



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 10, 2020 – 02:28 AM BST

PDB ID : 6VKK
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 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 : 2.13.1
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) : 2.13.1

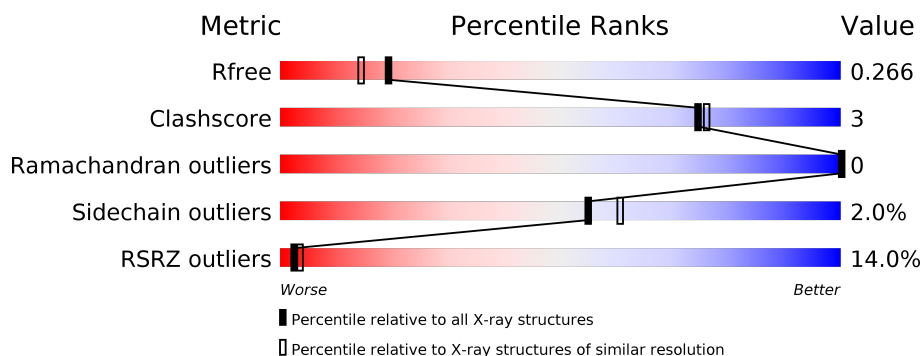
1 Overall quality at a glance

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}	130704	5197 (2.10-2.10)
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (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 on 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	<div> <div>9%</div> <div>85%</div> <div>8%</div> <div>7%</div> </div>
1	B	372	<div> <div>6%</div> <div>84%</div> <div>9%</div> <div>7%</div> </div>
1	C	372	<div> <div>15%</div> <div>83%</div> <div>8%</div> <div>9%</div> </div>
1	D	372	<div> <div>22%</div> <div>80%</div> <div>12%</div> <div>9%</div> </div>

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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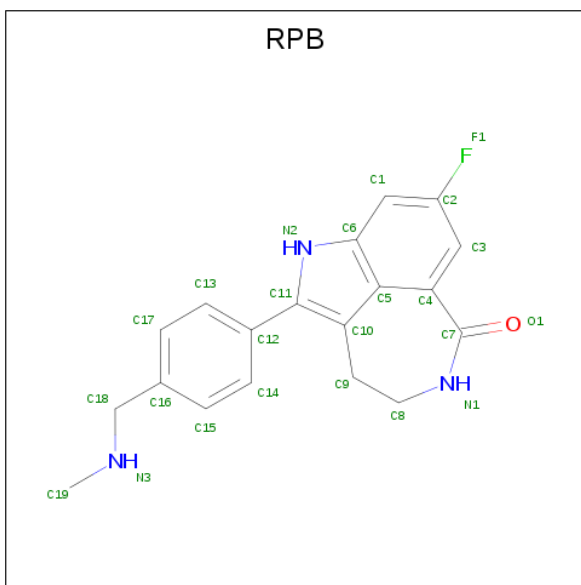
Chain	Residue	Modelled	Actual	Comment	Reference
A	762	ALA	VAL	variant	UNP P09874
D	640	MET	-	initiating methionine	UNP P09874
D	641	GLY	-	expression tag	UNP P09874
D	642	SER	-	expression tag	UNP P09874
D	643	SER	-	expression tag	UNP P09874
D	644	HIS	-	expression tag	UNP P09874
D	645	HIS	-	expression 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 (three-letter code: RPB) (formula: C₁₉H₁₈FN₃O) (labeled as "Ligand of Interest" by author).



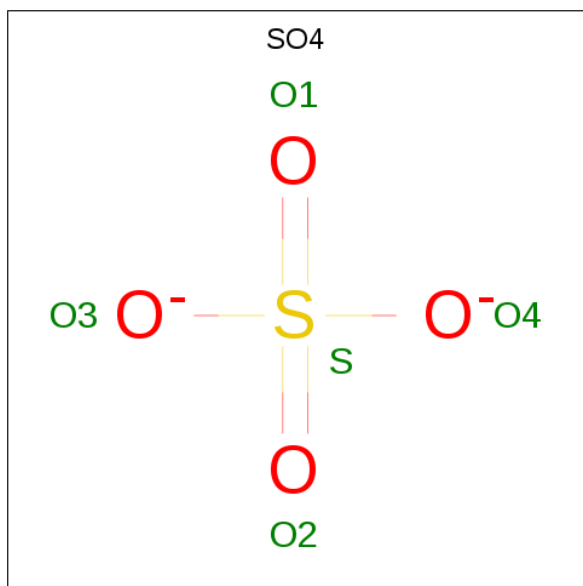
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	F	N	O	0	0
			24	19	1	3	1		
2	D	1	Total	C	F	N	O	0	0
			24	19	1	3	1		
2	C	1	Total	C	F	N	O	0	0
			24	19	1	3	1		
2	B	1	Total	C	F	N	O	0	0
			24	19	1	3	1		

- Molecule 3 is GLYCEROL (three-letter code: 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 (three-letter code: 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		

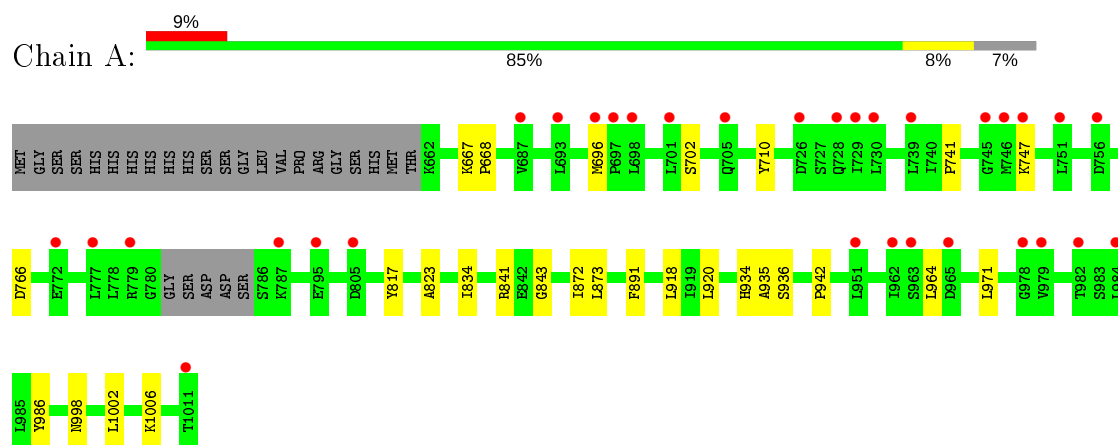
- Molecule 5 is water.

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

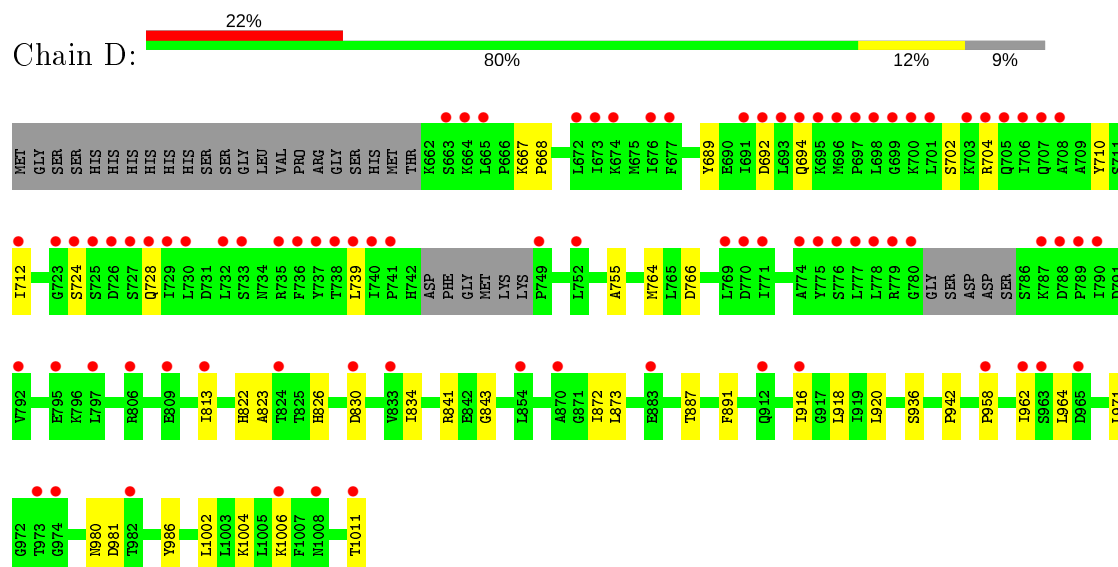
3 Residue-property plots [i](#)

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.

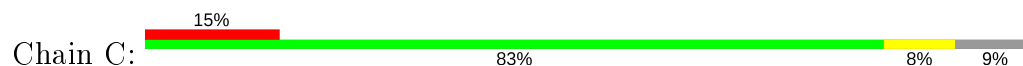
- Molecule 1: Poly [ADP-ribose] polymerase 1

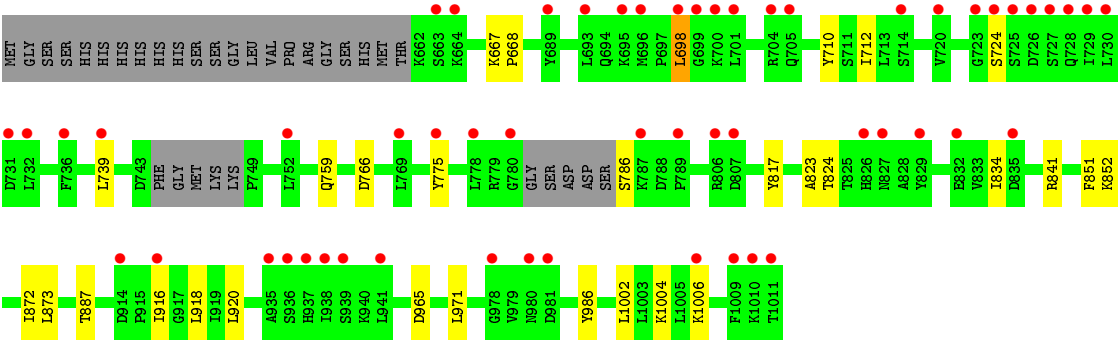


- Molecule 1: Poly [ADP-ribose] polymerase 1

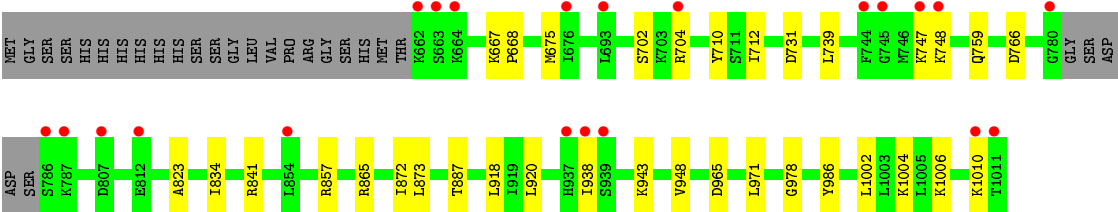
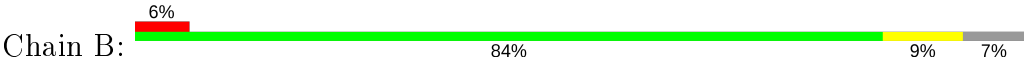


- Molecule 1: Poly [ADP-ribose] polymerase 1





● 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 47.92 – 2.10	Depositor EDS
% Data completeness (in resolution range)	99.1 (20.00-2.10) 99.2 (47.92-2.10)	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	4679 reflections (4.99%)	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 , 43.1	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: GOL, RPB, SO4

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	0.65	0/2770	0.74	0/3737
1	B	0.64	0/2778	0.73	1/3748 (0.0%)
1	C	0.65	0/2738	0.73	0/3695
1	D	0.64	0/2719	0.72	0/3669
All	All	0.64	0/11005	0.73	1/14849 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	857	ARG	CG-CD-NE	-5.06	101.18	111.80

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	16	0
1	B	2724	0	2775	19	0
1	C	2685	0	2729	16	0
1	D	2670	0	2718	27	0
2	A	24	0	18	0	0
2	B	24	0	18	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	24	0	18	1	0
2	D	24	0	18	0	0
3	A	6	0	8	1	0
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	70	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 3.

All (70) 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: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: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: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: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: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:B:938:ILE:CD1	1:B:948:VAL:HG21	2.39	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:852:LYS:NZ	5:C:1201:HOH:O	2.42	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:B:710:TYR:OH	1:B:766:ASP:OD1	2.21	0.49
1:D:689:TYR:HB3	1:D:764:MET:HE2	1.94	0.49
1:D:724:SER:HB3	1:D:728:GLN:NE2	2.28	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:C:872:ILE:HG21	1:C:920:LEU:HD11	1.96	0.48
1:B:872:ILE:HG21	1:B:920:LEU:HD11	1.95	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:D:712:ILE:CD1	1:D:739:LEU:HD12	2.40	0.48
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:D:755:ALA:HB1	1:D:887:THR:HG21	1.97	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:696:MET:HE3	1:A:741:PRO:HD2	1.99	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: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
1:A:667:LYS:HB3	1:A:668:PRO:HD3	1.97	0.44
1:D:964:LEU:HD23	1:D:964:LEU:C	2.38	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:964:LEU:HD23	1:A:964:LEU:C	2.39	0.43
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:759:GLN:N	5:B:1303:HOH:O	2.52	0.41
1:B:675:MET:CE	1:B:1004:LYS:HD2	2.50	0.41
1:B:834:ILE:HD11	1:B:1006:LYS:HB2	2.03	0.41
1:B:675:MET:HE3	1:B:675:MET:HB2	1.69	0.40
1:A:1002:LEU:HD23	1:A:1002:LEU:C	2.41	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	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 [i](#)

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%)	298 (98%)	5 (2%)	60	67
1	B	304/326 (93%)	297 (98%)	7 (2%)	50	55
1	C	300/326 (92%)	293 (98%)	7 (2%)	50	55
1	D	298/326 (91%)	293 (98%)	5 (2%)	60	67
All	All	1205/1304 (92%)	1181 (98%)	24 (2%)	55	60

All (24) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	702	SER
1	A	747	LYS
1	A	817	TYR
1	A	971	LEU
1	A	998	ASN
1	D	702	SER
1	D	704	ARG
1	D	830	ASP
1	D	971	LEU
1	D	1011	THR
1	C	698	LEU
1	C	724	SER
1	C	786	SER
1	C	817	TYR
1	C	824	THR
1	C	887	THR
1	C	971	LEU
1	B	702	SER
1	B	704	ARG
1	B	731	ASP
1	B	747	LYS
1	B	748	LYS
1	B	971	LEU
1	B	1010	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	705	GLN
1	A	998	ASN
1	D	728	GLN

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Mol	Chain	Res	Type
1	D	742	HIS
1	D	822	HIS
1	D	846	GLN
1	D	980	ASN
1	B	912	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 ⓘ

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	C	1102	-	4,4,4	0.39	0	6,6,6	0.05	0
4	SO4	B	1204	-	4,4,4	0.38	0	6,6,6	0.05	0
2	RPB	D	1101	-	25,27,27	0.66	0	28,39,39	0.82	2 (7%)
4	SO4	B	1203	-	4,4,4	0.37	0	6,6,6	0.09	0
2	RPB	B	1202	-	25,27,27	0.65	0	28,39,39	0.81	2 (7%)
3	GOL	B	1201	-	5,5,5	0.10	0	5,5,5	0.27	0
4	SO4	D	1103	-	4,4,4	0.35	0	6,6,6	0.06	0
4	SO4	C	1104	-	4,4,4	0.38	0	6,6,6	0.06	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	GOL	D	1102	-	5,5,5	0.09	0	5,5,5	0.24	0
4	SO4	A	1104	-	4,4,4	0.36	0	6,6,6	0.04	0
4	SO4	C	1103	-	4,4,4	0.38	0	6,6,6	0.06	0
3	GOL	A	1102	-	5,5,5	0.10	0	5,5,5	0.22	0
4	SO4	A	1103	-	4,4,4	0.39	0	6,6,6	0.06	0
2	RPB	C	1101	-	25,27,27	0.67	0	28,39,39	0.79	2 (7%)
2	RPB	A	1101	-	25,27,27	0.70	0	28,39,39	0.84	2 (7%)
4	SO4	A	1105	-	4,4,4	0.38	0	6,6,6	0.05	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	D	1101	-	-	2/6/17/17	0/3/4/4
2	RPB	B	1202	-	-	1/6/17/17	0/3/4/4
3	GOL	B	1201	-	-	2/4/4/4	-
3	GOL	D	1102	-	-	2/4/4/4	-
3	GOL	A	1102	-	-	2/4/4/4	-
2	RPB	C	1101	-	-	1/6/17/17	0/3/4/4
2	RPB	A	1101	-	-	1/6/17/17	0/3/4/4

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	1101	RPB	C11-N2-C6	2.62	109.29	103.90
2	A	1101	RPB	C11-N2-C6	2.61	109.25	103.90
2	B	1202	RPB	C11-N2-C6	2.59	109.22	103.90
2	C	1101	RPB	C11-N2-C6	2.59	109.21	103.90
2	C	1101	RPB	O1-C7-N1	-2.14	119.92	122.18
2	A	1101	RPB	O1-C7-N1	-2.13	119.93	122.18
2	B	1202	RPB	O1-C7-N1	-2.10	119.97	122.18
2	D	1101	RPB	O1-C7-N1	-2.05	120.02	122.18

There are no chirality outliers.

All (11) torsion outliers are listed below:

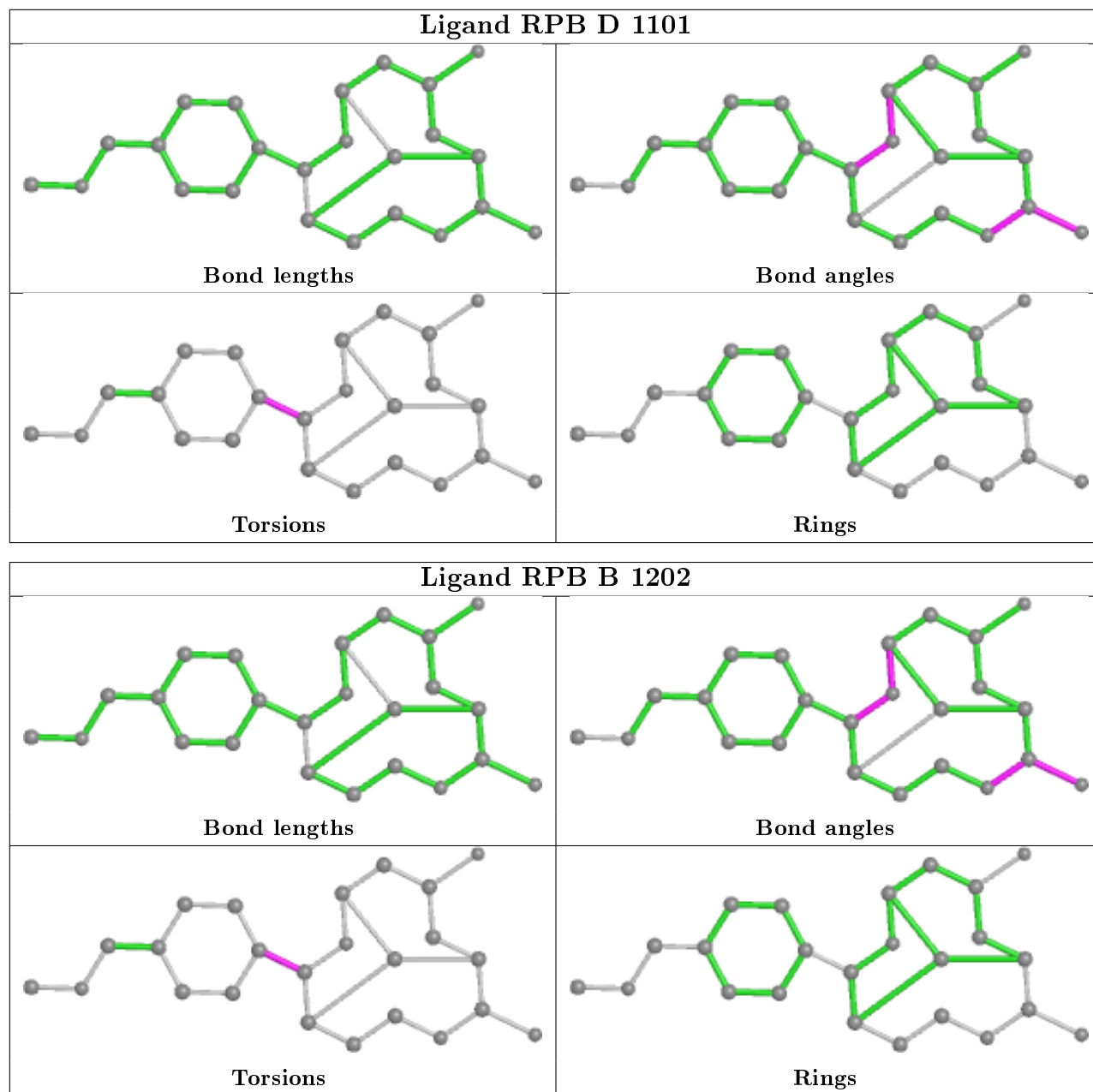
Mol	Chain	Res	Type	Atoms
3	B	1201	GOL	O1-C1-C2-C3
3	D	1102	GOL	O1-C1-C2-C3
3	A	1102	GOL	O1-C1-C2-C3
3	D	1102	GOL	O1-C1-C2-O2
3	A	1102	GOL	O1-C1-C2-O2
3	B	1201	GOL	O1-C1-C2-O2
2	D	1101	RPB	N2-C11-C12-C13
2	D	1101	RPB	N2-C11-C12-C14
2	B	1202	RPB	N2-C11-C12-C14
2	C	1101	RPB	N2-C11-C12-C14
2	A	1101	RPB	N2-C11-C12-C14

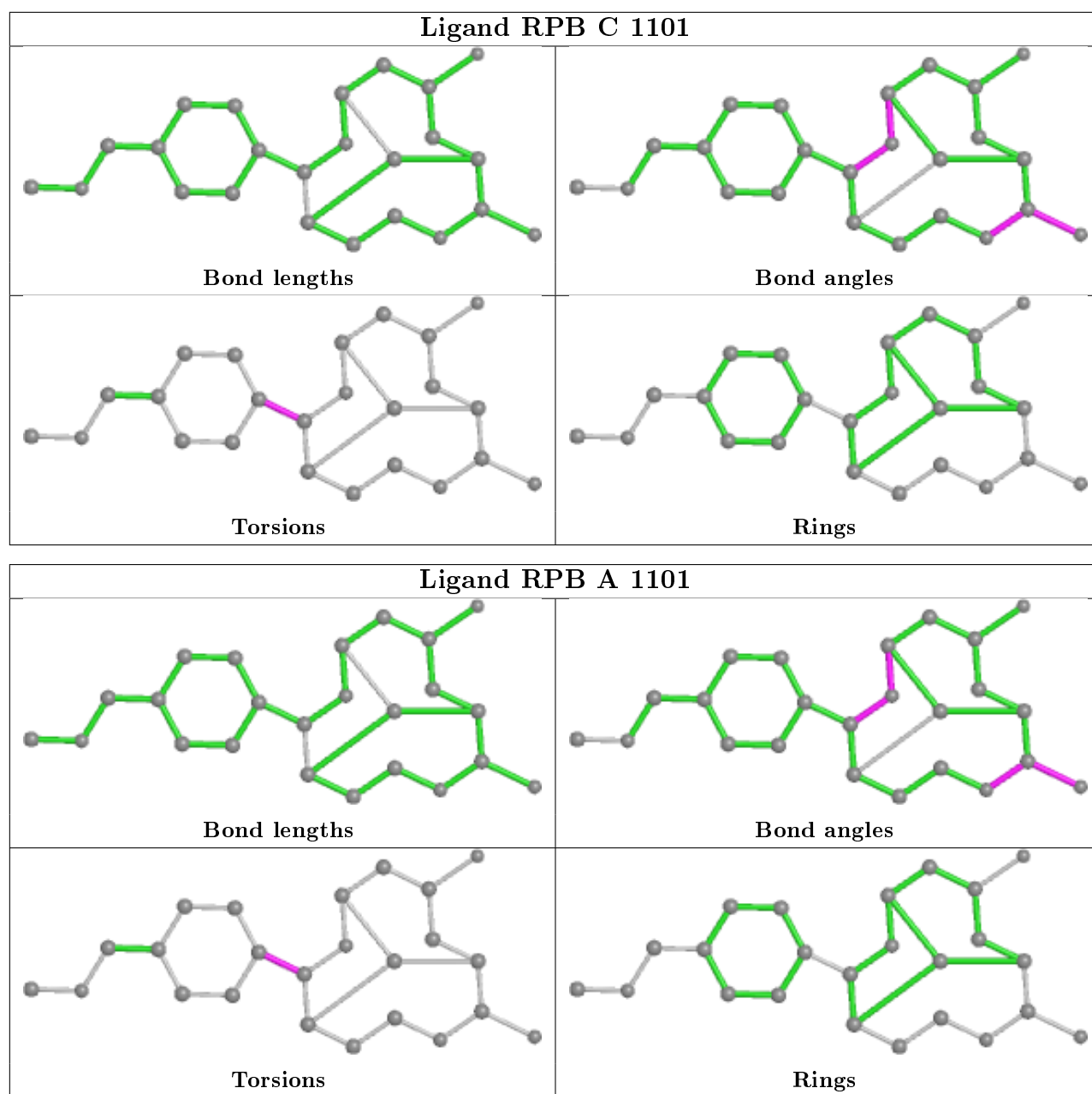
There are no ring outliers.

4 monomers are involved in 5 short contacts:

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

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	345/372 (92%)	0.90	32 (9%) 8 11	30, 50, 83, 105	0
1	B	345/372 (92%)	0.84	21 (6%) 21 26	31, 48, 77, 105	0
1	C	340/372 (91%)	1.16	55 (16%) 1 2	36, 61, 94, 119	0
1	D	339/372 (91%)	1.45	83 (24%) 0 0	37, 70, 109, 136	0
All	All	1369/1488 (92%)	1.08	191 (13%) 2 3	30, 55, 97, 136	0

All (191) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	1011	THR	10.8
1	D	693	LEU	7.8
1	A	1011	THR	7.8
1	C	937	HIS	7.5
1	C	1011	THR	7.5
1	D	706	ILE	7.4
1	D	775	TYR	6.6
1	D	696	MET	6.6
1	D	691	ILE	6.4
1	D	778	LEU	6.3
1	C	939	SER	6.2
1	C	938	ILE	5.9
1	C	727	SER	5.7
1	C	732	LEU	5.7
1	D	705	GLN	5.6
1	D	701	LEU	5.5
1	D	730	LEU	5.3
1	C	807	ASP	5.2
1	D	694	GLN	5.2
1	D	692	ASP	5.0
1	B	938	ILE	5.0

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Mol	Chain	Res	Type	RSRZ
1	C	725	SER	4.9
1	D	699	GLY	4.9
1	D	774	ALA	4.9
1	C	739	LEU	4.9
1	D	740	ILE	4.7
1	D	712	ILE	4.4
1	C	787	LYS	4.4
1	C	1010	LYS	4.4
1	D	732	LEU	4.3
1	C	724	SER	4.3
1	A	728	GLN	4.2
1	C	664	LYS	4.2
1	C	696	MET	4.2
1	C	728	GLN	4.2
1	A	701	LEU	4.2
1	B	939	SER	4.2
1	D	725	SER	4.0
1	D	916	ILE	4.0
1	D	736	PHE	4.0
1	D	728	GLN	3.9
1	D	708	ALA	3.9
1	D	739	LEU	3.9
1	B	744	PHE	3.8
1	D	792	VAL	3.8
1	B	787	LYS	3.7
1	D	806	ARG	3.7
1	B	664	LYS	3.7
1	D	674	LYS	3.7
1	D	698	LEU	3.6
1	D	729	ILE	3.6
1	D	777	LEU	3.6
1	D	780	GLY	3.5
1	D	733	SER	3.5
1	B	807	ASP	3.5
1	D	824	THR	3.4
1	A	747	LYS	3.4
1	B	937	HIS	3.4
1	D	1011	THR	3.3
1	D	672	LEU	3.3
1	C	726	ASP	3.3
1	D	963	SER	3.3
1	B	1010	LYS	3.3

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Mol	Chain	Res	Type	RSRZ
1	C	980	ASN	3.2
1	C	723	GLY	3.2
1	A	730	LEU	3.2
1	D	665	LEU	3.2
1	C	663	SER	3.2
1	C	700	LYS	3.2
1	D	830	ASP	3.2
1	D	727	SER	3.2
1	A	698	LEU	3.2
1	D	790	ILE	3.2
1	D	700	LYS	3.2
1	D	965	ASP	3.1
1	C	730	LEU	3.1
1	D	724	SER	3.1
1	B	663	SER	3.1
1	C	705	GLN	3.1
1	A	696	MET	3.1
1	D	749	PRO	3.1
1	D	779	ARG	3.1
1	D	912	GLN	3.0
1	D	982	THR	3.0
1	D	752	LEU	3.0
1	C	829	TYR	3.0
1	A	705	GLN	3.0
1	C	914	ASP	3.0
1	D	741	PRO	3.0
1	D	738	THR	3.0
1	D	770	ASP	3.0
1	D	677	PHE	2.9
1	D	663	SER	2.9
1	D	726	ASP	2.9
1	D	973	THR	2.9
1	D	769	LEU	2.9
1	B	747	LYS	2.9
1	A	746	MET	2.9
1	D	789	PRO	2.9
1	C	698	LEU	2.9
1	D	703	LYS	2.9
1	C	978	GLY	2.9
1	D	737	TYR	2.9
1	C	701	LEU	2.9
1	C	916	ILE	2.8

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Mol	Chain	Res	Type	RSRZ
1	C	936	SER	2.8
1	A	729	ILE	2.8
1	A	805	ASP	2.8
1	D	974	GLY	2.8
1	A	751	LEU	2.8
1	C	736	PHE	2.8
1	D	704	ARG	2.8
1	C	778	LEU	2.7
1	C	827	ASN	2.7
1	A	697	PRO	2.7
1	C	789	PRO	2.7
1	A	787	LYS	2.7
1	C	981	ASP	2.7
1	D	833	VAL	2.7
1	D	676	ILE	2.7
1	D	1006	LYS	2.7
1	D	787	LYS	2.6
1	D	735	ARG	2.6
1	B	748	LYS	2.6
1	C	699	GLY	2.6
1	A	951	LEU	2.6
1	A	772	GLU	2.6
1	D	776	SER	2.6
1	C	720	VAL	2.6
1	B	786	SER	2.6
1	C	689	TYR	2.5
1	A	982	THR	2.5
1	D	673	ILE	2.5
1	B	676	ILE	2.5
1	A	963	SER	2.5
1	B	780	GLY	2.5
1	A	962	ILE	2.5
1	D	795	GLU	2.5
1	C	806	ARG	2.5
1	D	788	ASP	2.5
1	D	697	PRO	2.4
1	A	965	ASP	2.4
1	A	687	VAL	2.4
1	C	731	ASP	2.4
1	C	826	HIS	2.4
1	D	809	GLU	2.4
1	C	714	SER	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	704	ARG	2.4
1	D	695	LYS	2.3
1	D	958	PRO	2.3
1	D	883	GLU	2.3
1	C	695	LYS	2.3
1	A	745	GLY	2.3
1	D	723	GLY	2.3
1	A	756	ASP	2.3
1	B	854	LEU	2.3
1	A	795	GLU	2.3
1	B	812	GLU	2.3
1	D	771	ILE	2.3
1	C	729	ILE	2.3
1	A	739	LEU	2.3
1	C	693	LEU	2.2
1	A	726	ASP	2.2
1	D	797	LEU	2.2
1	D	1008	ASN	2.2
1	D	707	GLN	2.2
1	C	769	LEU	2.2
1	C	832	GLU	2.2
1	C	835	ASP	2.2
1	A	984	LEU	2.2
1	D	854	LEU	2.2
1	C	752	LEU	2.2
1	C	780	GLY	2.2
1	C	704	ARG	2.1
1	A	777	LEU	2.1
1	C	1009	PHE	2.1
1	C	1006	LYS	2.1
1	D	813	ILE	2.1
1	A	693	LEU	2.1
1	A	978	GLY	2.1
1	D	962	ILE	2.1
1	C	941	LEU	2.1
1	B	693	LEU	2.1
1	C	935	ALA	2.1
1	D	664	LYS	2.1
1	A	979	VAL	2.0
1	D	870	ALA	2.0
1	B	745	GLY	2.0
1	C	775	TYR	2.0

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Mol	Chain	Res	Type	RSRZ
1	B	662	LYS	2.0
1	A	779	ARG	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 monosaccharides in this entry.

6.4 Ligands [i](#)

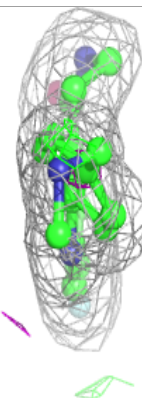
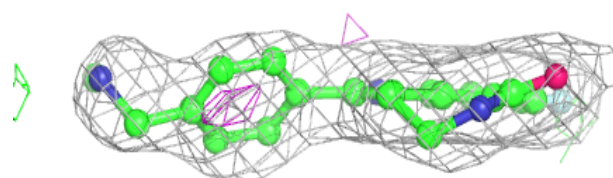
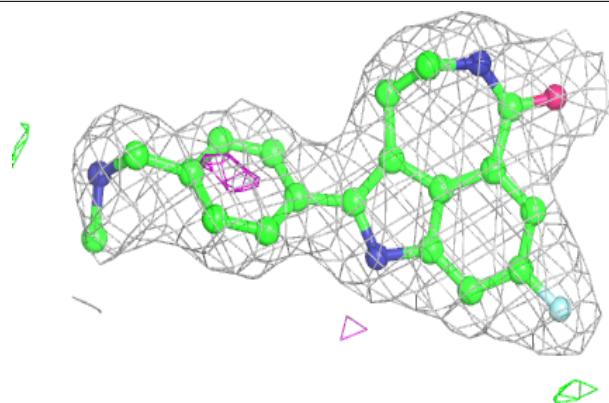
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	GOL	A	1102	6/6	0.64	0.31	63,63,66,68	0
3	GOL	D	1102	6/6	0.73	0.26	58,59,60,61	0
3	GOL	B	1201	6/6	0.79	0.30	58,60,61,62	0
4	SO4	C	1104	5/5	0.89	0.16	80,81,81,81	0
4	SO4	A	1105	5/5	0.92	0.16	90,91,92,92	0
4	SO4	B	1204	5/5	0.93	0.18	86,87,88,89	0
4	SO4	D	1103	5/5	0.93	0.13	64,65,67,69	0
2	RPB	C	1101	24/24	0.94	0.15	38,40,53,57	0
2	RPB	B	1202	24/24	0.94	0.15	34,36,48,52	0
4	SO4	A	1103	5/5	0.95	0.15	85,85,85,86	0
4	SO4	C	1102	5/5	0.95	0.11	79,80,80,81	0
2	RPB	D	1101	24/24	0.95	0.14	38,39,47,49	0
4	SO4	C	1103	5/5	0.96	0.10	68,68,72,72	0
4	SO4	A	1104	5/5	0.97	0.11	48,51,52,53	0
2	RPB	A	1101	24/24	0.97	0.15	31,33,38,39	0
4	SO4	B	1203	5/5	0.97	0.13	47,48,52,53	0

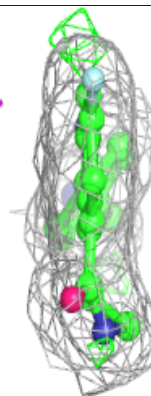
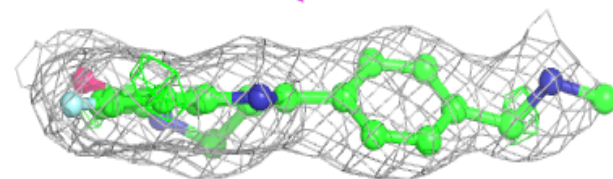
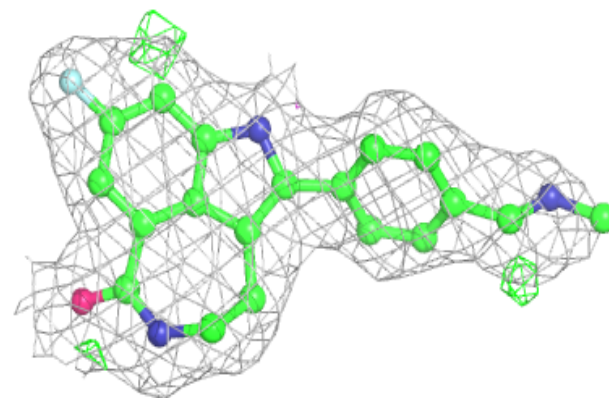
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation 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)

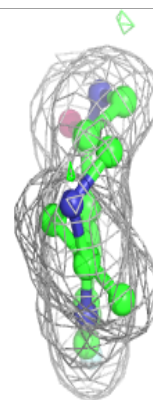
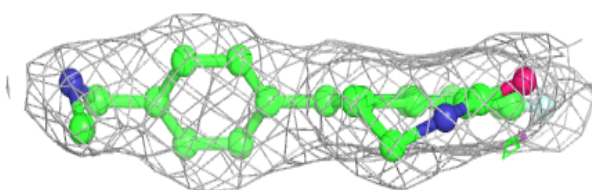
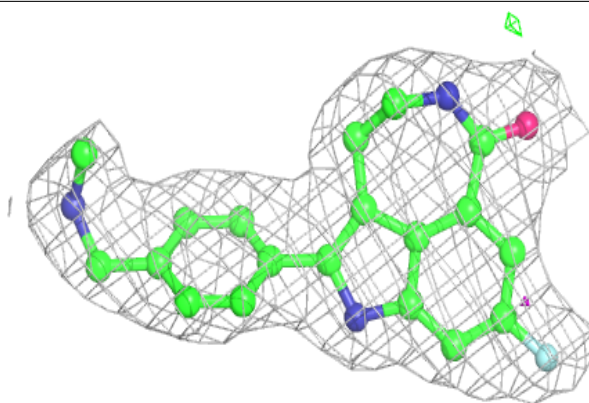
**Electron density around RPB B 1202:**

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

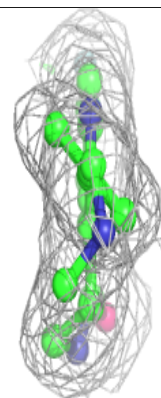
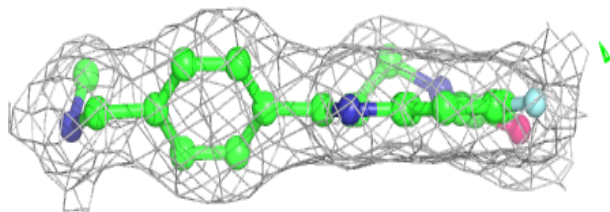
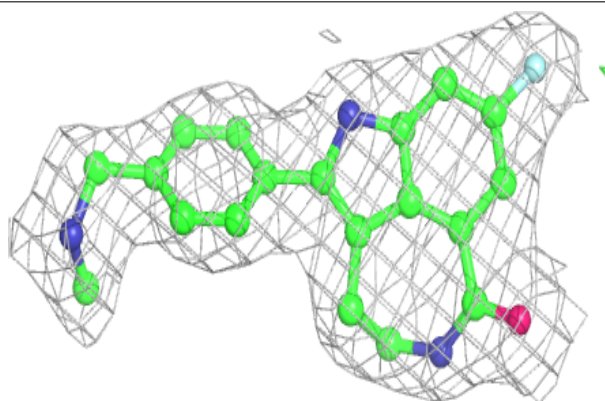


Electron density around RPB D 1101:

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

**Electron density around RPB A 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.