



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 04:14 AM UTC

PDB ID : 4NA4 / pdb_00004na4
Title : Crystal structure of mouse poly(ADP-ribose) glycohydrolase (PARG) catalytic domain with ADP-HPD
Authors : Wang, Z.; Cheng, Z.; Xu, W.
Deposited on : 2013-10-21
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

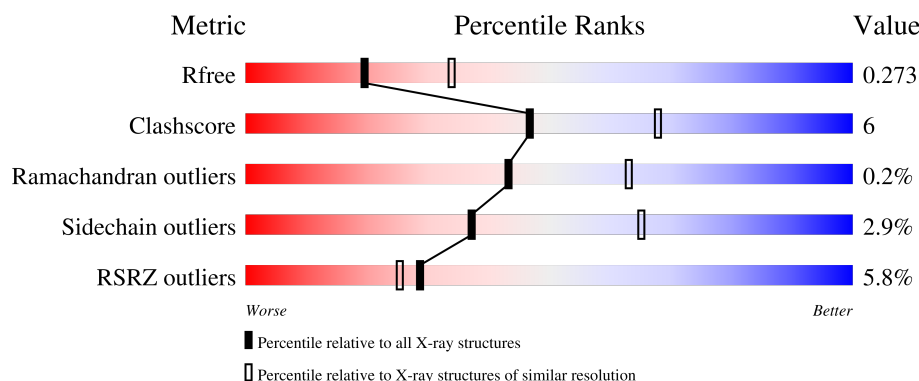
1 Overall quality at a glance

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	522	
1	B	522	
1	C	522	

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.

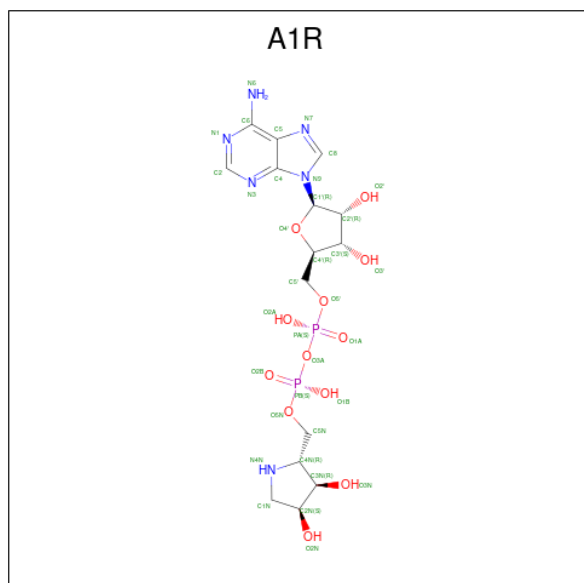
- Molecule 1 is a protein called Poly(ADP-ribose) glycohydrolase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	505	Total 4102	C 2621	N 714	O 744	S 14	Se 9	0	0	0
1	B	494	Total 4016	C 2565	N 700	O 728	S 14	Se 9	0	0	0
1	C	505	Total 4101	C 2619	N 714	O 745	S 14	Se 9	0	0	0

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	438	GLY	-	expression tag	UNP O88622
B	438	GLY	-	expression tag	UNP O88622
C	438	GLY	-	expression tag	UNP O88622

- Molecule 2 is 5'-O-[(S)-{[(S)-{[(2R,3R,4S)-3,4-DIHYDROXYPYRROLIDIN-2-YL]METHOXY}](HYDROXY)PHOSPHORYL]OXY}](HYDROXY)PHOSPHORYL]ADENOSINE (CCD ID: A1R) (formula: C₁₅H₂₄N₆O₁₂P₂).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			35	15	6	12	2		
2	B	1	Total	C	N	O	P	0	0
			35	15	6	12	2		
2	C	1	Total	C	N	O	P	0	0
			35	15	6	12	2		

- Molecule 3 is IODIDE ION (CCD ID: IOD) (formula: I).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	2	Total	I	0	0
			2	2		
3	B	1	Total	I	0	0
			1	1		
3	C	2	Total	I	0	0
			2	2		

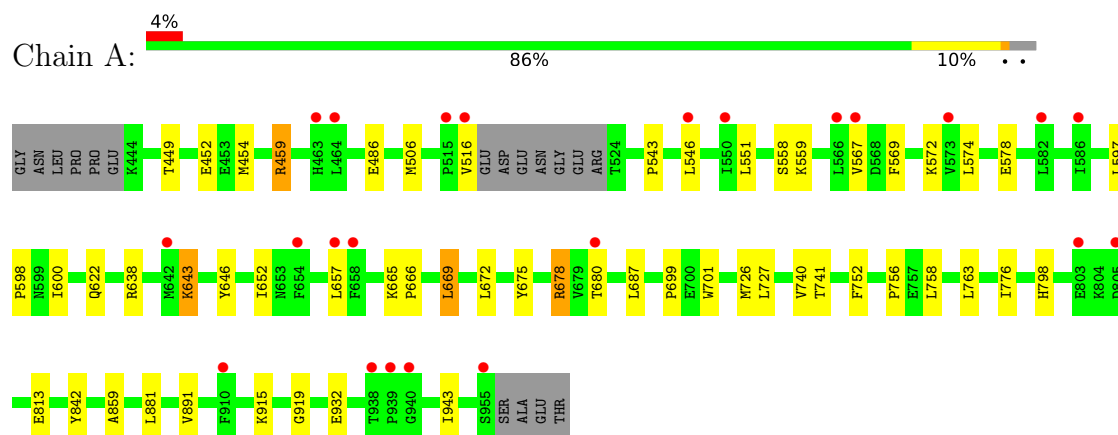
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	45	Total	O	0	0
			45	45		
4	B	6	Total	O	0	0
			6	6		
4	C	41	Total	O	0	0
			41	41		

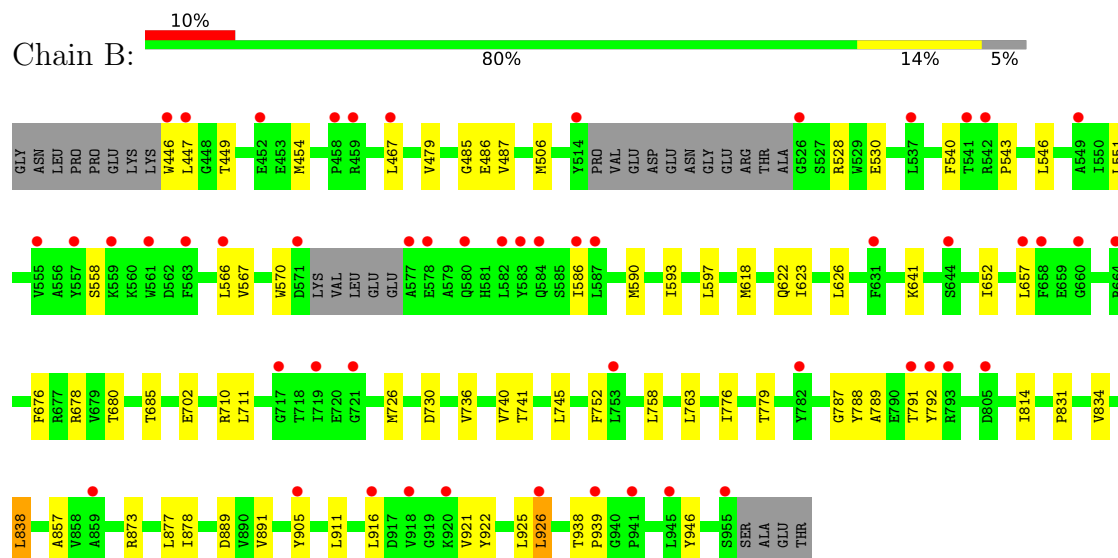
3 Residue-property plots [i](#)

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.

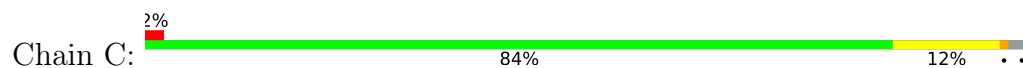
- Molecule 1: Poly(ADP-ribose) glycohydrolase

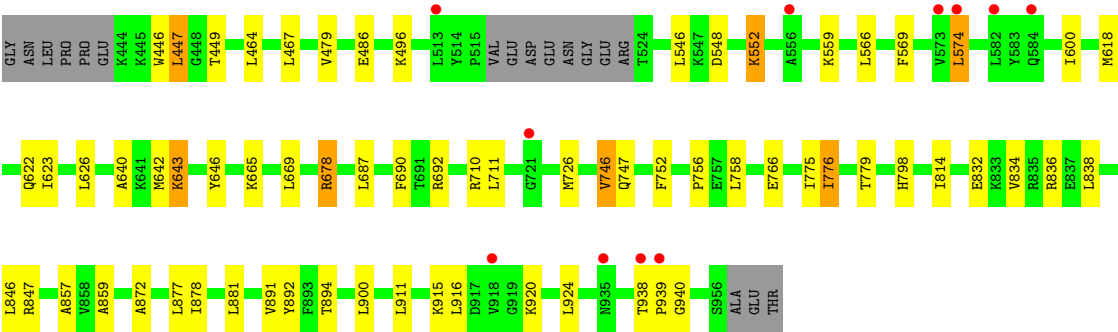


- Molecule 1: Poly(ADP-ribose) glycohydrolase



- Molecule 1: Poly(ADP-ribose) glycohydrolase





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	188.95Å 55.57Å 165.99Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.00 – 2.50 40.00 – 2.50	Depositor EDS
% Data completeness (in resolution range)	98.7 (40.00-2.50) 99.3 (40.00-2.50)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.71 (at 2.48Å)	Xtriage
Refinement program	REFMAC 5.5.0110	Depositor
R, R_{free}	0.242 , 0.282 0.236 , 0.273	Depositor DCC
R_{free} test set	3130 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	55.9	Xtriage
Anisotropy	0.306	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 52.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	12421	wwPDB-VP
Average B, all atoms (Å ²)	76.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 68.61 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 4.2432e-06. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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: IOD, A1R

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	0.49	0/4195	0.69	0/5663
1	B	0.41	0/4107	0.66	0/5543
1	C	0.49	0/4194	0.68	0/5661
All	All	0.46	0/12496	0.68	0/16867

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	4102	0	4072	32	0
1	B	4016	0	3972	57	0
1	C	4101	0	4068	50	0
2	A	35	0	22	0	0
2	B	35	0	22	1	0
2	C	35	0	22	2	0
3	A	2	0	0	0	0
3	B	1	0	0	0	0
3	C	2	0	0	0	0
4	A	45	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	6	0	0	1	0
4	C	41	0	0	1	0
All	All	12421	0	12178	139	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 6.

All (139) 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:C:779:THR:HG22	4:C:1107:HOH:O	1.72	0.89
1:B:618:MSE:HE1	1:B:626:LEU:HD12	1.56	0.87
1:C:726:MSE:HE2	1:C:859:ALA:HB2	1.56	0.85
1:C:618:MSE:CE	1:C:626:LEU:HD12	2.08	0.82
1:B:726:MSE:HE3	1:B:857:ALA:HB3	1.62	0.81
1:C:746:VAL:HG13	2:C:1001:A1R:O1A	1.80	0.80
1:A:726:MSE:HE1	1:A:891:VAL:HB	1.64	0.78
1:A:726:MSE:HE2	1:A:859:ALA:HB2	1.69	0.75
1:C:726:MSE:HE1	1:C:891:VAL:HB	1.68	0.75
1:B:618:MSE:HE1	1:B:626:LEU:CD1	2.16	0.74
1:C:938:THR:HG22	1:C:940:GLY:H	1.52	0.74
1:C:838:LEU:HD22	1:C:878:ILE:HG23	1.70	0.74
1:C:726:MSE:HE1	1:C:891:VAL:CG2	2.19	0.72
1:C:911:LEU:HD23	1:C:916:LEU:HD12	1.73	0.71
1:B:877:LEU:HD23	1:B:925:LEU:HD21	1.74	0.69
1:B:590:MSE:HE2	1:B:676:PHE:HB3	1.75	0.69
1:C:618:MSE:CE	1:C:626:LEU:CD1	2.71	0.69
1:B:838:LEU:HD13	1:B:878:ILE:HG23	1.75	0.68
1:C:618:MSE:HE3	1:C:626:LEU:HD12	1.76	0.68
1:B:726:MSE:HE1	1:B:891:VAL:CG2	2.26	0.66
1:C:746:VAL:HG13	1:C:747:GLN:H	1.61	0.65
1:A:932:GLU:HG2	1:A:943:ILE:HG22	1.77	0.65
1:C:726:MSE:HE1	1:C:891:VAL:CB	2.26	0.64
1:B:618:MSE:HE2	1:B:623:ILE:HG13	1.80	0.63
1:B:758:LEU:HD22	1:B:776:ILE:HD12	1.81	0.63
1:C:618:MSE:HE3	1:C:626:LEU:CD1	2.30	0.61
1:C:618:MSE:HE2	1:C:623:ILE:CG1	2.30	0.61
1:B:449:THR:HG21	1:B:710:ARG:HD2	1.80	0.61
1:B:467:LEU:O	1:B:479:VAL:HG11	2.00	0.61
1:A:678:ARG:NH2	1:A:798:HIS:O	2.34	0.60
1:C:877:LEU:O	1:C:881:LEU:HD13	2.02	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:546:LEU:HD23	1:B:566:LEU:HD21	1.83	0.60
1:A:726:MSE:HE1	1:A:891:VAL:CB	2.31	0.59
1:B:726:MSE:HE3	1:B:857:ALA:CB	2.33	0.59
1:C:618:MSE:HE2	1:C:623:ILE:HG12	1.84	0.59
1:C:618:MSE:HE1	1:C:626:LEU:CD1	2.31	0.59
1:B:740:VAL:HG13	1:B:741:THR:HG23	1.82	0.59
1:A:638:ARG:NH2	1:A:763:LEU:O	2.35	0.59
1:C:692:ARG:NH2	1:C:766:GLU:O	2.36	0.58
1:C:467:LEU:O	1:C:479:VAL:HG11	2.04	0.57
1:C:569:PHE:CE1	1:C:574:LEU:HD13	2.39	0.57
1:C:618:MSE:HE1	1:C:626:LEU:HD12	1.86	0.57
1:B:745:LEU:HD21	1:B:792:TYR:CD1	2.40	0.57
1:B:657:LEU:HD11	1:B:741:THR:HA	1.87	0.57
1:A:600:ILE:HG22	1:A:622:GLN:HG2	1.87	0.56
1:C:690:PHE:CD2	1:C:776:ILE:HD13	2.41	0.56
1:C:726:MSE:HE3	1:C:857:ALA:HB3	1.88	0.55
1:C:872:ALA:HB1	1:C:900:LEU:HD21	1.87	0.55
1:A:543:PRO:HB2	1:A:567:VAL:HG12	1.88	0.55
1:B:922:TYR:O	1:B:926:LEU:HD23	2.07	0.55
1:A:665:LYS:O	1:A:669:LEU:HD22	2.07	0.54
1:B:593:ILE:HD13	1:B:680:THR:HG22	1.89	0.54
1:C:746:VAL:HG13	1:C:747:GLN:N	2.22	0.54
1:C:746:VAL:CG1	2:C:1001:A1R:O1A	2.53	0.54
1:A:726:MSE:HE1	1:A:891:VAL:CG2	2.37	0.54
1:B:485:GLY:O	1:B:685:THR:HG21	2.07	0.54
1:B:758:LEU:HD11	1:B:814:ILE:CD1	2.38	0.53
1:A:657:LEU:HD21	1:A:672:LEU:HD12	1.90	0.53
1:B:831:PRO:HG3	1:B:926:LEU:HD13	1.90	0.53
1:A:752:PHE:O	1:A:756:PRO:HA	2.08	0.52
1:B:788:TYR:H	1:B:791:THR:HG23	1.73	0.52
1:B:454:MSE:HE1	1:B:889:ASP:HB3	1.92	0.52
1:C:752:PHE:O	1:C:756:PRO:HA	2.10	0.52
1:A:740:VAL:HG13	1:A:741:THR:HG23	1.91	0.51
1:C:779:THR:HG21	1:C:814:ILE:HD12	1.93	0.51
1:B:779:THR:HG21	1:B:814:ILE:HD12	1.92	0.51
1:C:640:ALA:HB3	1:C:643:LYS:HB2	1.93	0.51
1:C:726:MSE:HE1	1:C:891:VAL:HG21	1.92	0.51
1:A:643:LYS:HD3	1:A:646:TYR:HB2	1.93	0.51
1:B:618:MSE:HE2	1:B:623:ILE:CG1	2.40	0.51
1:B:551:LEU:HD22	1:B:558:SER:HA	1.93	0.50
1:C:920:LYS:O	1:C:924:LEU:HD13	2.11	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:543:PRO:CB	1:A:567:VAL:HG12	2.41	0.49
1:A:459:ARG:N	1:A:459:ARG:HD3	2.27	0.49
1:B:726:MSE:HE1	1:B:891:VAL:HB	1.94	0.49
1:C:642:MET:HA	1:C:642:MET:HE2	1.95	0.49
1:B:487:VAL:CG2	1:B:685:THR:HG22	2.44	0.48
1:C:449:THR:HG21	1:C:710:ARG:HD2	1.94	0.48
1:B:506:MSE:HE1	1:B:597:LEU:HD11	1.95	0.48
1:B:922:TYR:CZ	1:B:926:LEU:HD21	2.48	0.47
1:A:699:PRO:HD3	1:A:842:TYR:CE2	2.50	0.47
1:A:551:LEU:HD22	1:A:558:SER:HA	1.96	0.47
1:A:675:TYR:CG	1:A:756:PRO:HG2	2.51	0.46
1:C:938:THR:HG23	1:C:939:PRO:HD2	1.96	0.46
1:B:543:PRO:HD3	1:B:570:TRP:CD2	2.51	0.46
1:B:726:MSE:HE1	1:B:891:VAL:HG23	1.97	0.46
1:C:446:TRP:O	1:C:447:LEU:HD12	2.16	0.46
1:B:911:LEU:HD22	1:B:916:LEU:HD12	1.98	0.46
1:B:788:TYR:N	1:B:791:THR:HG23	2.32	0.45
1:C:665:LYS:O	1:C:669:LEU:HD23	2.17	0.45
1:C:726:MSE:HE3	1:C:857:ALA:CB	2.47	0.45
1:B:543:PRO:HB2	1:B:567:VAL:HG22	1.98	0.45
1:B:758:LEU:HD23	1:B:776:ILE:HG21	1.99	0.44
1:B:586:ILE:CG2	1:B:590:MSE:HE1	2.47	0.44
1:B:711:LEU:C	1:B:711:LEU:HD13	2.42	0.44
1:C:836:ARG:HD3	1:C:836:ARG:C	2.41	0.44
1:B:922:TYR:CE1	1:B:926:LEU:HD21	2.52	0.44
1:C:746:VAL:CG1	1:C:747:GLN:N	2.80	0.44
1:B:911:LEU:CD2	1:B:916:LEU:HD12	2.48	0.44
1:A:652:ILE:HG12	1:A:763:LEU:HD13	2.00	0.44
1:A:449:THR:HB	1:A:454:MSE:HE2	1.99	0.43
1:C:678:ARG:NH2	1:C:798:HIS:O	2.51	0.43
1:C:834:VAL:O	1:C:838:LEU:HD23	2.17	0.43
1:B:487:VAL:HG22	1:B:685:THR:HG22	1.99	0.43
1:A:516:VAL:O	1:A:516:VAL:HG12	2.17	0.43
1:B:586:ILE:HG22	1:B:590:MSE:CE	2.49	0.43
1:C:758:LEU:HD23	1:C:776:ILE:HG21	2.01	0.43
1:A:569:PHE:CZ	1:A:574:LEU:HD11	2.54	0.43
1:B:873:ARG:HB3	1:B:946:TYR:CE1	2.54	0.43
1:B:447:LEU:HD22	1:B:905:TYR:CD2	2.53	0.43
1:A:506:MSE:HE1	1:A:597:LEU:HD11	2.01	0.43
1:B:726:MSE:HE1	1:B:891:VAL:CB	2.49	0.43
1:C:548:ASP:O	1:C:552:LYS:HD3	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:574:LEU:HD22	1:A:578:GLU:HB3	2.01	0.42
1:A:597:LEU:N	1:A:598:PRO:HD2	2.35	0.42
1:A:701:TRP:O	1:A:919:GLY:HA2	2.20	0.42
1:A:657:LEU:HD21	1:A:672:LEU:CD1	2.50	0.42
1:C:600:ILE:HG22	1:C:622:GLN:HG2	2.02	0.41
1:A:758:LEU:HD23	1:A:776:ILE:HG21	2.02	0.41
1:B:652:ILE:HG12	1:B:763:LEU:HD13	2.02	0.41
1:B:618:MSE:HE3	1:B:622:GLN:HB3	2.03	0.41
1:B:740:VAL:HG21	1:B:752:PHE:HB3	2.03	0.41
1:C:643:LYS:HD2	1:C:646:TYR:HB2	2.03	0.41
1:B:736:VAL:HG22	4:B:1102:HOH:O	2.20	0.41
1:B:834:VAL:O	1:B:838:LEU:HD23	2.20	0.41
1:B:788:TYR:OH	2:B:1001:A1R:H5'1	2.21	0.41
1:B:911:LEU:HD13	1:B:921:VAL:HG21	2.02	0.41
1:B:447:LEU:HD13	1:B:905:TYR:HB3	2.03	0.40
1:C:642:MET:O	1:C:643:LYS:C	2.64	0.40
1:B:787:GLY:CA	1:B:791:THR:HG23	2.52	0.40
1:C:892:TYR:CE2	1:C:894:THR:HG22	2.56	0.40
1:A:726:MSE:HE2	1:A:859:ALA:CB	2.46	0.40
1:B:730:ASP:OD1	1:B:730:ASP:C	2.65	0.40
1:B:938:THR:HG23	1:B:939:PRO:HD2	2.03	0.40
1:C:775:ILE:HD13	1:C:847:ARG:CZ	2.52	0.40
1:A:727:LEU:HD23	1:A:813:GLU:CD	2.47	0.40
1:B:454:MSE:CE	1:B:889:ASP:HB3	2.51	0.40
1:C:911:LEU:CD2	1:C:916:LEU:HD12	2.47	0.40
1:A:665:LYS:N	1:A:666:PRO:CD	2.85	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	501/522 (96%)	487 (97%)	13 (3%)	1 (0%)	43	63
1	B	488/522 (94%)	459 (94%)	28 (6%)	1 (0%)	43	63
1	C	501/522 (96%)	485 (97%)	15 (3%)	1 (0%)	43	63
All	All	1490/1566 (95%)	1431 (96%)	56 (4%)	3 (0%)	43	63

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	643	LYS
1	C	643	LYS
1	B	789	ALA

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	445/450 (99%)	433 (97%)	12 (3%)	39	67
1	B	435/450 (97%)	425 (98%)	10 (2%)	44	72
1	C	445/450 (99%)	428 (96%)	17 (4%)	29	56
All	All	1325/1350 (98%)	1286 (97%)	39 (3%)	37	65

All (39) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	452	GLU
1	A	459	ARG
1	A	486	GLU
1	A	546	LEU
1	A	559	LYS
1	A	572	LYS
1	A	669	LEU
1	A	678	ARG
1	A	680	THR
1	A	687	LEU

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Mol	Chain	Res	Type
1	A	881	LEU
1	A	915	LYS
1	B	446	TRP
1	B	486	GLU
1	B	528	ARG
1	B	530	GLU
1	B	540	PHE
1	B	641	LYS
1	B	678	ARG
1	B	702	GLU
1	B	838	LEU
1	B	926	LEU
1	C	447	LEU
1	C	464	LEU
1	C	486	GLU
1	C	496	LYS
1	C	546	LEU
1	C	552	LYS
1	C	559	LYS
1	C	566	LEU
1	C	574	LEU
1	C	678	ARG
1	C	687	LEU
1	C	711	LEU
1	C	746	VAL
1	C	776	ILE
1	C	832	GLU
1	C	846	LEU
1	C	915	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	533	GLN
1	A	603	GLN
1	B	511	GLN
1	B	554	ASN
1	B	808	GLN
1	B	854	ASN
1	B	862	ASN
1	B	930	ASN
1	C	538	ASN

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Mol	Chain	Res	Type
1	C	610	GLN
1	C	629	ASN
1	C	808	GLN
1	C	854	ASN
1	C	951	HIS

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](#)

Of 8 ligands modelled in this entry, 5 are monoatomic - leaving 3 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	A1R	C	1001	-	38,38,38	0.89	1 (2%)	50,58,58	1.70	8 (16%)
2	A1R	A	1001	-	38,38,38	1.09	4 (10%)	50,58,58	1.78	11 (22%)
2	A1R	B	1001	-	38,38,38	0.89	2 (5%)	50,58,58	1.88	11 (22%)

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	A1R	C	1001	-	-	7/22/51/51	0/4/4/4
2	A1R	A	1001	-	-	6/22/51/51	0/4/4/4
2	A1R	B	1001	-	-	7/22/51/51	0/4/4/4

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1001	A1R	PA-O3A	2.55	1.62	1.59
2	A	1001	A1R	C8-N9	-2.47	1.33	1.37
2	A	1001	A1R	C5-N7	-2.44	1.34	1.39
2	B	1001	A1R	C5-N7	-2.41	1.34	1.39
2	A	1001	A1R	C8-N7	2.27	1.36	1.31
2	C	1001	A1R	C8-N7	2.22	1.35	1.31
2	B	1001	A1R	C8-N7	2.02	1.35	1.31

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1001	A1R	C5-C4-N3	-5.94	118.53	126.72
2	A	1001	A1R	N3-C2-N1	-5.24	120.66	128.58
2	C	1001	A1R	C5-C4-N3	-5.20	119.56	126.72
2	A	1001	A1R	C5-C4-N3	-5.05	119.76	126.72
2	B	1001	A1R	N3-C2-N1	-5.01	120.99	128.58
2	C	1001	A1R	N3-C2-N1	-4.68	121.49	128.58
2	B	1001	A1R	C1N-C2N-C3N	4.24	107.85	103.40
2	B	1001	A1R	N3-C4-N9	4.02	134.00	127.17
2	B	1001	A1R	C2-N3-C4	3.73	120.95	111.83
2	C	1001	A1R	N9-C8-N7	-3.69	108.70	113.94
2	C	1001	A1R	C2-N3-C4	3.67	120.80	111.83
2	A	1001	A1R	C2-N3-C4	3.58	120.58	111.83
2	A	1001	A1R	C1N-C2N-C3N	3.56	107.14	103.40
2	A	1001	A1R	N9-C8-N7	-3.30	109.25	113.94
2	C	1001	A1R	N3-C4-N9	3.30	132.78	127.17
2	B	1001	A1R	N9-C8-N7	-3.24	109.34	113.94
2	A	1001	A1R	C4-C5-N7	-3.17	106.96	110.58
2	C	1001	A1R	C4-C5-N7	-2.80	107.38	110.58
2	C	1001	A1R	C4-N9-C8	2.78	108.66	105.74
2	A	1001	A1R	N3-C4-N9	2.71	131.77	127.17
2	C	1001	A1R	C5-N7-C8	2.64	107.60	103.45
2	A	1001	A1R	C5-N7-C8	2.59	107.52	103.45
2	A	1001	A1R	C5-C4-N9	2.44	108.47	105.81
2	B	1001	A1R	C5-N7-C8	2.42	107.25	103.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1001	A1R	C3'-C2'-C1'	2.27	105.77	101.46
2	A	1001	A1R	C3'-C2'-C1'	2.23	105.68	101.46
2	B	1001	A1R	C4-C5-N7	-2.17	108.10	110.58
2	B	1001	A1R	C5'-C4'-C3'	-2.10	107.67	115.21
2	A	1001	A1R	O2A-PA-O1A	2.06	122.03	112.44
2	B	1001	A1R	C4-N9-C8	2.01	107.85	105.74

There are no chirality outliers.

All (20) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1001	A1R	C5N-O5N-PB-O3A
2	A	1001	A1R	C5N-O5N-PB-O2B
2	B	1001	A1R	C5'-O5'-PA-O1A
2	B	1001	A1R	C5'-O5'-PA-O2A
2	B	1001	A1R	C5'-O5'-PA-O3A
2	B	1001	A1R	PA-O3A-PB-O5N
2	B	1001	A1R	C5N-O5N-PB-O2B
2	B	1001	A1R	N4N-C4N-C5N-O5N
2	B	1001	A1R	C3N-C4N-C5N-O5N
2	C	1001	A1R	C5N-O5N-PB-O3A
2	C	1001	A1R	C5N-O5N-PB-O1B
2	C	1001	A1R	C5N-O5N-PB-O2B
2	A	1001	A1R	PA-O3A-PB-O5N
2	C	1001	A1R	PA-O3A-PB-O5N
2	C	1001	A1R	N4N-C4N-C5N-O5N
2	A	1001	A1R	C5N-O5N-PB-O1B
2	C	1001	A1R	C2'-C1'-N9-C8
2	A	1001	A1R	PB-O3A-PA-O1A
2	C	1001	A1R	PB-O3A-PA-O1A
2	A	1001	A1R	C2'-C1'-N9-C8

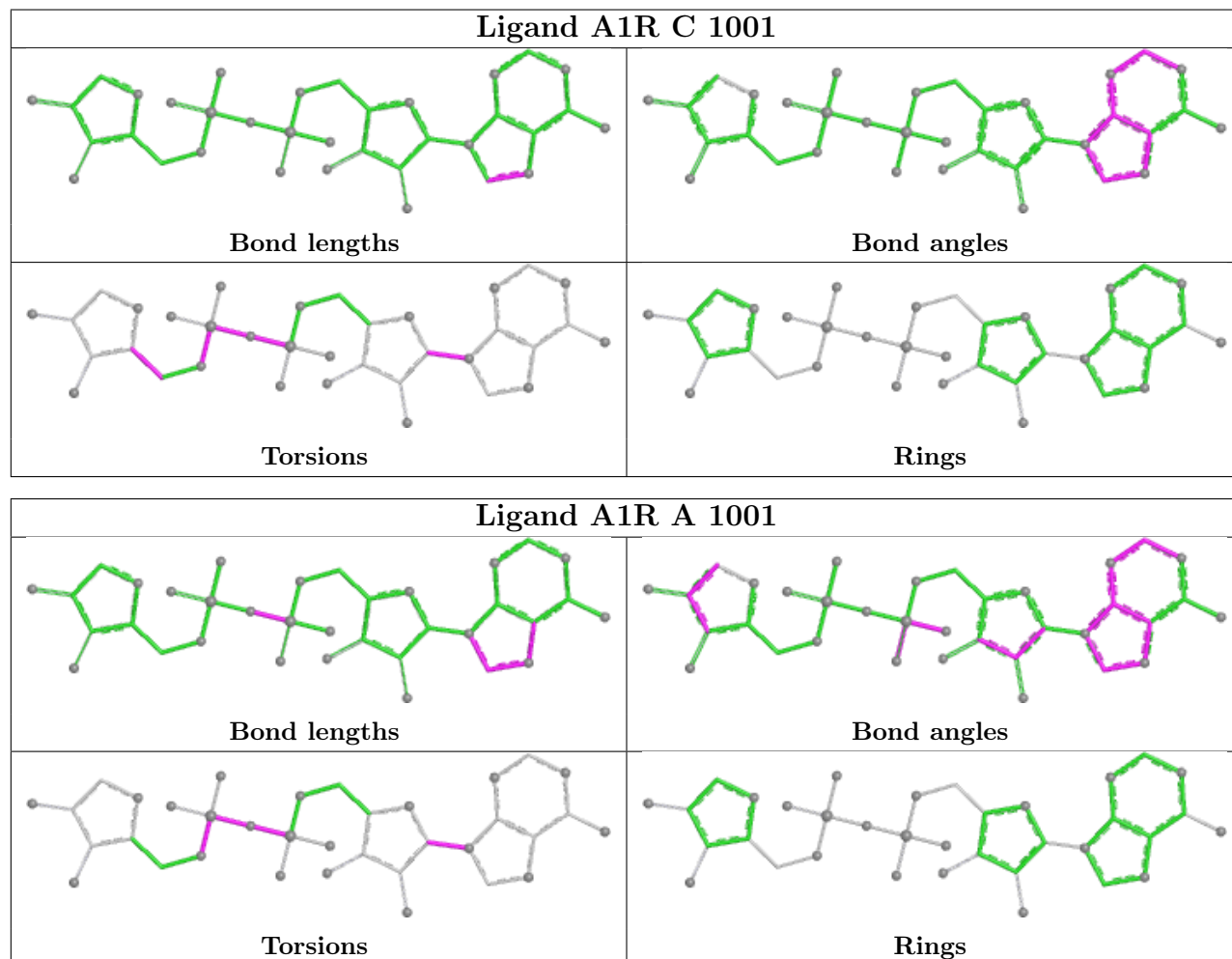
There are no ring outliers.

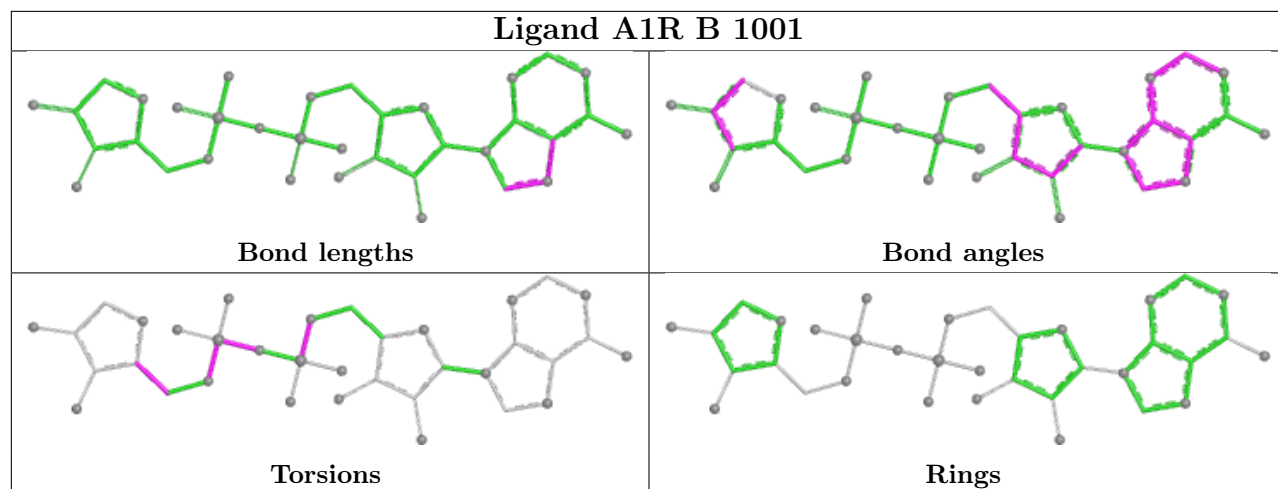
2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	1001	A1R	2	0
2	B	1001	A1R	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	496/522 (95%)	0.36	23 (4%) 37 33	27, 53, 101, 137	0
1	B	485/522 (92%)	0.90	52 (10%) 11 9	40, 106, 225, 331	0
1	C	496/522 (95%)	0.09	11 (2%) 62 58	26, 51, 92, 136	0
All	All	1477/1566 (94%)	0.45	86 (5%) 29 25	26, 62, 173, 331	0

All (86) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	515	PRO	5.7
1	B	582	LEU	5.5
1	B	514	TYR	5.1
1	B	577	ALA	4.8
1	B	658	PHE	4.5
1	C	582	LEU	4.3
1	B	526	GLY	4.3
1	A	546	LEU	4.1
1	B	916	LEU	4.0
1	B	559	LYS	4.0
1	B	905	TYR	4.0
1	A	516	VAL	3.7
1	A	566	LEU	3.6
1	A	658	PHE	3.6
1	B	578	GLU	3.4
1	A	573	VAL	3.3
1	C	938	THR	3.3
1	B	793	ARG	3.2
1	A	464	LEU	3.2
1	C	918	VAL	3.2
1	B	955	SER	3.1
1	B	657	LEU	3.1
1	C	721	GLY	3.1

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Mol	Chain	Res	Type	RSRZ
1	C	939	PRO	3.0
1	B	918	VAL	2.9
1	B	459	ARG	2.9
1	A	550	ILE	2.9
1	A	657	LEU	2.9
1	A	805	ASP	2.8
1	B	537	LEU	2.8
1	A	910	PHE	2.7
1	B	458	PRO	2.7
1	B	660	GLY	2.7
1	A	654	PHE	2.6
1	A	939	PRO	2.6
1	B	587	LEU	2.6
1	A	680	THR	2.6
1	A	463	HIS	2.6
1	B	557	TYR	2.6
1	B	792	TYR	2.6
1	B	561	TRP	2.6
1	B	563	PHE	2.6
1	A	586	ILE	2.6
1	B	719	ILE	2.6
1	A	582	LEU	2.6
1	B	580	GLN	2.6
1	B	859	ALA	2.5
1	B	446	TRP	2.5
1	B	571	ASP	2.5
1	B	926	LEU	2.5
1	B	945	LEU	2.5
1	B	721	GLY	2.5
1	B	555	VAL	2.5
1	B	583	TYR	2.4
1	B	644	SER	2.4
1	B	586	ILE	2.4
1	C	935	ASN	2.4
1	B	664	ARG	2.4
1	C	556	ALA	2.4
1	B	541	THR	2.3
1	B	717	GLY	2.3
1	B	447	LEU	2.3
1	B	566	LEU	2.3
1	C	513	LEU	2.3
1	C	573	VAL	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	467	LEU	2.2
1	B	753	LEU	2.2
1	B	791	THR	2.2
1	C	584	GLN	2.2
1	B	805	ASP	2.1
1	B	939	PRO	2.1
1	B	542	ARG	2.1
1	B	782	TYR	2.1
1	B	920	LYS	2.1
1	B	941	PRO	2.1
1	A	567	VAL	2.1
1	A	940	GLY	2.1
1	B	452	GLU	2.1
1	B	549	ALA	2.1
1	C	574	LEU	2.1
1	A	955	SER	2.1
1	B	584	GLN	2.0
1	B	631	PHE	2.0
1	A	803	GLU	2.0
1	A	938	THR	2.0
1	A	642	MET	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.

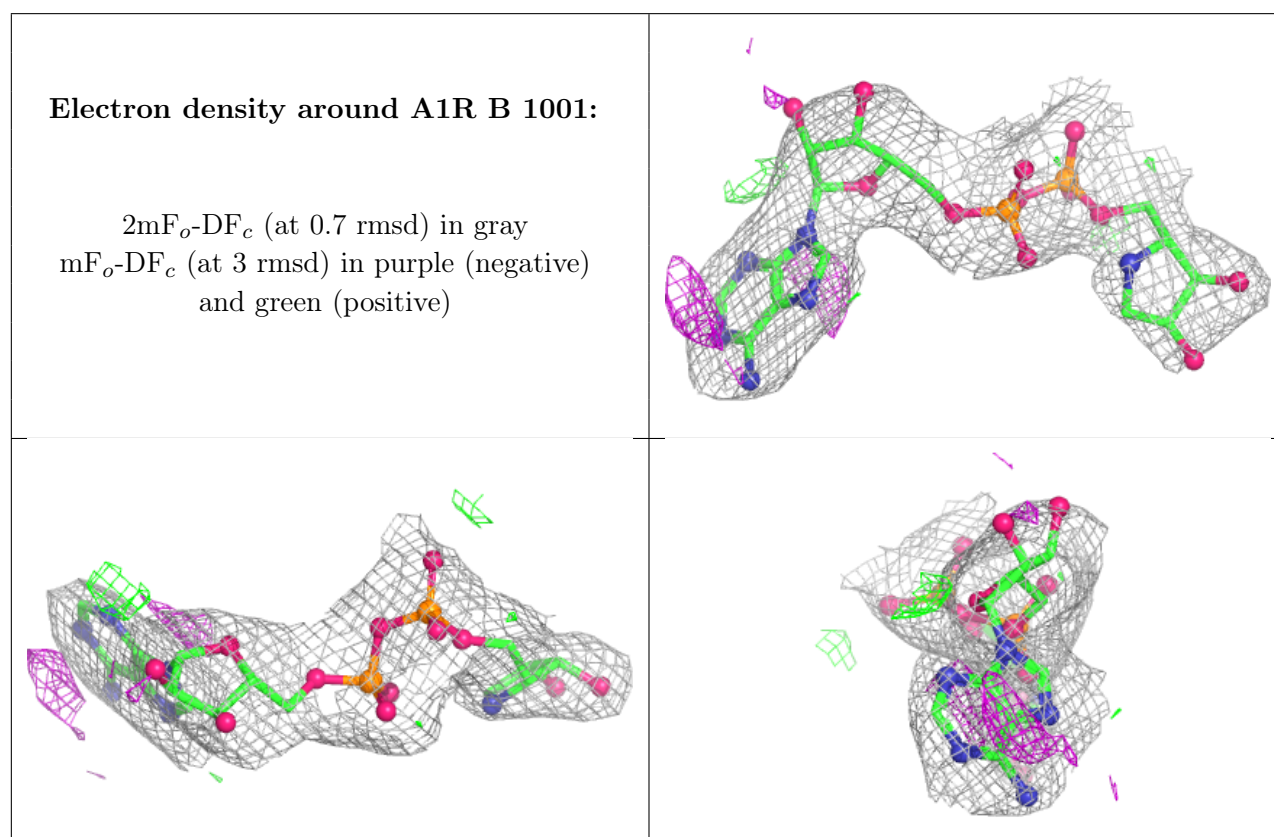
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	A1R	B	1001	35/35	0.86	0.12	45,62,67,71	0
3	IOD	B	1002	1/1	0.88	0.12	113,113,113,113	0

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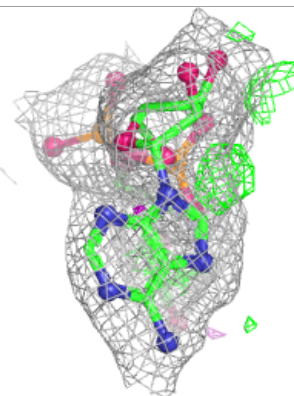
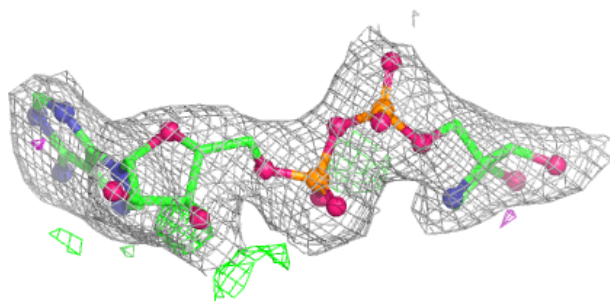
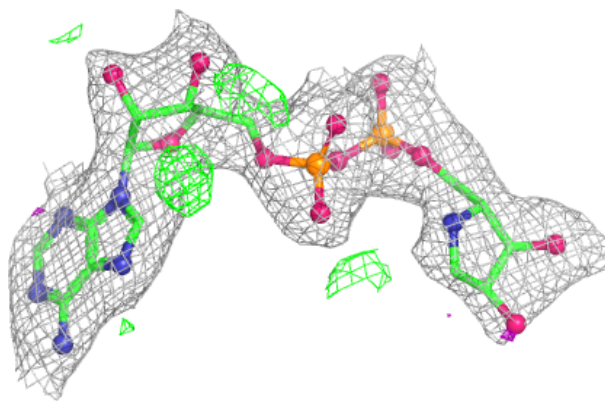
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	IOD	C	1003	1/1	0.93	0.38	121,121,121,121	0
2	A1R	A	1001	35/35	0.94	0.08	27,34,41,48	0
2	A1R	C	1001	35/35	0.95	0.07	26,34,39,41	0
3	IOD	C	1002	1/1	0.96	0.08	68,68,68,68	0
3	IOD	A	1003	1/1	0.97	0.12	66,66,66,66	0
3	IOD	A	1002	1/1	0.97	0.23	88,88,88,88	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.

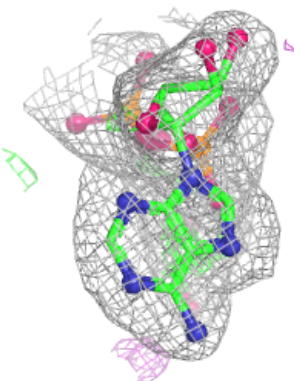
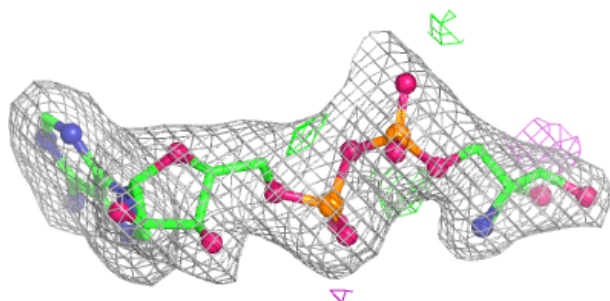
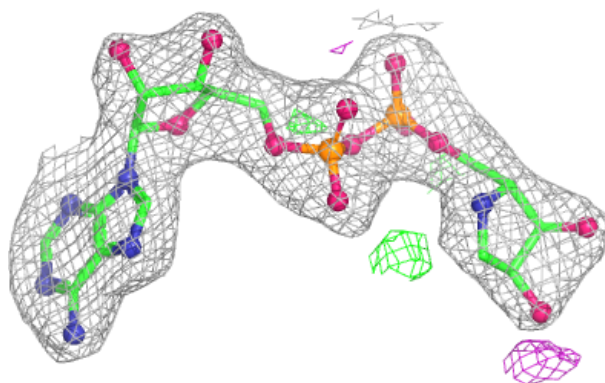


Electron density around A1R A 1001:

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

**Electron density around A1R C 1001:**

$2mF_o-DF_c$ (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.