



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 07:37 AM UTC

PDB ID : 4NA0 / pdb_00004na0
Title : Crystal structure of mouse poly(ADP-ribose) glycohydrolase (PARG) catalytic domain with ADPRibose
Authors : Wang, Z.; Cheng, Z.; Xu, W.
Deposited on : 2013-10-21
Resolution : 2.40 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

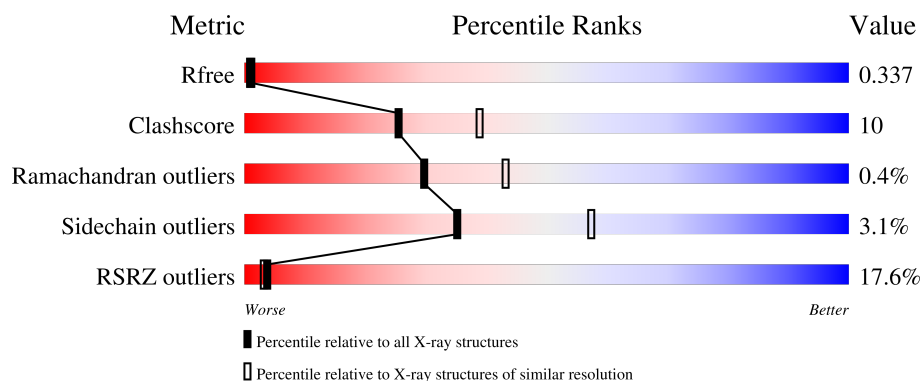
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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	4912 (2.40-2.40)
Clashscore	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)
RSRZ outliers	180081	4916 (2.40-2.40)

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	4% 83% 12% • •
1	B	522	11% 77% 18% • •
1	C	522	35% 72% 22% • •

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 12337 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) glycohydrolase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	501	Total	C	N	O	S	Se	0	0	0
			4074	2603	710	738	14	9			
1	B	502	Total	C	N	O	S	Se	0	0	0
			4079	2605	710	741	14	9			
1	C	501	Total	C	N	O	S	Se	0	0	0
			4070	2598	709	741	13	9			

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 IODIDE ION (CCD ID: IOD) (formula: I).

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

- Molecule 3 is [(2R,3S,4R,5R)-5-(6-AMINOPURIN-9-YL)-3,4-DIHYDROXY-OXOLAN-2-YL]METHYL [HYDROXY-[(2R,3S,4R,5S)-3,4,5-TRIHIDROXYOXOLAN-2-YL]METHOXY]PHOSPHORYL] HYDROGEN PHOSPHATE (CCD ID: AR6) (formula: C₁₅H₂₃N₅O₁₄P₂).

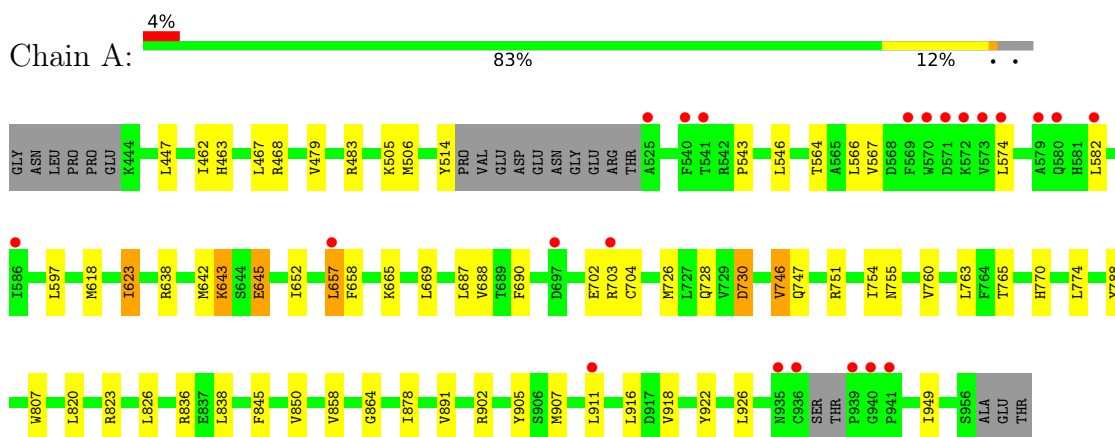


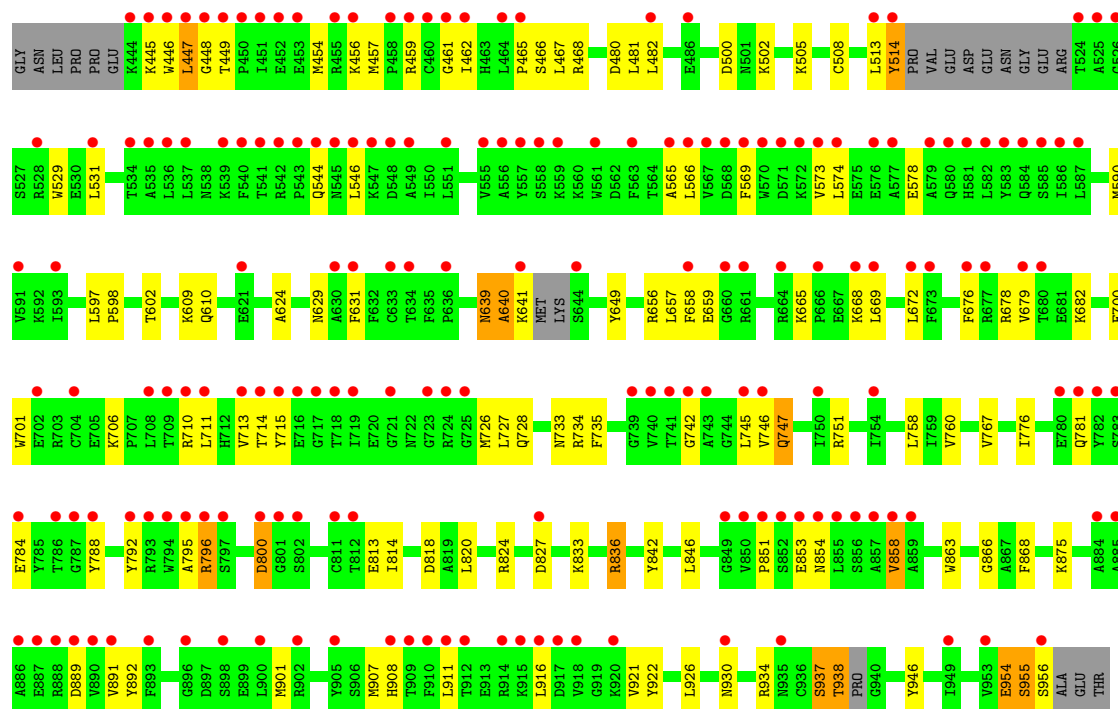
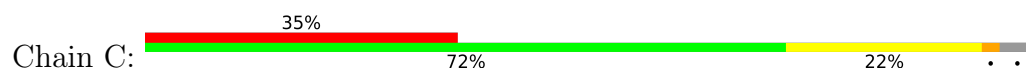
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total 36	C 15	N 5	O 14	P 2	0	0
3	B	1	Total 36	C 15	N 5	O 14	P 2	0	0
3	C	1	Total 36	C 15	N 5	O 14	P 2	0	0

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) glycohydrolase





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	188.30Å 55.66Å 166.15Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.40 50.00 – 2.40	Depositor EDS
% Data completeness (in resolution range)	97.7 (50.00-2.40) 97.6 (50.00-2.40)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.94 (at 2.39Å)	Xtriage
Refinement program	REFMAC 5.5.0110	Depositor
R, R_{free}	0.298 , 0.342 0.294 , 0.337	Depositor DCC
R_{free} test set	3419 reflections (4.95%)	wwPDB-VP
Wilson B-factor (Å ²)	50.2	Xtriage
Anisotropy	0.339	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 43.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	12337	wwPDB-VP
Average B, all atoms (Å ²)	70.0	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 70.75 % 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 2.9603e-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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: IOD, AR6

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	0.48	0/4165	0.71	0/5617
1	B	0.48	0/4170	0.70	0/5627
1	C	0.49	0/4159	0.72	3/5610 (0.1%)
All	All	0.48	0/12494	0.71	3/16854 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	C	0	1

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	701	TRP	N-CA-C	7.20	118.91	111.14
1	C	640	ALA	N-CA-C	5.71	116.93	107.73
1	C	639	ASN	N-CA-C	5.16	121.86	114.39

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	700	GLU	Peptide

5.2 Too-close contacts ⓘ

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	4074	0	4042	60	0
1	B	4079	0	4042	69	0
1	C	4070	0	4030	106	0
2	A	2	0	0	2	0
2	B	2	0	0	0	0
2	C	2	0	0	1	0
3	A	36	0	20	2	0
3	B	36	0	20	2	0
3	C	36	0	21	6	0
All	All	12337	0	12175	236	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 10.

All (236) 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:A:907:MSE:HE1	1:A:949:ILE:HG21	1.22	1.09
1:C:447:LEU:CD2	1:C:713:VAL:HG23	1.86	1.05
1:B:726:MSE:HE3	1:B:859:ALA:HB2	1.39	1.04
1:C:711:LEU:HD21	1:C:713:VAL:HG13	1.41	1.00
1:A:618:MSE:HE3	1:A:623:ILE:CD1	1.94	0.98
1:A:907:MSE:HE3	1:A:911:LEU:HD11	1.49	0.93
1:C:713:VAL:HG12	1:C:892:TYR:HB3	1.51	0.92
1:C:447:LEU:HD23	1:C:713:VAL:HG23	1.54	0.90
1:C:447:LEU:HD22	1:C:447:LEU:N	1.87	0.90
1:C:447:LEU:HD21	1:C:713:VAL:HG23	1.52	0.89
1:C:911:LEU:HD21	1:C:921:VAL:HG22	1.55	0.88
1:B:447:LEU:HG	1:B:901:MSE:HE3	1.57	0.86
1:C:447:LEU:HD23	1:C:713:VAL:CG2	2.07	0.85
1:B:728:GLN:OE1	1:B:751:ARG:NH2	2.14	0.81
1:A:728:GLN:OE1	1:A:751:ARG:NH2	2.14	0.81
1:A:907:MSE:HE1	1:A:949:ILE:CG2	2.09	0.79
1:B:447:LEU:HG	1:B:901:MSE:CE	2.11	0.79
1:C:711:LEU:HD21	1:C:713:VAL:CG1	2.12	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:858:VAL:HG12	1:C:889:ASP:O	1.84	0.78
1:A:467:LEU:O	1:A:479:VAL:HG11	1.83	0.78
1:A:907:MSE:CE	1:A:949:ILE:HG21	2.11	0.77
1:B:726:MSE:CE	1:B:859:ALA:HB2	2.16	0.76
1:C:447:LEU:CD2	1:C:447:LEU:N	2.51	0.73
1:C:624:ALA:HB1	1:C:679:VAL:HG11	1.69	0.73
1:B:629:ASN:OD1	1:B:634:THR:HG21	1.90	0.72
1:C:711:LEU:CD2	1:C:713:VAL:HG13	2.18	0.72
1:C:447:LEU:HD21	1:C:901:MSE:HG2	1.73	0.71
1:C:514:TYR:CE2	1:C:531:LEU:HD22	2.26	0.71
1:C:746:VAL:HG13	1:C:788:TYR:OH	1.90	0.71
1:B:723:GLY:HA2	1:B:726:MSE:HE2	1.73	0.70
1:A:618:MSE:CE	1:A:623:ILE:CD1	2.70	0.70
1:A:746:VAL:HG13	1:A:747:GLN:H	1.56	0.70
1:C:447:LEU:CD2	1:C:713:VAL:CG2	2.65	0.70
1:B:746:VAL:HG22	1:B:788:TYR:OH	1.90	0.69
1:B:709:THR:HG21	1:B:888:ARG:O	1.91	0.69
1:A:618:MSE:HE3	1:A:623:ILE:HD13	1.72	0.69
1:B:692:ARG:NH2	1:B:766:GLU:O	2.26	0.68
1:A:820:LEU:HD11	1:A:836:ARG:HG2	1.76	0.67
1:C:746:VAL:HG11	3:C:1003:AR6:O2A	1.96	0.65
1:C:665:LYS:O	1:C:669:LEU:HD23	1.97	0.65
1:A:514:TYR:C	2:A:1002:IOD:I	3.10	0.65
1:C:818:ASP:O	1:C:836:ARG:NH2	2.30	0.64
1:A:618:MSE:HE3	1:A:623:ILE:HD11	1.77	0.64
1:A:623:ILE:HD11	1:A:688:VAL:HG21	1.80	0.63
1:A:746:VAL:HG13	1:A:747:GLN:N	2.14	0.63
1:A:907:MSE:HE3	1:A:911:LEU:CD1	2.26	0.62
1:B:746:VAL:HG13	1:B:747:GLN:N	2.14	0.62
1:C:447:LEU:HD21	1:C:901:MSE:CG	2.29	0.62
1:C:781:GLN:N	1:C:800:ASP:OD2	2.32	0.62
1:B:657:LEU:HD21	1:B:672:LEU:HD12	1.81	0.62
1:C:715:TYR:H	1:C:901:MSE:HE2	1.63	0.62
1:B:838:LEU:HD23	1:B:878:ILE:HG23	1.82	0.62
1:C:824:ARG:HB3	1:C:827:ASP:HB2	1.82	0.61
1:C:668:LYS:NZ	1:C:742:GLY:O	2.34	0.61
1:B:837:GLU:OE2	1:B:875:LYS:NZ	2.25	0.61
1:A:618:MSE:CE	1:A:623:ILE:HD11	2.31	0.60
1:B:597:LEU:HD22	1:B:629:ASN:ND2	2.16	0.60
1:A:687:LEU:HD12	1:A:807:TRP:O	2.00	0.60
1:A:618:MSE:HE2	1:A:690:PHE:CE1	2.37	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:704:CYS:HB3	1:A:918:VAL:HG23	1.83	0.59
1:C:446:TRP:C	1:C:447:LEU:HD22	2.28	0.59
1:A:657:LEU:HD12	1:A:669:LEU:HD21	1.85	0.59
1:C:715:TYR:N	1:C:901:MSE:HE2	2.18	0.59
1:C:784:GLU:O	1:C:795:ALA:HB3	2.01	0.59
1:B:487:VAL:HG21	1:B:683:LYS:HB2	1.84	0.58
1:A:618:MSE:HE3	1:A:623:ILE:CG1	2.33	0.58
1:C:858:VAL:CG1	1:C:889:ASP:O	2.51	0.58
1:C:911:LEU:HD21	1:C:921:VAL:CG2	2.30	0.58
1:A:746:VAL:HG22	1:A:788:TYR:OH	2.04	0.58
1:C:954:GLU:O	1:C:955:SER:C	2.46	0.57
1:A:447:LEU:HD13	1:A:905:TYR:CD2	2.40	0.57
1:C:566:LEU:HD13	1:C:658:PHE:CD1	2.39	0.57
1:A:462:ILE:HD11	1:A:850:VAL:HG13	1.86	0.57
1:C:457:MSE:SE	1:C:461:GLY:HA2	2.54	0.57
1:B:867:ALA:HB3	3:B:1003:AR6:O5D	2.05	0.57
1:B:727:LEU:HD13	1:B:813:GLU:OE2	2.05	0.57
1:C:590:MSE:HE1	1:C:631:PHE:CG	2.40	0.56
1:B:746:VAL:HG13	1:B:747:GLN:H	1.69	0.56
1:C:624:ALA:CB	1:C:679:VAL:HG11	2.35	0.56
1:A:657:LEU:HD12	1:A:669:LEU:CD2	2.35	0.56
1:B:863:TRP:O	1:B:875:LYS:HG2	2.06	0.55
1:A:642:MET:HG2	1:A:643:LYS:N	2.22	0.55
1:C:480:ASP:OD2	1:C:481:LEU:HD12	2.06	0.55
1:A:638:ARG:NH2	1:A:763:LEU:O	2.39	0.55
1:C:598:PRO:O	1:C:602:THR:HG22	2.06	0.55
1:A:765:THR:HG21	1:A:774:LEU:HD22	1.89	0.55
1:C:863:TRP:O	1:C:875:LYS:HG2	2.07	0.54
1:C:851:PRO:HB2	1:C:854:ASN:HD22	1.72	0.54
1:C:937:SER:O	1:C:938:THR:HG23	2.07	0.54
1:A:746:VAL:HG13	3:A:1003:AR6:O2A	2.08	0.54
1:B:616:VAL:O	1:B:616:VAL:HG13	2.08	0.54
1:B:664:ARG:NH1	1:B:790:GLU:O	2.41	0.54
1:B:820:LEU:HD11	1:B:836:ARG:HD2	1.88	0.54
1:C:569:PHE:CE2	1:C:574:LEU:HD11	2.43	0.54
1:A:623:ILE:HD13	1:A:760:VAL:HG11	1.90	0.54
1:A:726:MSE:SE	1:A:891:VAL:HG21	2.58	0.54
1:C:728:GLN:OE1	1:C:751:ARG:NH2	2.40	0.54
1:B:485:GLY:O	1:B:685:THR:HG21	2.08	0.54
1:B:657:LEU:HD21	1:B:672:LEU:CD1	2.37	0.54
1:C:820:LEU:HD11	1:C:836:ARG:HG2	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:911:LEU:HD11	1:C:916:LEU:HD23	1.90	0.54
1:C:462:ILE:HD12	1:C:462:ILE:C	2.33	0.53
1:A:826:LEU:O	1:A:826:LEU:HD23	2.08	0.53
1:A:618:MSE:HE3	1:A:623:ILE:HG12	1.91	0.53
1:B:914:ARG:O	1:B:915:LYS:HG2	2.08	0.53
1:C:513:LEU:O	1:C:514:TYR:CD2	2.62	0.52
1:B:700:GLU:CD	1:B:700:GLU:H	2.16	0.52
1:C:866:GLY:HA3	3:C:1003:AR6:O1A	2.09	0.52
1:A:618:MSE:HE2	1:A:690:PHE:HE1	1.73	0.52
1:A:911:LEU:HD22	1:A:916:LEU:HD12	1.91	0.52
1:C:456:LYS:CE	1:C:726:MSE:HE2	2.40	0.52
1:A:704:CYS:SG	1:A:918:VAL:HG21	2.50	0.51
1:C:639:ASN:O	1:C:640:ALA:HB2	2.09	0.51
1:A:746:VAL:CG1	1:A:747:GLN:N	2.74	0.51
1:B:642:MET:O	1:B:644:SER:N	2.44	0.51
1:C:665:LYS:HE2	2:C:1001:IOD:I	2.81	0.51
1:B:507:PRO:CB	1:B:634:THR:HG23	2.41	0.50
1:B:551:LEU:HD22	1:B:558:SER:HA	1.93	0.50
1:C:784:GLU:HB3	1:C:796:ARG:HD3	1.93	0.50
1:A:564:THR:O	1:A:567:VAL:HG22	2.12	0.50
1:B:831:PRO:HG3	1:B:926:LEU:HD13	1.93	0.50
1:C:746:VAL:CG1	1:C:747:GLN:N	2.75	0.50
1:B:507:PRO:HB3	1:B:634:THR:HG23	1.94	0.50
1:C:500:ASP:O	1:C:505:LYS:NZ	2.44	0.50
1:C:449:THR:HG21	1:C:710:ARG:NE	2.27	0.49
1:A:754:ILE:HG13	1:A:755:ASN:HD22	1.78	0.49
1:C:454:MSE:HE1	1:C:889:ASP:HB3	1.93	0.49
1:A:566:LEU:HD13	1:A:658:PHE:CD1	2.46	0.49
1:A:543:PRO:HB2	1:A:567:VAL:HG12	1.94	0.49
1:C:610:GLN:HE21	1:C:767:VAL:HG13	1.78	0.49
1:B:652:ILE:HG12	1:B:763:LEU:HD13	1.93	0.49
1:C:922:TYR:CE2	1:C:926:LEU:HD11	2.48	0.49
1:C:746:VAL:HG12	1:C:747:GLN:N	2.28	0.49
1:C:866:GLY:HA3	3:C:1003:AR6:O3'	2.11	0.49
1:C:678:ARG:NH1	1:C:682:LYS:O	2.46	0.49
1:B:449:THR:HB	1:B:454:MSE:HE2	1.94	0.49
1:A:618:MSE:CE	1:A:623:ILE:HD13	2.38	0.49
3:C:1003:AR6:O1A	3:C:1003:AR6:C3'	2.60	0.48
1:B:938:THR:HG23	1:B:939:PRO:HD2	1.96	0.48
1:B:587:LEU:HB2	1:B:588:PRO:HD3	1.95	0.48
1:C:447:LEU:HD23	1:C:713:VAL:HG22	1.90	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:473:HIS:NE2	1:B:617:THR:OG1	2.36	0.48
1:B:752:PHE:O	1:B:756:PRO:HA	2.13	0.48
1:B:507:PRO:HG3	1:B:634:THR:CG2	2.44	0.48
1:A:574:LEU:CD1	1:A:582:LEU:HD22	2.44	0.47
1:A:746:VAL:HG22	1:A:788:TYR:CZ	2.49	0.47
1:C:733:ASN:HD22	1:C:735:PHE:H	1.61	0.47
1:A:730:ASP:OD2	1:A:730:ASP:C	2.56	0.47
1:C:514:TYR:CZ	1:C:531:LEU:HD22	2.49	0.47
1:B:746:VAL:HG22	1:B:788:TYR:CZ	2.50	0.47
1:A:652:ILE:HG12	1:A:763:LEU:HD13	1.95	0.47
1:A:462:ILE:HG22	1:A:463:HIS:N	2.30	0.47
1:C:657:LEU:HD11	1:C:672:LEU:CD1	2.45	0.47
1:A:845:PHE:CE1	1:A:858:VAL:HG11	2.50	0.46
1:C:711:LEU:C	1:C:711:LEU:HD23	2.40	0.46
1:A:907:MSE:HE2	1:A:949:ILE:HD13	1.96	0.46
1:C:573:VAL:HG12	1:C:573:VAL:O	2.15	0.46
1:B:866:GLY:HA3	3:B:1003:AR6:O5'	2.16	0.46
1:C:776:ILE:N	1:C:776:ILE:HD12	2.29	0.46
1:A:864:GLY:HA2	3:A:1003:AR6:O2B	2.15	0.46
1:B:484:ALA:HB2	1:B:808:GLN:HE22	1.81	0.46
1:C:597:LEU:HD22	1:C:629:ASN:ND2	2.30	0.46
1:B:945:LEU:HD11	1:B:949:ILE:HD11	1.98	0.46
1:C:842:TYR:CZ	1:C:846:LEU:HD22	2.50	0.46
1:C:746:VAL:O	1:C:747:GLN:C	2.58	0.46
1:C:447:LEU:HD21	1:C:901:MSE:SE	2.66	0.46
1:B:675:TYR:CG	1:B:756:PRO:HG2	2.51	0.46
1:C:454:MSE:HE2	1:C:891:VAL:HG23	1.97	0.46
1:C:784:GLU:HB3	1:C:796:ARG:CD	2.45	0.45
1:C:597:LEU:N	1:C:598:PRO:HD2	2.32	0.45
1:A:704:CYS:SG	1:A:918:VAL:CG2	3.04	0.45
1:A:770:HIS:CD2	1:A:836:ARG:HE	2.35	0.45
1:B:727:LEU:HD11	1:B:815:VAL:CG1	2.46	0.45
1:C:456:LYS:HE2	1:C:726:MSE:HE2	1.97	0.45
1:C:467:LEU:HD12	1:C:468:ARG:N	2.32	0.45
1:B:542:ARG:HB2	1:B:543:PRO:HD2	1.99	0.45
1:A:826:LEU:HD23	1:A:826:LEU:C	2.42	0.45
1:A:665:LYS:HD2	2:A:1001:IOD:I	2.87	0.44
1:C:668:LYS:HE3	1:C:745:LEU:HG	1.99	0.44
1:C:745:LEU:HD22	1:C:792:TYR:CG	2.52	0.44
1:A:506:MSE:HE1	1:A:597:LEU:HD11	1.99	0.44
1:B:610:GLN:O	1:B:611:LYS:HB2	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:873:ARG:NH2	1:B:903:ASP:OD2	2.47	0.44
1:C:565:ALA:HB3	1:C:658:PHE:O	2.18	0.44
1:B:776:ILE:N	1:B:776:ILE:HD12	2.32	0.44
1:C:590:MSE:HE3	1:C:676:PHE:CD1	2.53	0.44
1:C:796:ARG:HG2	1:C:796:ARG:HH11	1.82	0.44
1:C:514:TYR:CD1	1:C:514:TYR:C	2.95	0.44
1:C:796:ARG:HH11	1:C:796:ARG:CG	2.30	0.44
1:B:700:GLU:CD	1:B:700:GLU:N	2.76	0.44
1:C:727:LEU:HD13	1:C:813:GLU:HG2	2.00	0.43
1:C:569:PHE:CZ	1:C:574:LEU:HD11	2.53	0.43
1:B:701:TRP:O	1:B:919:GLY:HA2	2.17	0.43
1:B:819:ALA:HB2	1:B:863:TRP:CE2	2.52	0.43
1:C:656:ARG:NE	1:C:659:GLU:OE1	2.42	0.43
1:C:508:CYS:HA	1:C:529:TRP:CD2	2.54	0.43
1:C:955:SER:O	1:C:956:SER:CB	2.67	0.43
1:C:449:THR:HG21	1:C:710:ARG:CZ	2.49	0.43
1:C:640:ALA:O	1:C:641:LYS:C	2.61	0.43
1:C:500:ASP:HB3	1:C:502:LYS:H	1.83	0.43
1:C:574:LEU:HD22	1:C:578:GLU:HB3	2.01	0.43
1:B:838:LEU:CD2	1:B:878:ILE:HG23	2.48	0.42
1:C:911:LEU:CD1	1:C:916:LEU:HD23	2.49	0.42
1:B:597:LEU:N	1:B:598:PRO:HD2	2.35	0.42
1:C:609:LYS:HG2	1:C:649:TYR:OH	2.19	0.42
1:C:758:LEU:HD11	1:C:814:ILE:HD12	2.01	0.42
1:A:838:LEU:HD23	1:A:878:ILE:HG23	2.02	0.42
1:B:543:PRO:HG3	1:B:570:TRP:HB3	2.02	0.42
1:B:820:LEU:CD1	1:B:836:ARG:HD2	2.50	0.42
1:C:746:VAL:CG1	3:C:1003:AR6:O2A	2.65	0.42
1:B:563:PHE:O	1:B:567:VAL:HG23	2.19	0.42
1:B:726:MSE:HE3	1:B:859:ALA:CB	2.29	0.42
1:C:454:MSE:HE1	1:C:889:ASP:CB	2.50	0.42
1:C:456:LYS:NZ	1:C:726:MSE:HE2	2.35	0.42
1:A:922:TYR:CZ	1:A:926:LEU:HD11	2.55	0.41
1:C:868:PHE:CD1	3:C:1003:AR6:H5DA	2.55	0.41
1:C:454:MSE:HE2	1:C:891:VAL:CG2	2.50	0.41
1:C:465:PRO:O	1:C:466:SER:C	2.62	0.41
1:A:483:ARG:HA	1:A:483:ARG:NE	2.35	0.41
1:B:546:LEU:HD22	1:B:550:ILE:CD1	2.51	0.41
1:A:505:LYS:NZ	1:A:645:GLU:OE1	2.52	0.41
1:B:457:MSE:SE	1:B:461:GLY:CA	3.18	0.41
1:B:765:THR:HG21	1:B:774:LEU:HD22	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:877:LEU:HD23	1:B:925:LEU:HD21	2.03	0.41
1:B:623:ILE:HG12	1:B:760:VAL:HG11	2.01	0.41
1:B:641:LYS:O	1:B:642:MET:HE2	2.21	0.41
1:C:907:MSE:HE3	1:C:946:TYR:HA	2.02	0.41
1:B:446:TRP:C	1:B:901:MSE:HE3	2.46	0.41
1:B:746:VAL:CG1	1:B:747:GLN:N	2.83	0.41
1:C:448:GLY:HA3	1:C:711:LEU:O	2.21	0.41
1:C:454:MSE:CE	1:C:891:VAL:HG23	2.51	0.41
1:C:711:LEU:HD13	1:C:908:HIS:ND1	2.36	0.41
1:C:590:MSE:HE3	1:C:676:PHE:CE1	2.56	0.40
1:B:727:LEU:HD11	1:B:815:VAL:HB	2.03	0.40
1:B:831:PRO:CG	1:B:926:LEU:HD13	2.51	0.40
1:B:914:ARG:O	1:B:916:LEU:HD12	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	495/522 (95%)	473 (96%)	20 (4%)	2 (0%)	30	43
1	B	496/522 (95%)	482 (97%)	14 (3%)	0	100	100
1	C	493/522 (94%)	464 (94%)	25 (5%)	4 (1%)	16	25
All	All	1484/1566 (95%)	1419 (96%)	59 (4%)	6 (0%)	30	43

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	643	LYS
1	C	937	SER
1	C	954	GLU
1	C	747	GLN

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Mol	Chain	Res	Type
1	C	955	SER
1	A	645	GLU

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	441/450 (98%)	431 (98%)	10 (2%)	44	66
1	B	442/450 (98%)	431 (98%)	11 (2%)	42	64
1	C	441/450 (98%)	421 (96%)	20 (4%)	24	42
All	All	1324/1350 (98%)	1283 (97%)	41 (3%)	35	57

All (41) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	468	ARG
1	A	546	LEU
1	A	623	ILE
1	A	657	LEU
1	A	702	GLU
1	A	703	ARG
1	A	730	ASP
1	A	746	VAL
1	A	823	ARG
1	A	902	ARG
1	B	459	ARG
1	B	496	LYS
1	B	504	VAL
1	B	510	GLU
1	B	544	GLN
1	B	546	LEU
1	B	582	LEU
1	B	634	THR
1	B	700	GLU
1	B	746	VAL

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Mol	Chain	Res	Type
1	B	942	ASP
1	C	445	LYS
1	C	447	LEU
1	C	459	ARG
1	C	482	LEU
1	C	514	TYR
1	C	544	GLN
1	C	546	LEU
1	C	706	LYS
1	C	714	THR
1	C	734	ARG
1	C	760	VAL
1	C	796	ARG
1	C	800	ASP
1	C	833	LYS
1	C	836	ARG
1	C	853	GLU
1	C	858	VAL
1	C	930	ASN
1	C	934	ARG
1	C	938	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	544	GLN
1	A	545	ASN
1	A	653	ASN
1	A	755	ASN
1	A	770	HIS
1	A	862	ASN
1	B	545	ASN
1	B	603	GLN
1	B	614	HIS
1	B	693	GLN
1	B	770	HIS
1	B	781	GLN
1	B	808	GLN
1	B	854	ASN
1	B	879	GLN
1	C	538	ASN
1	C	544	GLN

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Mol	Chain	Res	Type
1	C	554	ASN
1	C	603	GLN
1	C	610	GLN
1	C	733	ASN
1	C	808	GLN
1	C	854	ASN
1	C	879	GLN
1	C	935	ASN

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 9 ligands modelled in this entry, 6 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	$\# Z > 2$
3	AR6	B	1003	-	39,39,39	2.75	8 (20%)	56,60,60	2.30	15 (26%)
3	AR6	C	1003	-	39,39,39	2.55	6 (15%)	56,60,60	2.77	17 (30%)
3	AR6	A	1003	-	39,39,39	2.68	7 (17%)	56,60,60	2.32	15 (26%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral

centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	AR6	B	1003	-	-	9/22/54/54	0/4/4/4
3	AR6	C	1003	-	-	11/22/54/54	0/4/4/4
3	AR6	A	1003	-	-	8/22/54/54	0/4/4/4

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1003	AR6	PA-O3A	13.92	1.74	1.59
3	A	1003	AR6	PA-O3A	13.53	1.74	1.59
3	C	1003	AR6	PA-O3A	12.34	1.72	1.59
3	C	1003	AR6	C6-N6	6.60	1.51	1.34
3	B	1003	AR6	C6-N6	5.89	1.49	1.34
3	A	1003	AR6	C6-N6	5.71	1.48	1.34
3	C	1003	AR6	PA-O2A	4.81	1.67	1.50
3	B	1003	AR6	PA-O2A	4.46	1.66	1.50
3	A	1003	AR6	PA-O2A	4.16	1.65	1.50
3	B	1003	AR6	PA-O5'	2.94	1.70	1.59
3	A	1003	AR6	PA-O5'	2.83	1.70	1.59
3	B	1003	AR6	PA-O1A	2.70	1.67	1.55
3	C	1003	AR6	C8-N7	2.53	1.36	1.31
3	C	1003	AR6	PA-O1A	2.51	1.67	1.55
3	A	1003	AR6	PA-O1A	2.50	1.66	1.55
3	B	1003	AR6	C8-N7	2.45	1.36	1.31
3	A	1003	AR6	C5-N7	-2.33	1.34	1.39
3	C	1003	AR6	PA-O5'	2.21	1.68	1.59
3	B	1003	AR6	C8-N9	-2.18	1.33	1.37
3	B	1003	AR6	C5-N7	-2.18	1.35	1.39
3	A	1003	AR6	PB-O3A	2.17	1.61	1.59

All (47) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	1003	AR6	O5'-C5'-C4'	10.26	143.91	108.99
3	A	1003	AR6	PA-O5'-C5'	-8.72	71.38	121.35
3	B	1003	AR6	PA-O5'-C5'	-8.68	71.64	121.35
3	C	1003	AR6	PA-O5'-C5'	-8.56	72.28	121.35
3	C	1003	AR6	O1A-PA-O5'	6.59	137.43	107.57
3	A	1003	AR6	C5-C4-N3	-5.87	118.63	126.72
3	B	1003	AR6	O5'-C5'-C4'	-5.83	89.14	108.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	1003	AR6	C5-C4-N3	-4.99	119.84	126.72
3	B	1003	AR6	C5-C4-N3	-4.97	119.87	126.72
3	C	1003	AR6	O1A-PA-O2A	-4.85	89.89	112.44
3	C	1003	AR6	N3-C2-N1	-4.76	121.38	128.58
3	B	1003	AR6	N3-C2-N1	-4.71	121.45	128.58
3	B	1003	AR6	O1A-PA-O5'	-4.70	86.25	107.57
3	A	1003	AR6	O5'-C5'-C4'	-4.62	93.25	108.99
3	A	1003	AR6	N3-C2-N1	-4.50	121.78	128.58
3	A	1003	AR6	O1A-PA-O5'	-4.36	87.79	107.57
3	B	1003	AR6	O5'-PA-O2A	4.19	125.55	108.94
3	C	1003	AR6	O5'-PA-O2A	-3.77	93.99	108.94
3	A	1003	AR6	N3-C4-N9	3.73	133.51	127.17
3	A	1003	AR6	O5'-PA-O2A	3.60	123.20	108.94
3	C	1003	AR6	N9-C8-N7	-3.57	108.88	113.94
3	A	1003	AR6	C2-N3-C4	3.56	120.53	111.83
3	C	1003	AR6	C2-N3-C4	3.37	120.06	111.83
3	B	1003	AR6	C2-N3-C4	3.30	119.89	111.83
3	A	1003	AR6	N9-C8-N7	-3.28	109.28	113.94
3	A	1003	AR6	O1A-PA-O3A	-3.22	98.58	107.27
3	B	1003	AR6	C4-C5-N7	-3.12	107.01	110.58
3	C	1003	AR6	N3-C4-N9	2.86	132.04	127.17
3	C	1003	AR6	C4-C5-N7	-2.83	107.34	110.58
3	C	1003	AR6	O3A-PB-O2B	-2.80	102.27	110.70
3	C	1003	AR6	C5-N7-C8	2.77	107.81	103.45
3	B	1003	AR6	N9-C8-N7	-2.71	110.09	113.94
3	A	1003	AR6	C4-C5-N7	-2.69	107.51	110.58
3	A	1003	AR6	C5-N7-C8	2.62	107.56	103.45
3	B	1003	AR6	N3-C4-N9	2.61	131.60	127.17
3	B	1003	AR6	O1D-C1D-O4D	-2.60	107.81	111.12
3	C	1003	AR6	O4'-C1'-N9	2.54	112.97	108.09
3	B	1003	AR6	C5-C4-N9	2.50	108.53	105.81
3	B	1003	AR6	C3'-C2'-C1'	2.48	106.15	101.46
3	B	1003	AR6	O1A-PA-O3A	-2.37	100.87	107.27
3	C	1003	AR6	O1A-PA-O3A	2.33	113.56	107.27
3	A	1003	AR6	C3'-C2'-C1'	2.30	105.82	101.46
3	A	1003	AR6	O1A-PA-O2A	-2.29	101.80	112.44
3	B	1003	AR6	C5-N7-C8	2.23	106.96	103.45
3	C	1003	AR6	C5-C4-N9	2.12	108.12	105.81
3	A	1003	AR6	C6-C5-C4	2.01	119.92	117.18
3	C	1003	AR6	C4-N9-C8	2.00	107.84	105.74

There are no chirality outliers.

All (28) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1003	AR6	C5'-O5'-PA-O2A
3	B	1003	AR6	PB-O3A-PA-O5'
3	B	1003	AR6	C5'-O5'-PA-O2A
3	B	1003	AR6	C5D-O5D-PB-O2B
3	B	1003	AR6	C5D-O5D-PB-O3A
3	C	1003	AR6	C5'-O5'-PA-O3A
3	C	1003	AR6	C5D-O5D-PB-O2B
3	C	1003	AR6	O4D-C4D-C5D-O5D
3	C	1003	AR6	C4'-C5'-O5'-PA
3	A	1003	AR6	C3D-C4D-C5D-O5D
3	C	1003	AR6	C3'-C4'-C5'-O5'
3	C	1003	AR6	O4'-C4'-C5'-O5'
3	C	1003	AR6	C3D-C4D-C5D-O5D
3	B	1003	AR6	O4D-C4D-C5D-O5D
3	B	1003	AR6	C3D-C4D-C5D-O5D
3	A	1003	AR6	O4D-C4D-C5D-O5D
3	A	1003	AR6	PB-O3A-PA-O5'
3	C	1003	AR6	PA-O3A-PB-O5D
3	C	1003	AR6	C2'-C1'-N9-C8
3	A	1003	AR6	C5D-O5D-PB-O2B
3	B	1003	AR6	C5D-O5D-PB-O1B
3	C	1003	AR6	C5'-O5'-PA-O2A
3	A	1003	AR6	O4'-C4'-C5'-O5'
3	A	1003	AR6	PA-O3A-PB-O2B
3	B	1003	AR6	PB-O3A-PA-O2A
3	A	1003	AR6	PA-O3A-PB-O1B
3	B	1003	AR6	O4'-C4'-C5'-O5'
3	C	1003	AR6	O4'-C1'-N9-C8

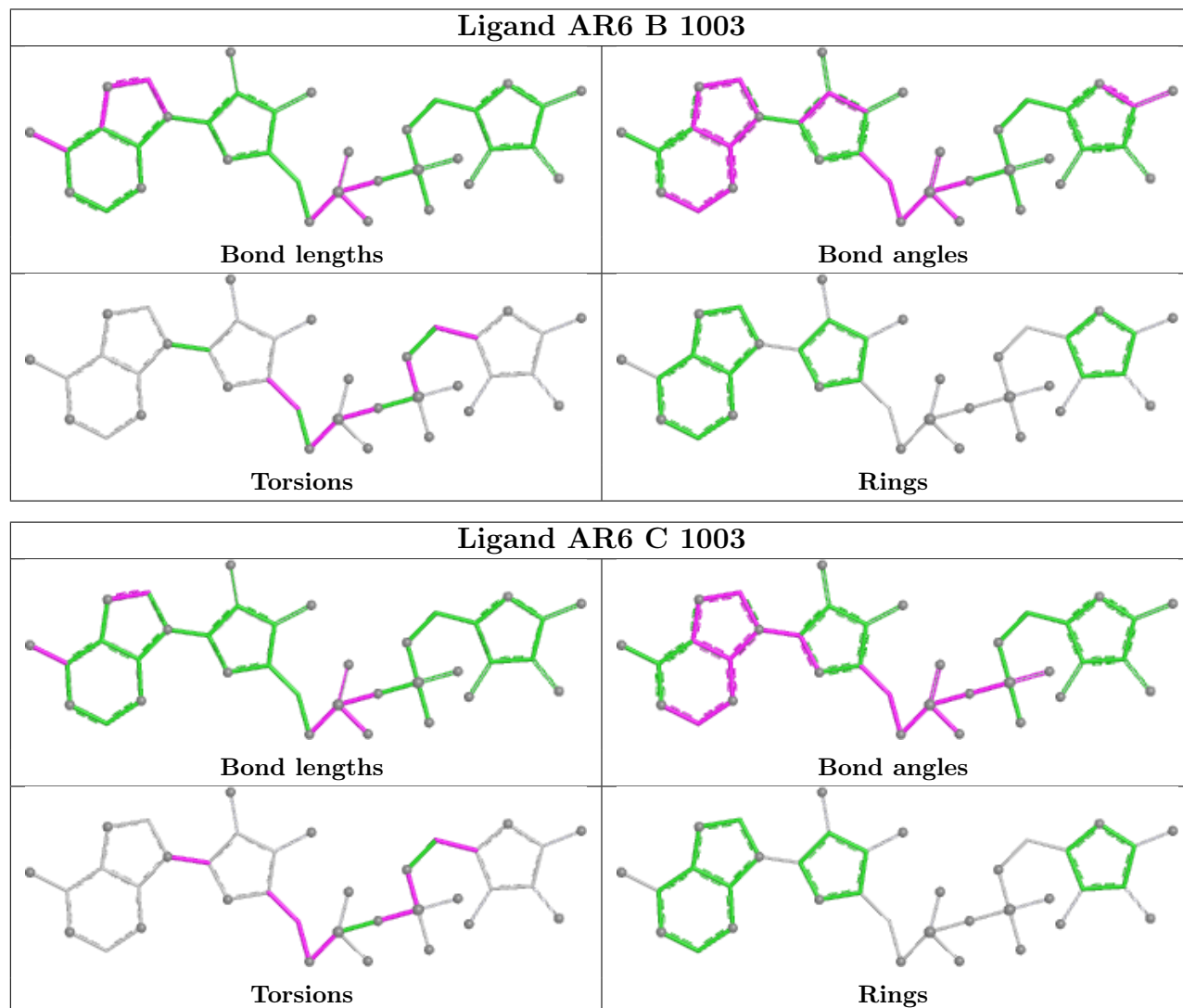
There are no ring outliers.

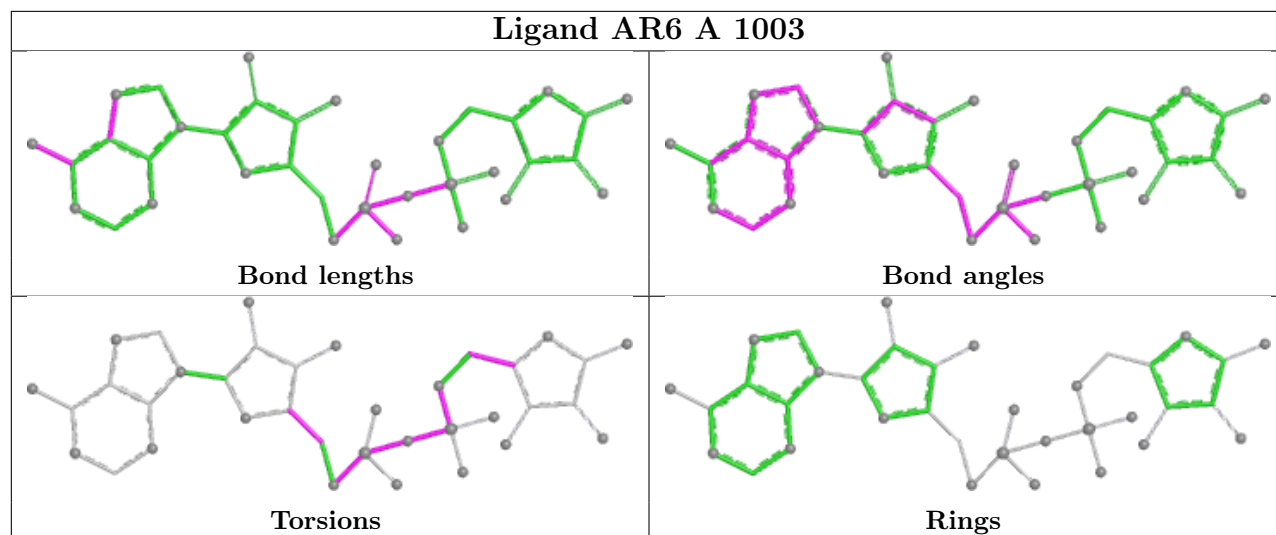
3 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	1003	AR6	2	0
3	C	1003	AR6	6	0
3	A	1003	AR6	2	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	492/522 (94%)	0.55	22 (4%) 38 34	24, 56, 106, 174	0
1	B	493/522 (94%)	0.85	56 (11%) 10 7	24, 61, 130, 194	0
1	C	492/522 (94%)	1.51	182 (36%) 1 0	20, 73, 159, 254	0
All	All	1477/1566 (94%)	0.97	260 (17%) 4 3	20, 62, 136, 254	0

All (260) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	587	LEU	6.7
1	C	857	ALA	6.4
1	C	916	LEU	6.0
1	B	811	CYS	5.7
1	C	884	ALA	5.5
1	C	658	PHE	5.5
1	C	849	GLY	5.5
1	C	524	THR	5.4
1	C	586	ILE	5.4
1	C	514	TYR	5.4
1	C	582	LEU	5.3
1	C	525	ALA	4.8
1	C	918	VAL	4.8
1	C	570	TRP	4.8
1	C	792	TYR	4.7
1	C	563	PHE	4.7
1	C	540	PHE	4.7
1	C	566	LEU	4.6
1	C	450	PRO	4.6
1	C	851	PRO	4.6
1	C	912	THR	4.6
1	C	889	ASP	4.6
1	B	567	VAL	4.3

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Mol	Chain	Res	Type	RSRZ
1	C	782	TYR	4.3
1	C	811	CYS	4.2
1	C	794	TRP	4.2
1	C	446	TRP	4.1
1	C	559	LYS	4.1
1	C	717	GLY	4.1
1	A	573	VAL	4.1
1	C	513	LEU	4.1
1	C	710	ARG	4.0
1	C	571	ASP	3.9
1	C	787	GLY	3.9
1	C	561	TRP	3.8
1	C	660	GLY	3.8
1	C	547	LYS	3.8
1	C	486	GLU	3.8
1	C	741	THR	3.7
1	C	636	PRO	3.7
1	C	888	ARG	3.7
1	A	541	THR	3.6
1	C	725	GLY	3.6
1	A	582	LEU	3.6
1	A	570	TRP	3.6
1	C	569	PHE	3.6
1	B	462	ILE	3.6
1	C	449	THR	3.6
1	C	455	ARG	3.5
1	C	891	VAL	3.5
1	C	745	LEU	3.5
1	C	852	SER	3.5
1	C	812	THR	3.4
1	C	574	LEU	3.4
1	C	709	THR	3.4
1	C	591	VAL	3.4
1	C	541	THR	3.3
1	C	666	PRO	3.3
1	C	679	VAL	3.3
1	C	902	ARG	3.3
1	C	784	GLU	3.3
1	C	853	GLU	3.3
1	C	885	ALA	3.3
1	C	886	ALA	3.3
1	B	545	ASN	3.3

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Mol	Chain	Res	Type	RSRZ
1	B	464	LEU	3.3
1	B	570	TRP	3.3
1	C	890	VAL	3.3
1	C	856	SER	3.3
1	C	459	ARG	3.3
1	C	573	VAL	3.3
1	C	584	GLN	3.3
1	C	633	CYS	3.3
1	C	859	ALA	3.3
1	C	893	PHE	3.2
1	C	458	PRO	3.2
1	C	911	LEU	3.2
1	C	567	VAL	3.2
1	C	905	TYR	3.2
1	C	453	GLU	3.2
1	A	586	ILE	3.2
1	C	800	ASP	3.2
1	C	750	ILE	3.2
1	A	935	ASN	3.2
1	B	935	ASN	3.2
1	C	900	LEU	3.2
1	C	953	VAL	3.2
1	B	560	LYS	3.1
1	A	939	PRO	3.1
1	C	557	TYR	3.1
1	C	447	LEU	3.1
1	C	854	ASN	3.1
1	B	540	PHE	3.1
1	A	574	LEU	3.1
1	C	448	GLY	3.1
1	B	582	LEU	3.1
1	C	536	LEU	3.1
1	C	551	LEU	3.1
1	C	644	SER	3.1
1	B	459	ARG	3.1
1	C	565	ALA	3.0
1	C	930	ASN	3.0
1	C	451	ILE	3.0
1	C	462	ILE	2.9
1	C	555	VAL	2.9
1	B	541	THR	2.9
1	B	581	HIS	2.9

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Mol	Chain	Res	Type	RSRZ
1	C	714	THR	2.9
1	C	535	ALA	2.9
1	C	542	ARG	2.9
1	C	537	LEU	2.9
1	C	715	TYR	2.9
1	B	586	ILE	2.9
1	B	941	PRO	2.9
1	B	583	TYR	2.9
1	C	796	ARG	2.8
1	C	460	CYS	2.8
1	C	631	PHE	2.8
1	C	788	TYR	2.8
1	B	566	LEU	2.8
1	C	556	ALA	2.8
1	C	528	ARG	2.8
1	C	673	PHE	2.8
1	C	526	GLY	2.8
1	A	941	PRO	2.8
1	C	850	VAL	2.7
1	A	936	CYS	2.7
1	B	898	SER	2.7
1	B	574	LEU	2.7
1	C	444	LYS	2.7
1	C	452	GLU	2.7
1	C	580	GLN	2.7
1	B	660	GLY	2.7
1	C	754	ILE	2.7
1	C	783	SER	2.7
1	A	579	ALA	2.7
1	C	855	LEU	2.7
1	C	543	PRO	2.6
1	B	536	LEU	2.6
1	C	464	LEU	2.6
1	C	482	LEU	2.6
1	B	487	VAL	2.6
1	C	558	SER	2.6
1	C	742	GLY	2.6
1	B	803	GLU	2.6
1	C	585	SER	2.6
1	C	577	ALA	2.6
1	C	680	THR	2.6
1	A	572	LYS	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	934	ARG	2.6
1	B	939	PRO	2.6
1	A	569	PHE	2.6
1	C	935	ASN	2.6
1	C	534	THR	2.6
1	C	583	TYR	2.6
1	C	896	GLY	2.5
1	C	456	LYS	2.5
1	C	915	LYS	2.5
1	A	697	ASP	2.5
1	B	702	GLU	2.5
1	C	546	LEU	2.5
1	B	463	HIS	2.5
1	C	539	LYS	2.5
1	C	718	THR	2.5
1	C	465	PRO	2.5
1	C	739	GLY	2.5
1	B	853	GLU	2.5
1	C	545	ASN	2.5
1	C	621	GLU	2.5
1	C	641	LYS	2.5
1	C	746	VAL	2.5
1	C	858	VAL	2.5
1	B	824	ARG	2.5
1	C	724	ARG	2.5
1	C	802	SER	2.5
1	B	571	ASP	2.4
1	C	920	LYS	2.4
1	C	914	ARG	2.4
1	C	740	VAL	2.4
1	C	898	SER	2.4
1	A	540	PHE	2.4
1	B	524	THR	2.4
1	C	716	GLU	2.4
1	C	908	HIS	2.4
1	C	713	VAL	2.4
1	B	561	TRP	2.4
1	B	940	GLY	2.4
1	A	571	ASP	2.4
1	B	494	HIS	2.4
1	B	546	LEU	2.4
1	C	576	GLU	2.4

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Mol	Chain	Res	Type	RSRZ
1	C	544	GLN	2.3
1	C	708	LEU	2.3
1	C	827	ASP	2.3
1	B	572	LYS	2.3
1	A	703	ARG	2.3
1	A	657	LEU	2.3
1	A	911	LEU	2.3
1	B	568	ASP	2.3
1	B	642	MET	2.3
1	C	795	ALA	2.3
1	C	723	GLY	2.3
1	C	668	LYS	2.3
1	C	630	ALA	2.3
1	B	678	ARG	2.3
1	C	909	THR	2.3
1	C	956	SER	2.3
1	B	759	ILE	2.3
1	C	531	LEU	2.3
1	C	917	ASP	2.3
1	C	702	GLU	2.3
1	B	573	VAL	2.3
1	A	580	GLN	2.2
1	C	581	HIS	2.2
1	A	940	GLY	2.2
1	C	719	ILE	2.2
1	A	525	ALA	2.2
1	B	884	ALA	2.2
1	C	579	ALA	2.2
1	C	743	ALA	2.2
1	C	781	GLN	2.2
1	C	461	GLY	2.2
1	B	937	SER	2.2
1	B	539	LYS	2.2
1	B	915	LYS	2.2
1	C	549	ALA	2.2
1	C	672	LEU	2.2
1	C	548	ASP	2.2
1	C	887	GLU	2.2
1	C	572	LYS	2.2
1	B	485	GLY	2.1
1	C	676	PHE	2.1
1	B	479	VAL	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	669	LEU	2.1
1	C	593	ILE	2.1
1	C	949	ILE	2.1
1	B	576	GLU	2.1
1	C	664	ARG	2.1
1	C	704	CYS	2.1
1	C	797	SER	2.1
1	B	490	PRO	2.1
1	B	745	LEU	2.1
1	C	634	THR	2.1
1	B	532	ILE	2.1
1	B	559	LYS	2.1
1	B	535	ALA	2.1
1	C	711	LEU	2.1
1	B	534	THR	2.1
1	C	786	THR	2.1
1	C	445	LYS	2.1
1	C	661	ARG	2.0
1	C	721	GLY	2.0
1	C	780	GLU	2.0
1	C	801	GLY	2.0
1	B	671	THR	2.0
1	C	568	ASP	2.0
1	C	677	ARG	2.0
1	C	793	ARG	2.0
1	C	910	PHE	2.0
1	B	804	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.

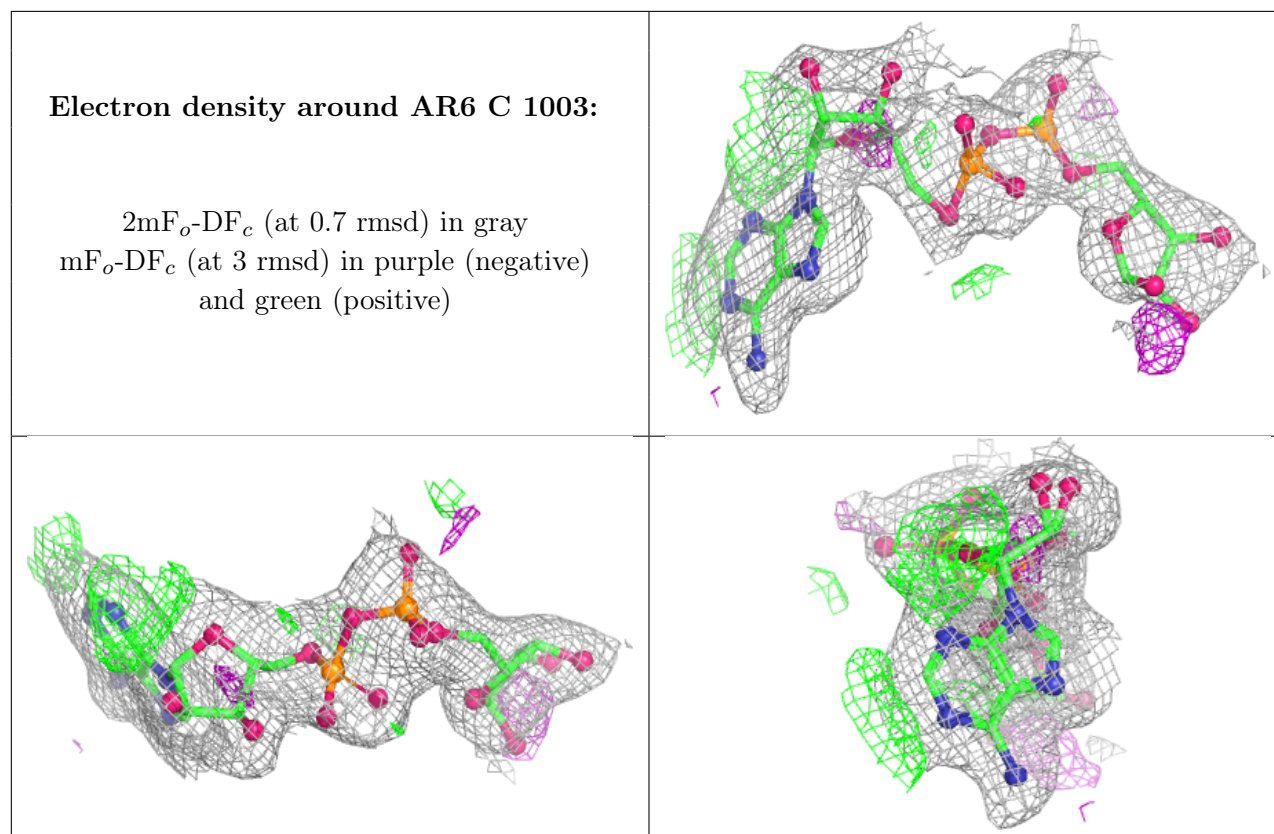
6.4 Ligands [i](#)

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.

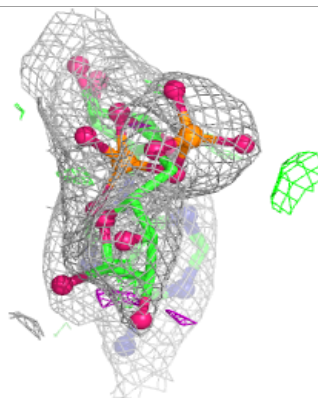
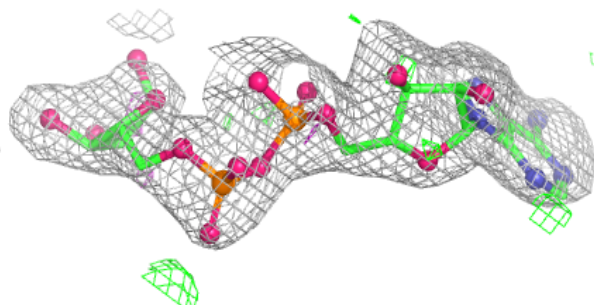
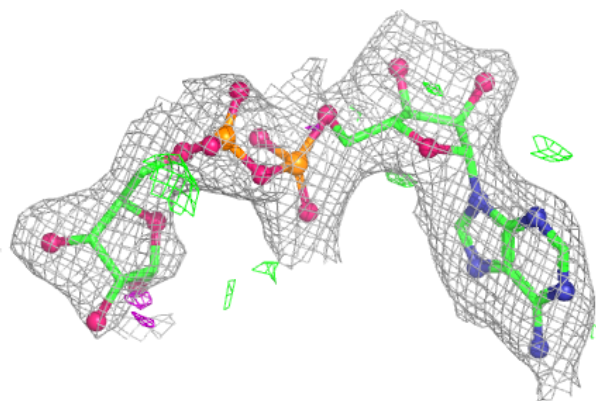
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	IOD	A	1002	1/1	0.79	0.19	139,139,139,139	0
2	IOD	C	1002	1/1	0.81	0.29	175,175,175,175	0
3	AR6	C	1003	36/36	0.87	0.12	23,40,50,51	0
3	AR6	B	1003	36/36	0.91	0.10	26,38,47,52	0
2	IOD	A	1001	1/1	0.92	0.08	78,78,78,78	0
2	IOD	C	1001	1/1	0.94	0.12	98,98,98,98	0
2	IOD	B	1001	1/1	0.94	0.11	75,75,75,75	0
3	AR6	A	1003	36/36	0.95	0.08	24,34,41,44	0
2	IOD	B	1002	1/1	0.96	0.17	93,93,93,93	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.

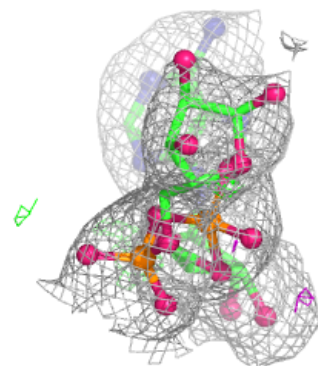
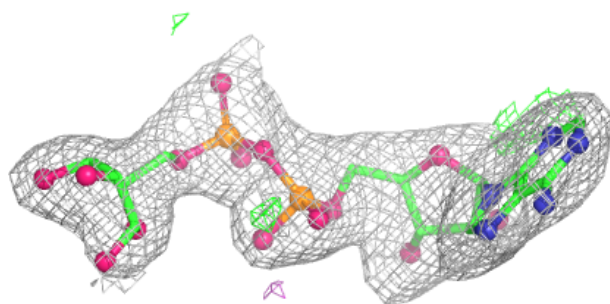
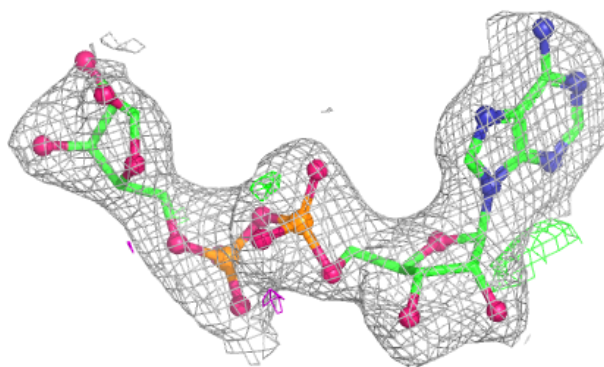


Electron density around AR6 B 1003:

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

**Electron density around AR6 A 1003:**

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



6.5 Other polymers ⓘ

There are no such residues in this entry.