Full wwPDB X-ray Structure Validation Report ⓘ

Oct 15, 2023 – 12:29 PM EDT

PDB ID	:	1U2R
Title	:	Crystal Structure of ADP-ribosylated Ribosomal Translocase from Saccharomyces cerevisiae
Authors	:	Jorgensen, R.; Yates, S.P.; Nilsson, J.; Prentice, G.A.; Teal, D.J.; Merrill, A.R.; Andersen, G.R.
Deposited on	:	2004-07-20
Resolution	:	2.60 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:

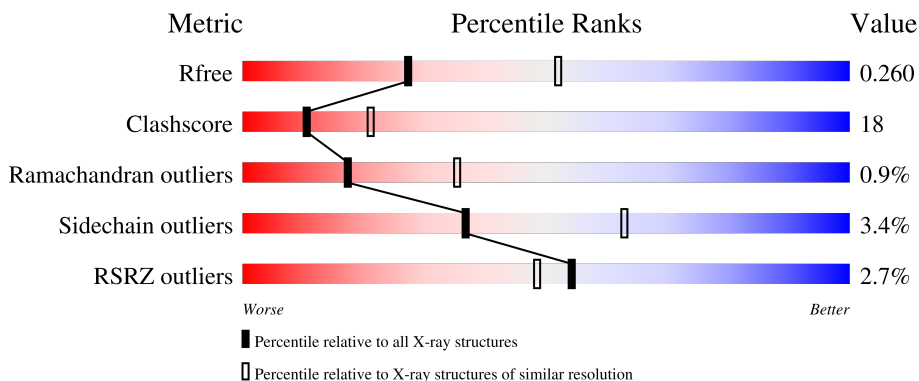|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.60 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	Percentile Ranks	Value
Rfree		0.260
Clashscore		18
Ramachandran outliers		0.9%
Sidechain outliers		3.4%
RSRZ outliers		2.7%

Worse .... *Better*

▮ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (2.60-2.60)

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 <=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	842	3% / 65% / 30% / · ·

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	APR	A	1699	X	-	-	X
4	SO1	A	1700	X	-	-	-

2 Entry composition ⓘ

There are 6 unique types of molecules in this entry. The entry contains 6670 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 Elongation factor 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	819	Total 6386	C 4064	N 1088	O 1204	S 30	0	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	699	DDE	HIS	modified residue	UNP P32324

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total 1	Mg 1	0	0

- Molecule 3 is ADENOSINE-5-DIPHOSPHORIBOSE (three-letter code: APR) (formula: $C_{15}H_{23}N_5O_{14}P_2$).
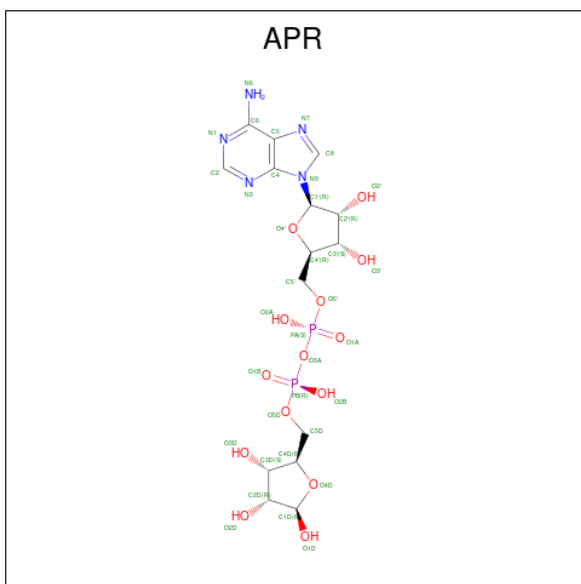
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			35	15	5	13	2		

- Molecule 4 is [1R-(1.ALPHA.,3A.BETA.,4.BETA.,4A.BETA.,7.BETA.,7A.ALPHA.,8A.BETA.)]8A-[(6-DEOXY-4-O-METHYL-BETA-D-ALTROPYRANOSYLOXY)METHYL]-4-FORMYL-4,4A,5,6,7,7A,8,8A-OCTAHYDRO-7-METHYL-3-(1-METHYLETHYL)-1,4-METHANO-S-INDACENE-3A(1H)-CARBOXYLIC ACID (three-letter code: SO1) (formula: $C_{27}H_{42}O_8$).
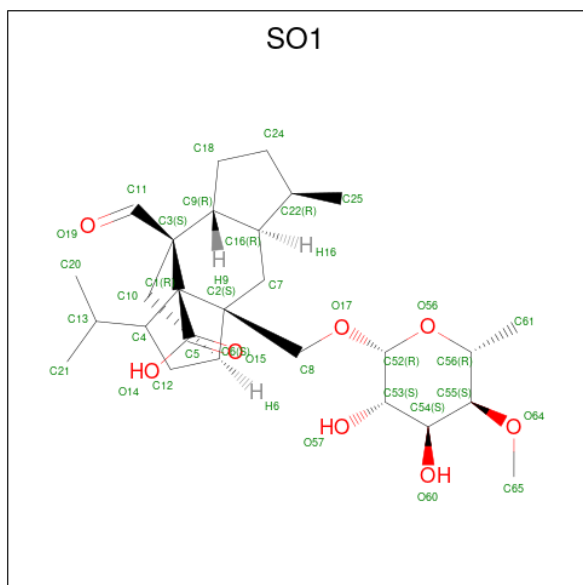
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			35	27	8		

- Molecule 5 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula: $C_{10}H_{15}N_5O_{11}P_2$).

GDP
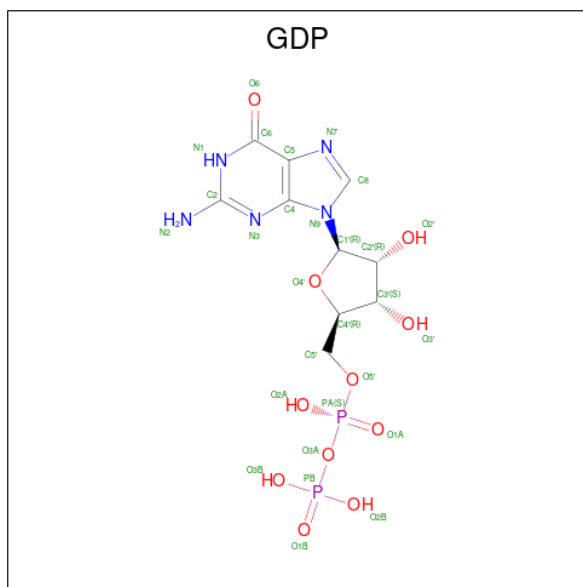
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
5	A	1	28	10	5	11	2	0	0

• Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
6	A	185	185	185	0	0

3 Residue-property plots ⓘ

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: Elongation factor 2

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α, β, γ	119.72Å　　151.00Å　　65.17Å 90.00°　　　90.00°　　　90.00°	Depositor
Resolution (Å)	35.00　–　2.60 34.03　–　2.60	Depositor EDS
% Data completeness (in resolution range)	99.6 (35.00-2.60) 99.6 (34.03-2.60)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	0.06	Depositor
$< I/\sigma(I) >$ [1]	3.70 (at 2.61Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.227　,　0.262 0.219　,　0.260	Depositor DCC
R_{free} test set	1130 reflections (3.04%)	wwPDB-VP
Wilson B-factor (Å^2)	47.4	Xtriage
Anisotropy	0.329	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 40.9	EDS
L-test for twinning[2]	$< |L| > = 0.49, < L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	6670	wwPDB-VP
Average B, all atoms (Å^2)	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.56% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.
[2]Theoretical values of $< |L| >$, $< L^2 >$ 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: APR, DDE, SO1, GDP, MG

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	0.38	0/6486	0.62	0/8779

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	6386	0	6453	237	0
2	A	1	0	0	0	0
3	A	35	0	19	5	0
4	A	35	0	40	2	0
5	A	28	0	12	3	0
6	A	185	0	0	19	0
All	All	6670	0	6524	240	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 18.

All (240) 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:109:VAL:HG21	1:A:138:GLN:HG2	1.37	1.03
1:A:126:LEU:HD11	1:A:156:VAL:HG23	1.43	0.99
1:A:27:HIS:CD2	1:A:138:GLN:HB2	2.07	0.89
1:A:126:LEU:HD11	1:A:156:VAL:CG2	2.03	0.87
1:A:463:LEU:HD21	1:A:467:GLY:HA3	1.55	0.85
1:A:694:HIS:O	1:A:700:ARG:HD3	1.81	0.81
1:A:109:VAL:CG2	1:A:138:GLN:HG2	2.11	0.80
1:A:813:SER:O	1:A:817:GLU:HG3	1.84	0.77
3:A:1699:APR:H8	3:A:1699:APR:H5R2	1.65	0.77
1:A:22:MET:SD	1:A:102:LEU:HD12	2.26	0.76
1:A:34:THR:HG23	5:A:1920:GDP:O2A	1.86	0.75
1:A:603:ASN:HB2	6:A:2052:HOH:O	1.86	0.74
1:A:576:LEU:HD21	1:A:842:LEU:HG	1.69	0.74
1:A:781:THR:HG22	6:A:2010:HOH:O	1.89	0.72
1:A:353:ALA:CB	1:A:370:LYS:HG2	2.20	0.72
1:A:378:LEU:H	1:A:471:THR:HG22	1.55	0.71
1:A:464:LEU:O	1:A:465:LYS:HB2	1.90	0.71
1:A:32:LYS:O	1:A:36:THR:HG23	1.92	0.70
1:A:28:VAL:HG12	6:A:2035:HOH:O	1.92	0.70
1:A:223:ARG:HH11	1:A:223:ARG:HG2	1.57	0.69
1:A:189:VAL:CG1	1:A:200:VAL:HG13	2.22	0.69
1:A:374:PRO:O	1:A:404:THR:HG23	1.92	0.68
1:A:630:ALA:O	1:A:633:ILE:HG23	1.94	0.67
1:A:324:MET:HE2	1:A:324:MET:HA	1.76	0.65
1:A:88:GLU:CD	1:A:223:ARG:HH21	1.99	0.65
1:A:297:PRO:HD2	6:A:2065:HOH:O	1.95	0.65
1:A:829:LYS:HA	1:A:829:LYS:HE3	1.78	0.65
1:A:103:ILE:HD12	1:A:122:THR:HG22	1.77	0.65
1:A:67:GLY:HA3	6:A:2007:HOH:O	1.97	0.64
1:A:237:LYS:O	1:A:241:MET:HG2	1.97	0.64
1:A:763:THR:N	1:A:764:PRO:HD3	2.12	0.64
1:A:731:VAL:HG12	1:A:770:ALA:O	1.97	0.64
1:A:829:LYS:CE	1:A:830:GLU:H	2.11	0.64
1:A:627:VAL:O	1:A:631:ARG:HG3	1.98	0.63
1:A:86:VAL:HG13	1:A:93:THR:HG21	1.81	0.63
1:A:520:THR:HG22	1:A:530:VAL:HG22	1.81	0.62
1:A:633:ILE:HD12	1:A:635:CYS:N	2.14	0.62
1:A:126:LEU:CD1	1:A:156:VAL:HG23	2.25	0.62
1:A:433:ARG:HB3	1:A:457:VAL:CG1	2.30	0.62
1:A:120:ARG:HH12	1:A:481:MET:CE	2.13	0.62
3:A:1699:APR:H8	3:A:1699:APR:C5D	2.30	0.61
1:A:804:LEU:N	6:A:1962:HOH:O	2.31	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:120:ARG:NH1	1:A:481:MET:HE1	2.14	0.61
1:A:576:LEU:HD11	1:A:585:ARG:HD3	1.82	0.61
1:A:718:LEU:HB3	1:A:835:TRP:HB3	1.82	0.61
1:A:564:ARG:HG3	1:A:682:ARG:HB2	1.83	0.60
1:A:694:HIS:CD2	1:A:696:ASP:H	2.19	0.60
1:A:734:GLN:HG3	1:A:767:THR:HG22	1.83	0.60
1:A:284:LEU:HD13	1:A:324:MET:CE	2.32	0.59
1:A:379:MET:HB2	1:A:402:ALA:HB3	1.84	0.59
1:A:202:VAL:HG12	1:A:209:VAL:CG2	2.33	0.58
1:A:615:ARG:HG2	1:A:619:MET:HE3	1.85	0.58
1:A:545:LEU:HA	1:A:549:HIS:HB2	1.85	0.58
1:A:365:ASN:O	1:A:369:ILE:HG12	2.03	0.58
1:A:3:ALA:HA	1:A:46:ILE:O	2.05	0.57
1:A:581:ASN:O	1:A:582:LYS:HB2	2.05	0.57
1:A:737:GLU:HB2	1:A:766:PHE:CE2	2.39	0.57
1:A:500:ASP:CB	1:A:552:VAL:HG11	2.35	0.57
1:A:386:VAL:HG11	1:A:437:MET:CE	2.34	0.57
1:A:497:ASN:HB3	1:A:500:ASP:OD2	2.04	0.57
1:A:296:ILE:O	1:A:300:LEU:HD13	2.05	0.57
1:A:106:PRO:HB3	1:A:108:HIS:NE2	2.21	0.56
1:A:223:ARG:HA	1:A:241:MET:HE2	1.88	0.56
1:A:284:LEU:HD13	1:A:324:MET:HE1	1.88	0.56
1:A:785:ARG:HD3	6:A:2067:HOH:O	2.05	0.56
1:A:223:ARG:HG2	1:A:223:ARG:NH1	2.21	0.56
1:A:129:VAL:HG11	1:A:181:THR:CG2	2.36	0.56
1:A:500:ASP:HB3	1:A:552:VAL:HG11	1.87	0.56
1:A:725:GLN:HA	6:A:1962:HOH:O	2.05	0.56
1:A:413:ILE:HB	1:A:427:PHE:HB2	1.88	0.55
1:A:89:ILE:HG12	1:A:340:LEU:HD23	1.88	0.55
1:A:108:HIS:CE1	1:A:114:GLU:HB2	2.42	0.55
1:A:88:GLU:OE2	1:A:223:ARG:NH2	2.39	0.55
1:A:369:ILE:HD12	1:A:401:PHE:HB3	1.90	0.54
1:A:615:ARG:HG2	1:A:619:MET:CE	2.36	0.54
1:A:829:LYS:HE3	1:A:830:GLU:H	1.71	0.54
1:A:26:ALA:HB3	1:A:32:LYS:HB2	1.88	0.54
1:A:284:LEU:CD1	1:A:324:MET:HE1	2.37	0.54
1:A:279:ASP:HB3	1:A:280:PRO:HD3	1.89	0.54
1:A:804:LEU:HG	6:A:1962:HOH:O	2.06	0.54
1:A:194:ASP:HB2	1:A:197:LEU:HD13	1.89	0.54
1:A:296:ILE:HB	1:A:297:PRO:HD3	1.89	0.54
1:A:806:SER:HB2	1:A:813:SER:HB2	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:42:ARG:HB2	6:A:2039:HOH:O	2.07	0.54
1:A:28:VAL:HG22	1:A:138:GLN:OE1	2.08	0.53
1:A:108:HIS:HE1	1:A:114:GLU:HB2	1.72	0.53
1:A:360:PRO:O	1:A:363:ASP:HB3	2.08	0.53
1:A:646:VAL:C	1:A:647:ILE:HD12	2.29	0.53
1:A:109:VAL:HG11	1:A:142:VAL:CG2	2.38	0.53
1:A:520:THR:HA	1:A:529:ILE:O	2.08	0.53
1:A:120:ARG:NH1	1:A:481:MET:CE	2.72	0.53
1:A:129:VAL:HG11	1:A:181:THR:HG23	1.91	0.52
1:A:250:PHE:O	1:A:252:PRO:HD3	2.10	0.52
1:A:471:THR:HG23	1:A:471:THR:O	2.08	0.52
1:A:515:ASP:HB3	1:A:518:VAL:CG1	2.39	0.52
1:A:500:ASP:CG	1:A:552:VAL:HG11	2.29	0.52
1:A:718:LEU:HD12	1:A:722:PRO:HG2	1.92	0.52
1:A:751:ARG:HD3	1:A:814:LYS:NZ	2.24	0.52
1:A:569:SER:O	1:A:720:ALA:HB1	2.10	0.52
1:A:378:LEU:H	1:A:471:THR:CG2	2.21	0.51
1:A:829:LYS:HE2	1:A:830:GLU:H	1.74	0.51
1:A:21:ASN:ND2	1:A:453:ILE:HD13	2.25	0.51
1:A:489:VAL:HG22	1:A:781:THR:HG21	1.91	0.51
1:A:576:LEU:HD13	1:A:587:TYR:CE1	2.46	0.51
1:A:189:VAL:HG13	1:A:200:VAL:HG13	1.92	0.51
1:A:358:GLU:OE2	1:A:479:LYS:HA	2.11	0.51
1:A:745:SER:O	1:A:749:LYS:HG3	2.10	0.51
1:A:470:THR:HG21	1:A:475:ALA:HB1	1.93	0.51
1:A:607:ASN:HB2	1:A:610:ASP:OD2	2.11	0.51
1:A:426:LEU:HD12	1:A:427:PHE:H	1.76	0.51
1:A:345:PRO:O	1:A:349:GLN:HG3	2.12	0.50
1:A:576:LEU:HD21	1:A:585:ARG:NH1	2.27	0.50
1:A:785:ARG:HG3	1:A:785:ARG:HH11	1.75	0.50
1:A:360:PRO:HB2	1:A:363:ASP:HB2	1.94	0.50
1:A:481:MET:HE2	1:A:481:MET:HA	1.94	0.50
1:A:386:VAL:HG11	1:A:437:MET:HE1	1.93	0.50
1:A:414:GLN:HB2	1:A:477:ASN:HD21	1.77	0.50
1:A:576:LEU:HD21	1:A:585:ARG:HH11	1.77	0.50
1:A:693:LEU:HB3	1:A:700:ARG:HD2	1.92	0.50
1:A:539:GLU:O	1:A:543:GLN:HG3	2.12	0.50
1:A:411:VAL:HG12	1:A:412:ARG:N	2.27	0.49
1:A:503:LYS:HD2	1:A:552:VAL:HG21	1.94	0.49
1:A:224:GLN:HA	6:A:2033:HOH:O	2.12	0.49
1:A:200:VAL:O	1:A:200:VAL:HG22	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:202:VAL:CG1	1:A:209:VAL:CG2	2.91	0.49
1:A:706:ILE:HB	1:A:707:PRO:HD3	1.94	0.49
1:A:153:PRO:HD2	1:A:200:VAL:HG22	1.95	0.48
1:A:271:ARG:HG3	1:A:271:ARG:HH11	1.78	0.48
1:A:774:VAL:HG11	4:A:1700:SO1:H121	1.94	0.48
1:A:186:ASN:HB3	1:A:201:GLN:OE1	2.14	0.48
1:A:699:DDE:HAC3	3:A:1699:APR:O2B	2.13	0.48
1:A:461:GLN:H	1:A:461:GLN:CD	2.16	0.48
1:A:646:VAL:HG23	1:A:667:PHE:CD2	2.49	0.48
1:A:16:VAL:HG11	1:A:450:ALA:O	2.13	0.48
1:A:433:ARG:HB3	1:A:457:VAL:HG11	1.95	0.48
1:A:120:ARG:HH12	1:A:481:MET:HE1	1.76	0.48
1:A:109:VAL:CG1	1:A:142:VAL:CG2	2.92	0.48
1:A:237:LYS:HA	1:A:240:MET:HB2	1.95	0.48
1:A:552:VAL:HG13	1:A:553:PRO:HD2	1.95	0.48
1:A:807:ASP:OD1	1:A:809:LEU:N	2.44	0.48
1:A:110:ASP:OD2	1:A:112:SER:HB3	2.14	0.47
1:A:823:ARG:HE	1:A:832:VAL:HG22	1.80	0.47
1:A:784:LEU:HD23	1:A:794:PRO:HD3	1.96	0.47
1:A:232:LYS:HG3	6:A:2137:HOH:O	2.13	0.47
1:A:565:GLU:O	1:A:681:MET:HA	2.14	0.47
1:A:823:ARG:NH1	1:A:829:LYS:O	2.47	0.47
1:A:16:VAL:O	1:A:345:PRO:HD2	2.14	0.47
1:A:699:DDE:HAD2	1:A:699:DDE:HAA3	1.78	0.47
1:A:481:MET:CE	1:A:481:MET:HA	2.45	0.47
1:A:360:PRO:HD2	1:A:363:ASP:HB2	1.96	0.46
1:A:454:ILE:HG13	1:A:455:GLY:N	2.30	0.46
1:A:631:ARG:NH1	6:A:2003:HOH:O	2.47	0.46
1:A:80:GLU:HA	1:A:96:ASN:O	2.15	0.46
1:A:106:PRO:HB3	1:A:108:HIS:CD2	2.50	0.46
1:A:202:VAL:HG12	1:A:209:VAL:HG23	1.98	0.46
1:A:221:THR:OG1	1:A:224:GLN:HG3	2.15	0.46
1:A:378:LEU:N	1:A:471:THR:HG22	2.29	0.46
1:A:809:LEU:O	1:A:811:PRO:HD3	2.16	0.46
1:A:785:ARG:HG3	1:A:786:GLN:N	2.31	0.46
1:A:84:GLU:HG3	1:A:85:ASP:N	2.30	0.46
1:A:411:VAL:HG12	1:A:412:ARG:H	1.80	0.46
1:A:434:VAL:HG12	1:A:445:ILE:HG22	1.98	0.46
1:A:175:TYR:OH	1:A:246:GLY:HA2	2.17	0.45
1:A:267:LYS:HA	1:A:268:PRO:HD3	1.81	0.45
1:A:515:ASP:O	1:A:518:VAL:HG12	2.15	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:202:VAL:CG1	1:A:209:VAL:HG22	2.47	0.45
1:A:42:ARG:HG2	1:A:331:ALA:CB	2.47	0.45
1:A:733:ILE:O	1:A:767:THR:HA	2.17	0.45
1:A:751:ARG:HD3	1:A:814:LYS:HZ2	1.82	0.44
1:A:172:GLU:HA	1:A:274:ASN:HD21	1.82	0.44
1:A:391:LYS:HD3	6:A:2028:HOH:O	2.17	0.44
1:A:524:GLU:HG3	6:A:1993:HOH:O	2.17	0.44
1:A:77:LEU:HB2	1:A:100:ILE:HB	1.99	0.44
1:A:126:LEU:HD11	1:A:156:VAL:HG21	1.93	0.44
1:A:515:ASP:HB3	1:A:518:VAL:HG12	2.00	0.44
1:A:81:MET:HG3	1:A:339:VAL:HG11	1.99	0.43
1:A:214:GLY:HA3	6:A:1939:HOH:O	2.17	0.43
1:A:600:ALA:HA	6:A:2052:HOH:O	2.18	0.43
1:A:715:ALA:HB2	1:A:838:TYR:HB2	2.00	0.43
1:A:633:ILE:O	1:A:633:ILE:HG13	2.18	0.43
1:A:29:ASP:HA	5:A:1920:GDP:H5'	2.00	0.43
1:A:559:PRO:HB2	4:A:1700:SO1:H201	2.00	0.43
1:A:28:VAL:O	1:A:29:ASP:HB2	2.18	0.43
1:A:260:LYS:HE2	1:A:260:LYS:HB3	1.80	0.43
1:A:353:ALA:HB3	1:A:370:LYS:HG2	1.99	0.43
1:A:109:VAL:HG12	1:A:142:VAL:HG22	1.99	0.43
1:A:153:PRO:HD2	1:A:200:VAL:CG2	2.49	0.43
1:A:410:LYS:HB2	6:A:2122:HOH:O	2.18	0.43
1:A:763:THR:HG22	1:A:763:THR:O	2.19	0.43
1:A:369:ILE:HD13	1:A:402:ALA:HB2	2.01	0.43
1:A:718:LEU:HA	1:A:722:PRO:HG3	2.00	0.42
1:A:108:HIS:CE1	1:A:112:SER:HG	2.36	0.42
1:A:235:VAL:HG12	1:A:239:LYS:HB3	2.01	0.42
1:A:564:ARG:HG3	1:A:682:ARG:CB	2.47	0.42
1:A:426:LEU:HD12	1:A:427:PHE:N	2.34	0.42
1:A:25:ILE:HG23	1:A:142:VAL:HB	2.00	0.42
1:A:699:DDE:HD2	3:A:1699:APR:O2D	2.20	0.42
1:A:763:THR:N	1:A:764:PRO:CD	2.79	0.42
1:A:810:ASP:O	1:A:816:GLY:HA3	2.19	0.42
1:A:159:LYS:HG3	5:A:1920:GDP:C2	2.53	0.42
1:A:829:LYS:HE3	1:A:829:LYS:CA	2.48	0.42
1:A:197:LEU:N	1:A:197:LEU:HD12	2.34	0.42
1:A:386:VAL:HG11	1:A:437:MET:HE3	2.01	0.42
1:A:491:VAL:HG21	1:A:542:LEU:HD11	2.01	0.42
1:A:287:ALA:HA	1:A:292:LYS:HD2	2.02	0.42
1:A:388:THR:HG21	1:A:395:TYR:CD1	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:417:ASN:HB2	1:A:425:ASP:OD2	2.20	0.42
1:A:414:GLN:CB	1:A:477:ASN:HD21	2.31	0.41
1:A:454:ILE:HG13	1:A:455:GLY:H	1.84	0.41
1:A:284:LEU:HD13	1:A:324:MET:HE3	2.02	0.41
1:A:694:HIS:CD2	1:A:699:DDE:HD2	2.55	0.41
1:A:737:GLU:HB2	1:A:766:PHE:HE2	1.84	0.41
1:A:478:MET:O	1:A:479:LYS:C	2.58	0.41
1:A:284:LEU:HD11	1:A:303:LEU:CD1	2.50	0.41
1:A:418:TYR:CD1	1:A:418:TYR:C	2.94	0.41
1:A:565:GLU:CD	1:A:676:ILE:HB	2.41	0.41
1:A:155:VAL:CG1	1:A:156:VAL:N	2.84	0.41
1:A:378:LEU:HD11	1:A:380:LEU:HB2	2.02	0.41
1:A:380:LEU:HD13	1:A:456:LEU:HD11	2.01	0.41
1:A:658:GLU:OE1	1:A:700:ARG:NH2	2.54	0.41
1:A:744:TYR:CE1	1:A:754:VAL:HG21	2.55	0.41
1:A:666:ALA:CB	1:A:709:MET:HB3	2.51	0.41
1:A:722:PRO:O	1:A:723:LYS:HD2	2.20	0.41
1:A:39:LEU:HB3	1:A:77:LEU:HD21	2.03	0.41
1:A:357:TYR:OH	1:A:476:HIS:HB2	2.20	0.41
1:A:579:SER:HB3	1:A:708:THR:OG1	2.20	0.41
1:A:607:ASN:HA	1:A:608:PRO:HD3	1.83	0.41
1:A:256:LYS:NZ	6:A:2133:HOH:O	2.44	0.41
1:A:552:VAL:CG1	1:A:553:PRO:HD2	2.50	0.41
1:A:807:ASP:HA	1:A:808:PRO:HD3	1.96	0.41
1:A:27:HIS:CD2	1:A:136:CYS:HB2	2.57	0.40
1:A:386:VAL:HA	1:A:387:PRO:HD3	1.87	0.40
1:A:636:PHE:CE1	1:A:645:LEU:HD21	2.56	0.40
1:A:110:ASP:O	1:A:111:PHE:HB2	2.21	0.40
1:A:230:ALA:C	1:A:232:LYS:H	2.23	0.40
3:A:1699:APR:H8	3:A:1699:APR:H5'2	2.03	0.40
1:A:235:VAL:CG1	1:A:239:LYS:HB3	2.51	0.40
1:A:484:SER:HB3	1:A:533:THR:HG23	2.03	0.40
1:A:710:ARG:NH1	1:A:714:TYR:OH	2.54	0.40
1:A:146:ALA:HA	1:A:151:ILE:HD12	2.04	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	812/842 (96%)	768 (95%)	37 (5%)	7 (1%)	17	35

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	764	PRO
1	A	391	LYS
1	A	465	LYS
1	A	425	ASP
1	A	479	LYS
1	A	498	ALA
1	A	359	GLY

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	696/714 (98%)	672 (97%)	24 (3%)	37	63

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

Mol	Chain	Res	Type
1	A	28	VAL
1	A	109	VAL
1	A	138	GLN
1	A	165	LEU

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Mol	Chain	Res	Type
1	A	183	GLU
1	A	194	ASP
1	A	248	SER
1	A	352	ARG
1	A	438	MET
1	A	457	VAL
1	A	460	ASP
1	A	471	THR
1	A	476	HIS
1	A	477	ASN
1	A	490	GLN
1	A	522	MET
1	A	596	GLU
1	A	599	LEU
1	A	633	ILE
1	A	677	PHE
1	A	718	LEU
1	A	738	GLN
1	A	758	GLU
1	A	829	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	21	ASN
1	A	27	HIS
1	A	101	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

1 non-standard protein/DNA/RNA residue is 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	$\#|Z| > 2$
1	DDE	A	699	3,1	14,20,21	1.18	1 (7%)	14,28,30	2.05	6 (42%)

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
1	DDE	A	699	3,1	-	1/20/21/23	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	699	DDE	CAT-CE1	3.32	1.55	1.50

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	699	DDE	OAG-CBI-CBW	-3.70	115.81	120.49
1	A	699	DDE	OAG-CBI-NAD	3.15	128.48	123.00
1	A	699	DDE	CAT-CE1-ND1	2.99	130.90	122.54
1	A	699	DDE	CAC-NCB-CBW	2.82	117.53	110.51
1	A	699	DDE	CAU-CBW-CBI	-2.72	105.81	111.20
1	A	699	DDE	CAC-NCB-CAB	-2.15	102.23	108.10

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	699	DDE	CE1-CAT-CAU-CBW

There are no ring outliers.

1 monomer is involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	699	DDE	4	0

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 4 ligands modelled in this entry, 1 is 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	APR	A	1699	1	33,38,39	1.73	6 (18%)	37,58,60	2.20	11 (29%)
5	GDP	A	1920	2	24,30,30	1.08	3 (12%)	30,47,47	0.82	1 (3%)
4	SO1	A	1700	-	35,39,39	2.02	9 (25%)	39,64,64	2.16	7 (17%)

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	APR	A	1699	1	1/1/9/10	6/18/51/54	0/4/4/4
5	GDP	A	1920	2	-	0/12/32/32	0/3/3/3
4	SO1	A	1700	-	1/1/15/16	7/21/104/104	0/7/5/5

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1700	SO1	C7-C2	6.30	1.64	1.54
3	A	1699	APR	O5'-C5'	-6.27	1.20	1.44
4	A	1700	SO1	C12-C4	-5.02	1.42	1.54
4	A	1700	SO1	C1-C5	3.88	1.59	1.50
3	A	1699	APR	C2-N1	3.49	1.40	1.33
4	A	1700	SO1	C55-C56	3.27	1.58	1.52
3	A	1699	APR	PA-O2A	-3.13	1.40	1.55
5	A	1920	GDP	C6-N1	2.82	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1699	APR	PB-O2B	-2.75	1.42	1.55
4	A	1700	SO1	O56-C52	2.69	1.48	1.41
4	A	1700	SO1	C10-C3	2.58	1.59	1.55
3	A	1699	APR	O4'-C4'	2.54	1.50	1.45
4	A	1700	SO1	C8-C2	2.37	1.57	1.53
4	A	1700	SO1	C52-C53	2.35	1.59	1.52
4	A	1700	SO1	C10-C6	2.32	1.58	1.53
5	A	1920	GDP	O3'-C3'	2.13	1.48	1.43
5	A	1920	GDP	C5-C4	-2.13	1.37	1.43
3	A	1699	APR	O4D-C4D	2.00	1.47	1.44

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1700	SO1	C1-C4-C13	9.00	128.11	118.44
4	A	1700	SO1	C10-C6-C2	6.49	111.97	104.16
3	A	1699	APR	O4'-C4'-C5'	-6.03	89.54	109.37
3	A	1699	APR	PB-O3A-PA	-4.52	117.33	132.83
4	A	1700	SO1	C7-C2-C6	4.27	120.27	112.17
3	A	1699	APR	C1D-C2D-C3D	4.06	107.81	101.63
3	A	1699	APR	O5'-C5'-C4'	3.97	122.65	108.99
3	A	1699	APR	C3'-C2'-C1'	3.83	106.75	100.98
3	A	1699	APR	O2D-C2D-C3D	-3.76	104.13	111.27
4	A	1700	SO1	C18-C9-C16	-3.63	98.44	103.64
3	A	1699	APR	C1D-O4D-C4D	3.29	115.83	108.16
3	A	1699	APR	C1'-N9-C4	-3.05	121.28	126.64
3	A	1699	APR	C5-C6-N6	2.69	124.43	120.35
3	A	1699	APR	O4D-C1D-C2D	-2.47	101.22	105.99
4	A	1700	SO1	C12-C6-C10	-2.23	106.14	107.91
5	A	1920	GDP	O3'-C3'-C4'	-2.23	104.61	111.05
4	A	1700	SO1	O17-C52-C53	2.16	111.67	108.30
4	A	1700	SO1	C24-C18-C9	-2.10	100.98	105.13
3	A	1699	APR	C5'-C4'-C3'	-2.03	107.58	115.18

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	A	1699	APR	C1D
4	A	1700	SO1	C4

All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1699	APR	C5D-O5D-PB-O3A
4	A	1700	SO1	C2-C1-C5-O14
4	A	1700	SO1	C2-C1-C5-O15
3	A	1699	APR	C3'-C4'-C5'-O5'
3	A	1699	APR	O4'-C4'-C5'-O5'
3	A	1699	APR	O4D-C4D-C5D-O5D
3	A	1699	APR	C3D-C4D-C5D-O5D
4	A	1700	SO1	C21-C13-C4-C12
4	A	1700	SO1	C20-C13-C4-C1
4	A	1700	SO1	C21-C13-C4-C1
4	A	1700	SO1	C20-C13-C4-C12
3	A	1699	APR	C5D-O5D-PB-O2B
4	A	1700	SO1	C1-C2-C8-O17

There are no ring outliers.

3 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1699	APR	5	0
5	A	1920	GDP	3	0
4	A	1700	SO1	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 then 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.

Ligand APR A 1699

Bond lengths

Bond angles

Torsions

Rings

Ligand GDP A 1920

Bond lengths

Bond angles

Torsions

Rings

Ligand SO1 A 1700

Bond lengths

Bond angles

Torsions

Rings
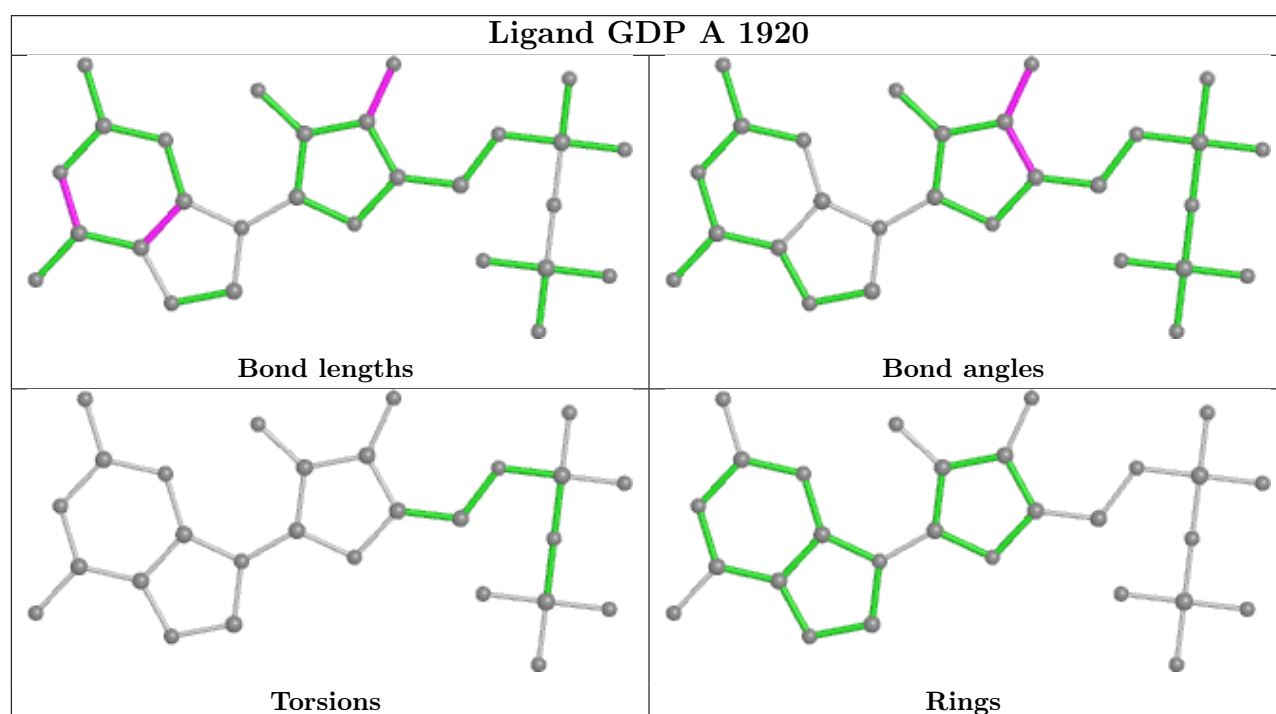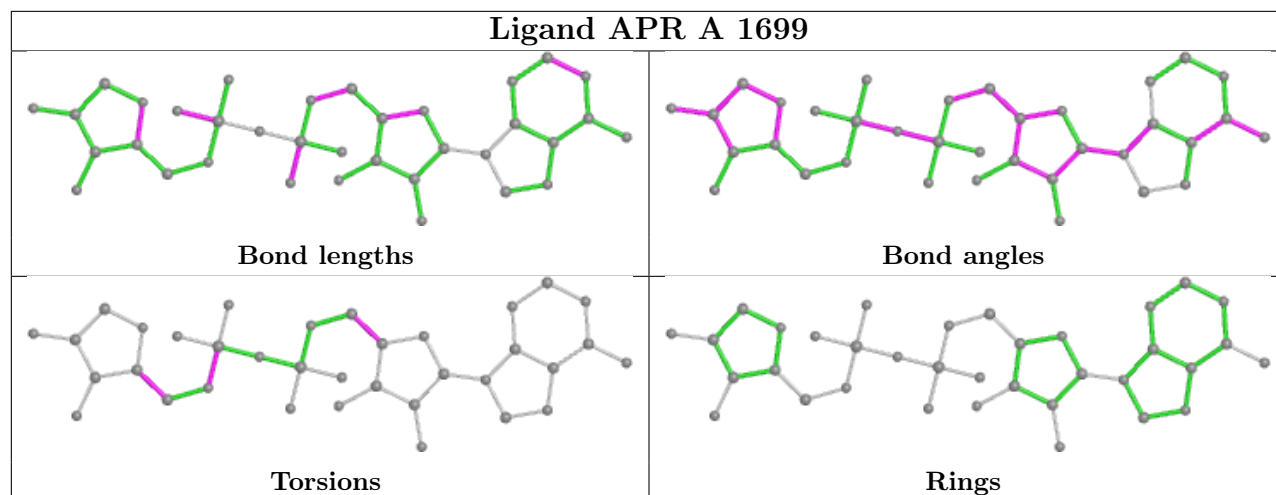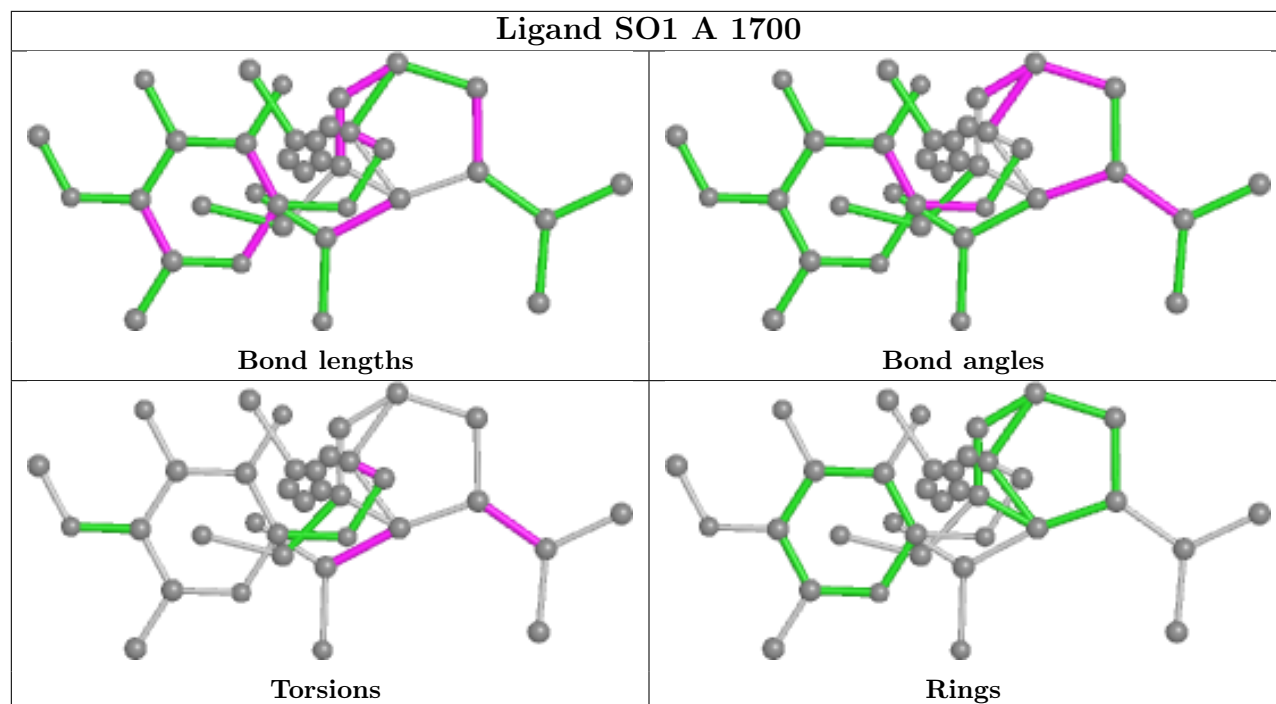
5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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	818/842 (97%)	-0.08	22 (2%)	54	48	24, 46, 74, 92	0

All (22) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	763	THR	3.8
1	A	696	ASP	3.1
1	A	422	LYS	2.9
1	A	473	GLU	2.8
1	A	417	ASN	2.8
1	A	501	LEU	2.7
1	A	391	LYS	2.7
1	A	424	ASP	2.6
1	A	426	LEU	2.4
1	A	767	THR	2.4
1	A	483	PHE	2.3
1	A	168	GLN	2.3
1	A	195	GLU	2.3
1	A	423	LYS	2.2
1	A	427	PHE	2.2
1	A	107	GLY	2.2
1	A	419	VAL	2.1
1	A	125	ALA	2.1
1	A	124	GLY	2.1
1	A	418	TYR	2.1
1	A	167	LEU	2.0
1	A	765	LEU	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains (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
1	DDE	A	699	20/21	0.90	0.25	57,84,90,91	0

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(Å^2)	Q<0.9
3	APR	A	1699	35/36	0.73	0.54	48,117,128,128	0
2	MG	A	843	1/1	0.89	0.07	62,62,62,62	0
4	SO1	A	1700	35/35	0.96	0.15	32,35,39,43	0
5	GDP	A	1920	28/28	0.96	0.13	46,49,52,55	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.
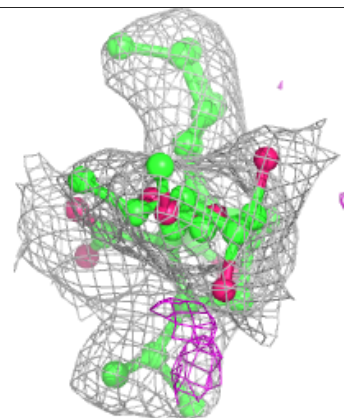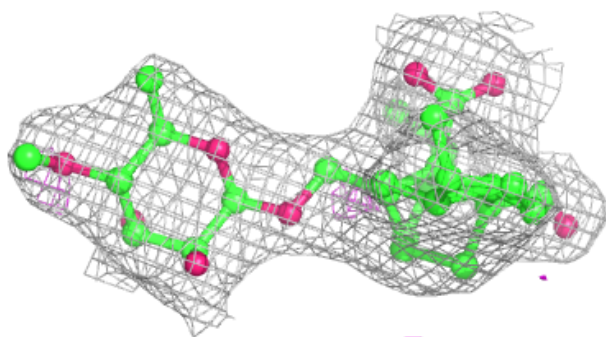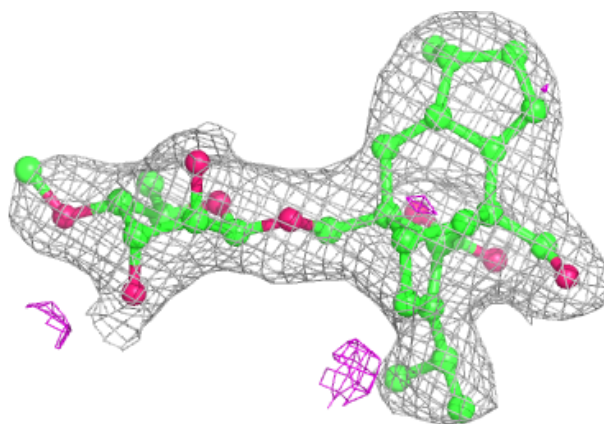
Electron density around APR A 1699:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
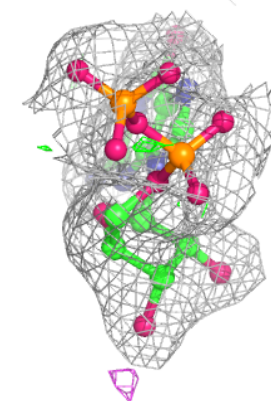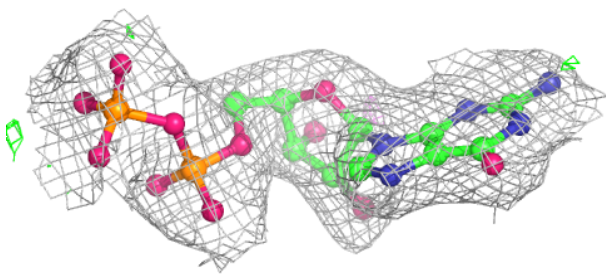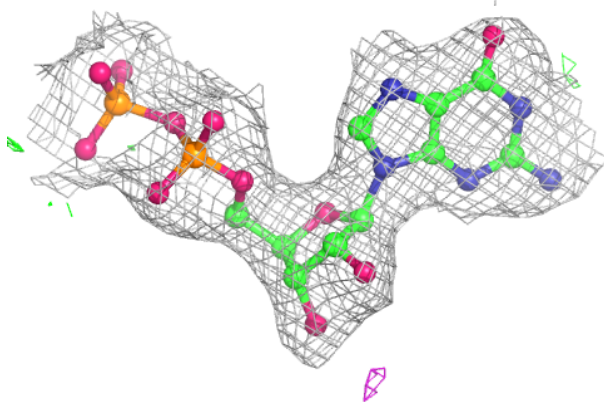mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
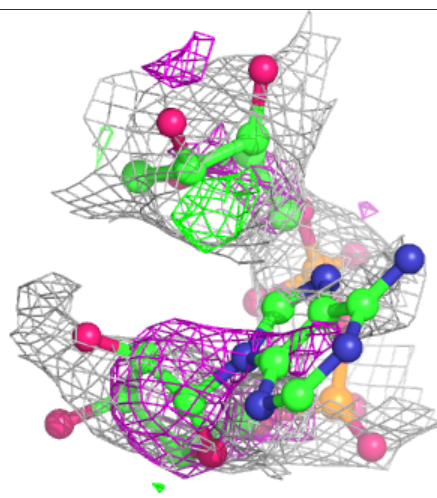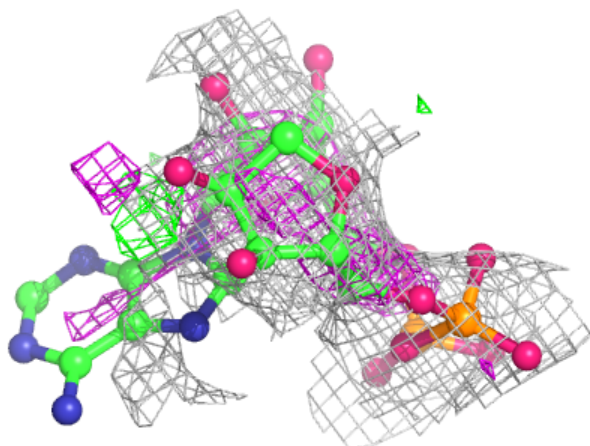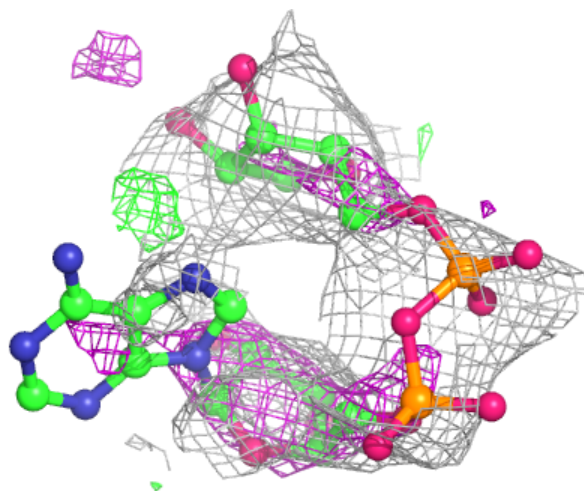
Electron density around SO1 A 1700:

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

Electron density around GDP A 1920:

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

6.5 Other polymers (i)

There are no such residues in this entry.