	UNP P09874
A	652	GLY	-	expression tag	UNP P09874
A	653	LEU	-	expression tag	UNP P09874
A	654	VAL	-	expression tag	UNP P09874
A	655	PRO	-	expression tag	UNP P09874
A	656	ARG	-	expression tag	UNP P09874
A	657	GLY	-	expression tag	UNP P09874
A	658	SER	-	expression tag	UNP P09874
A	659	HIS	-	expression tag	UNP P09874
A	660	MET	-	expression tag	UNP P09874

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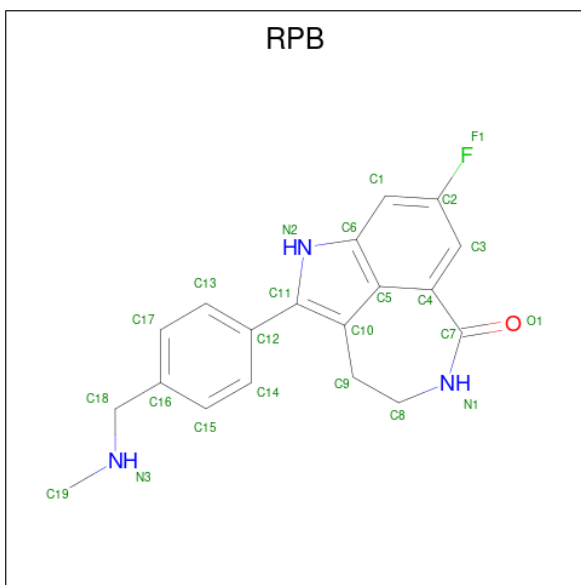
Chain	Residue	Modelled	Actual	Comment	Reference
A	762	ALA	VAL	variant	UNP P09874
D	640	MET	-	initiating methionine	UNP P09874
D	641	GLY	-	expression tag	UNP P09874
D	642	SER	-	expression tag	UNP P09874
D	643	SER	-	expression tag	UNP P09874
D	644	HIS	-	expression tag	UNP P09874
D	645	HIS	-	expression tag	UNP P09874
D	646	HIS	-	expression tag	UNP P09874
D	647	HIS	-	expression tag	UNP P09874
D	648	HIS	-	expression tag	UNP P09874
D	649	HIS	-	expression tag	UNP P09874
D	650	SER	-	expression tag	UNP P09874
D	651	SER	-	expression tag	UNP P09874
D	652	GLY	-	expression tag	UNP P09874
D	653	LEU	-	expression tag	UNP P09874
D	654	VAL	-	expression tag	UNP P09874
D	655	PRO	-	expression tag	UNP P09874
D	656	ARG	-	expression tag	UNP P09874
D	657	GLY	-	expression tag	UNP P09874
D	658	SER	-	expression tag	UNP P09874
D	659	HIS	-	expression tag	UNP P09874
D	660	MET	-	expression tag	UNP P09874
D	762	ALA	VAL	variant	UNP P09874
C	640	MET	-	initiating methionine	UNP P09874
C	641	GLY	-	expression tag	UNP P09874
C	642	SER	-	expression tag	UNP P09874
C	643	SER	-	expression tag	UNP P09874
C	644	HIS	-	expression tag	UNP P09874
C	645	HIS	-	expression tag	UNP P09874
C	646	HIS	-	expression tag	UNP P09874
C	647	HIS	-	expression tag	UNP P09874
C	648	HIS	-	expression tag	UNP P09874
C	649	HIS	-	expression tag	UNP P09874
C	650	SER	-	expression tag	UNP P09874
C	651	SER	-	expression tag	UNP P09874
C	652	GLY	-	expression tag	UNP P09874
C	653	LEU	-	expression tag	UNP P09874
C	654	VAL	-	expression tag	UNP P09874
C	655	PRO	-	expression tag	UNP P09874
C	656	ARG	-	expression tag	UNP P09874
C	657	GLY	-	expression tag	UNP P09874
C	658	SER	-	expression tag	UNP P09874

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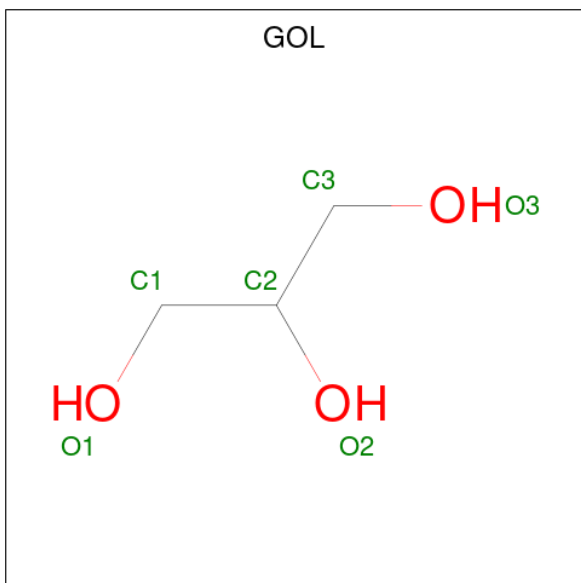
Chain	Residue	Modelled	Actual	Comment	Reference
C	659	HIS	-	expression tag	UNP P09874
C	660	MET	-	expression tag	UNP P09874
C	762	ALA	VAL	variant	UNP P09874
B	640	MET	-	initiating methionine	UNP P09874
B	641	GLY	-	expression tag	UNP P09874
B	642	SER	-	expression tag	UNP P09874
B	643	SER	-	expression tag	UNP P09874
B	644	HIS	-	expression tag	UNP P09874
B	645	HIS	-	expression tag	UNP P09874
B	646	HIS	-	expression tag	UNP P09874
B	647	HIS	-	expression tag	UNP P09874
B	648	HIS	-	expression tag	UNP P09874
B	649	HIS	-	expression tag	UNP P09874
B	650	SER	-	expression tag	UNP P09874
B	651	SER	-	expression tag	UNP P09874
B	652	GLY	-	expression tag	UNP P09874
B	653	LEU	-	expression tag	UNP P09874
B	654	VAL	-	expression tag	UNP P09874
B	655	PRO	-	expression tag	UNP P09874
B	656	ARG	-	expression tag	UNP P09874
B	657	GLY	-	expression tag	UNP P09874
B	658	SER	-	expression tag	UNP P09874
B	659	HIS	-	expression tag	UNP P09874
B	660	MET	-	expression tag	UNP P09874
B	762	ALA	VAL	variant	UNP P09874

- Molecule 2 is Rucaparib (CCD ID: RPB) (formula: $C_{19}H_{18}FN_3O$) (labeled as "Ligand of Interest" by depositor).



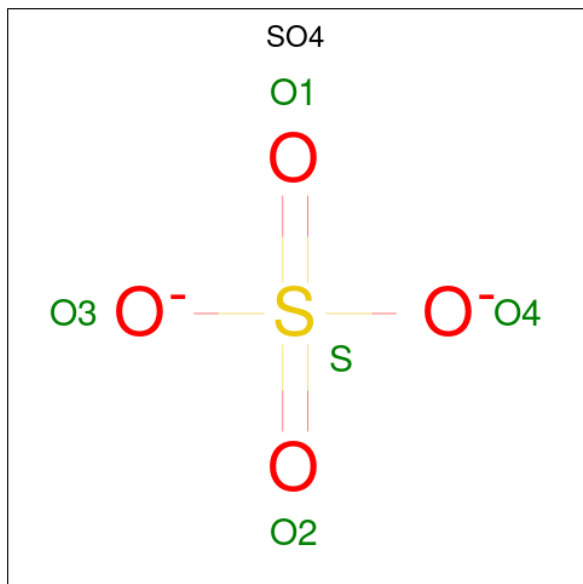
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	F	N	O	0	0
			24	19	1	3	1		
2	D	1	Total	C	F	N	O	0	0
			24	19	1	3	1		
2	C	1	Total	C	F	N	O	0	0
			24	19	1	3	1		
2	B	1	Total	C	F	N	O	0	0
			24	19	1	3	1		

- Molecule 3 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



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

- Molecule 4 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	O	S	0	0
			5	4	1		
4	A	1	Total	O	S	0	0
			5	4	1		
4	A	1	Total	O	S	0	0
			5	4	1		
4	D	1	Total	O	S	0	0
			5	4	1		
4	C	1	Total	O	S	0	0
			5	4	1		
4	C	1	Total	O	S	0	0
			5	4	1		
4	C	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total	O	S	0	0
			5	4	1		

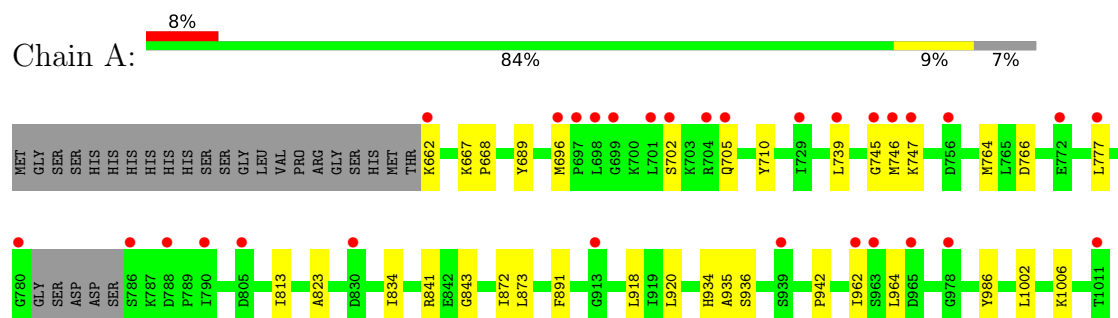
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	52	Total 52	O 52	0	0
5	D	33	Total 33	O 33	0	0
5	C	30	Total 30	O 30	0	0
5	B	54	Total 54	O 54	0	0

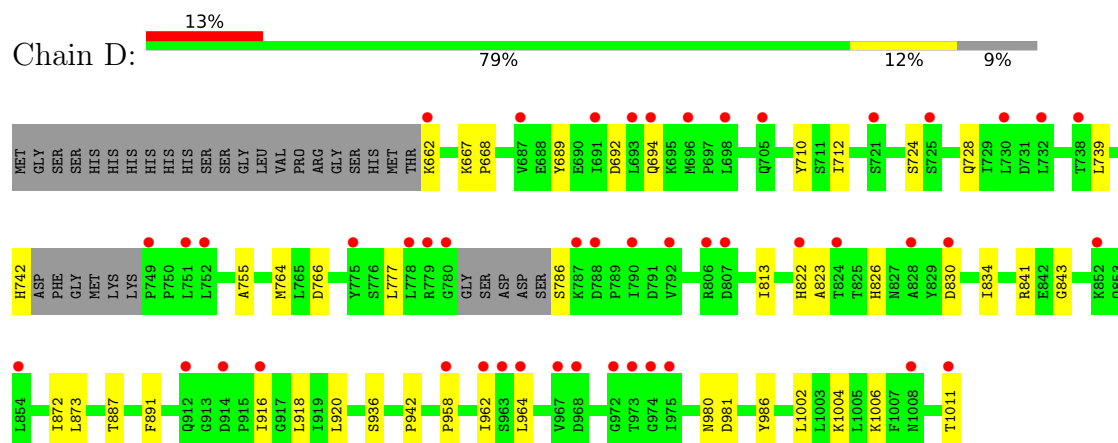
3 Residue-property plots [i](#)

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.

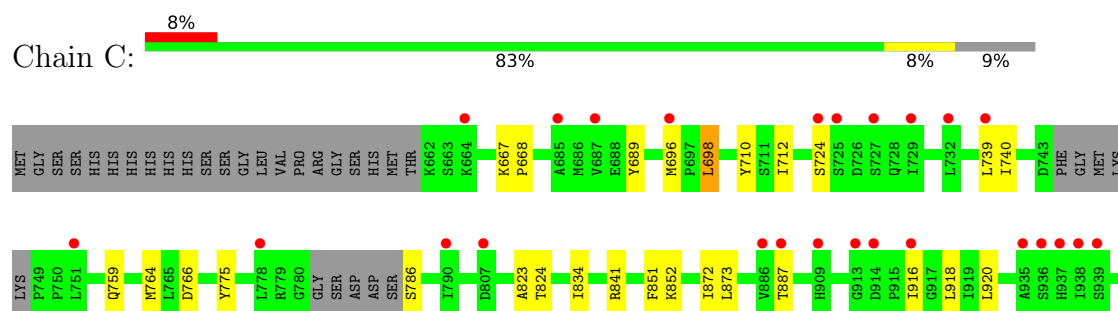
- Molecule 1: Poly [ADP-ribose] polymerase 1

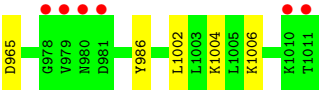


- Molecule 1: Poly [ADP-ribose] polymerase 1

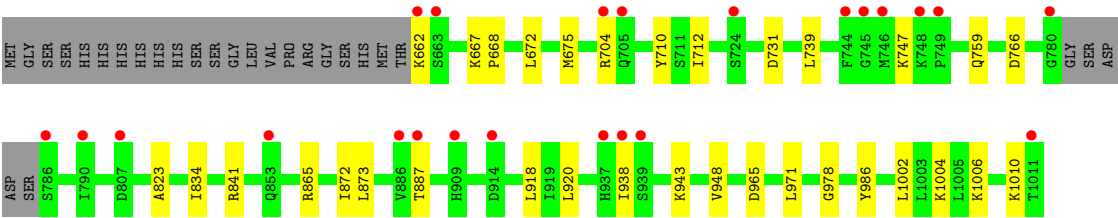
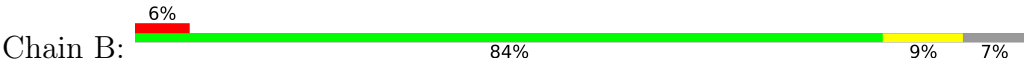


- Molecule 1: Poly [ADP-ribose] polymerase 1





● Molecule 1: Poly [ADP-ribose] polymerase 1



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	104.27Å 107.90Å 142.84Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.10 20.00 – 2.10	Depositor EDS
% Data completeness (in resolution range)	99.1 (20.00-2.10) 99.1 (20.00-2.10)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.12 (at 2.10Å)	Xtriage
Refinement program	REFMAC 5.8.0257	Depositor
R, R_{free}	0.239 , 0.261 0.245 , 0.266	Depositor DCC
R_{free} test set	4709 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å ²)	41.1	Xtriage
Anisotropy	0.197	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 35.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.010 for k,h,-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	11126	wwPDB-VP
Average B, all atoms (Å ²)	59.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.74% 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: RPB, SO4, GOL

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	1.00	0/2770	1.40	0/3737
1	B	0.99	0/2778	1.38	0/3748
1	C	0.99	0/2738	1.39	0/3695
1	D	0.99	0/2719	1.38	0/3669
All	All	0.99	0/11005	1.39	0/14849

There are no bond length outliers.

There are no bond angle outliers.

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	2719	0	2769	19	0
1	B	2724	0	2775	23	0
1	C	2685	0	2729	19	0
1	D	2670	0	2718	30	0
2	A	24	0	18	0	0
2	B	24	0	18	1	0
2	C	24	0	18	1	0
2	D	24	0	18	0	0
3	A	6	0	8	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	6	0	8	0	0
3	D	6	0	8	2	0
4	A	15	0	0	0	0
4	B	10	0	0	0	0
4	C	15	0	0	0	0
4	D	5	0	0	0	0
5	A	52	0	0	0	0
5	B	54	0	0	3	0
5	C	30	0	0	1	0
5	D	33	0	0	0	0
All	All	11126	0	11087	83	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 4.

All (83) 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:D:692:ASP:OD1	1:D:694:GLN:HG2	1.81	0.79
1:D:712:ILE:HD12	1:D:739:LEU:HD12	1.65	0.78
1:B:712:ILE:HD12	1:B:739:LEU:HD22	1.73	0.70
1:A:689:TYR:HB3	1:A:764:MET:HE2	1.74	0.69
1:A:841:ARG:HD2	1:A:873:LEU:O	1.92	0.69
1:C:841:ARG:HD2	1:C:873:LEU:O	1.92	0.69
1:D:841:ARG:HD2	1:D:873:LEU:O	1.92	0.68
1:B:675:MET:HE1	1:B:1004:LYS:CD	2.23	0.68
1:B:841:ARG:HD2	1:B:873:LEU:O	1.92	0.68
1:C:712:ILE:HD12	1:C:739:LEU:HD22	1.77	0.67
1:B:675:MET:HE1	1:B:1004:LYS:HD2	1.77	0.66
1:C:689:TYR:HB3	1:C:764:MET:HE2	1.79	0.65
1:D:689:TYR:HB3	1:D:764:MET:HE2	1.79	0.64
1:D:958:PRO:HG2	1:B:978:GLY:O	1.97	0.64
1:B:759:GLN:HG3	2:B:1202:RPB:H191	1.83	0.60
1:A:934:HIS:CG	1:D:981:ASP:HA	2.39	0.58
1:A:935:ALA:HB3	1:D:980:ASN:HD21	1.69	0.58
1:C:851:PHE:CZ	1:B:943:LYS:HE3	2.40	0.56
1:D:822:HIS:HE1	1:D:826:HIS:O	1.88	0.56
1:D:742:HIS:CE1	1:D:764:MET:HE1	2.41	0.55
1:A:918:LEU:HD22	1:A:1002:LEU:HD21	1.88	0.55
1:D:918:LEU:HD22	1:D:1002:LEU:HD21	1.89	0.55
1:B:675:MET:HE1	1:B:1004:LYS:HD3	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:918:LEU:HD22	1:C:1002:LEU:HD21	1.90	0.53
1:C:698:LEU:HD22	1:C:775:TYR:CG	2.44	0.53
1:B:918:LEU:HD22	1:B:1002:LEU:HD21	1.90	0.53
1:C:852:LYS:NZ	5:C:1201:HOH:O	2.42	0.52
1:B:938:ILE:CD1	1:B:948:VAL:HG21	2.39	0.52
1:B:865:ARG:NH2	5:B:1301:HOH:O	2.42	0.52
1:D:872:ILE:HG21	1:D:920:LEU:HD11	1.93	0.50
1:C:698:LEU:HD22	1:C:775:TYR:CD1	2.46	0.50
1:D:724:SER:HB3	1:D:728:GLN:NE2	2.28	0.49
1:B:710:TYR:OH	1:B:766:ASP:OD1	2.21	0.49
1:D:843:GLY:H	3:D:1102:GOL:H2	1.78	0.49
1:A:891:PHE:HA	1:A:936:SER:O	2.12	0.49
1:A:942:PRO:HA	1:B:965:ASP:OD1	2.13	0.49
1:D:964:LEU:C	1:D:964:LEU:HD23	2.38	0.49
1:A:746:MET:HE2	1:A:746:MET:N	2.28	0.48
1:C:872:ILE:HG21	1:C:920:LEU:HD11	1.96	0.48
1:D:843:GLY:H	3:D:1102:GOL:C2	2.27	0.48
1:D:891:PHE:HA	1:D:936:SER:O	2.14	0.48
1:B:872:ILE:HG21	1:B:920:LEU:HD11	1.95	0.48
1:D:712:ILE:CD1	1:D:739:LEU:HD12	2.40	0.48
1:A:964:LEU:C	1:A:964:LEU:HD23	2.39	0.47
1:D:916:ILE:HD11	1:D:1004:LYS:HD2	1.95	0.47
1:B:667:LYS:HB3	1:B:668:PRO:HD3	1.97	0.47
1:D:710:TYR:OH	1:D:766:ASP:OD1	2.23	0.47
1:C:823:ALA:HB1	1:C:986:TYR:CZ	2.49	0.47
1:D:813:ILE:HD12	1:D:962:ILE:CD1	2.45	0.47
1:D:823:ALA:HB1	1:D:986:TYR:CZ	2.49	0.47
1:B:823:ALA:HB1	1:B:986:TYR:CZ	2.50	0.46
1:C:916:ILE:HD11	1:C:1004:LYS:HD2	1.97	0.46
1:A:1002:LEU:C	1:A:1002:LEU:HD23	2.41	0.45
1:D:755:ALA:HB1	1:D:887:THR:HG21	1.97	0.45
1:A:745:GLY:C	1:A:746:MET:HE2	2.41	0.45
1:D:667:LYS:HB3	1:D:668:PRO:HD3	1.98	0.45
1:C:667:LYS:HB3	1:C:668:PRO:HD3	1.98	0.45
1:A:872:ILE:HG21	1:A:920:LEU:HD11	1.98	0.45
1:A:823:ALA:HB1	1:A:986:TYR:CZ	2.51	0.45
1:D:916:ILE:HD11	1:D:1004:LYS:CD	2.46	0.45
1:D:942:PRO:HA	1:C:965:ASP:OD1	2.17	0.45
1:C:696:MET:HE1	1:C:740:ILE:HG23	1.98	0.44
1:B:887:THR:HB	5:B:1303:HOH:O	2.17	0.44
1:A:710:TYR:OH	1:A:766:ASP:OD1	2.23	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:742:HIS:HE1	1:D:764:MET:HE1	1.82	0.44
1:A:667:LYS:HB3	1:A:668:PRO:HD3	1.97	0.44
1:B:1002:LEU:C	1:B:1002:LEU:HD23	2.42	0.44
1:A:696:MET:HE2	1:A:705:GLN:NE2	2.33	0.44
1:D:1002:LEU:HD23	1:D:1002:LEU:C	2.42	0.44
1:C:1002:LEU:C	1:C:1002:LEU:HD23	2.42	0.44
1:D:958:PRO:CG	1:B:978:GLY:O	2.65	0.44
1:C:916:ILE:HD11	1:C:1004:LYS:CD	2.48	0.44
1:A:834:ILE:HD11	1:A:1006:LYS:HB2	2.00	0.43
1:A:843:GLY:H	3:A:1102:GOL:H2	1.83	0.43
1:A:934:HIS:ND1	1:D:981:ASP:HA	2.34	0.43
1:C:710:TYR:OH	1:C:766:ASP:OD1	2.22	0.43
1:B:672:LEU:HA	1:B:675:MET:HE3	2.01	0.42
1:D:834:ILE:HD11	1:D:1006:LYS:HB2	2.02	0.42
1:C:834:ILE:HD11	1:C:1006:LYS:HB2	2.01	0.42
1:C:759:GLN:NE2	2:C:1101:RPB:H191	2.34	0.42
1:B:971:LEU:HD12	1:B:971:LEU:C	2.45	0.41
1:B:759:GLN:N	5:B:1303:HOH:O	2.52	0.41
1:B:834:ILE:HD11	1:B:1006:LYS:HB2	2.03	0.41

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	341/372 (92%)	338 (99%)	3 (1%)	0	100	100
1	B	342/372 (92%)	340 (99%)	2 (1%)	0	100	100
1	C	335/372 (90%)	331 (99%)	4 (1%)	0	100	100
1	D	333/372 (90%)	331 (99%)	2 (1%)	0	100	100
All	All	1351/1488 (91%)	1340 (99%)	11 (1%)	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	303/326 (93%)	296 (98%)	7 (2%)	44	51
1	B	304/326 (93%)	299 (98%)	5 (2%)	55	64
1	C	300/326 (92%)	295 (98%)	5 (2%)	53	62
1	D	298/326 (91%)	293 (98%)	5 (2%)	53	62
All	All	1205/1304 (92%)	1183 (98%)	22 (2%)	51	60

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	662	LYS
1	A	702	SER
1	A	739	LEU
1	A	747	LYS
1	A	777	LEU
1	A	813	ILE
1	A	962	ILE
1	D	662	LYS
1	D	777	LEU
1	D	786	SER
1	D	830	ASP
1	D	1011	THR
1	C	698	LEU
1	C	724	SER
1	C	786	SER
1	C	824	THR
1	C	887	THR
1	B	662	LYS
1	B	704	ARG
1	B	731	ASP
1	B	747	LYS
1	B	1010	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	705	GLN
1	A	793	ASN
1	A	909	HIS
1	A	998	ASN
1	D	717	GLN
1	D	728	GLN
1	D	767	ASN
1	D	822	HIS
1	D	846	GLN
1	D	909	HIS
1	D	980	ASN
1	C	717	GLN
1	C	759	GLN
1	C	980	ASN
1	C	1008	ASN
1	B	717	GLN
1	B	909	HIS
1	B	912	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

16 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
4	SO4	A	1104	-	4,4,4	0.33	0	6,6,6	0.08	0
2	RPB	A	1101	-	27,27,27	0.22	0	31,39,39	0.84	1 (3%)
3	GOL	B	1201	-	5,5,5	0.09	0	5,5,5	0.26	0
4	SO4	A	1103	-	4,4,4	0.34	0	6,6,6	0.09	0
4	SO4	B	1203	-	4,4,4	0.34	0	6,6,6	0.11	0
3	GOL	A	1102	-	5,5,5	0.11	0	5,5,5	0.22	0
4	SO4	B	1204	-	4,4,4	0.34	0	6,6,6	0.08	0
3	GOL	D	1102	-	5,5,5	0.10	0	5,5,5	0.23	0
4	SO4	A	1105	-	4,4,4	0.33	0	6,6,6	0.07	0
4	SO4	C	1102	-	4,4,4	0.34	0	6,6,6	0.08	0
2	RPB	C	1101	-	27,27,27	0.19	0	31,39,39	0.85	2 (6%)
4	SO4	C	1104	-	4,4,4	0.33	0	6,6,6	0.08	0
2	RPB	B	1202	-	27,27,27	0.20	0	31,39,39	0.89	1 (3%)
4	SO4	D	1103	-	4,4,4	0.31	0	6,6,6	0.08	0
2	RPB	D	1101	-	27,27,27	0.19	0	31,39,39	0.87	1 (3%)
4	SO4	C	1103	-	4,4,4	0.33	0	6,6,6	0.09	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	RPB	A	1101	-	-	0/7/17/17	0/3/4/4
3	GOL	B	1201	-	-	2/4/4/4	-
3	GOL	A	1102	-	-	2/4/4/4	-
3	GOL	D	1102	-	-	2/4/4/4	-
2	RPB	C	1101	-	-	0/7/17/17	0/3/4/4
2	RPB	B	1202	-	-	0/7/17/17	0/3/4/4
2	RPB	D	1101	-	-	0/7/17/17	0/3/4/4

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1202	RPB	C9-C10-C5	-3.22	120.42	127.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	1101	RPB	C9-C10-C5	-3.04	120.79	127.25
2	A	1101	RPB	C9-C10-C5	-2.95	120.99	127.25
2	C	1101	RPB	C9-C10-C5	-2.75	121.41	127.25
2	C	1101	RPB	C1-C6-C5	-2.21	120.70	123.15

There are no chirality outliers.

All (6) torsion outliers are listed below:

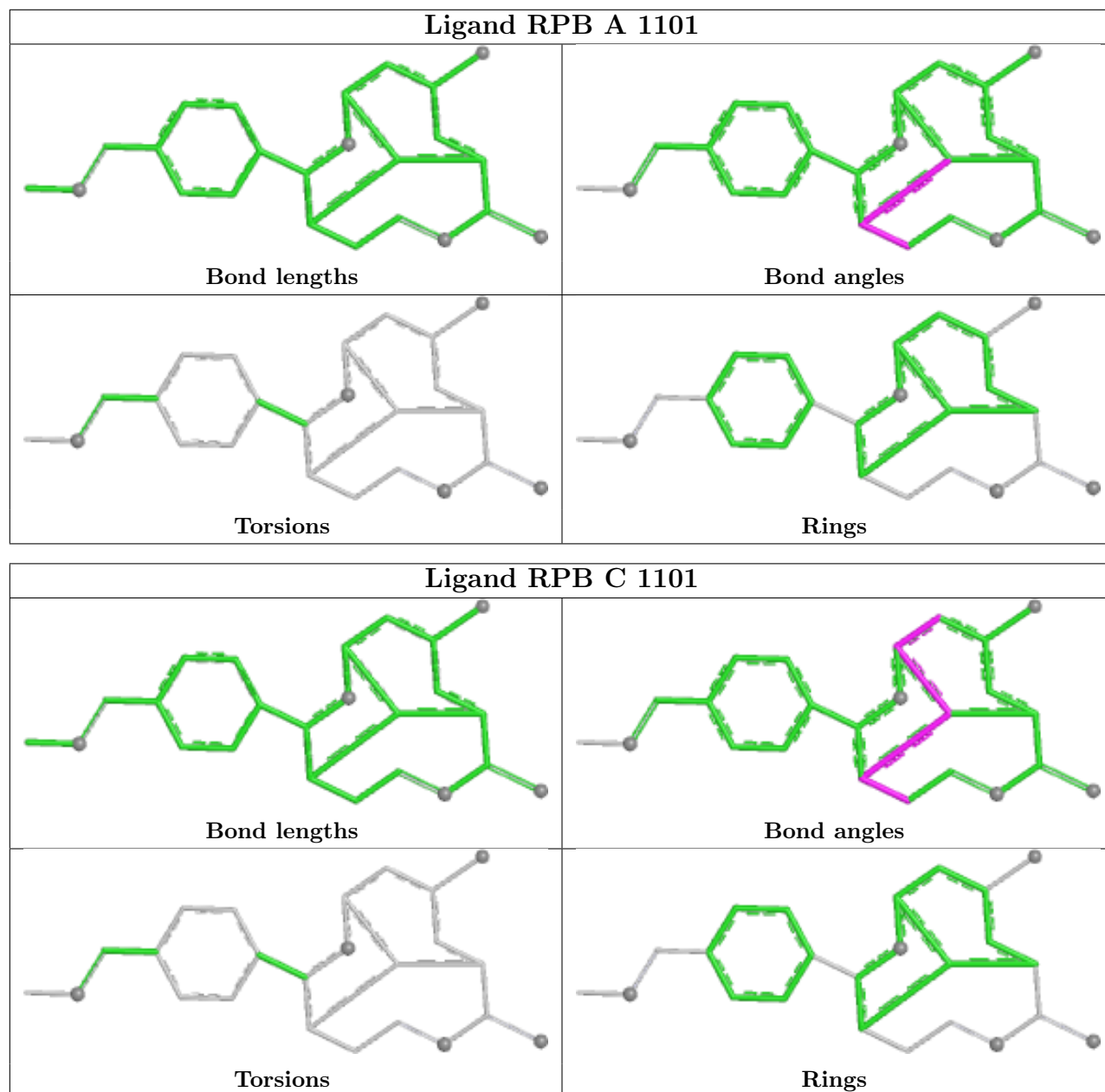
Mol	Chain	Res	Type	Atoms
3	B	1201	GOL	O1-C1-C2-C3
3	A	1102	GOL	O1-C1-C2-C3
3	D	1102	GOL	O1-C1-C2-C3
3	A	1102	GOL	O1-C1-C2-O2
3	D	1102	GOL	O1-C1-C2-O2
3	B	1201	GOL	O1-C1-C2-O2

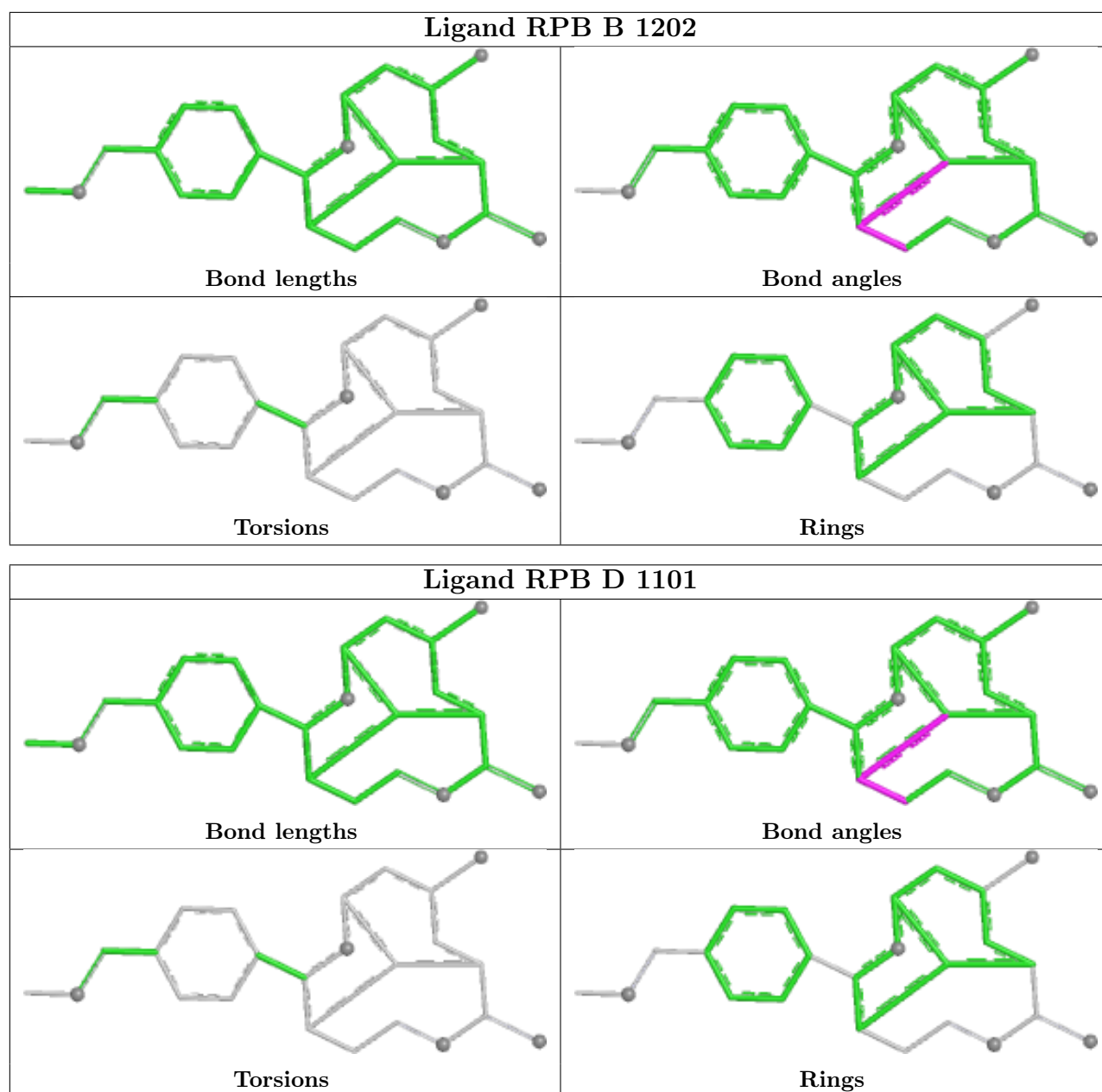
There are no ring outliers.

4 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1102	GOL	1	0
3	D	1102	GOL	2	0
2	C	1101	RPB	1	0
2	B	1202	RPB	1	0

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





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [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	345/372 (92%)	0.61	30 (8%) 16 16	30, 50, 83, 105	0
1	B	345/372 (92%)	0.52	23 (6%) 24 25	26, 48, 77, 105	1 (0%)
1	C	340/372 (91%)	0.82	31 (9%) 15 15	35, 61, 94, 119	1 (0%)
1	D	339/372 (91%)	0.99	47 (13%) 6 6	37, 70, 109, 136	0
All	All	1369/1488 (92%)	0.73	131 (9%) 13 14	26, 55, 97, 136	2 (0%)

All (131) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	938	ILE	5.7
1	A	701	LEU	4.6
1	A	780	GLY	4.2
1	C	937	HIS	4.1
1	A	1011	THR	4.1
1	B	1011	THR	4.0
1	D	790	ILE	4.0
1	A	698	LEU	3.9
1	C	1011	THR	3.8
1	D	780	GLY	3.7
1	B	937	HIS	3.7
1	B	938	ILE	3.7
1	C	935	ALA	3.7
1	A	705	GLN	3.5
1	C	727	SER	3.5
1	A	746	MET	3.4
1	A	913	GLY	3.4
1	D	963	SER	3.3
1	C	725	SER	3.3
1	A	805	ASP	3.3
1	D	691	ILE	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	965	ASP	3.2
1	A	702	SER	3.2
1	D	828	ALA	3.1
1	C	807	ASP	3.1
1	C	939	SER	3.1
1	B	746	MET	3.1
1	C	729	ILE	3.1
1	D	687	VAL	3.1
1	D	824	THR	3.0
1	C	724	SER	2.9
1	D	973	THR	2.9
1	A	697	PRO	2.9
1	C	936	SER	2.9
1	D	962	ILE	2.9
1	C	916	ILE	2.8
1	D	1008	ASN	2.8
1	B	939	SER	2.8
1	C	696	MET	2.8
1	D	975	ILE	2.8
1	A	699	GLY	2.8
1	A	729	ILE	2.8
1	D	730	LEU	2.8
1	C	909[A]	HIS	2.7
1	C	981	ASP	2.7
1	A	745	GLY	2.7
1	C	1010	LYS	2.7
1	A	772	GLU	2.7
1	A	662	LYS	2.7
1	D	830	ASP	2.7
1	B	744	PHE	2.7
1	A	962	ILE	2.7
1	C	732	LEU	2.6
1	A	747	LYS	2.6
1	B	662	LYS	2.6
1	C	886	VAL	2.6
1	D	1011	THR	2.6
1	A	777	LEU	2.6
1	D	788	ASP	2.6
1	A	756	ASP	2.6
1	D	725	SER	2.6
1	D	732	LEU	2.6
1	D	778	LEU	2.6

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Mol	Chain	Res	Type	RSRZ
1	C	914	ASP	2.5
1	A	696	MET	2.5
1	A	786	SER	2.5
1	D	751	LEU	2.5
1	B	704	ARG	2.5
1	B	807	ASP	2.5
1	C	978	GLY	2.5
1	C	887	THR	2.4
1	D	958	PRO	2.4
1	B	886	VAL	2.4
1	B	914	ASP	2.4
1	D	721	SER	2.4
1	D	738	THR	2.4
1	D	705	GLN	2.4
1	D	749	PRO	2.4
1	A	704	ARG	2.4
1	D	806	ARG	2.4
1	A	963	SER	2.4
1	A	739	LEU	2.3
1	A	978	GLY	2.3
1	D	964	LEU	2.3
1	D	974	GLY	2.3
1	C	687	VAL	2.3
1	D	752	LEU	2.3
1	B	745	GLY	2.3
1	D	775	TYR	2.3
1	B	909	HIS	2.2
1	B	705	GLN	2.2
1	D	822	HIS	2.2
1	A	790	ILE	2.2
1	D	792	VAL	2.2
1	D	967	VAL	2.2
1	C	778	LEU	2.2
1	D	779	ARG	2.2
1	B	749	PRO	2.2
1	A	788	ASP	2.2
1	C	979	VAL	2.2
1	B	780	GLY	2.2
1	D	698	LEU	2.2
1	C	751	LEU	2.2
1	B	748	LYS	2.2
1	D	968	ASP	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	853	GLN	2.1
1	D	854	LEU	2.1
1	C	913	GLY	2.1
1	D	787	LYS	2.1
1	B	663	SER	2.1
1	B	724	SER	2.1
1	C	980	ASN	2.1
1	D	807	ASP	2.1
1	D	914	ASP	2.1
1	D	852	LYS	2.1
1	C	664	LYS	2.1
1	D	693	LEU	2.1
1	C	739	LEU	2.1
1	D	696	MET	2.1
1	D	912	GLN	2.1
1	D	916	ILE	2.1
1	B	790	ILE	2.1
1	A	939	SER	2.1
1	A	830	ASP	2.0
1	D	694	GLN	2.0
1	B	887	THR	2.0
1	D	972	GLY	2.0
1	C	790	ILE	2.0
1	B	786	SER	2.0
1	C	685	ALA	2.0
1	D	662	LYS	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](#)

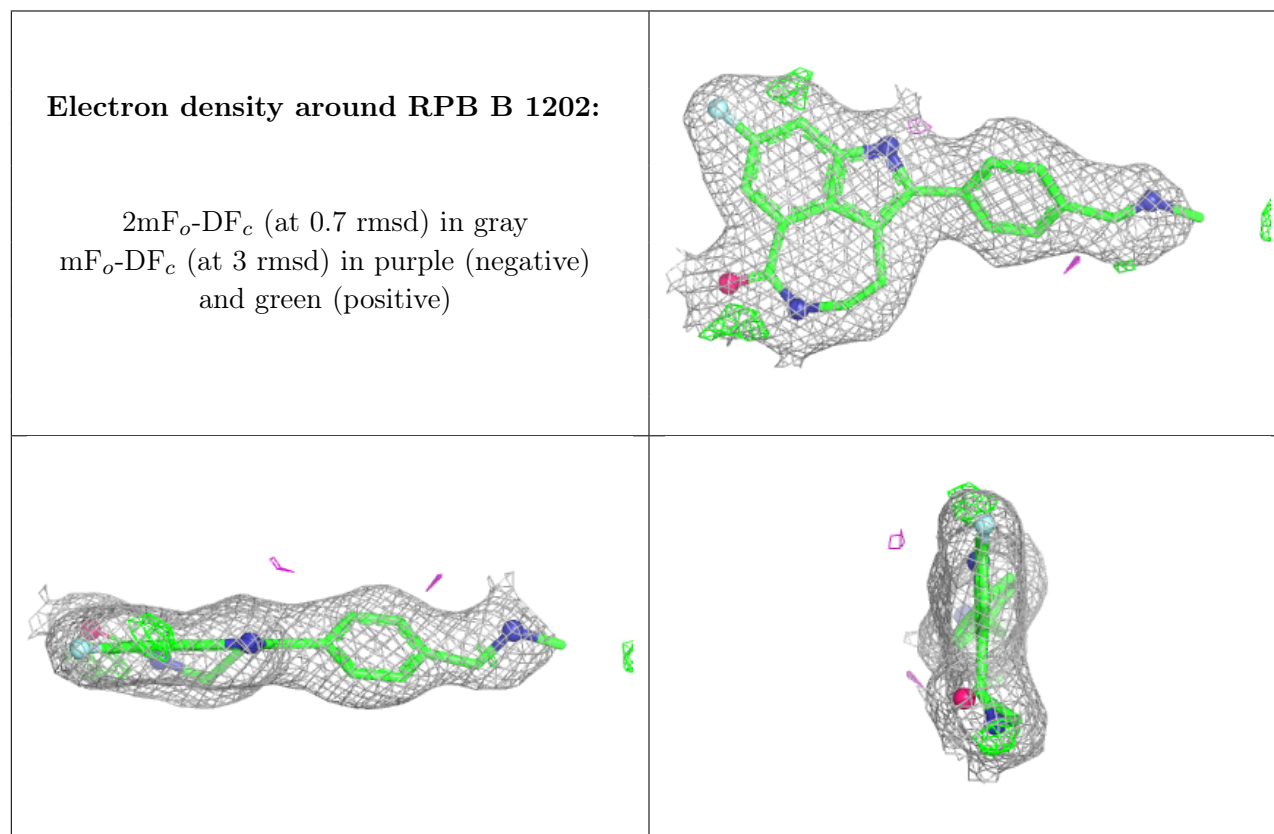
There are no oligosaccharides in this entry.

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.

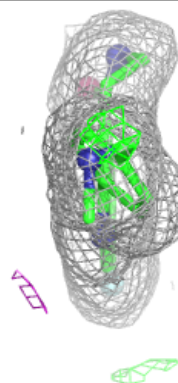
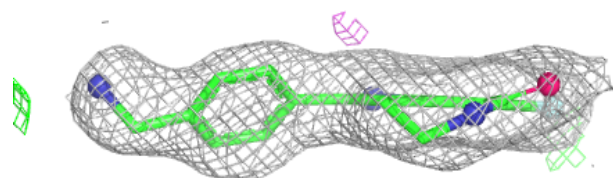
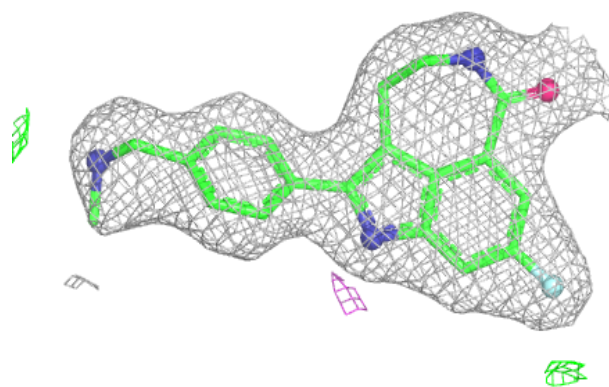
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	GOL	A	1102	6/6	0.64	0.26	63,63,66,68	0
3	GOL	D	1102	6/6	0.73	0.20	58,59,60,61	0
4	SO4	C	1104	5/5	0.77	0.09	80,81,81,81	0
4	SO4	A	1103	5/5	0.78	0.09	85,85,85,86	0
4	SO4	B	1204	5/5	0.78	0.09	86,87,88,89	0
4	SO4	A	1105	5/5	0.80	0.09	90,91,92,92	0
4	SO4	C	1102	5/5	0.82	0.09	79,80,80,81	0
3	GOL	B	1201	6/6	0.87	0.14	58,60,61,62	0
4	SO4	D	1103	5/5	0.88	0.14	64,65,67,69	0
2	RPB	B	1202	24/24	0.91	0.09	34,36,48,52	0
4	SO4	B	1203	5/5	0.92	0.12	47,48,52,53	0
4	SO4	C	1103	5/5	0.92	0.10	68,68,72,72	0
2	RPB	C	1101	24/24	0.93	0.08	38,40,53,57	0
2	RPB	D	1101	24/24	0.94	0.07	38,39,47,49	0
2	RPB	A	1101	24/24	0.94	0.07	31,33,38,39	0
4	SO4	A	1104	5/5	0.96	0.14	48,51,52,53	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.

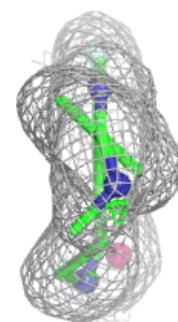
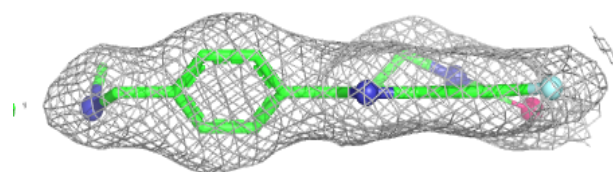
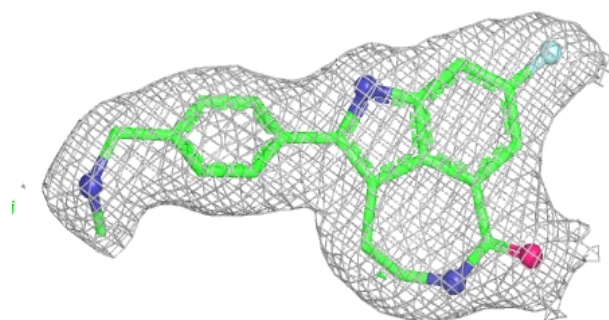


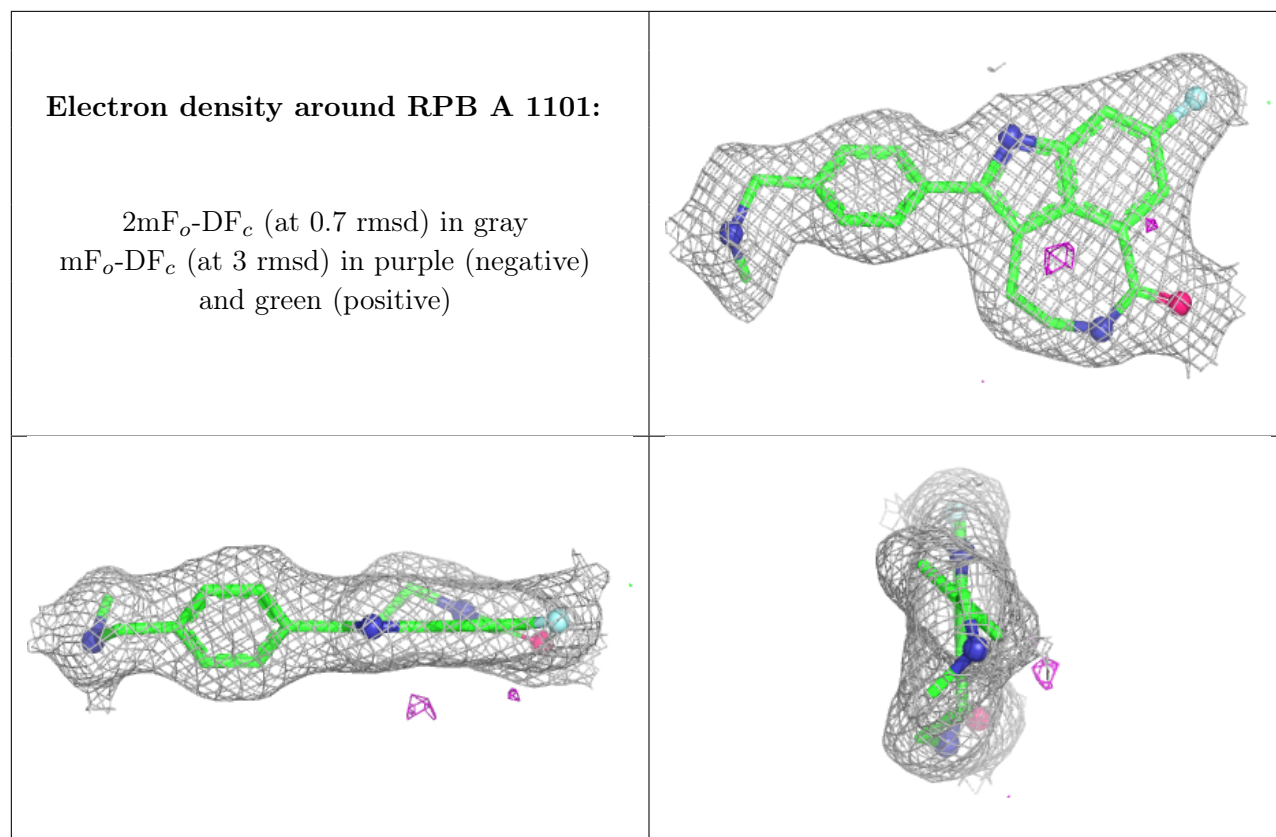
Electron density around RPB C 1101:

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

**Electron density around RPB D 1101:**

$2mF_o-DF_c$ (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.