Full wwPDB X-ray Structure Validation Report ⓘ

Oct 22, 2024 – 10:14 AM EDT

PDB ID	:	9AZK
Title	:	Macrocyclic inhibitors targeting the prime site of the fibrinolytic serine protease plasmin
Authors	:	Guojie, W.
Deposited on	:	2024-03-11
Resolution	:	2.10 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The 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:

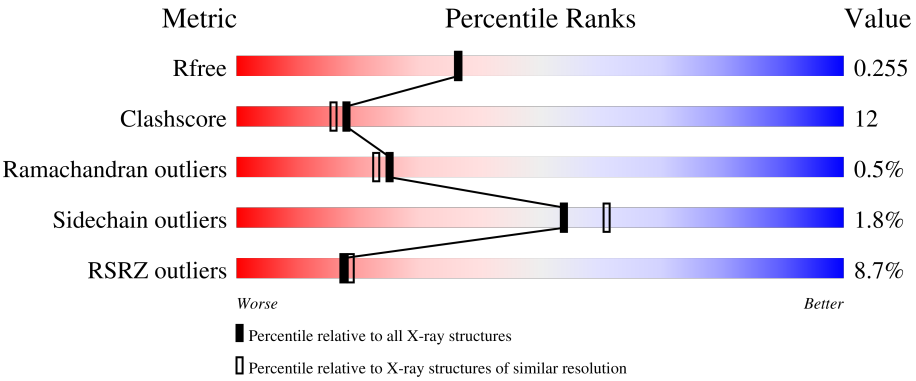
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

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 2.10 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	164625	6234 (2.10-2.10)
Clashscore	180529	6893 (2.10-2.10)
Ramachandran outliers	177936	6839 (2.10-2.10)
Sidechain outliers	177891	6840 (2.10-2.10)
RSRZ outliers	164620	6234 (2.10-2.10)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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	250	6% 78% 20%
1	B	250	5% 76% 22%
1	C	250	5% 71% 26%
1	D	250	8% 74% 22%
1	E	250	6% 75% 22%

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Mol	Chain	Length	Quality of chain
1	F	250	

2 Entry composition

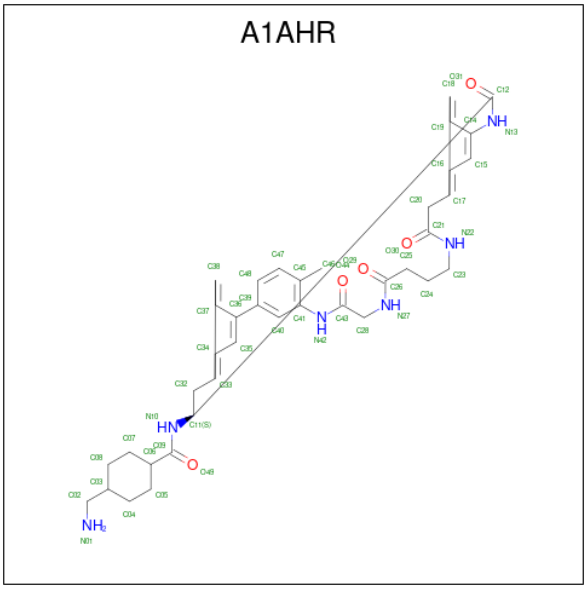
There are 3 unique types of molecules in this entry. The entry contains 12542 atoms, of which 276 are hydrogens and 0 are deuteriums.

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 Plasminogen.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	246	Total	C	N	O	S	1	7	0
			1914	1223	329	347	15			
1	B	246	Total	C	N	O	S	0	4	0
			1907	1215	333	345	14			
1	C	244	Total	C	N	O	S	0	4	0
			1892	1204	330	344	14			
1	D	244	Total	C	N	O	S	1	4	0
			1888	1204	327	343	14			
1	E	245	Total	C	N	O	S	1	9	0
			1915	1223	329	348	15			
1	F	239	Total	C	N	O	S	1	7	0
			1847	1180	315	337	15			

- Molecule 2 is (1r,4S)-4-(aminomethyl)-N-[(24S)-5-methyl-8,11,16,23-tetraoxo-7,10,15,22-tetraazatetracyclo[24.2.2.2 18,21 .1 2,6]tritriaconta-1(28),2(33),3,5,18,20,26,29,31-nonaen-24-yl]cyclohexane-1-carboxamide (three-letter code: A1AHR) (formula: $C_{38}H_{46}N_6O_5$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	H	N	O	0	0
			95	38	46	6	5		
2	B	1	Total	C	H	N	O	0	0
			95	38	46	6	5		
2	C	1	Total	C	H	N	O	0	0
			95	38	46	6	5		
2	D	1	Total	C	H	N	O	0	0
			95	38	46	6	5		
2	E	1	Total	C	H	N	O	0	0
			95	38	46	6	5		
2	F	1	Total	C	H	N	O	0	0
			95	38	46	6	5		

- Molecule 3 is water.

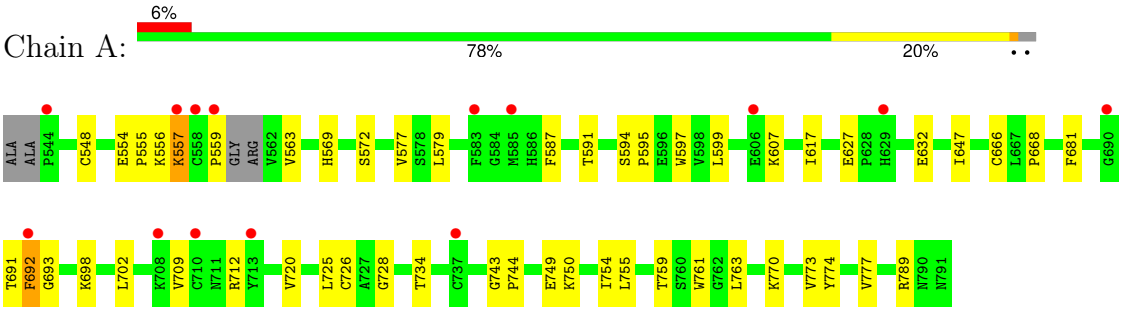
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	144	Total	O	0	0
			144	144		
3	B	128	Total	O	0	0
			128	128		
3	C	117	Total	O	0	0
			117	117		
3	D	79	Total	O	0	0
			79	79		
3	E	92	Total	O	0	0
			92	92		
3	F	49	Total	O	0	0
			49	49		

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.

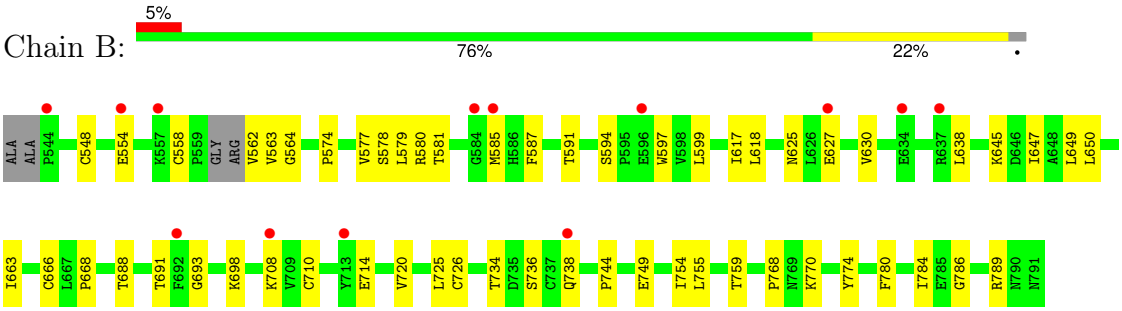
• Molecule 1: Plasminogen

Chain A:



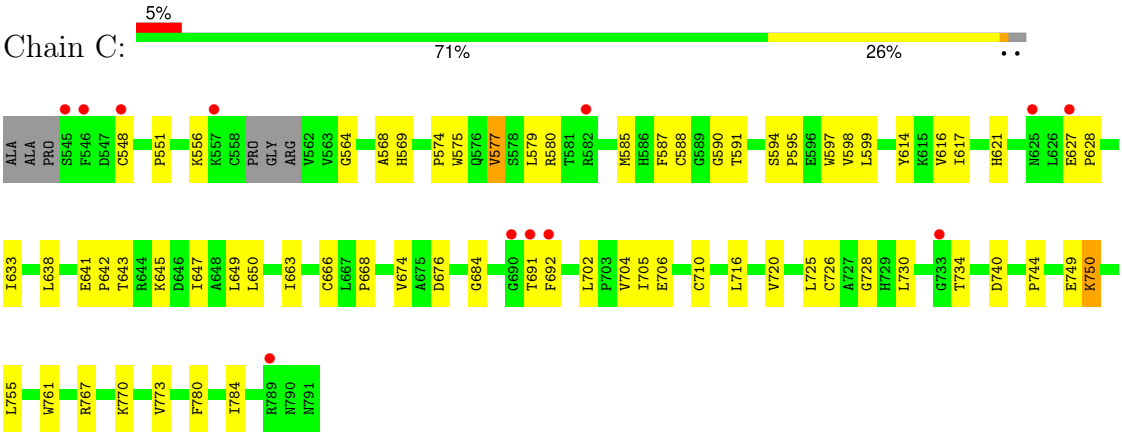
• Molecule 1: Plasminogen

Chain B:



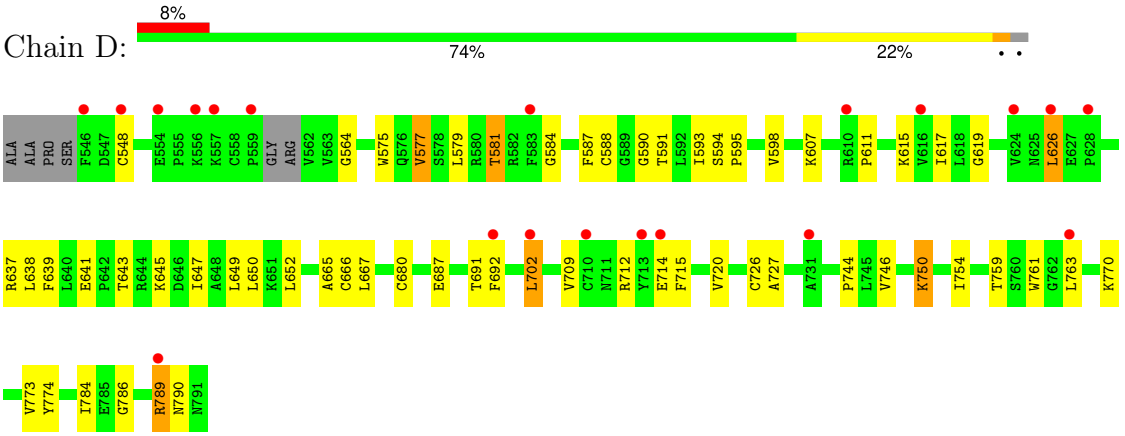
• Molecule 1: Plasminogen

Chain C:



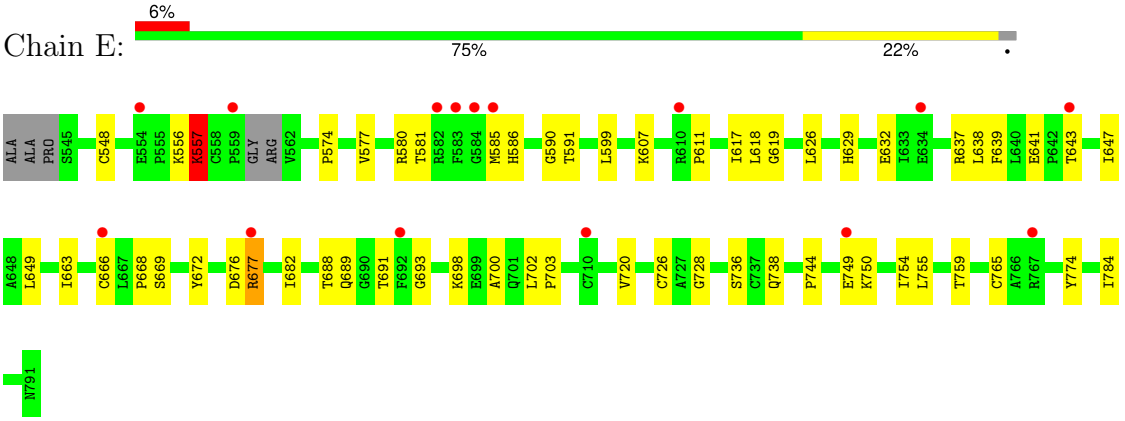
• Molecule 1: Plasminogen

Chain D:



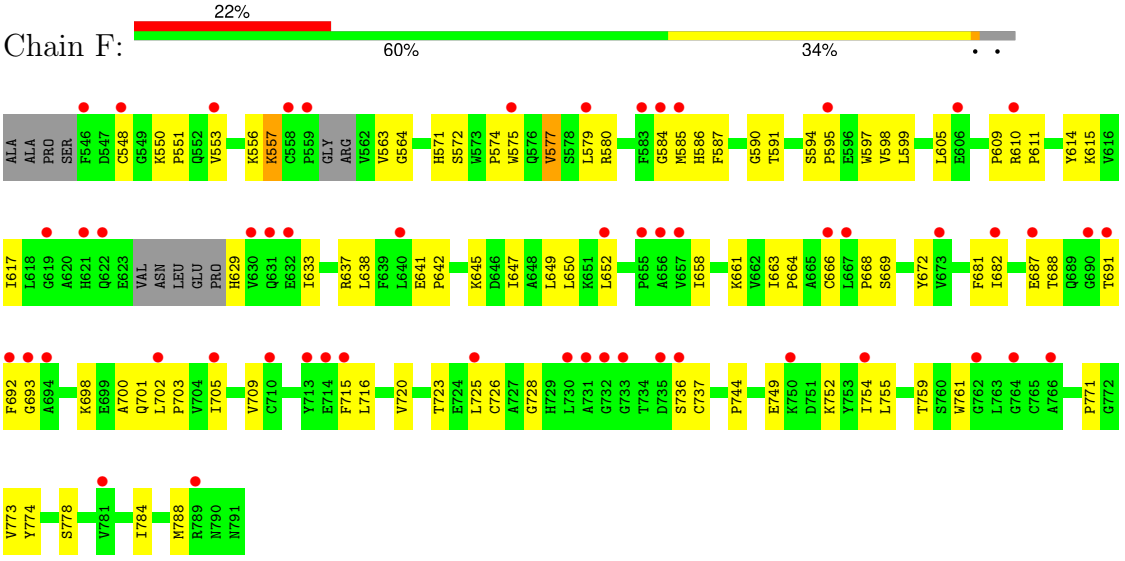
• Molecule 1: Plasminogen

Chain E:



• Molecule 1: Plasminogen

Chain F:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	74.85Å 128.88Å 79.08Å 90.00° 108.06° 90.00°	Depositor
Resolution (Å)	47.76 – 2.10 47.76 – 2.10	Depositor EDS
% Data completeness (in resolution range)	99.8 (47.76-2.10) 99.7 (47.76-2.10)	Depositor EDS
R_{merge}	0.22	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.61 (at 2.10Å)	Xtriage
Refinement program	PHENIX 1.19.2_4158	Depositor
R, R_{free}	0.237 , 0.255 0.237 , 0.255	Depositor DCC
R_{free} test set	4065 reflections (4.90%)	wwPDB-VP
Wilson B-factor (Å^2)	28.5	Xtriage
Anisotropy	0.404	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 45.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	12542	wwPDB-VP
Average B, all atoms (Å^2)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.00% 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: A1AHR

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	0.64	0/1985	0.67	0/2699
1	B	0.62	0/1969	0.67	0/2678
1	C	0.63	0/1952	0.65	0/2652
1	D	0.64	0/1949	0.64	0/2651
1	E	0.68	0/1991	0.68	0/2707
1	F	0.69	0/1914	0.65	0/2602
All	All	0.65	0/11760	0.66	0/15989

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

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	1914	0	1906	34	3
1	B	1907	0	1891	40	3
1	C	1892	0	1874	47	0
1	D	1888	0	1868	46	0
1	E	1915	0	1908	42	0
1	F	1847	0	1825	66	0
2	A	49	46	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	49	46	0	1	0
2	C	49	46	0	0	0
2	D	49	46	0	2	0
2	E	49	46	0	3	0
2	F	49	46	0	1	0
3	A	144	0	0	2	0
3	B	128	0	0	1	0
3	C	117	0	0	0	0
3	D	79	0	0	2	0
3	E	92	0	0	2	0
3	F	49	0	0	2	0
All	All	12266	276	11272	274	3

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 12.

All (274) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:581:THR:HG23	1:D:584:GLY:HA3	1.21	1.18
1:D:581:THR:CG2	1:D:584:GLY:HA3	1.92	0.98
1:F:584:GLY:HA2	1:F:615:LYS:HE2	1.56	0.85
1:D:581:THR:HG23	1:D:584:GLY:CA	2.07	0.84
1:B:581:THR:CG2	1:B:585:MET:HG2	2.10	0.81
1:E:682[B]:ILE:HD11	1:E:700:ALA:HB3	1.66	0.78
1:F:615:LYS:HE3	1:F:617:ILE:HD11	1.66	0.77
1:E:738:GLN:HB3	2:E:801:A1AHR:C19	2.15	0.76
1:B:581:THR:HG23	1:B:585:MET:HG2	1.67	0.75
1:F:579:LEU:HG	1:F:587:PHE:CZ	2.24	0.72
1:E:580:ARG:HG2	1:E:586:HIS:HA	1.70	0.72
1:F:598:VAL:HG23	1:F:652:LEU:HD11	1.72	0.72
1:F:749:GLU:OE1	1:F:754[B]:ILE:HB	1.92	0.69
1:A:691:THR:O	1:A:692:PHE:HB3	1.95	0.67
1:A:789:ARG:HG3	3:A:1008:HOH:O	1.94	0.67
1:F:556:LYS:O	1:F:557:LYS:HG2	1.96	0.66
1:D:581:THR:O	1:D:615:LYS:HE2	1.96	0.65
1:F:749:GLU:OE1	1:F:754[A]:ILE:HB	1.95	0.65
1:E:693:GLY:HA3	1:E:698:LYS:HD2	1.79	0.65
1:F:594[B]:SER:OG	1:F:595:PRO:HD2	1.96	0.65
1:A:749:GLU:HB2	1:A:754[A]:ILE:HD13	1.78	0.65
1:D:763:LEU:HD12	1:D:770:LYS:HD2	1.77	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:709:VAL:HG22	1:A:712:ARG:HH21	1.62	0.65
1:D:786:GLY:HA2	1:D:789:ARG:HD2	1.78	0.64
1:F:591:THR:OG1	1:F:744:PRO:HB3	1.98	0.63
1:C:720:VAL:HG21	1:C:726:CYS:SG	2.40	0.62
1:B:738:GLN:HB3	2:B:801:A1AHR:C15	2.30	0.62
1:B:720:VAL:HG21	1:B:726:CYS:SG	2.40	0.61
1:D:789:ARG:HG2	1:D:790:ASN:N	2.15	0.61
1:F:594[B]:SER:HB3	1:F:597:TRP:HB2	1.82	0.61
1:F:649:LEU:HD11	1:F:784:ILE:HG23	1.83	0.60
1:E:682[B]:ILE:CD1	1:E:700:ALA:HB3	2.30	0.60
1:D:702:LEU:HD13	1:D:727:ALA:HB1	1.84	0.60
1:E:677:ARG:HE	1:E:677:ARG:HA	1.66	0.60
1:F:693:GLY:HA3	1:F:698:LYS:HD2	1.83	0.60
1:A:702:LEU:HD22	1:A:728:GLY:HA2	1.84	0.59
1:F:658:ILE:HD12	1:F:664:PRO:HD3	1.84	0.59
1:F:577:VAL:HG22	1:F:590:GLY:HA3	1.86	0.58
1:B:585:MET:O	1:B:585:MET:HG3	2.04	0.57
1:B:627:GLU:HG2	1:B:630:VAL:HG23	1.86	0.57
1:D:579:LEU:HG	1:D:587:PHE:CZ	2.39	0.57
1:C:649:LEU:HD11	1:C:784:ILE:HG23	1.87	0.57
1:E:557:LYS:HD2	1:E:557:LYS:O	2.04	0.57
1:D:641:GLU:HB2	1:D:647:ILE:HG23	1.87	0.56
1:D:591:THR:OG1	1:D:744:PRO:HB3	2.05	0.56
1:F:691:THR:O	1:F:692:PHE:HB3	2.05	0.56
1:A:693:GLY:HA3	1:A:698:LYS:HD2	1.88	0.56
1:A:594[A]:SER:OG	1:A:595:PRO:HD2	2.06	0.56
1:D:593:ILE:HB	1:D:667:LEU:HD21	1.88	0.56
1:C:691:THR:O	1:C:692:PHE:HB3	2.06	0.56
1:E:556:LYS:O	1:E:557:LYS:HG3	2.06	0.56
1:E:611:PRO:HG3	1:E:638:LEU:HG	1.89	0.55
1:F:594[A]:SER:HB2	1:F:597:TRP:HB2	1.88	0.55
1:E:676:ASP:OD1	1:E:677:ARG:HG2	2.06	0.55
1:F:610:ARG:HH11	1:F:611:PRO:HD2	1.71	0.55
1:F:666:CYS:HB2	1:F:754[A]:ILE:HD13	1.87	0.55
1:D:587:PHE:O	1:D:588:CYS:SG	2.65	0.55
1:D:607:LYS:HE2	2:D:801:A1AHR:O44	2.07	0.55
1:C:580:ARG:HD2	1:C:617:ILE:HG13	1.88	0.55
1:C:556:LYS:HD2	1:C:569:HIS:CE1	2.42	0.55
1:B:599:LEU:HD21	1:B:647:ILE:HD11	1.89	0.54
1:F:666:CYS:SG	1:F:752:LYS:HE2	2.47	0.54
1:A:668:PRO:HD3	1:A:755:LEU:O	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:599:LEU:HD21	1:C:647:ILE:HD11	1.89	0.54
1:C:761:TRP:CZ2	1:C:773:VAL:HG21	2.42	0.54
1:B:786:GLY:HA2	1:B:789:ARG:NH1	2.22	0.53
1:E:599:LEU:HD21	1:E:647:ILE:HD11	1.90	0.53
1:B:581:THR:HG23	1:B:585:MET:CG	2.39	0.53
1:E:759:THR:HA	1:E:774:TYR:CD2	2.44	0.53
1:C:674:VAL:HG11	1:C:704:VAL:HG21	1.91	0.53
1:E:676:ASP:O	1:E:677:ARG:HB2	2.08	0.53
1:F:638:LEU:HD22	1:F:650:LEU:HD22	1.90	0.53
1:C:579:LEU:HD11	1:C:650:LEU:HD11	1.89	0.52
1:F:577:VAL:HG22	1:F:590:GLY:CA	2.39	0.52
1:F:584:GLY:HA2	1:F:615:LYS:CE	2.36	0.52
1:B:581:THR:HG21	1:B:585:MET:HG2	1.91	0.52
1:B:638:LEU:HD22	1:B:650:LEU:HD22	1.90	0.52
1:E:720:VAL:HG21	1:E:726:CYS:SG	2.50	0.52
1:E:556:LYS:C	1:E:557:LYS:HG3	2.30	0.52
1:F:682[B]:ILE:HD13	1:F:702:LEU:HD12	1.91	0.52
1:B:578:SER:HB3	1:B:617:ILE:HB	1.91	0.51
1:F:682[A]:ILE:HD13	1:F:702:LEU:HD12	1.91	0.51
1:C:591:THR:OG1	1:C:744:PRO:HB3	2.10	0.51
1:E:702:LEU:HD22	1:E:728:GLY:HA2	1.93	0.51
1:E:577:VAL:HG22	1:E:590:GLY:C	2.31	0.51
1:B:591:THR:OG1	1:B:744:PRO:HB3	2.11	0.51
1:C:749:GLU:O	1:C:750:LYS:HB2	2.10	0.50
1:E:591:THR:OG1	1:E:744:PRO:HB3	2.10	0.50
1:A:761:TRP:CZ2	1:A:773:VAL:HG21	2.46	0.50
1:E:688:THR:HB	1:E:691:THR:OG1	2.11	0.50
1:B:577:VAL:HG22	1:B:618:LEU:CD2	2.42	0.50
1:D:611:PRO:HB3	1:D:638:LEU:HG	1.92	0.50
1:D:548:CYS:C	1:D:666:CYS:SG	2.89	0.50
1:E:738:GLN:HB3	2:E:801:A1AHR:C18	2.42	0.50
1:A:743:GLY:HA3	3:A:938:HOH:O	2.10	0.50
1:F:580:ARG:HG2	1:F:586:HIS:HA	1.93	0.50
1:D:750:LYS:NZ	1:D:750:LYS:HB3	2.26	0.50
1:A:548:CYS:C	1:A:666:CYS:SG	2.90	0.49
1:F:629:HIS:N	3:F:901:HOH:O	2.44	0.49
1:C:587:PHE:O	1:C:588:CYS:SG	2.70	0.49
1:E:585:MET:HB3	3:E:906:HOH:O	2.12	0.49
1:C:638:LEU:HD22	1:C:650:LEU:HD22	1.94	0.49
1:E:581:THR:HG23	3:E:906:HOH:O	2.12	0.49
1:C:668:PRO:HD3	1:C:755:LEU:O	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:548:CYS:C	1:F:666:CYS:SG	2.91	0.49
1:F:649:LEU:HD11	1:F:784:ILE:HA	1.94	0.49
1:F:564:GLY:H	1:F:691:THR:CB	2.25	0.49
1:A:557:LYS:HB3	1:A:559:PRO:HD3	1.95	0.48
1:A:591:THR:OG1	1:A:744:PRO:HB3	2.12	0.48
1:C:564:GLY:H	1:C:691:THR:HG21	1.78	0.48
1:C:676:ASP:HB2	1:C:706:GLU:HB3	1.93	0.48
1:F:716:LEU:HD12	1:F:720:VAL:CG2	2.43	0.48
1:B:688:THR:HB	1:B:691:THR:OG1	2.14	0.48
1:E:682[B]:ILE:HD12	1:E:702:LEU:HD12	1.95	0.48
1:D:617:ILE:HG21	1:D:626:LEU:HD21	1.96	0.48
1:E:682[B]:ILE:HD13	1:E:682[B]:ILE:H	1.78	0.48
1:C:627:GLU:H	1:C:627:GLU:CD	2.15	0.48
1:C:577:VAL:HG22	1:C:590:GLY:HA3	1.96	0.48
1:F:591:THR:HG21	1:F:755:LEU:HD22	1.95	0.48
1:B:579:LEU:HG	1:B:587:PHE:CZ	2.49	0.48
1:A:556:LYS:HB3	1:A:569:HIS:CD2	2.48	0.48
1:A:557:LYS:HD2	1:A:681:PHE:HZ	1.78	0.48
1:B:638:LEU:CD2	1:B:650:LEU:HD22	2.44	0.48
1:C:594[B]:SER:OG	1:C:597:TRP:HB2	2.13	0.48
1:F:571:HIS:CE1	1:F:661:LYS:HD3	2.49	0.47
1:C:616:VAL:HG22	1:C:633:ILE:O	2.15	0.47
1:C:577:VAL:HG22	1:C:590:GLY:CA	2.44	0.47
1:A:579[A]:LEU:HG	1:A:587:PHE:CZ	2.49	0.47
1:D:575:TRP:CG	1:D:665:ALA:HB2	2.49	0.47
1:C:580:ARG:HD2	1:C:617:ILE:CG1	2.44	0.47
1:E:607:LYS:HA	1:F:609:PRO:HG3	1.97	0.47
1:F:574:PRO:HB2	1:F:663:ILE:H	1.79	0.47
1:D:637:ARG:HD3	1:D:639:PHE:CZ	2.50	0.47
1:D:759:THR:HA	1:D:774:TYR:CD2	2.50	0.47
1:E:617:ILE:HD12	1:E:632:GLU:HG2	1.97	0.47
1:F:669:SER:OG	1:F:672:TYR:HB2	2.15	0.47
1:A:557:LYS:HD2	1:A:681:PHE:CZ	2.50	0.46
1:B:574:PRO:HB2	1:B:663:ILE:H	1.80	0.46
1:F:645:LYS:NZ	1:F:723:THR:HG21	2.30	0.46
1:F:705:ILE:HD12	1:F:771:PRO:HB3	1.97	0.46
1:A:594[B]:SER:HG	1:A:597:TRP:HD1	1.62	0.46
1:D:564:GLY:H	1:D:691:THR:HG21	1.79	0.46
1:F:759:THR:HA	1:F:774:TYR:CD2	2.50	0.46
1:C:577:VAL:HG21	1:C:598:VAL:HG11	1.97	0.46
1:B:668:PRO:HD3	1:B:755:LEU:O	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:594[A]:SER:HB3	1:D:595:PRO:HD2	1.96	0.46
1:D:643:THR:OG1	1:D:645:LYS:HG2	2.15	0.46
1:B:759:THR:HA	1:B:774:TYR:CD2	2.50	0.46
1:C:702:LEU:HD21	1:C:734:THR:HG22	1.97	0.46
1:A:709:VAL:O	1:A:712:ARG:HG3	2.14	0.46
1:C:627:GLU:HB3	1:C:628:PRO:HD2	1.97	0.46
1:E:668:PRO:HD3	1:E:755:LEU:O	2.15	0.46
1:E:619:GLY:O	1:E:629:HIS:HE1	1.99	0.46
1:F:682[A]:ILE:HG12	1:F:700:ALA:HB3	1.97	0.46
1:F:682[A]:ILE:CG1	1:F:700:ALA:HB3	2.46	0.46
1:D:720:VAL:HG21	1:D:726:CYS:SG	2.56	0.46
1:E:607:LYS:HG3	2:E:801:A1AHR:C47	2.46	0.46
1:F:585:MET:HE2	1:F:585:MET:HA	1.98	0.46
1:A:702:LEU:HD21	1:A:734:THR:HG22	1.96	0.46
1:B:564:GLY:H	1:B:691:THR:HG21	1.81	0.46
1:C:548:CYS:C	1:C:666:CYS:SG	2.94	0.46
1:D:761:TRP:CZ2	1:D:773:VAL:HG21	2.51	0.46
1:F:682[B]:ILE:HG12	1:F:700:ALA:HB3	1.97	0.45
1:A:599:LEU:HD21	1:A:647:ILE:HD11	1.98	0.45
1:E:749:GLU:OE1	1:E:754[A]:ILE:HD12	2.15	0.45
1:F:605:LEU:HA	1:F:614:TYR:OH	2.16	0.45
1:B:580:ARG:HD2	1:B:617:ILE:HG13	1.98	0.45
1:A:563:VAL:HG13	1:A:691:THR:HG21	1.98	0.45
1:A:607:LYS:HG3	2:A:801:A1AHR:C45	2.46	0.45
1:B:617:ILE:HG23	1:B:630:VAL:CG1	2.47	0.45
1:C:580:ARG:CD	1:C:617:ILE:HG13	2.47	0.45
1:F:682[B]:ILE:CG1	1:F:700:ALA:HB3	2.46	0.45
1:F:688:THR:HB	1:F:691:THR:OG1	2.17	0.45
1:A:755:LEU:HG	1:A:777:VAL:HG21	1.99	0.45
1:C:710:CYS:SG	1:C:716:LEU:HD12	2.57	0.45
1:A:557:LYS:C	1:A:559:PRO:HD3	2.38	0.44
1:B:548:CYS:C	1:B:666:CYS:SG	2.96	0.44
1:C:702:LEU:HD22	1:C:728:GLY:HA2	1.99	0.44
1:A:720:VAL:HG21	1:A:726:CYS:SG	2.57	0.44
1:D:687:GLU:HB3	3:D:906:HOH:O	2.18	0.44
1:D:759:THR:HG1	1:D:774:TYR:HE2	1.63	0.44
1:F:709:VAL:O	1:F:715:PHE:HD2	2.01	0.44
1:A:627:GLU:H	1:A:627:GLU:CD	2.20	0.44
1:A:555:PRO:HA	1:A:572:SER:HB2	1.99	0.44
1:B:768:PRO:O	1:B:770:LYS:HG2	2.18	0.44
1:D:564:GLY:N	1:D:691:THR:HG21	2.32	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:599:LEU:HD11	1:C:647:ILE:HG12	2.00	0.44
1:E:641:GLU:CD	1:E:643:THR:H	2.21	0.44
1:D:637:ARG:HD3	1:D:639:PHE:HZ	1.82	0.44
1:C:568:ALA:O	1:C:621:HIS:HE1	2.01	0.43
1:D:680:CYS:HB3	1:D:746:VAL:O	2.18	0.43
1:F:551:PRO:HG3	1:F:575:TRP:CH2	2.52	0.43
1:F:668:PRO:HG2	1:F:778:SER:HA	1.99	0.43
1:A:763:LEU:HD12	1:A:770:LYS:HD2	2.01	0.43
1:F:761:TRP:CZ2	1:F:773:VAL:HG21	2.53	0.43
1:C:594[A]:SER:OG	1:C:595:PRO:HD2	2.19	0.43
1:F:633:ILE:HD12	1:F:652:LEU:HD22	1.98	0.43
1:D:577:VAL:HG22	1:D:590:GLY:CA	2.49	0.43
1:F:550:LYS:HB2	3:F:902:HOH:O	2.18	0.43
1:D:607:LYS:HG3	2:D:801:A1AHR:C47	2.49	0.43
1:F:703:PRO:HG2	1:F:728:GLY:O	2.18	0.43
1:C:684:GLY:HA3	1:C:740:ASP:OD1	2.19	0.43
1:C:725:LEU:C	1:C:725:LEU:HD12	2.39	0.43
1:B:759:THR:HG1	1:B:774:TYR:HE2	1.67	0.43
1:D:638:LEU:HD22	1:D:650:LEU:HD22	2.00	0.43
1:F:585:MET:HA	1:F:585:MET:CE	2.49	0.43
1:C:643:THR:OG1	1:C:645:LYS:HG2	2.18	0.42
1:C:767:ARG:NH2	1:C:770:LYS:HE2	2.33	0.42
1:B:725:LEU:HD12	1:B:725:LEU:C	2.40	0.42
1:C:580:ARG:HA	1:C:585:MET:O	2.20	0.42
1:E:548:CYS:C	1:E:666:CYS:SG	2.98	0.42
1:E:618:LEU:HD12	1:E:618:LEU:N	2.34	0.42
1:F:599:LEU:HD11	1:F:647:ILE:HG12	2.00	0.42
1:F:761:TRP:CH2	1:F:773:VAL:HG21	2.53	0.42
1:C:705:ILE:HD13	1:C:730:LEU:HD21	2.00	0.42
1:E:580:ARG:NH1	1:E:626:LEU:HD11	2.35	0.42
1:B:714:GLU:CD	1:B:714:GLU:H	2.23	0.42
1:D:548:CYS:O	1:D:666:CYS:SG	2.78	0.42
1:E:689:GLN:NE2	1:E:765:CYS:HB2	2.35	0.42
1:F:553:VAL:O	1:F:572:SER:HA	2.19	0.42
1:F:681:PHE:CE2	1:F:701:GLN:HB2	2.55	0.42
1:A:759:THR:HA	1:A:774:TYR:CD2	2.54	0.42
1:A:617:ILE:CD1	1:A:632:GLU:HG2	2.50	0.42
1:C:580:ARG:NE	1:C:617:ILE:HG13	2.35	0.42
1:F:641:GLU:HA	1:F:642:PRO:HD3	1.93	0.42
1:A:691:THR:O	1:A:692:PHE:CB	2.65	0.41
1:E:580:ARG:HH22	1:E:626:LEU:HD21	1.84	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:702:LEU:HD23	1:F:702:LEU:HA	1.90	0.41
1:D:709:VAL:O	1:D:715:PHE:HD2	2.04	0.41
1:F:720:VAL:HG21	1:F:726:CYS:SG	2.60	0.41
1:D:702:LEU:O	1:D:702:LEU:HD12	2.20	0.41
1:E:649:LEU:HD11	1:E:784:ILE:HG23	2.02	0.41
1:F:594[A]:SER:CB	1:F:788[A]:MET:HE3	2.51	0.41
1:B:710:CYS:SG	1:B:720:VAL:HG21	2.60	0.41
1:C:564:GLY:H	1:C:691:THR:CB	2.33	0.41
1:F:563:VAL:HG13	1:F:691:THR:HG21	2.03	0.41
1:D:643:THR:HG1	1:D:645:LYS:HG2	1.85	0.41
1:B:594[B]:SER:HG	1:B:597:TRP:HD1	1.68	0.41
1:C:645:LYS:HG3	1:C:780:PHE:CZ	2.55	0.41
1:B:562:VAL:N	3:B:911:HOH:O	2.53	0.41
1:C:551:PRO:HG3	1:C:575:TRP:CH2	2.56	0.41
1:C:587:PHE:HZ	1:C:614:TYR:CD1	2.39	0.41
1:F:652:LEU:HD12	1:F:652:LEU:H	1.84	0.41
1:A:725:LEU:C	1:A:725:LEU:HD12	2.40	0.41
1:B:563:VAL:O	1:B:734:THR:HA	2.21	0.41
1:B:645:LYS:HG3	1:B:780:PHE:CE1	2.56	0.41
1:B:649:LEU:HD11	1:B:784:ILE:HA	2.02	0.41
1:B:693:GLY:HA3	1:B:698:LYS:HD2	2.03	0.41
1:E:574:PRO:HB2	1:E:663:ILE:H	1.85	0.41
1:E:637:ARG:HB3	1:E:639:PHE:CE1	2.55	0.41
1:C:641:GLU:HG2	1:C:642:PRO:HD2	2.02	0.41
1:D:594[A]:SER:HB3	1:D:595:PRO:CD	2.51	0.41
1:C:574:PRO:HB2	1:C:663:ILE:H	1.86	0.40
1:E:669:SER:OG	1:E:672:TYR:HB2	2.21	0.40
1:B:579:LEU:HD12	1:B:579:LEU:HA	1.93	0.40
1:B:594[B]:SER:OG	1:B:597:TRP:HB2	2.21	0.40
1:B:749:GLU:OE1	1:B:754[B]:ILE:HD12	2.21	0.40
1:C:579:LEU:HD23	1:C:579:LEU:HA	1.88	0.40
1:D:577:VAL:HG22	1:D:590:GLY:HA3	2.04	0.40
1:D:598:VAL:HG23	1:D:652:LEU:HD11	2.03	0.40
1:B:574:PRO:HB2	1:B:663:ILE:N	2.36	0.40
1:D:714:GLU:H	1:D:714:GLU:CD	2.25	0.40
1:F:725:LEU:HD12	1:F:725:LEU:C	2.41	0.40
1:D:649:LEU:HD11	1:D:784:ILE:HA	2.04	0.40
1:D:789:ARG:HG2	1:D:790:ASN:H	1.83	0.40
1:D:619:GLY:HA2	3:D:913:HOH:O	2.21	0.40
1:E:677:ARG:HH21	1:E:703:PRO:CB	2.34	0.40
1:F:587:PHE:CD1	2:F:801:A1AHR:C48	3.04	0.40

All (3) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:554:GLU:OE1	1:B:554:GLU:OE1[1_655]	0.52	1.68
1:A:554:GLU:CD	1:B:554:GLU:OE1[1_655]	1.68	0.52
1:A:554:GLU:OE1	1:B:554:GLU:CD[1_655]	1.75	0.45

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	249/250 (100%)	240 (96%)	7 (3%)	2 (1%)	16	13
1	B	246/250 (98%)	239 (97%)	7 (3%)	0	100	100
1	C	243/250 (97%)	231 (95%)	11 (4%)	1 (0%)	30	29
1	D	244/250 (98%)	227 (93%)	16 (7%)	1 (0%)	30	29
1	E	249/250 (100%)	238 (96%)	9 (4%)	2 (1%)	16	13
1	F	240/250 (96%)	226 (94%)	13 (5%)	1 (0%)	30	29
All	All	1471/1500 (98%)	1401 (95%)	63 (4%)	7 (0%)	25	23

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	557	LYS
1	F	557	LYS
1	C	750	LYS
1	A	692	PHE
1	D	750	LYS
1	E	750	LYS
1	A	750	LYS

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	214/210 (102%)	212 (99%)	2 (1%)	75	82
1	B	212/210 (101%)	208 (98%)	4 (2%)	52	59
1	C	210/210 (100%)	209 (100%)	1 (0%)	86	91
1	D	209/210 (100%)	202 (97%)	7 (3%)	33	36
1	E	215/210 (102%)	212 (99%)	3 (1%)	62	70
1	F	204/210 (97%)	199 (98%)	5 (2%)	42	47
All	All	1264/1260 (100%)	1242 (98%)	22 (2%)	54	63

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	557	LYS
1	A	577	VAL
1	B	558	CYS
1	B	625	ASN
1	B	708	LYS
1	B	736	SER
1	C	577	VAL
1	D	577	VAL
1	D	581	THR
1	D	626	LEU
1	D	692	PHE
1	D	702	LEU
1	D	712	ARG
1	D	789	ARG
1	E	557	LYS
1	E	677	ARG
1	E	736	SER
1	F	577	VAL
1	F	637	ARG
1	F	687	GLU
1	F	736	SER
1	F	737	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	625	ASN
1	A	721	GLN
1	A	790	ASN
1	B	625	ASN
1	B	701	GLN
1	C	701	GLN
1	C	790	ASN
1	D	701	GLN
1	D	738	GLN
1	D	790	ASN
1	E	629	HIS
1	F	571	HIS
1	F	603	HIS
1	F	671	ASN
1	F	769	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry

6 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	A1AHR	D	801	-	52,53,53	1.75	10 (19%)	71,72,72	2.41	14 (19%)
2	A1AHR	B	801	-	52,53,53	1.77	10 (19%)	71,72,72	1.54	17 (23%)
2	A1AHR	C	801	-	52,53,53	1.78	10 (19%)	71,72,72	1.17	5 (7%)
2	A1AHR	E	801	-	52,53,53	1.71	10 (19%)	71,72,72	1.26	6 (8%)
2	A1AHR	F	801	-	52,53,53	1.80	10 (19%)	71,72,72	1.79	11 (15%)
2	A1AHR	A	801	-	52,53,53	1.78	10 (19%)	71,72,72	2.07	11 (15%)

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	A1AHR	D	801	-	-	8/46/56/56	0/4/5/5
2	A1AHR	B	801	-	-	9/46/56/56	0/4/5/5
2	A1AHR	C	801	-	-	1/46/56/56	0/4/5/5
2	A1AHR	E	801	-	-	4/46/56/56	0/4/5/5
2	A1AHR	F	801	-	-	7/46/56/56	0/4/5/5
2	A1AHR	A	801	-	-	5/46/56/56	0/4/5/5

All (60) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	801	A1AHR	C21-N22	5.25	1.45	1.33
2	F	801	A1AHR	C09-N10	5.21	1.45	1.34
2	F	801	A1AHR	C26-N27	5.14	1.45	1.33
2	B	801	A1AHR	C09-N10	5.13	1.45	1.34
2	C	801	A1AHR	C26-N27	5.01	1.45	1.33
2	A	801	A1AHR	C43-N42	4.95	1.46	1.35
2	D	801	A1AHR	C21-N22	4.89	1.45	1.33
2	A	801	A1AHR	C09-N10	4.88	1.44	1.34
2	B	801	A1AHR	C26-N27	4.87	1.44	1.33
2	F	801	A1AHR	C21-N22	4.84	1.44	1.33
2	C	801	A1AHR	C43-N42	4.83	1.46	1.35
2	D	801	A1AHR	C26-N27	4.81	1.44	1.33
2	F	801	A1AHR	C43-N42	4.80	1.45	1.35
2	E	801	A1AHR	C09-N10	4.80	1.44	1.34
2	E	801	A1AHR	C26-N27	4.74	1.44	1.33
2	C	801	A1AHR	C21-N22	4.72	1.44	1.33
2	E	801	A1AHR	C21-N22	4.72	1.44	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	801	A1AHR	C09-N10	4.69	1.44	1.34
2	D	801	A1AHR	C43-N42	4.62	1.45	1.35
2	B	801	A1AHR	C21-N22	4.58	1.44	1.33
2	A	801	A1AHR	C26-N27	4.54	1.44	1.33
2	B	801	A1AHR	C43-N42	4.40	1.45	1.35
2	D	801	A1AHR	C12-N13	4.13	1.45	1.35
2	D	801	A1AHR	C09-N10	4.01	1.42	1.34
2	C	801	A1AHR	C12-N13	4.00	1.44	1.35
2	E	801	A1AHR	C43-N42	3.99	1.44	1.35
2	F	801	A1AHR	C12-N13	3.98	1.44	1.35
2	B	801	A1AHR	C12-N13	3.81	1.44	1.35
2	E	801	A1AHR	C12-N13	3.71	1.44	1.35
2	A	801	A1AHR	C12-N13	3.61	1.43	1.35
2	D	801	A1AHR	O49-C09	-3.44	1.16	1.23
2	B	801	A1AHR	O49-C09	-3.03	1.17	1.23
2	B	801	A1AHR	O31-C12	-3.03	1.17	1.23
2	A	801	A1AHR	O31-C12	-2.96	1.17	1.23
2	C	801	A1AHR	O31-C12	-2.94	1.17	1.23
2	E	801	A1AHR	O31-C12	-2.78	1.18	1.23
2	A	801	A1AHR	O49-C09	-2.75	1.18	1.23
2	A	801	A1AHR	O29-C26	-2.75	1.17	1.23
2	D	801	A1AHR	O31-C12	-2.74	1.18	1.23
2	E	801	A1AHR	O49-C09	-2.74	1.18	1.23
2	C	801	A1AHR	O49-C09	-2.73	1.18	1.23
2	E	801	A1AHR	O44-C43	-2.71	1.17	1.23
2	F	801	A1AHR	O31-C12	-2.70	1.18	1.23
2	C	801	A1AHR	O29-C26	-2.68	1.18	1.23
2	C	801	A1AHR	O44-C43	-2.64	1.18	1.23
2	F	801	A1AHR	O49-C09	-2.63	1.18	1.23
2	B	801	A1AHR	O29-C26	-2.55	1.18	1.23
2	A	801	A1AHR	O44-C43	-2.55	1.18	1.23
2	C	801	A1AHR	O30-C21	-2.53	1.18	1.23
2	E	801	A1AHR	O29-C26	-2.51	1.18	1.23
2	A	801	A1AHR	O30-C21	-2.48	1.18	1.23
2	B	801	A1AHR	O44-C43	-2.47	1.18	1.23
2	F	801	A1AHR	O44-C43	-2.47	1.18	1.23
2	D	801	A1AHR	O44-C43	-2.47	1.18	1.23
2	F	801	A1AHR	O29-C26	-2.45	1.18	1.23
2	D	801	A1AHR	O30-C21	-2.41	1.18	1.23
2	E	801	A1AHR	O30-C21	-2.39	1.18	1.23
2	B	801	A1AHR	O30-C21	-2.38	1.18	1.23
2	D	801	A1AHR	O29-C26	-2.37	1.18	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	801	A1AHR	O30-C21	-2.13	1.19	1.23

All (64) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	801	A1AHR	C14-N13-C12	12.98	157.03	127.37
2	D	801	A1AHR	C11-N10-C09	10.98	145.25	121.65
2	D	801	A1AHR	C06-C09-N10	8.53	130.87	116.19
2	F	801	A1AHR	C41-N42-C43	7.20	150.75	126.61
2	D	801	A1AHR	O49-C09-N10	-6.50	111.32	122.96
2	F	801	A1AHR	C28-C43-N42	5.73	129.23	114.84
2	D	801	A1AHR	C32-C11-N10	5.68	122.59	110.83
2	D	801	A1AHR	C33-C32-C11	-5.03	99.99	113.36
2	E	801	A1AHR	C20-C21-N22	4.82	122.75	116.06
2	F	801	A1AHR	O44-C43-N42	-4.69	115.23	123.64
2	E	801	A1AHR	C14-N13-C12	-3.99	118.25	127.37
2	B	801	A1AHR	C14-N13-C12	-3.99	118.27	127.37
2	A	801	A1AHR	C24-C25-C26	-3.63	103.13	113.19
2	A	801	A1AHR	C23-N22-C21	3.43	129.21	122.82
2	F	801	A1AHR	C25-C26-N27	3.40	122.53	116.34
2	B	801	A1AHR	C06-C09-N10	3.22	121.73	116.19
2	F	801	A1AHR	C47-C45-C41	3.19	120.49	117.50
2	D	801	A1AHR	C25-C26-N27	3.11	122.00	116.34
2	A	801	A1AHR	O31-C12-N13	-2.90	117.79	123.92
2	D	801	A1AHR	C47-C45-C41	2.85	120.17	117.50
2	D	801	A1AHR	O49-C09-C06	-2.84	117.80	122.19
2	B	801	A1AHR	C08-C03-C04	2.84	116.23	109.29
2	A	801	A1AHR	C43-C28-N27	-2.79	104.91	113.04
2	B	801	A1AHR	O49-C09-C06	-2.75	117.95	122.19
2	A	801	A1AHR	C20-C17-C18	-2.71	116.90	120.89
2	D	801	A1AHR	C04-C05-C06	-2.71	106.42	111.18
2	F	801	A1AHR	C05-C06-C09	-2.65	105.20	110.79
2	D	801	A1AHR	C32-C11-C12	-2.63	103.57	110.30
2	B	801	A1AHR	C11-C12-N13	2.60	122.81	115.28
2	B	801	A1AHR	C04-C03-C02	-2.59	103.87	111.79
2	B	801	A1AHR	C08-C07-C06	-2.57	106.65	111.18
2	B	801	A1AHR	C25-C26-N27	2.55	120.98	116.34
2	B	801	A1AHR	C47-C45-C41	2.51	119.85	117.50
2	B	801	A1AHR	C37-C36-C39	-2.49	116.95	121.25
2	B	801	A1AHR	C32-C11-C12	-2.48	103.97	110.30
2	E	801	A1AHR	C23-N22-C21	-2.45	118.26	122.82
2	B	801	A1AHR	C20-C21-N22	2.42	119.42	116.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	801	A1AHR	C32-C11-C12	-2.42	104.11	110.30
2	F	801	A1AHR	C20-C17-C16	-2.41	117.34	120.89
2	D	801	A1AHR	C12-C11-N10	-2.41	104.59	111.11
2	A	801	A1AHR	C45-C41-N42	2.41	122.66	118.82
2	E	801	A1AHR	C33-C32-C11	-2.40	106.97	113.36
2	A	801	A1AHR	C47-C45-C41	2.38	119.73	117.50
2	C	801	A1AHR	C28-C43-N42	2.36	120.76	114.84
2	A	801	A1AHR	C11-C12-N13	2.35	122.09	115.28
2	F	801	A1AHR	O44-C43-C28	-2.34	115.54	120.75
2	D	801	A1AHR	C08-C07-C06	-2.33	107.07	111.18
2	C	801	A1AHR	C47-C45-C41	2.30	119.65	117.50
2	B	801	A1AHR	C33-C32-C11	-2.29	107.26	113.36
2	B	801	A1AHR	C24-C23-N22	-2.24	105.90	112.20
2	A	801	A1AHR	C28-C43-N42	2.21	120.37	114.84
2	B	801	A1AHR	C23-N22-C21	-2.20	118.73	122.82
2	E	801	A1AHR	C47-C45-C41	2.19	119.56	117.50
2	A	801	A1AHR	C33-C32-C11	-2.19	107.53	113.36
2	F	801	A1AHR	C15-C14-N13	-2.16	113.17	120.41
2	C	801	A1AHR	C33-C32-C11	-2.15	107.63	113.36
2	D	801	A1AHR	C35-C36-C39	-2.12	117.60	121.25
2	F	801	A1AHR	O29-C26-C25	-2.10	118.21	122.02
2	B	801	A1AHR	O31-C12-N13	-2.09	119.51	123.92
2	E	801	A1AHR	O30-C21-N22	-2.06	118.98	123.03
2	B	801	A1AHR	O29-C26-C25	-2.06	118.29	122.02
2	F	801	A1AHR	C32-C11-C12	-2.03	105.09	110.30
2	D	801	A1AHR	C45-C41-N42	2.03	122.07	118.82
2	C	801	A1AHR	C19-C14-N13	-2.01	113.67	120.41

There are no chirality outliers.

All (34) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	801	A1AHR	C24-C23-N22-C21
2	E	801	A1AHR	N22-C23-C24-C25
2	B	801	A1AHR	C05-C06-C09-N10
2	F	801	A1AHR	C24-C25-C26-N27
2	D	801	A1AHR	C24-C25-C26-N27
2	F	801	A1AHR	C24-C25-C26-O29
2	D	801	A1AHR	C24-C25-C26-O29
2	B	801	A1AHR	C05-C06-C09-O49
2	B	801	A1AHR	N27-C28-C43-N42
2	A	801	A1AHR	N01-C02-C03-C04

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Mol	Chain	Res	Type	Atoms
2	F	801	A1AHR	N01-C02-C03-C08
2	B	801	A1AHR	C24-C25-C26-N27
2	B	801	A1AHR	N27-C28-C43-O44
2	B	801	A1AHR	C24-C25-C26-O29
2	D	801	A1AHR	C05-C06-C09-N10
2	D	801	A1AHR	C05-C06-C09-O49
2	A	801	A1AHR	N01-C02-C03-C08
2	D	801	A1AHR	N01-C02-C03-C04
2	F	801	A1AHR	N01-C02-C03-C04
2	A	801	A1AHR	C23-C24-C25-C26
2	E	801	A1AHR	C19-C14-N13-C12
2	D	801	A1AHR	N22-C23-C24-C25
2	F	801	A1AHR	N22-C23-C24-C25
2	B	801	A1AHR	C18-C17-C20-C21
2	B	801	A1AHR	C19-C14-N13-C12
2	D	801	A1AHR	N01-C02-C03-C08
2	F	801	A1AHR	C40-C41-N42-C43
2	B	801	A1AHR	C16-C17-C20-C21
2	D	801	A1AHR	C45-C41-N42-C43
2	F	801	A1AHR	C45-C41-N42-C43
2	C	801	A1AHR	C45-C41-N42-C43
2	E	801	A1AHR	C17-C20-C21-O30
2	E	801	A1AHR	N01-C02-C03-C04
2	A	801	A1AHR	C45-C41-N42-C43

There are no ring outliers.

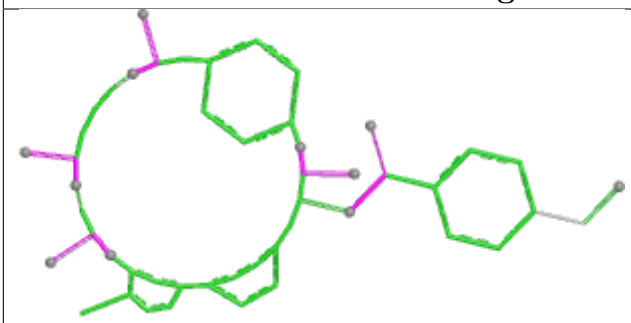
5 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	801	A1AHR	2	0
2	B	801	A1AHR	1	0
2	E	801	A1AHR	3	0
2	F	801	A1AHR	1	0
2	A	801	A1AHR	1	0

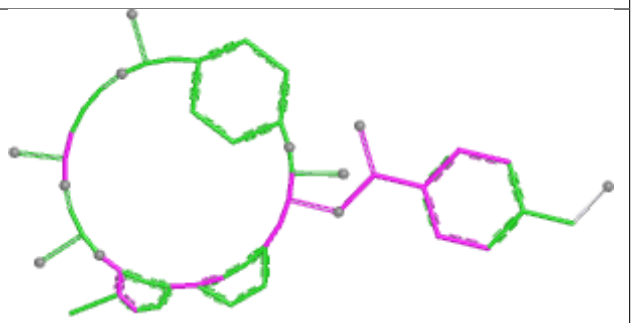
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less 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.

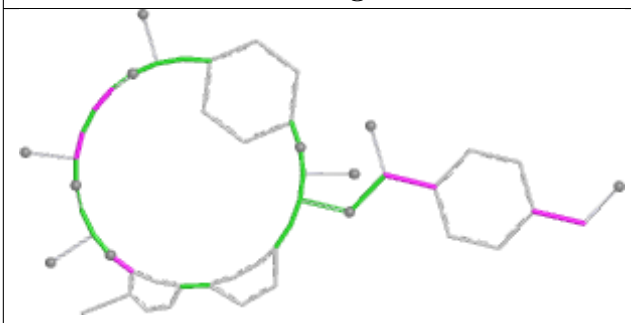
Ligand A1AHR D 801



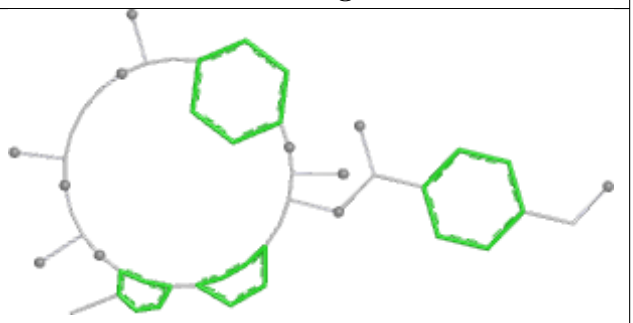
Bond lengths



Bond angles

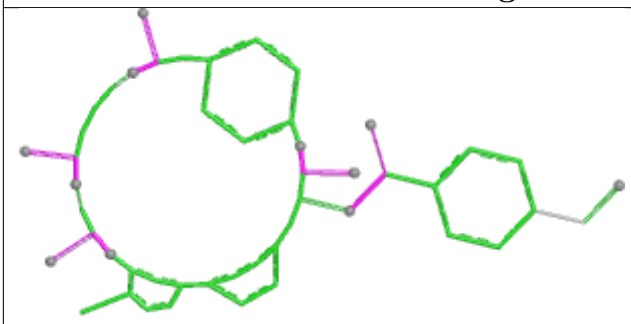


Torsions

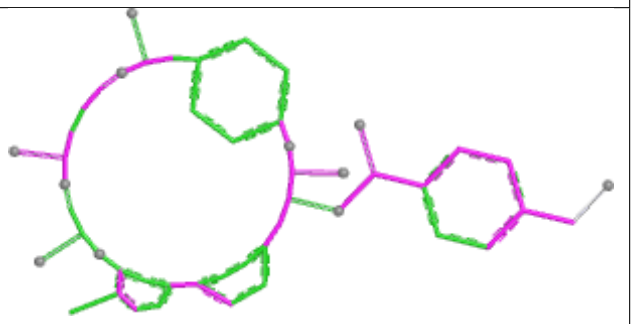


Rings

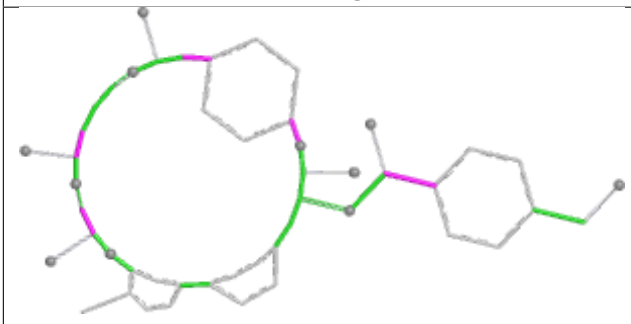
Ligand A1AHR B 801



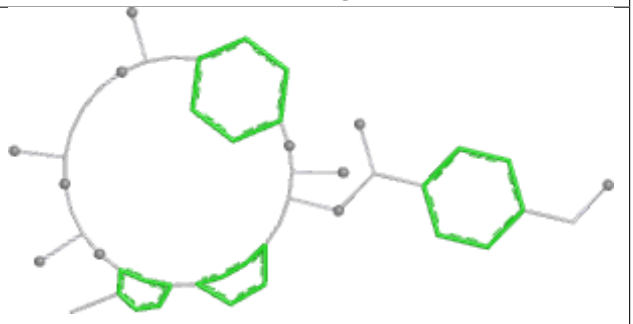
Bond lengths



Bond angles

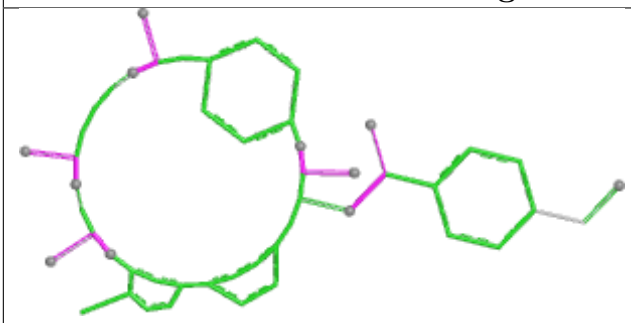


Torsions

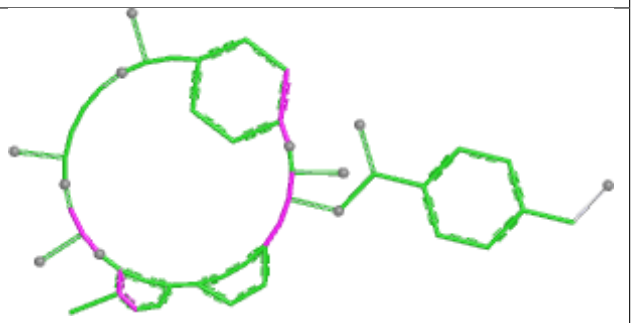


Rings

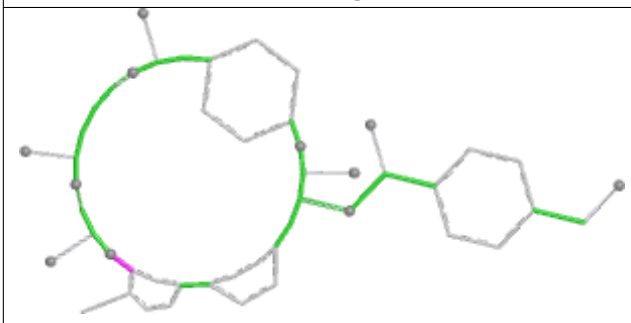
Ligand A1AHR C 801



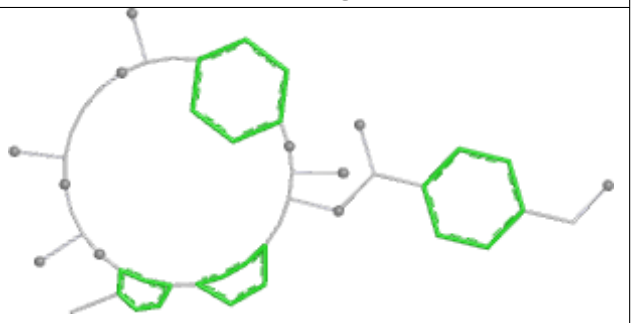
Bond lengths



Bond angles

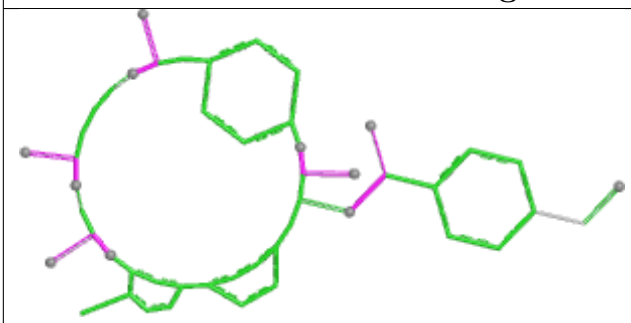


Torsions

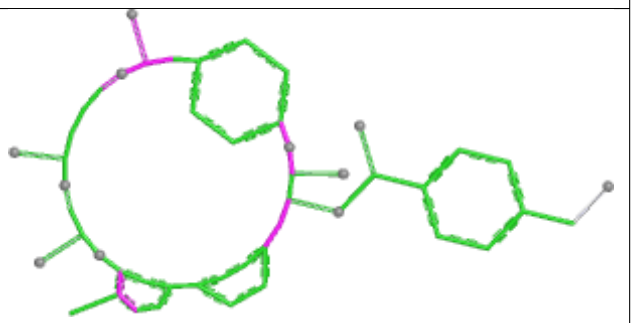


Rings

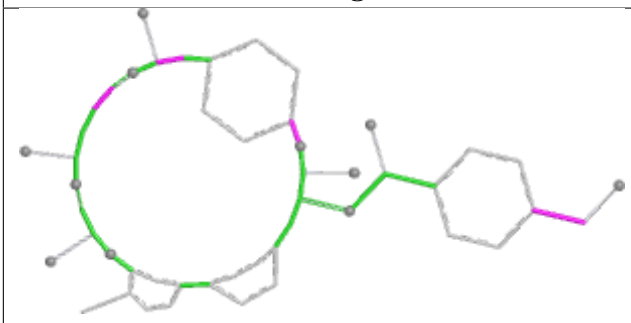
Ligand A1AHR E 801



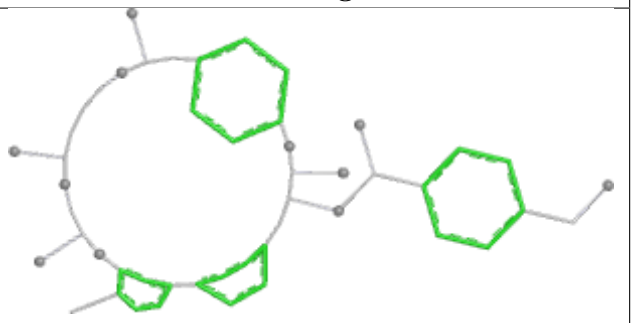
Bond lengths



Bond angles

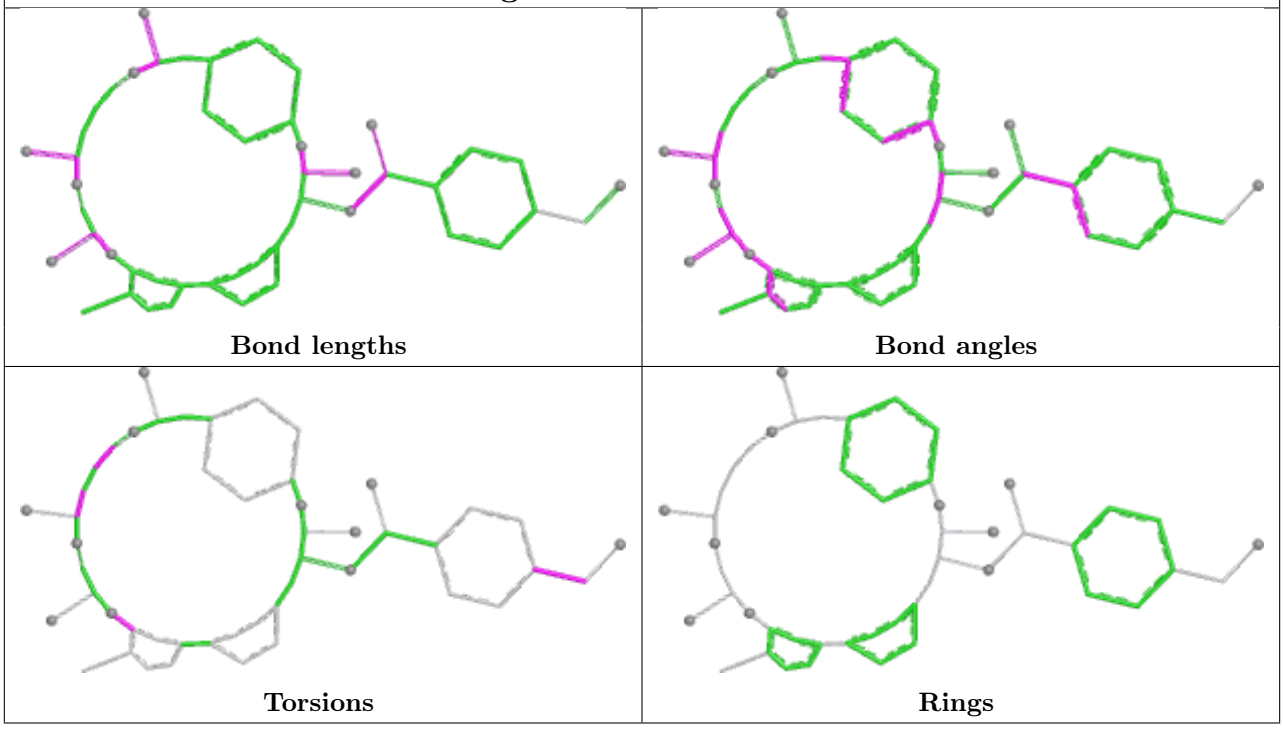


Torsions

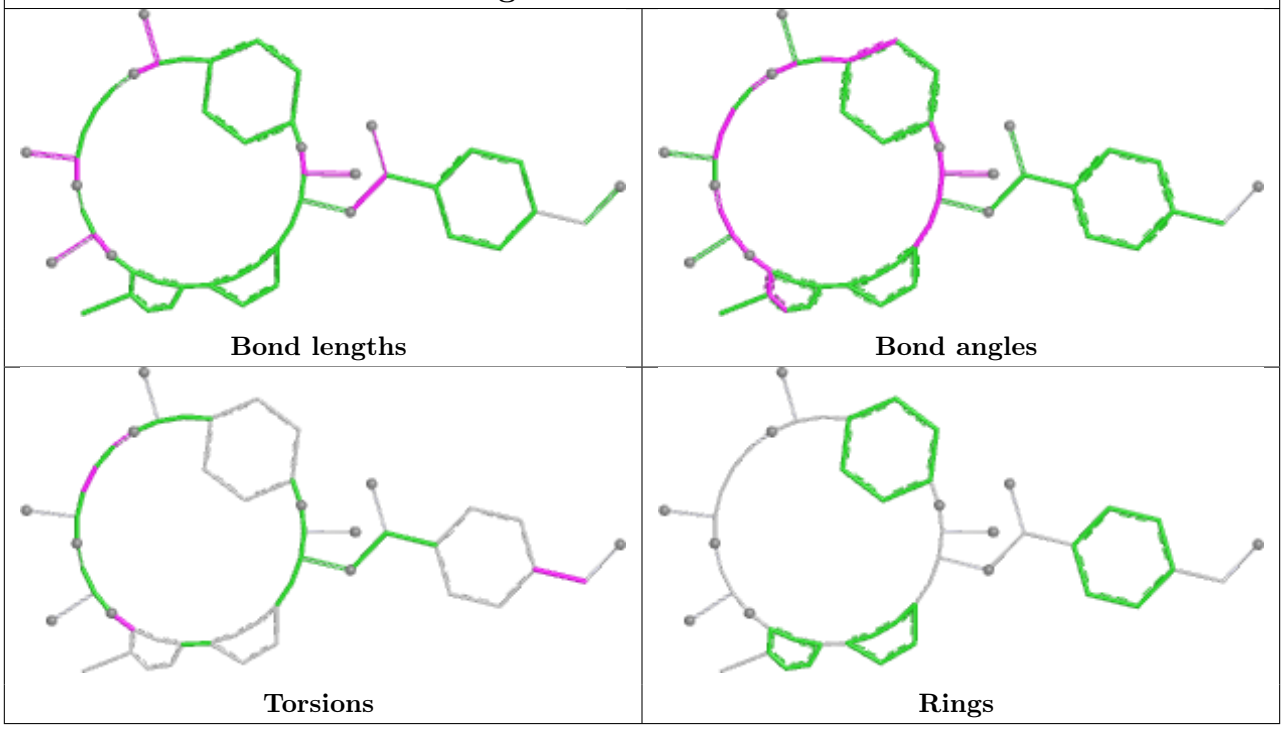


Rings

Ligand A1AHR F 801



Ligand A1AHR A 801



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, 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	246/250 (98%)	0.30	14 (5%)	30	33	11, 25, 48, 97	8 (3%)
1	B	246/250 (98%)	0.35	13 (5%)	33	35	11, 27, 47, 75	4 (1%)
1	C	244/250 (97%)	0.48	12 (4%)	36	38	19, 34, 59, 81	4 (1%)
1	D	244/250 (97%)	0.74	20 (8%)	19	21	23, 43, 73, 90	5 (2%)
1	E	245/250 (98%)	0.65	15 (6%)	28	30	20, 38, 63, 102	10 (4%)
1	F	239/250 (95%)	1.51	54 (22%)	3	3	32, 59, 91, 134	8 (3%)
All	All	1464/1500 (97%)	0.67	128 (8%)	17	19	11, 36, 74, 134	39 (2%)

All (128) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	692	PHE	5.2
1	E	583	PHE	5.2
1	E	692	PHE	4.6
1	B	544	PRO	4.2
1	B	692	PHE	4.1
1	D	692	PHE	4.0
1	E	585	MET	3.7
1	F	583	PHE	3.7
1	D	583	PHE	3.7
1	F	735	ASP	3.5
1	F	558	CYS	3.5
1	A	692	PHE	3.4
1	A	558	CYS	3.4
1	A	544	PRO	3.4
1	B	713	TYR	3.4
1	E	584	GLY	3.4
1	F	766	ALA	3.3
1	E	582	ARG	3.3
1	C	546	PHE	3.3

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Mol	Chain	Res	Type	RSRZ
1	F	730	LEU	3.2
1	A	629	HIS	3.2
1	F	553	VAL	3.1
1	D	554	GLU	3.1
1	F	687	GLU	3.1
1	F	702	LEU	3.1
1	A	583	PHE	3.0
1	E	610	ARG	3.0
1	D	628	PRO	3.0
1	F	691	THR	3.0
1	F	657	VAL	3.0
1	F	713	TYR	2.9
1	F	656	ALA	2.9
1	F	736	SER	2.9
1	F	666	CYS	2.9
1	F	682[A]	ILE	2.8
1	F	559	PRO	2.8
1	D	714	GLU	2.8
1	F	715	PHE	2.8
1	D	559	PRO	2.8
1	B	634	GLU	2.8
1	F	690	GLY	2.7
1	F	731	ALA	2.7
1	D	626	LEU	2.7
1	F	630	VAL	2.7
1	C	789	ARG	2.7
1	C	691	THR	2.7
1	F	585	MET	2.6
1	D	546	PHE	2.6
1	F	606	GLU	2.6
1	D	548	CYS	2.6
1	F	610	ARG	2.6
1	F	781	VAL	2.6
1	B	708	LYS	2.6
1	D	557	LYS	2.6
1	E	677	ARG	2.6
1	F	789	ARG	2.6
1	A	606	GLU	2.6
1	E	554	GLU	2.6
1	F	693	GLY	2.6
1	A	737	CYS	2.6
1	F	725	LEU	2.6

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Mol	Chain	Res	Type	RSRZ
1	F	750	LYS	2.5
1	B	585	MET	2.5
1	A	585	MET	2.5
1	A	713	TYR	2.5
1	F	754[A]	ILE	2.5
1	B	627	GLU	2.4
1	E	634	GLU	2.4
1	C	557	LYS	2.4
1	C	625	ASN	2.4
1	F	655	PRO	2.4
1	F	579	LEU	2.4
1	E	767	ARG	2.4
1	B	584	GLY	2.4
1	C	690	GLY	2.4
1	C	733	GLY	2.4
1	F	640	LEU	2.4
1	F	710	CYS	2.4
1	E	559	PRO	2.4
1	D	556	LYS	2.3
1	E	643	THR	2.3
1	F	673	VAL	2.3
1	F	584	GLY	2.3
1	F	764	GLY	2.3
1	C	627	GLU	2.3
1	A	690	GLY	2.3
1	F	619	GLY	2.3
1	F	546	PHE	2.3
1	A	557	LYS	2.3
1	F	667	LEU	2.3
1	F	694	ALA	2.3
1	A	710	CYS	2.3
1	A	559	PRO	2.3
1	F	621	HIS	2.3
1	D	789	ARG	2.3
1	D	763	LEU	2.3
1	F	631	GLN	2.3
1	E	749	GLU	2.2
1	C	582	ARG	2.2
1	B	554	GLU	2.2
1	D	731	ALA	2.2
1	F	762	GLY	2.2
1	D	616	VAL	2.2

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Mol	Chain	Res	Type	RSRZ
1	D	702	LEU	2.2
1	F	714[A]	GLU	2.2
1	D	610	ARG	2.2
1	B	738	GLN	2.2
1	F	595	PRO	2.2
1	B	637	ARG	2.2
1	C	692	PHE	2.1
1	F	732	GLY	2.1
1	F	733	GLY	2.1
1	D	710	CYS	2.1
1	D	624	VAL	2.1
1	F	705	ILE	2.1
1	B	596	GLU	2.1
1	C	548	CYS	2.1
1	A	708	LYS	2.1
1	F	622	GLN	2.1
1	F	575	TRP	2.1
1	F	632	GLU	2.1
1	E	666	CYS	2.1
1	E	710	CYS	2.1
1	C	545[A]	SER	2.1
1	D	713	TYR	2.0
1	B	557	LYS	2.0
1	F	652	LEU	2.0
1	F	548	CYS	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

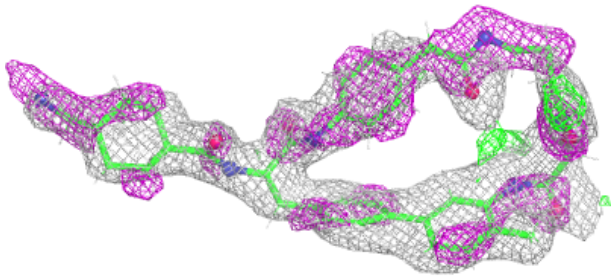
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

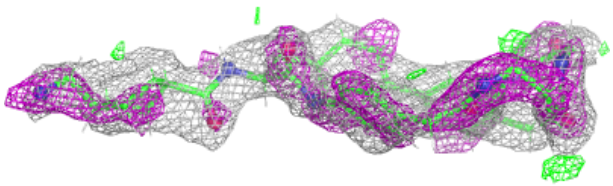
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	A1AHR	F	801	49/49	0.74	0.11	21,21,21,21	0
2	A1AHR	B	801	49/49	0.75	0.12	21,21,21,21	0
2	A1AHR	E	801	49/49	0.80	0.10	21,21,21,21	0
2	A1AHR	D	801	49/49	0.83	0.09	21,21,21,21	0
2	A1AHR	A	801	49/49	0.85	0.09	21,21,21,21	0
2	A1AHR	C	801	49/49	0.90	0.08	21,21,21,21	0

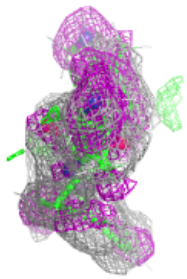
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around A1AHR F 801:

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

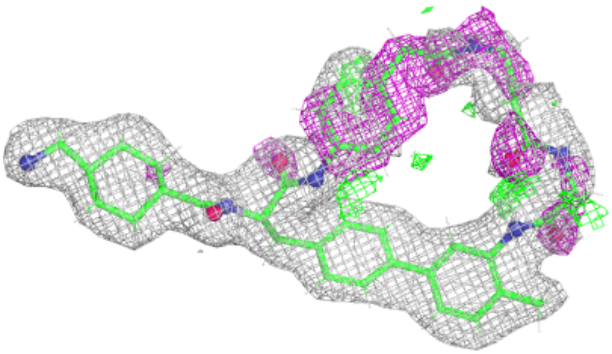


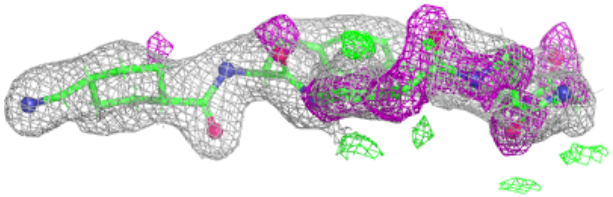


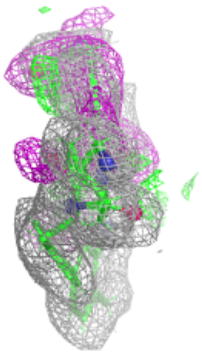


Electron density around A1AHR B 801:

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

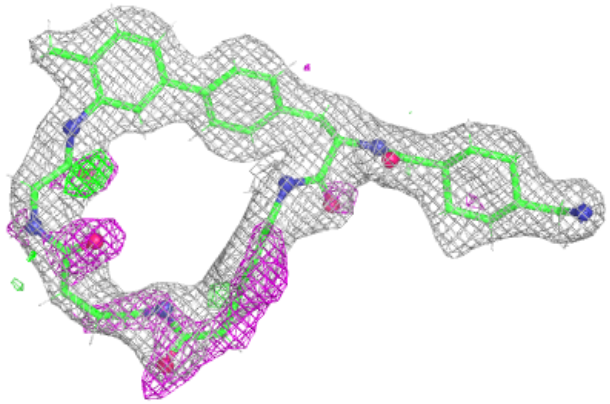


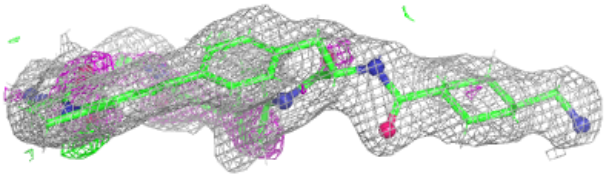


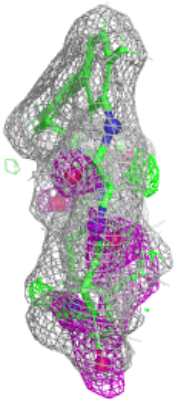


Electron density around A1AHR E 801:

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

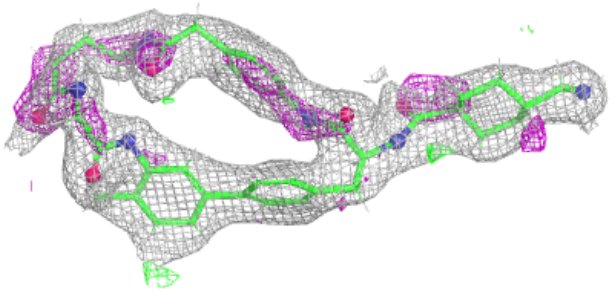


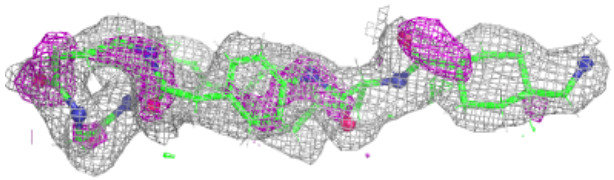


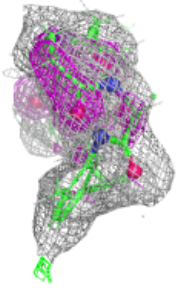


Electron density around A1AHR D 801:

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

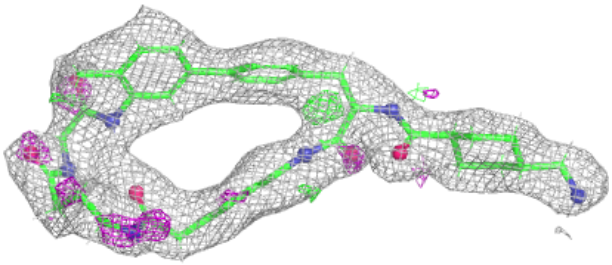


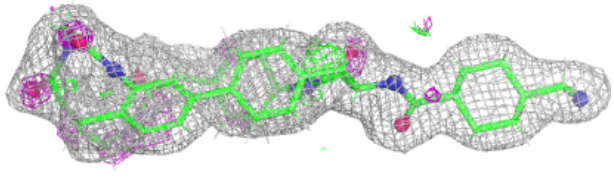


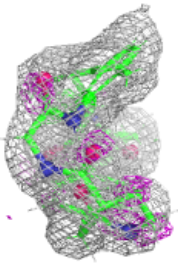


Electron density around A1AHR A 801:

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

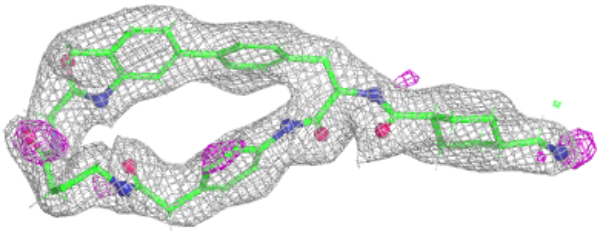


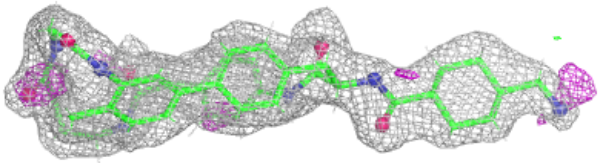


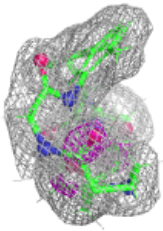


Electron density around A1AHR C 801:

$2mF_o$-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.