Full wwPDB X-ray Structure Validation Report ⓘ

Sep 6, 2023 – 03:20 AM EDT

PDB ID	:	4F0E
Title	:	Human ADP-RIBOSYLTRANSFERASE 7 (ARTD7/PARP15), CATALYTIC DOMAIN IN COMPLEX WITH STO1102
Authors	:	Karlberg, T.; Andersson, C.D.; Lindgren, A.; Thorsell, A.G.; Ekblad, T.; Spjut, S.; Weigelt, J.; Elofsson, M.; Linusson, A.; Schuler, H.
Deposited on	:	2012-05-04
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:

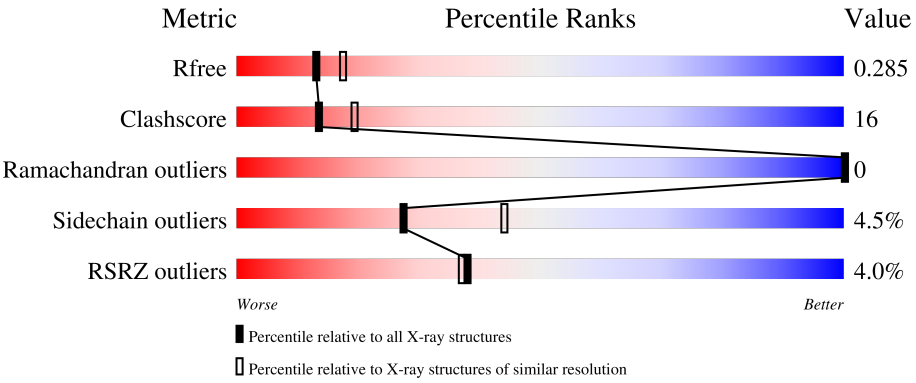
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

1 Overall quality at a glance (i)

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}	130704	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (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 <=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	200	66% 31%
1	B	200	68% 30%
1	C	200	10% 54% 40%
1	D	200	3% 67% 26%

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
2	0RU	C	701	-	-	X	-

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 6441 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

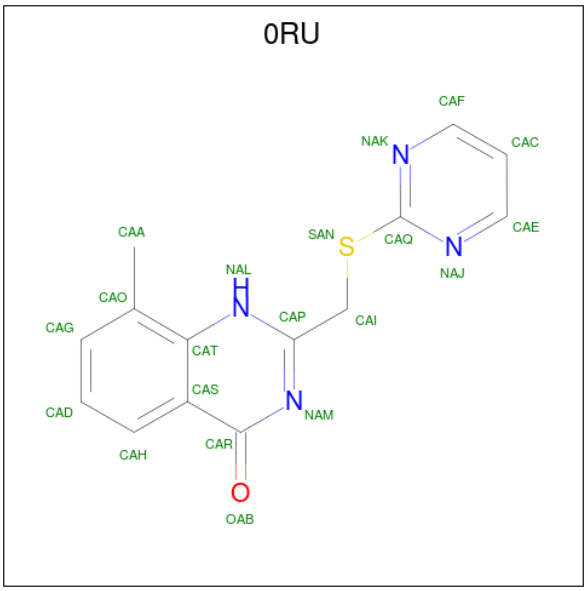
- Molecule 1 is a protein called Poly [ADP-ribose] polymerase 15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	198	Total	C	N	O	S	0	0	0
			1598	1013	278	300	7			
1	B	198	Total	C	N	O	S	0	0	0
			1596	1012	277	300	7			
1	C	193	Total	C	N	O	S	0	0	0
			1559	992	268	292	7			
1	D	191	Total	C	N	O	S	0	0	0
			1552	986	268	292	6			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	457	SER	-	expression tag	UNP Q460N3
A	458	MET	-	expression tag	UNP Q460N3
B	457	SER	-	expression tag	UNP Q460N3
B	458	MET	-	expression tag	UNP Q460N3
C	457	SER	-	expression tag	UNP Q460N3
C	458	MET	-	expression tag	UNP Q460N3
D	457	SER	-	expression tag	UNP Q460N3
D	458	MET	-	expression tag	UNP Q460N3

- Molecule 2 is 8-methyl-2-[(pyrimidin-2-ylsulfanyl)methyl]quinazolin-4(1H)-one (three-letter code: 0RU) (formula: $C_{14}H_{12}N_4OS$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C N O S 20 14 4 1 1	0	0
2	C	1	Total C N O S 20 14 4 1 1	0	0
2	D	1	Total C N O 13 10 2 1	0	0

- Molecule 3 is water.

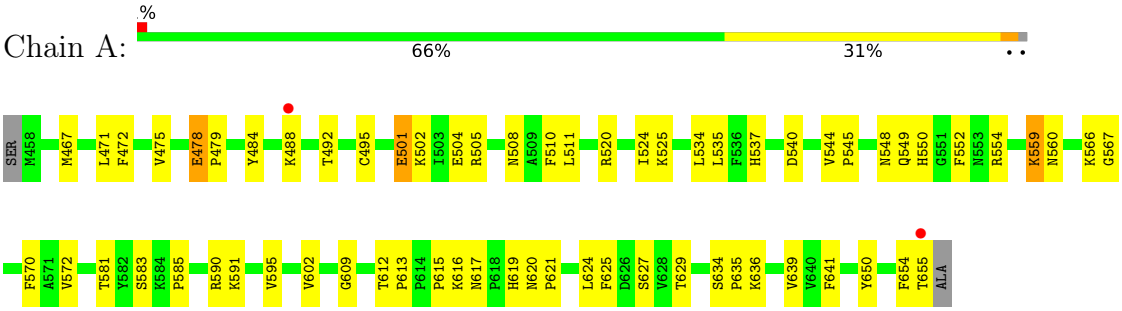
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	27	Total O 27 27	0	0
3	B	20	Total O 20 20	0	0
3	C	18	Total O 18 18	0	0
3	D	18	Total O 18 18	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

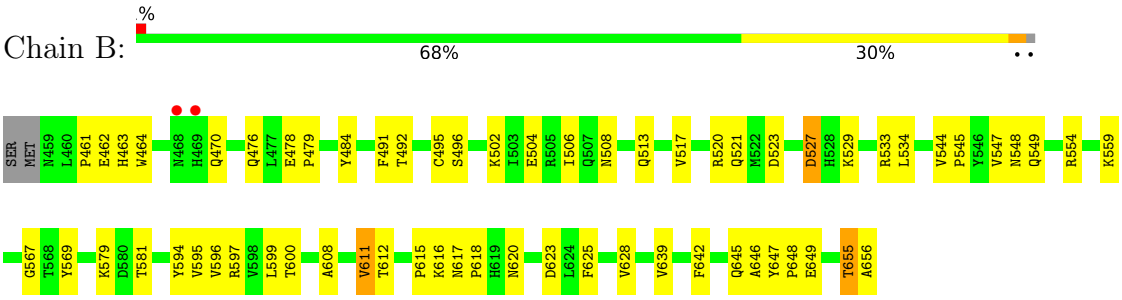
• Molecule 1: Poly [ADP-ribose] polymerase 15

Chain A:



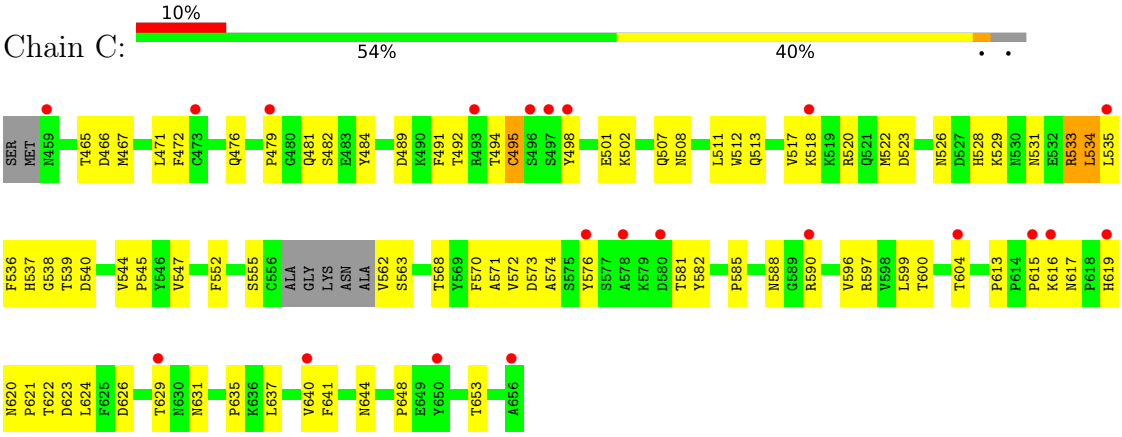
• Molecule 1: Poly [ADP-ribose] polymerase 15

Chain B:



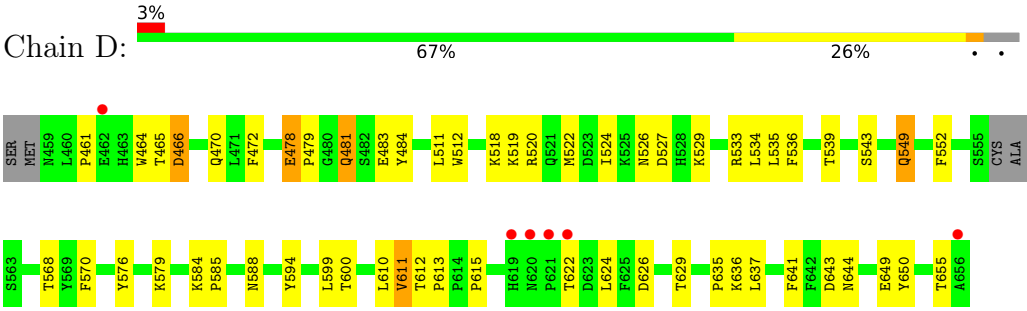
• Molecule 1: Poly [ADP-ribose] polymerase 15

Chain C:



• Molecule 1: Poly [ADP-ribose] polymerase 15

Chain D:


3%
67%
26%
SER MET N459 L460 P461 E462 H463 W464 T465 D466 Q470 L471 F472 E478 P479 G480 Q481 S482 E483 Y484 L511 W512 K518 K519 R520 Q521 M522 D523 I524 K525 N526 D527 H528 K529 R533 L534 L535 F536 T539 S543 Q549 F552 S555 CYS ALA GLY LYS ASN ALA VAL
S563 T568 Y569 F570 Y576 K579 K584 P585 N588 Y594 L599 T600 L610 V611 T612 P613 P614 P615 H619 N620 P621 T622 D623 L624 F625 D626 T629 P635 K636 L637 F641 F642 D643 N644 E649 Y650 T655 A656

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	69.68Å 45.38Å 123.39Å 90.00° 90.25° 90.00°	Depositor
Resolution (Å)	38.03 – 2.40 38.03 – 2.40	Depositor EDS
% Data completeness (in resolution range)	98.1 (38.03-2.40) 96.9 (38.03-2.40)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.58 (at 2.39Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7_650)	Depositor
R, R_{free}	0.220 , 0.287 0.220 , 0.285	Depositor DCC
R_{free} test set	1999 reflections (6.64%)	wwPDB-VP
Wilson B-factor (Å^2)	32.0	Xtriage
Anisotropy	0.869	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.38 , 35.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.43$, $< L^2 > = 0.25$	Xtriage
Estimated twinning fraction	0.419 for h,-k,-l	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	6441	wwPDB-VP
Average B, all atoms (Å^2)	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.07% of the height of the origin peak. No significant pseudotranslation is detected.*

[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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 0RU

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	0.26	0/1642	0.45	0/2227
1	B	0.25	0/1640	0.46	0/2223
1	C	0.25	0/1602	0.47	0/2171
1	D	0.26	0/1595	0.48	0/2161
All	All	0.26	0/6479	0.47	0/8782

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	D	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	527	ASP	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	1598	0	1529	47	0
1	B	1596	0	1528	43	0
1	C	1559	0	1487	74	0
1	D	1552	0	1481	37	0
2	A	20	0	12	3	0
2	C	20	0	12	10	0
2	D	13	0	7	2	0
3	A	27	0	0	4	0
3	B	20	0	0	8	0
3	C	18	0	0	7	0
3	D	18	0	0	2	0
All	All	6441	0	6056	199	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 16.

All (199) 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:526:ASN:HB3	1:C:529:LYS:HG3	1.21	1.17
1:D:533:ARG:HD2	1:D:600:THR:HG21	1.35	1.09
1:C:540:ASP:N	2:C:701:0RU:H3	1.89	0.88
1:C:501:GLU:HG2	1:C:502:LYS:HG2	1.59	0.84
1:C:526:ASN:CB	1:C:529:LYS:HG3	2.09	0.80
1:C:619:HIS:C	1:C:621:PRO:HD3	2.03	0.79
1:A:585:PRO:HA	1:A:590:ARG:O	1.83	0.77
1:C:562:VAL:HG22	1:C:563:SER:N	2.01	0.75
1:C:533:ARG:HD2	1:C:600:THR:HG21	1.69	0.74
1:C:616:LYS:HD2	1:C:623:ASP:HB3	1.72	0.72
1:C:562:VAL:HG22	1:C:563:SER:H	1.54	0.72
1:C:531:ASN:O	1:C:599:LEU:HA	1.92	0.70
1:A:479:PRO:HA	1:A:484:TYR:CD2	2.26	0.70
1:C:648:PRO:HG3	3:C:818:HOH:O	1.91	0.70
1:A:560:ASN:HB2	2:A:701:0RU:H7	1.73	0.69
1:A:591:LYS:HE3	1:A:654:PHE:CE1	2.28	0.68
1:A:581:THR:O	2:A:701:0RU:H1	1.92	0.68
1:D:522:MET:SD	1:D:599:LEU:HB3	2.34	0.68
1:C:535:LEU:HD22	1:C:572:VAL:HA	1.76	0.68
1:C:552:PHE:CD1	1:C:568:THR:HG21	2.31	0.66
1:C:637:LEU:HD21	2:C:701:0RU:H11	1.77	0.66
1:A:591:LYS:HE3	1:A:654:PHE:CZ	2.31	0.65
1:B:513:GLN:O	1:B:517:VAL:HG23	1.96	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:527:ASP:O	1:B:529:LYS:HG2	1.96	0.65
1:C:613:PRO:HG3	1:C:641:PHE:CD2	2.32	0.64
1:A:479:PRO:HA	1:A:484:TYR:CG	2.33	0.64
1:A:566:LYS:HZ2	1:A:609:GLY:HA2	1.64	0.63
1:B:642:PHE:HD2	3:B:712:HOH:O	1.80	0.63
1:B:628:VAL:HG22	1:B:639:VAL:HB	1.81	0.61
1:C:508:ASN:HB3	1:C:511:LEU:HB2	1.83	0.61
1:A:602:VAL:HG12	1:A:625:PHE:CD1	2.36	0.61
1:A:540:ASP:OD1	2:A:701:0RU:H3	2.01	0.60
1:D:518:LYS:HD3	1:D:644:ASN:O	2.01	0.60
1:C:540:ASP:H	2:C:701:0RU:H3	1.67	0.60
1:C:615:PRO:HA	1:C:624:LEU:HD23	1.82	0.60
1:C:585:PRO:HA	1:C:590:ARG:O	2.02	0.60
1:C:617:ASN:O	1:C:621:PRO:HA	2.02	0.60
1:C:526:ASN:HB3	1:C:529:LYS:CG	2.14	0.59
1:C:613:PRO:HG3	1:C:641:PHE:HD2	1.66	0.59
1:C:536:PHE:CE1	1:C:574:ALA:HB2	2.37	0.59
1:C:537:HIS:CE1	2:C:701:0RU:H4	2.36	0.59
1:A:544:VAL:N	1:A:545:PRO:HD2	2.16	0.59
1:B:529:LYS:NZ	3:B:710:HOH:O	2.35	0.59
1:B:533:ARG:HD2	1:B:600:THR:HG21	1.84	0.59
1:C:604:THR:O	1:C:629:THR:HG22	2.03	0.58
1:C:518:LYS:HD3	1:C:644:ASN:O	2.04	0.58
1:A:559:LYS:NZ	3:A:824:HOH:O	2.37	0.58
1:C:492:THR:HA	1:C:495:CYS:O	2.04	0.57
1:C:537:HIS:CD2	1:C:552:PHE:HE1	2.22	0.57
1:D:615:PRO:HA	1:D:624:LEU:HA	1.87	0.57
1:A:549:GLN:HB3	1:A:550:HIS:CD2	2.39	0.57
1:D:649:GLU:HG3	3:D:818:HOH:O	2.03	0.57
1:C:552:PHE:CZ	1:C:570:PHE:HE1	2.23	0.57
1:D:649:GLU:HG2	1:D:650:TYR:CE2	2.40	0.56
1:C:481:GLN:HG2	1:C:482:SER:N	2.19	0.56
1:A:615:PRO:HB3	1:A:621:PRO:O	2.06	0.56
1:B:506:ILE:HD12	1:B:648:PRO:HB2	1.85	0.56
1:C:648:PRO:CG	3:C:818:HOH:O	2.52	0.56
1:A:472:PHE:CZ	1:A:548:ASN:HB3	2.41	0.56
1:C:512:TRP:HH2	1:C:597:ARG:NH1	2.03	0.56
1:C:479:PRO:HA	1:C:484:TYR:CG	2.41	0.55
1:C:495:CYS:HB3	1:C:498:TYR:HD2	1.72	0.55
1:B:491:PHE:O	1:B:495:CYS:HB2	2.06	0.55
1:B:476:GLN:HG2	3:B:702:HOH:O	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:461:PRO:HG2	1:D:464:TRP:CE2	2.42	0.54
1:A:629:THR:OG1	1:A:635:PRO:HB3	2.08	0.54
1:A:479:PRO:HG2	1:B:559:LYS:O	2.06	0.54
1:C:626:ASP:O	3:C:811:HOH:O	2.18	0.54
1:C:637:LEU:HD21	2:C:701:0RU:CAD	2.37	0.54
1:D:478:GLU:O	1:D:481:GLN:HB2	2.08	0.54
1:B:554:ARG:HB2	1:B:567:GLY:HA2	1.89	0.54
1:B:523:ASP:CG	3:B:711:HOH:O	2.47	0.53
1:D:520:ARG:O	1:D:524:ILE:HG13	2.08	0.53
1:A:566:LYS:NZ	1:A:609:GLY:HA2	2.23	0.52
1:C:631:ASN:O	1:C:635:PRO:HG3	2.10	0.52
1:A:478:GLU:OE2	3:A:812:HOH:O	2.18	0.52
1:A:554:ARG:HB2	1:A:567:GLY:HA2	1.89	0.52
1:C:576:TYR:CE2	2:C:701:0RU:H11	2.44	0.52
1:D:526:ASN:HB3	1:D:529:LYS:HG3	1.90	0.52
1:A:627:SER:HB2	1:A:639:VAL:O	2.09	0.52
1:D:461:PRO:HG3	1:D:512:TRP:CZ2	2.44	0.52
1:A:619:HIS:C	1:A:621:PRO:HD3	2.30	0.52
1:D:533:ARG:HD2	1:D:600:THR:CG2	2.24	0.51
1:C:465:THR:HG22	1:C:466:ASP:O	2.09	0.51
1:C:617:ASN:O	1:C:621:PRO:CA	2.58	0.51
1:B:628:VAL:CG2	1:B:639:VAL:HB	2.41	0.51
1:A:492:THR:HA	1:A:495:CYS:O	2.11	0.51
1:C:479:PRO:HA	1:C:484:TYR:CD2	2.46	0.51
1:C:588:ASN:HB2	1:C:590:ARG:NH1	2.26	0.50
1:A:471:LEU:HD13	1:A:510:PHE:CZ	2.46	0.50
1:C:547:VAL:O	3:C:818:HOH:O	2.20	0.50
1:D:461:PRO:HD3	1:D:512:TRP:NE1	2.27	0.50
1:C:491:PHE:CE2	1:C:495:CYS:HB2	2.47	0.50
1:B:547:VAL:HB	1:B:594:TYR:OH	2.12	0.50
1:B:617:ASN:HB3	1:B:620:ASN:HB3	1.93	0.50
1:C:494:THR:HG21	1:C:573:ASP:HB3	1.94	0.49
1:C:534:LEU:HD12	1:C:597:ARG:HG2	1.94	0.49
1:D:629:THR:OG1	1:D:635:PRO:HB3	2.12	0.49
1:D:479:PRO:HA	1:D:484:TYR:CG	2.47	0.49
1:B:534:LEU:HD11	1:B:595:VAL:HG12	1.94	0.49
1:B:544:VAL:HB	1:B:545:PRO:HD3	1.94	0.49
1:C:472:PHE:HA	1:C:507:GLN:O	2.12	0.49
1:B:461:PRO:O	1:B:464:TRP:HB2	2.12	0.49
1:B:462:GLU:OE1	1:B:462:GLU:N	2.44	0.49
1:D:636:LYS:HG2	3:D:811:HOH:O	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:523:ASP:HA	3:B:711:HOH:O	2.12	0.48
1:D:611:VAL:HG12	1:D:612:THR:HG23	1.95	0.48
1:A:602:VAL:HG12	1:A:625:PHE:HD1	1.75	0.48
1:C:620:ASN:N	1:C:621:PRO:HD3	2.27	0.48
1:A:501:GLU:HG2	1:A:502:LYS:HG2	1.96	0.48
1:A:488:LYS:O	1:A:492:THR:HG23	2.14	0.48
1:C:522:MET:HG2	1:C:531:ASN:CG	2.34	0.47
1:B:599:LEU:HB2	1:B:645:GLN:HG3	1.95	0.47
1:C:528:HIS:N	1:C:528:HIS:CD2	2.81	0.47
1:C:520:ARG:HB2	3:C:817:HOH:O	2.14	0.47
1:C:572:VAL:HG21	1:C:635:PRO:O	2.14	0.47
1:C:613:PRO:HD3	1:C:641:PHE:HB2	1.95	0.47
1:A:525:LYS:HB3	1:A:525:LYS:HE2	1.67	0.47
1:D:643:ASP:O	1:D:644:ASN:HB2	2.15	0.47
1:C:501:GLU:HB3	1:C:653:THR:O	2.14	0.47
1:C:576:TYR:CE2	1:C:637:LEU:HD11	2.50	0.47
1:C:629:THR:OG1	1:C:635:PRO:HB3	2.15	0.46
1:A:534:LEU:O	1:A:535:LEU:HD23	2.14	0.46
1:B:599:LEU:HB2	1:B:645:GLN:CG	2.45	0.46
1:A:616:LYS:HD2	3:A:822:HOH:O	2.14	0.46
1:D:465:THR:HG22	1:D:466:ASP:O	2.16	0.46
1:D:522:MET:HE1	1:D:626:ASP:HB3	1.98	0.45
1:B:502:LYS:NZ	1:B:504:GLU:OE1	2.47	0.45
1:B:623:ASP:HB3	3:B:707:HOH:O	2.16	0.45
1:D:481:GLN:NE2	1:D:483:GLU:HB2	2.31	0.45
1:C:576:TYR:CD2	2:C:701:0RU:H11	2.52	0.45
1:C:544:VAL:HB	1:C:545:PRO:HD3	1.98	0.45
1:D:470:GLN:HE21	1:D:470:GLN:HB3	1.66	0.45
1:D:461:PRO:HG2	1:D:464:TRP:CZ2	2.52	0.45
1:A:615:PRO:HA	1:A:624:LEU:HA	1.99	0.44
1:B:616:LYS:HA	1:B:625:PHE:CE2	2.52	0.44
1:A:583:SER:O	1:A:591:LYS:NZ	2.49	0.44
1:B:479:PRO:HA	1:B:484:TYR:CD2	2.53	0.44
1:C:534:LEU:HA	1:C:596:VAL:O	2.17	0.44
1:C:615:PRO:CA	1:C:624:LEU:HD23	2.46	0.44
1:C:523:ASP:OD1	1:C:531:ASN:ND2	2.49	0.44
1:C:539:THR:C	2:C:701:0RU:H3	2.36	0.44
1:D:576:TYR:CE2	2:D:701:0RU:H11	2.53	0.44
1:B:579:LYS:HB3	1:B:581:THR:HG22	1.99	0.44
1:B:508:ASN:ND2	1:B:548:ASN:O	2.51	0.44
1:C:533:ARG:O	1:C:597:ARG:HA	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:576:TYR:O	1:D:579:LYS:HG3	2.17	0.44
1:A:537:HIS:CD2	1:A:552:PHE:HE1	2.36	0.44
1:B:596:VAL:HG13	1:B:647:TYR:O	2.18	0.44
1:C:513:GLN:O	1:C:517:VAL:HG23	2.17	0.44
1:D:472:PHE:CG	1:D:549:GLN:NE2	2.85	0.44
1:D:536:PHE:HA	1:D:594:TYR:O	2.18	0.43
1:A:505:ARG:NH2	3:A:809:HOH:O	2.50	0.43
1:A:617:ASN:HB3	1:A:620:ASN:HB3	1.99	0.43
1:C:489:ASP:HA	1:C:492:THR:OG1	2.19	0.43
1:D:552:PHE:HB3	1:D:568:THR:HG21	2.01	0.43
1:D:613:PRO:HD3	1:D:641:PHE:CD2	2.53	0.43
1:B:496:SER:CB	3:B:709:HOH:O	2.66	0.43
1:B:611:VAL:HG12	1:B:612:THR:HG23	2.00	0.43
1:A:613:PRO:HG3	1:A:641:PHE:CD2	2.54	0.43
1:A:636:LYS:HD3	1:A:636:LYS:HA	1.81	0.43
1:D:519:LYS:HG3	1:D:599:LEU:HD21	2.01	0.43
1:D:637:LEU:HD22	2:D:701:0RU:H11	2.00	0.43
1:C:535:LEU:HB3	1:C:571:ALA:O	2.19	0.43
1:A:655:THR:CG2	1:B:608:ALA:HB3	2.49	0.42
1:B:655:THR:HG23	1:B:656:ALA:N	2.34	0.42
1:D:576:TYR:CE2	1:D:637:LEU:HD21	2.54	0.42
1:B:491:PHE:HD2	1:B:492:THR:HG23	1.84	0.42
1:A:595:VAL:HB	1:A:650:TYR:HB2	2.01	0.42
1:C:582:TYR:CD1	2:C:701:0RU:CAT	3.02	0.42
1:D:461:PRO:HB2	1:D:464:TRP:CD1	2.54	0.42
1:A:535:LEU:HD12	1:A:570:PHE:HB2	2.01	0.42
1:B:463:HIS:ND1	3:B:715:HOH:O	2.37	0.42
1:A:520:ARG:O	1:A:524:ILE:HG13	2.20	0.42
1:A:613:PRO:HD3	1:A:641:PHE:HB2	2.02	0.42
1:D:584:LYS:HA	1:D:585:PRO:HD2	1.91	0.42
1:B:569:TYR:CD2	1:B:639:VAL:HG22	2.55	0.42
1:B:617:ASN:HA	1:B:618:PRO:HD3	1.92	0.42
1:C:622:THR:HG23	1:C:623:ASP:H	1.85	0.42
1:B:517:VAL:O	1:B:521:GLN:HG3	2.20	0.41
1:B:559:LYS:HD2	1:B:559:LYS:N	2.34	0.41
1:B:520:ARG:NH1	1:B:520:ARG:HG3	2.35	0.41
1:A:472:PHE:HZ	1:A:548:ASN:HB3	1.85	0.41
1:B:615:PRO:HB2	1:B:617:ASN:O	2.20	0.41
1:B:597:ARG:HG3	1:B:649:GLU:OE1	2.20	0.41
1:C:562:VAL:CG2	1:C:563:SER:N	2.72	0.41
1:B:597:ARG:O	1:B:646:ALA:HA	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:534:LEU:C	1:A:535:LEU:HD23	2.41	0.41
1:C:467:MET:N	3:C:813:HOH:O	2.53	0.41
1:D:636:LYS:O	1:D:637:LEU:HD23	2.21	0.41
1:A:508:ASN:CG	1:A:511:LEU:HG	2.40	0.41
1:A:572:VAL:HG21	1:A:635:PRO:O	2.21	0.40
1:C:544:VAL:N	1:C:545:PRO:CD	2.85	0.40
1:D:535:LEU:CB	1:D:570:PHE:HB3	2.51	0.40
1:A:475:VAL:O	1:A:504:GLU:HA	2.22	0.40
1:C:538:GLY:O	2:C:701:0RU:H5	2.21	0.40
1:C:604:THR:O	1:C:629:THR:N	2.55	0.40
1:C:640:VAL:HG13	3:C:807:HOH:O	2.21	0.40
1:D:610:LEU:HD22	1:D:612:THR:O	2.21	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	196/200 (98%)	188 (96%)	8 (4%)	0	100	100
1	B	196/200 (98%)	188 (96%)	8 (4%)	0	100	100
1	C	189/200 (94%)	175 (93%)	14 (7%)	0	100	100
1	D	187/200 (94%)	175 (94%)	12 (6%)	0	100	100
All	All	768/800 (96%)	726 (94%)	42 (6%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

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

resolution.

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	176/179 (98%)	170 (97%)	6 (3%)	37	56
1	B	175/179 (98%)	169 (97%)	6 (3%)	37	56
1	C	171/179 (96%)	164 (96%)	7 (4%)	30	48
1	D	171/179 (96%)	159 (93%)	12 (7%)	15	24
All	All	693/716 (97%)	662 (96%)	31 (4%)	27	44

All (31) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	467	MET
1	A	478	GLU
1	A	501	GLU
1	A	559	LYS
1	A	612	THR
1	A	634	SER
1	B	470	GLN
1	B	478	GLU
1	B	527	ASP
1	B	549	GLN
1	B	611	VAL
1	B	655	THR
1	C	471	LEU
1	C	476	GLN
1	C	495	CYS
1	C	533	ARG
1	C	534	LEU
1	C	555	SER
1	C	581	THR
1	D	466	ASP
1	D	478	GLU
1	D	481	GLN
1	D	511	LEU
1	D	534	LEU
1	D	539	THR
1	D	543	SER
1	D	549	GLN
1	D	588	ASN

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Mol	Chain	Res	Type
1	D	611	VAL
1	D	622	THR
1	D	655	THR

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

Mol	Chain	Res	Type
1	A	459	ASN
1	A	550	HIS
1	A	588	ASN
1	B	485	ASN
1	B	549	GLN
1	B	550	HIS
1	C	476	GLN
1	C	481	GLN
1	C	485	ASN
1	C	526	ASN
1	C	528	HIS
1	C	550	HIS
1	D	463	HIS
1	D	470	GLN
1	D	481	GLN
1	D	485	ASN
1	D	550	HIS
1	D	645	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

3 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	0RU	D	701	-	14,14,22	2.82	5 (35%)	18,20,30	0.80	0
2	0RU	A	701	-	21,22,22	2.39	5 (23%)	26,30,30	1.73	8 (30%)
2	0RU	C	701	-	21,22,22	2.34	5 (23%)	26,30,30	1.87	7 (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
2	0RU	D	701	-	-	-	0/2/2/3
2	0RU	A	701	-	-	2/3/5/5	0/3/3/3
2	0RU	C	701	-	-	3/3/5/5	0/3/3/3

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	701	0RU	OAB-CAR	9.20	1.39	1.23
2	D	701	0RU	OAB-CAR	9.04	1.39	1.23
2	C	701	0RU	OAB-CAR	8.91	1.39	1.23
2	A	701	0RU	CAS-CAT	-3.06	1.37	1.41
2	C	701	0RU	CAS-CAT	-3.05	1.37	1.41
2	D	701	0RU	CAS-CAT	-2.96	1.37	1.41
2	C	701	0RU	CAS-CAR	-2.49	1.44	1.48
2	A	701	0RU	CAT-CAO	2.44	1.43	1.40
2	D	701	0RU	CAT-CAO	2.17	1.43	1.40
2	C	701	0RU	CAT-CAO	2.17	1.43	1.40
2	D	701	0RU	CAS-CAR	-2.16	1.45	1.48
2	A	701	0RU	CAS-CAR	-2.15	1.45	1.48
2	A	701	0RU	CAR-NAM	-2.15	1.34	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	701	0RU	CAR-NAM	-2.08	1.34	1.39
2	C	701	0RU	CAR-NAM	-2.07	1.34	1.39

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	701	0RU	CAI-SAN-CAQ	5.01	108.09	101.63
2	A	701	0RU	CAI-SAN-CAQ	3.96	106.74	101.63
2	A	701	0RU	CAF-NAK-CAQ	3.46	120.13	114.94
2	C	701	0RU	CAE-NAJ-CAQ	3.29	119.87	114.94
2	C	701	0RU	CAF-NAK-CAQ	3.19	119.73	114.94
2	A	701	0RU	CAE-NAJ-CAQ	2.92	119.32	114.94
2	C	701	0RU	CAP-CAI-SAN	2.78	118.42	111.09
2	C	701	0RU	CAC-CAE-NAJ	-2.75	118.94	123.43
2	A	701	0RU	CAC-CAF-NAK	-2.64	119.12	123.43
2	C	701	0RU	CAC-CAF-NAK	-2.44	119.44	123.43
2	A	701	0RU	CAP-CAI-SAN	2.43	117.50	111.09
2	C	701	0RU	NAK-CAQ-NAJ	-2.42	122.88	126.85
2	A	701	0RU	NAK-CAQ-NAJ	-2.41	122.90	126.85
2	A	701	0RU	CAC-CAE-NAJ	-2.31	119.65	123.43
2	A	701	0RU	CAO-CAT-NAL	2.21	121.48	117.65

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	701	0RU	NAJ-CAQ-SAN-CAI
2	A	701	0RU	NAK-CAQ-SAN-CAI
2	C	701	0RU	CAP-CAI-SAN-CAQ
2	C	701	0RU	NAJ-CAQ-SAN-CAI
2	C	701	0RU	NAK-CAQ-SAN-CAI

There are no ring outliers.

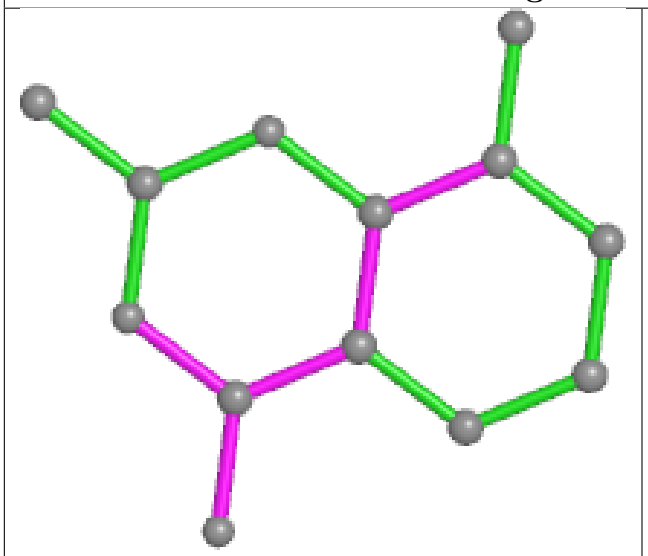
3 monomers are involved in 15 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	701	0RU	2	0
2	A	701	0RU	3	0
2	C	701	0RU	10	0

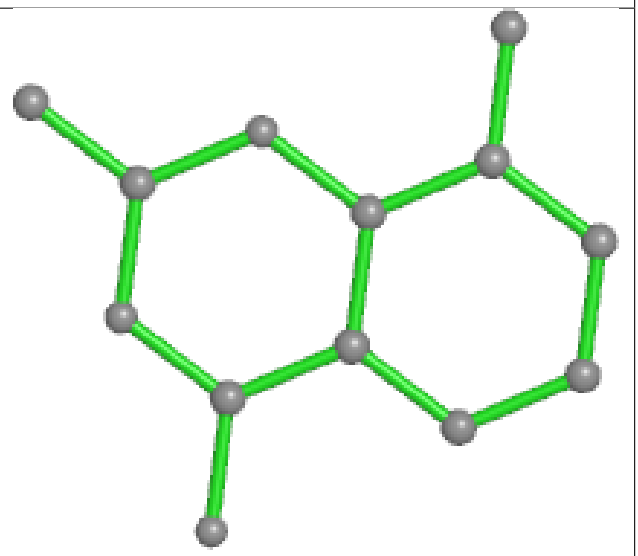
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths,

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.

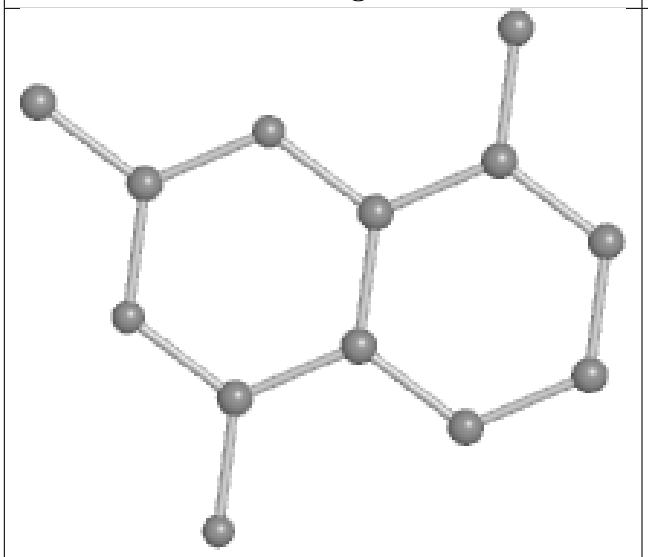
Ligand 0RU D 701



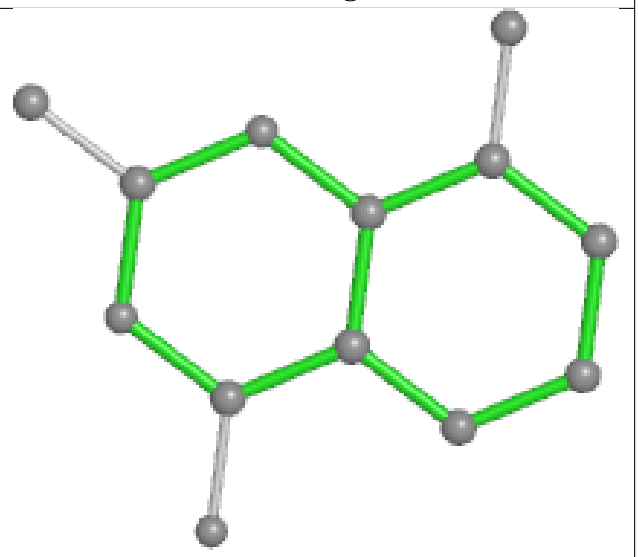
Bond lengths



Bond angles

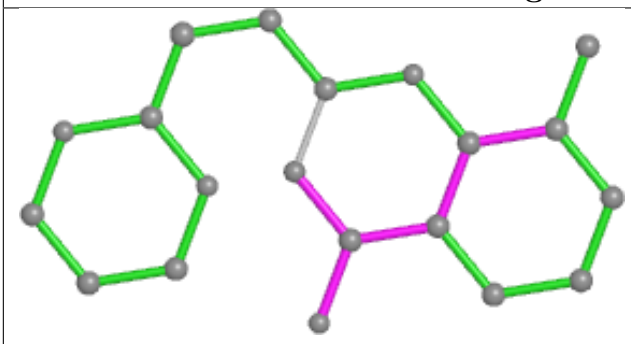


Torsions

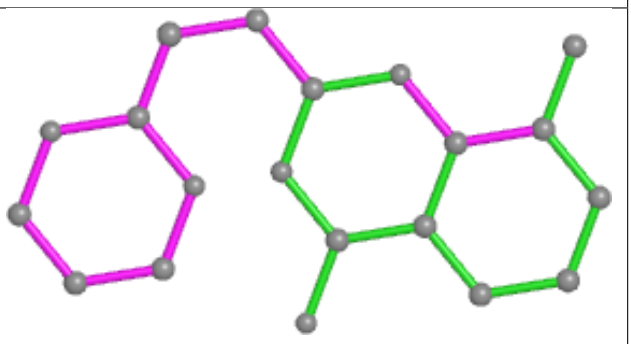


Rings

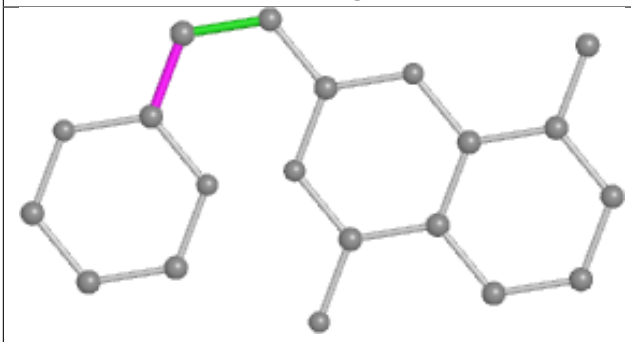
Ligand 0RU A 701



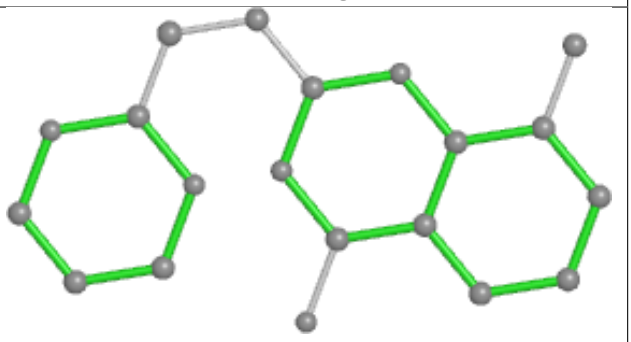
Bond lengths



Bond angles

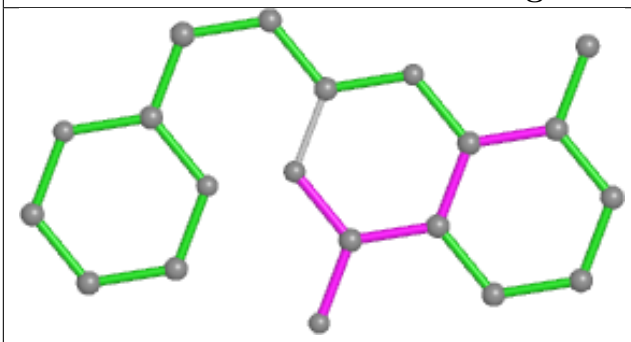


Torsions

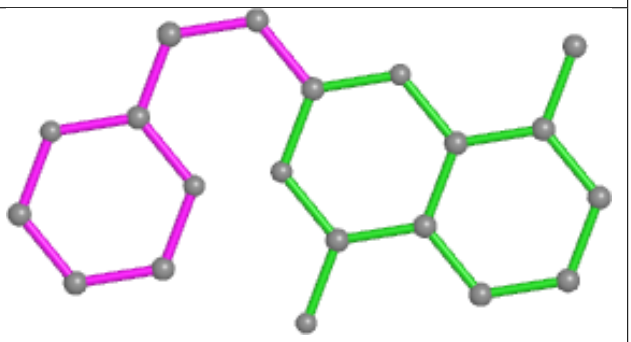


Rings

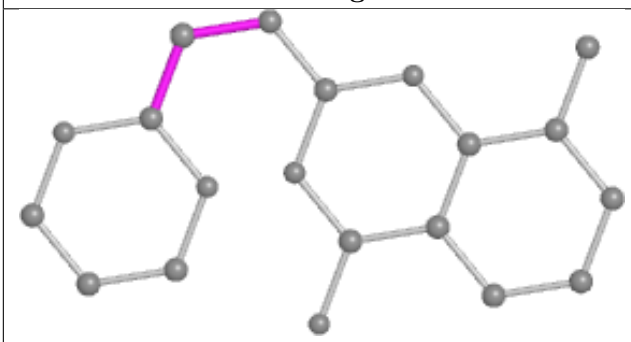
Ligand 0RU C 701



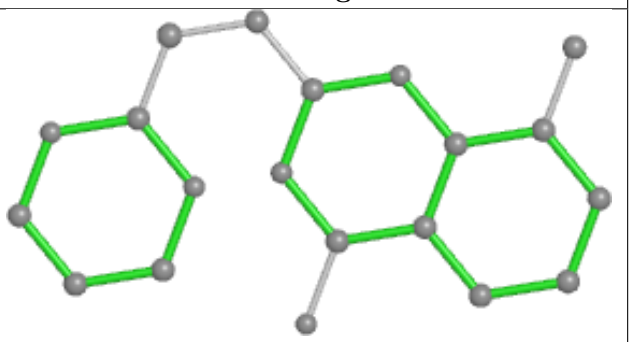
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers

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, 95^{th} 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	198/200 (99%)	-0.32	2 (1%) 82 80	18, 33, 56, 76	0
1	B	198/200 (99%)	-0.23	2 (1%) 82 80	25, 37, 52, 91	0
1	C	193/200 (96%)	0.73	21 (10%) 5 5	41, 63, 78, 83	0
1	D	191/200 (95%)	-0.32	6 (3%) 49 47	16, 29, 52, 81	0
All	All	780/800 (97%)	-0.04	31 (3%) 38 37	16, 38, 73, 91	0

All (31) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	656	ALA	5.0
1	D	619	HIS	4.0
1	C	459	ASN	3.2
1	C	650	TYR	3.0
1	D	620	ASN	3.0
1	C	615	PRO	2.9
1	C	656	ALA	2.9
1	C	473	CYS	2.8
1	C	479	PRO	2.8
1	B	468	ASN	2.7
1	C	640	VAL	2.7
1	C	619	HIS	2.4
1	C	580	ASP	2.3
1	C	578	ALA	2.3
1	C	590	ARG	2.3
1	C	576	TYR	2.3
1	C	496	SER	2.3
1	C	604	THR	2.2
1	C	629	THR	2.2
1	B	469	HIS	2.2
1	C	493	ARG	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	518	LYS	2.2
1	A	655	THR	2.2
1	D	622	THR	2.2
1	C	535	LEU	2.2
1	C	497	SER	2.2
1	D	462	GLU	2.1
1	A	488	LYS	2.1
1	D	621	PRO	2.1
1	C	498	TYR	2.1
1	C	616	LYS	2.1

6.2 Non-standard residues in protein, DNA, RNA chains (i)

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

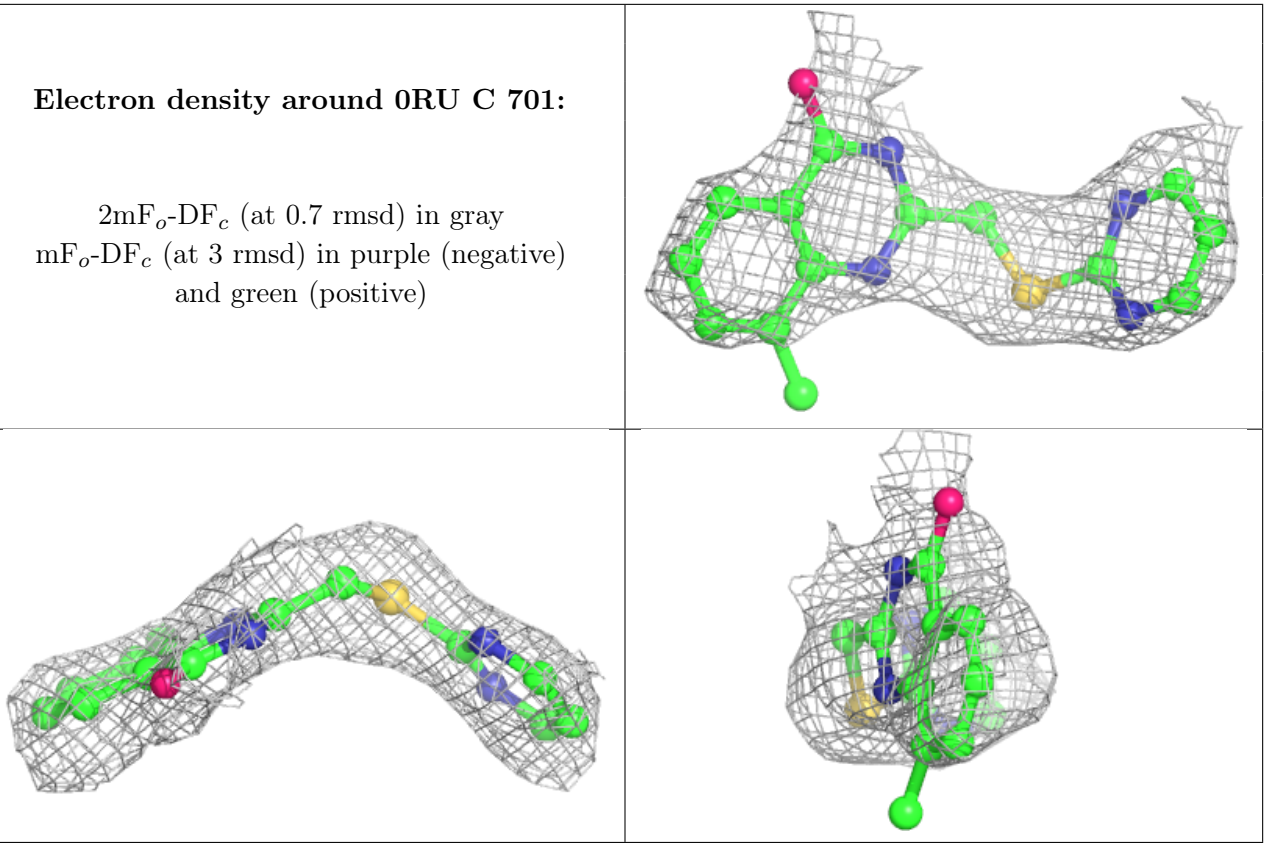
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' 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	0RU	C	701	20/20	0.85	0.21	59,67,73,74	0
2	0RU	A	701	20/20	0.92	0.13	26,37,47,65	0
2	0RU	D	701	13/20	0.96	0.11	18,20,24,26	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.

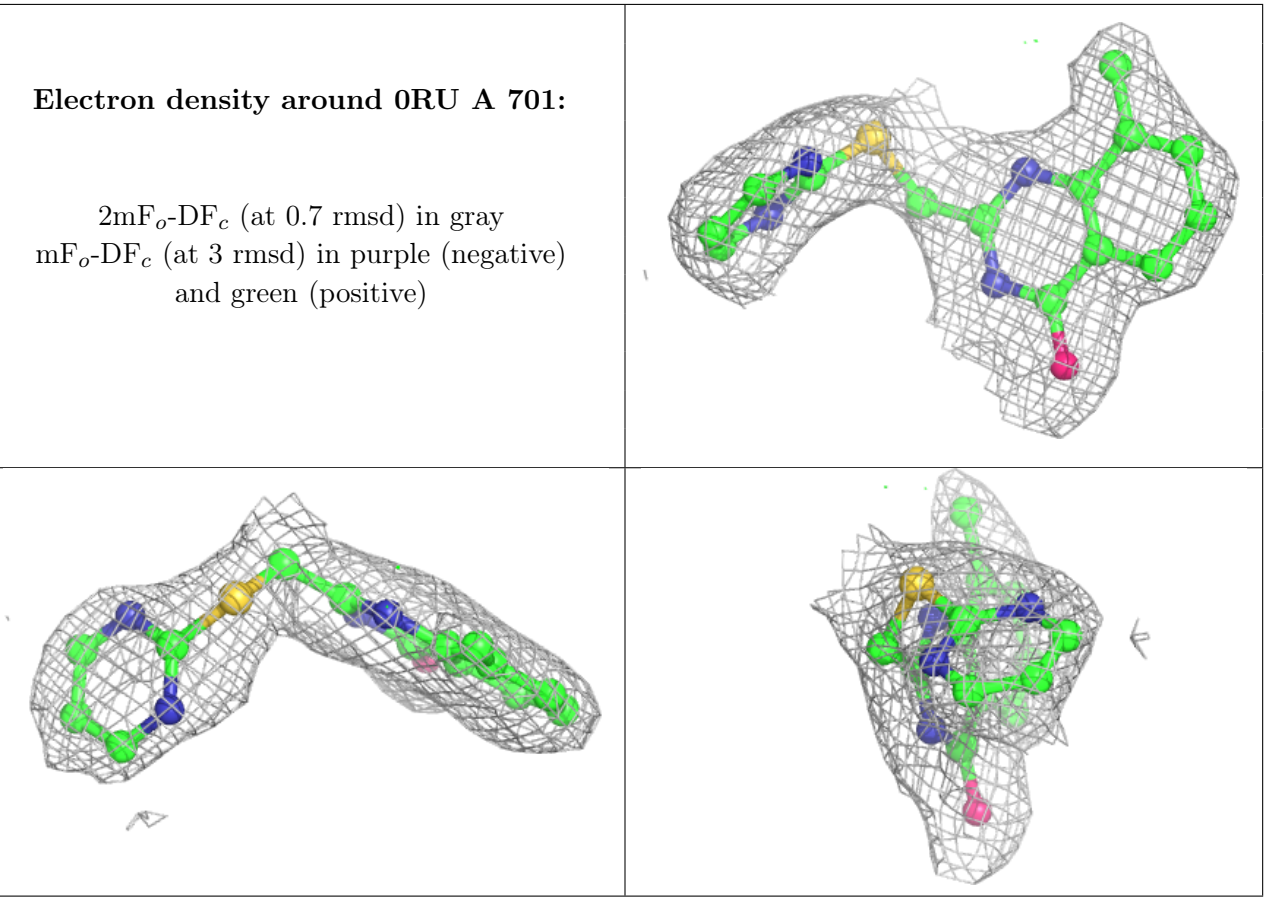
Electron density around 0RU C 701:

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



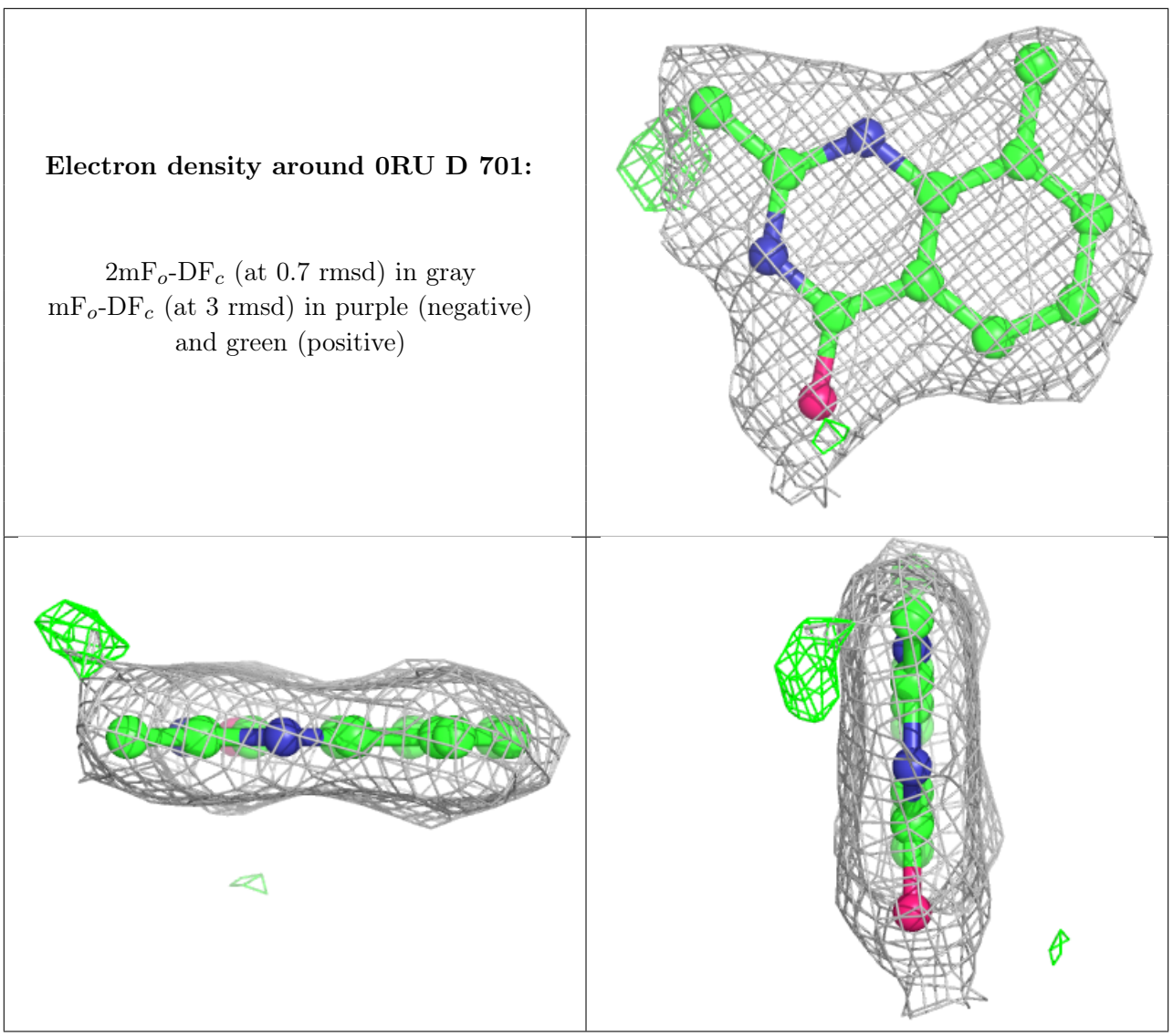
Electron density around 0RU A 701:

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



Electron density around 0RU D 701:

$2mF_o$-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.