Full wwPDB X-ray Structure Validation Report (i)

Sep 3, 2023 – 06:42 AM EDT

PDB ID	:	3SJO
Title	:	structure of EV71 3C in complex with Rupintrivir (AG7088)
Authors	:	Lu, G.; Qi, J.; Chen, Z.; Xu, X.; Gao, F.; Lin, D.; Qian, W.; Liu, H.; Jiang, H.; Yan, J.; Gao, G.F.
Deposited on	:	2011-06-21
Resolution	:	1.70 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 (i) 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 (i)) were used in the production of this report:

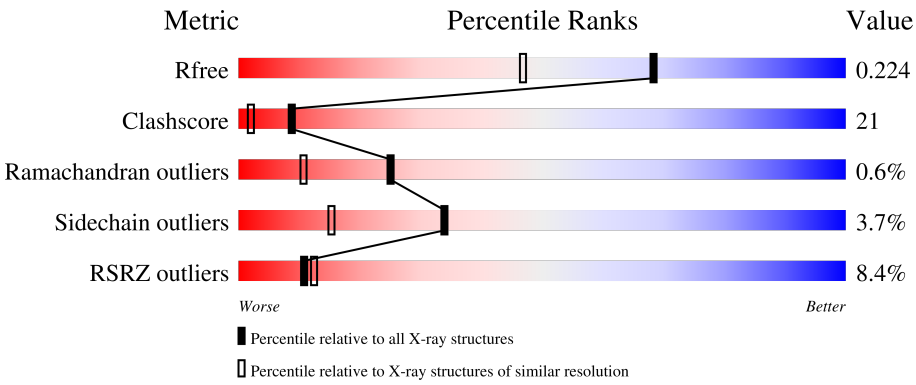
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (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 1.70 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	4298 (1.70-1.70)
Clashscore	141614	4695 (1.70-1.70)
Ramachandran outliers	138981	4610 (1.70-1.70)
Sidechain outliers	138945	4610 (1.70-1.70)
RSRZ outliers	127900	4222 (1.70-1.70)

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	190	3% 77% 16% • 6%
1	B	190	17% 59% 33% • • 6%
1	C	190	2% 76% 15% • 6%
1	D	190	3% 81% 11% • 6%
1	E	190	5% 73% 21% • 6%

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Mol	Chain	Length	Quality of chain
1	F	190	14% 62% 31% 6%
1	G	190	13% 67% 23% 6%
1	H	190	8% 68% 24% 6%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 12391 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 3C protease.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	179	1391	881	247	256	7	0	0	0
1	B	179	1391	881	247	256	7	0	0	0
1	C	179	1391	881	247	256	7	0	0	0
1	D	179	1391	881	247	256	7	0	0	0
1	E	179	1391	881	247	256	7	0	0	0
1	F	179	1391	881	247	256	7	0	0	0
1	G	179	1391	881	247	256	7	0	0	0
1	H	179	1391	881	247	256	7	0	0	0

There are 56 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	MET	-	initiating methionine	UNP E0WWC7
A	184	HIS	-	expression tag	UNP E0WWC7
A	185	HIS	-	expression tag	UNP E0WWC7
A	186	HIS	-	expression tag	UNP E0WWC7
A	187	HIS	-	expression tag	UNP E0WWC7
A	188	HIS	-	expression tag	UNP E0WWC7
A	189	HIS	-	expression tag	UNP E0WWC7
B	0	MET	-	initiating methionine	UNP E0WWC7
B	184	HIS	-	expression tag	UNP E0WWC7
B	185	HIS	-	expression tag	UNP E0WWC7
B	186	HIS	-	expression tag	UNP E0WWC7
B	187	HIS	-	expression tag	UNP E0WWC7
B	188	HIS	-	expression tag	UNP E0WWC7

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Chain	Residue	Modelled	Actual	Comment	Reference
B	189	HIS	-	expression tag	UNP E0WWC7
C	0	MET	-	initiating methionine	UNP E0WWC7
C	184	HIS	-	expression tag	UNP E0WWC7
C	185	HIS	-	expression tag	UNP E0WWC7
C	186	HIS	-	expression tag	UNP E0WWC7
C	187	HIS	-	expression tag	UNP E0WWC7
C	188	HIS	-	expression tag	UNP E0WWC7
C	189	HIS	-	expression tag	UNP E0WWC7
D	0	MET	-	initiating methionine	UNP E0WWC7
D	184	HIS	-	expression tag	UNP E0WWC7
D	185	HIS	-	expression tag	UNP E0WWC7
D	186	HIS	-	expression tag	UNP E0WWC7
D	187	HIS	-	expression tag	UNP E0WWC7
D	188	HIS	-	expression tag	UNP E0WWC7
D	189	HIS	-	expression tag	UNP E0WWC7
E	0	MET	-	initiating methionine	UNP E0WWC7
E	184	HIS	-	expression tag	UNP E0WWC7
E	185	HIS	-	expression tag	UNP E0WWC7
E	186	HIS	-	expression tag	UNP E0WWC7
E	187	HIS	-	expression tag	UNP E0WWC7
E	188	HIS	-	expression tag	UNP E0WWC7
E	189	HIS	-	expression tag	UNP E0WWC7
F	0	MET	-	initiating methionine	UNP E0WWC7
F	184	HIS	-	expression tag	UNP E0WWC7
F	185	HIS	-	expression tag	UNP E0WWC7
F	186	HIS	-	expression tag	UNP E0WWC7
F	187	HIS	-	expression tag	UNP E0WWC7
F	188	HIS	-	expression tag	UNP E0WWC7
F	189	HIS	-	expression tag	UNP E0WWC7
G	0	MET	-	initiating methionine	UNP E0WWC7
G	184	HIS	-	expression tag	UNP E0WWC7
G	185	HIS	-	expression tag	UNP E0WWC7
G	186	HIS	-	expression tag	UNP E0WWC7
G	187	HIS	-	expression tag	UNP E0WWC7
G	188	HIS	-	expression tag	UNP E0WWC7
G	189	HIS	-	expression tag	UNP E0WWC7
H	0	MET	-	initiating methionine	UNP E0WWC7
H	184	HIS	-	expression tag	UNP E0WWC7
H	185	HIS	-	expression tag	UNP E0WWC7
H	186	HIS	-	expression tag	UNP E0WWC7
H	187	HIS	-	expression tag	UNP E0WWC7
H	188	HIS	-	expression tag	UNP E0WWC7

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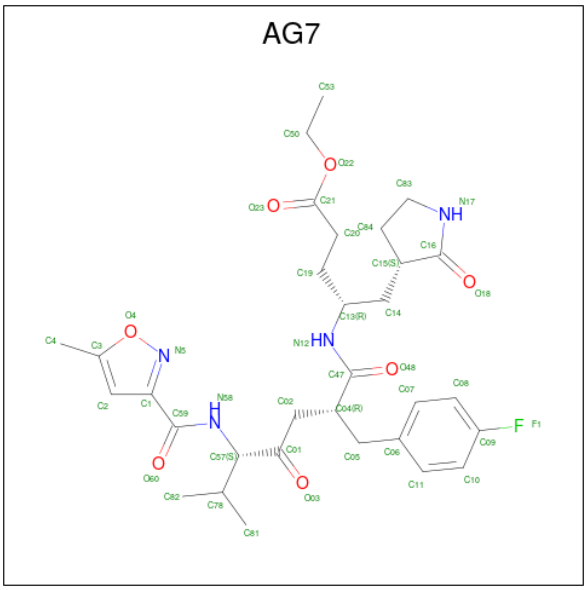
Chain	Residue	Modelled	Actual	Comment	Reference
H	189	HIS	-	expression tag	UNP E0WWC7

- Molecule 2 is 4-{2-(4-FLUORO-BENZYL)-6-METHYL-5-[(5-METHYL-ISOXAZOLE-3-CARBONYL)-AMINO]-4-OXO-HEPTANOYLAMINO}-5-(2-OXO-PYRROLIDIN-3-YL)-PENTANOIC ACID ETHYL ESTER (three-letter code: AG7) (formula: $C_{31}H_{41}FN_4O_7$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	F	N	O		
2	A	1	43	31	1	4	7	0	0
2	B	1	43	31	1	4	7	0	0
2	C	1	43	31	1	4	7	0	0
2	D	1	43	31	1	4	7	0	0
2	E	1	43	31	1	4	7	0	0
2	F	1	43	31	1	4	7	0	0
2	G	1	43	31	1	4	7	0	0
2	H	1	43	31	1	4	7	0	0

- Molecule 3 is water.

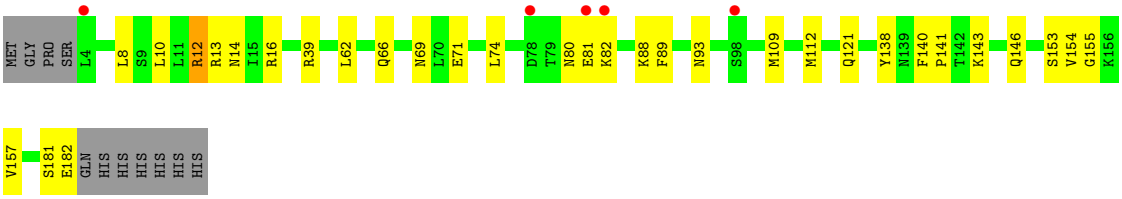
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
3	A	124	124	124	0	0
			Total	O		
3	B	97	97	97	0	0
			Total	O		
3	C	144	144	144	0	0
			Total	O		
3	D	137	137	137	0	0
			Total	O		
3	E	146	146	146	0	0
			Total	O		
3	F	106	106	106	0	0
			Total	O		
3	G	73	73	73	0	0
			Total	O		
3	H	92	92	92	0	0

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.

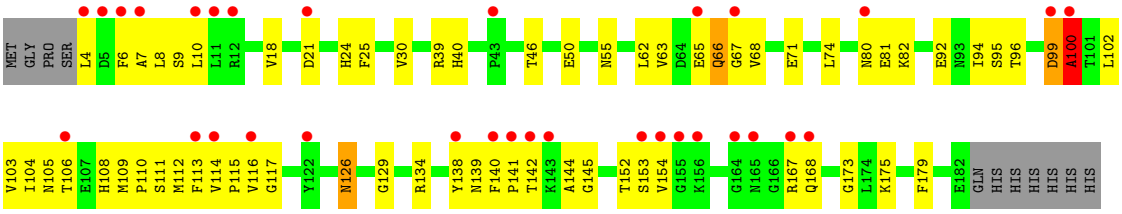
- Molecule 1: 3C protease

Chain A:



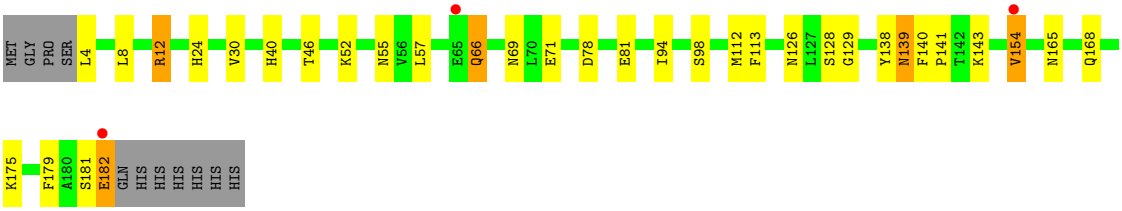
- Molecule 1: 3C protease

Chain B:



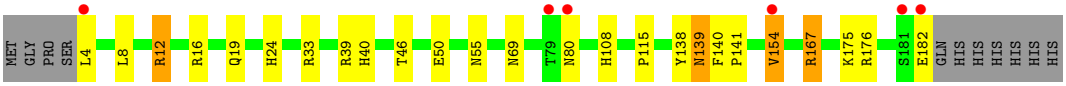
- Molecule 1: 3C protease

Chain C:



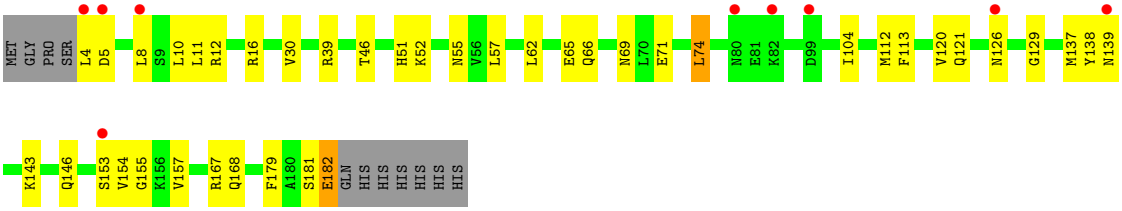
- Molecule 1: 3C protease

Chain D:



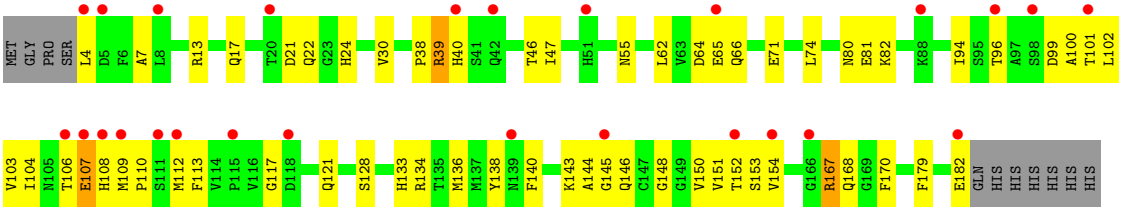
• Molecule 1: 3C protease

Chain E:



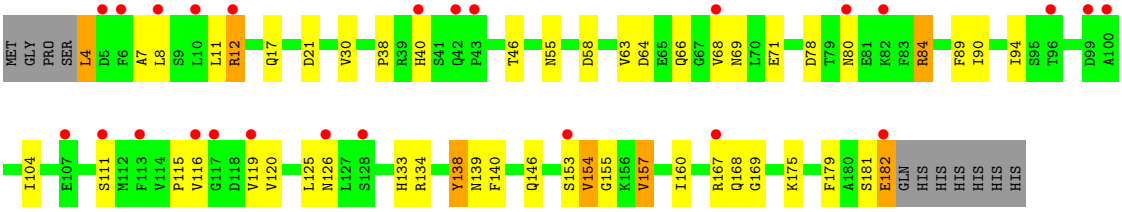
• Molecule 1: 3C protease

Chain F:



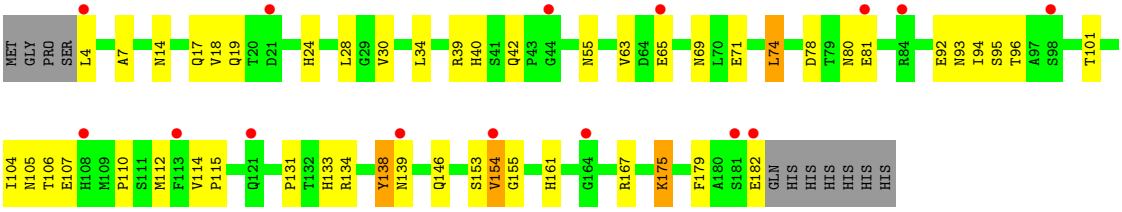
• Molecule 1: 3C protease

Chain G:



• Molecule 1: 3C protease

Chain H:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	41.26Å 82.17Å 97.95Å 89.96° 89.99° 90.13°	Depositor
Resolution (Å)	34.54 – 1.70 34.54 – 1.70	Depositor EDS
% Data completeness (in resolution range)	93.2 (34.54-1.70) 96.5 (34.54-1.70)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	0.05	Depositor
$< I/\sigma(I) >$ [1]	2.99 (at 1.70Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.5_2)	Depositor
R, R_{free}	0.205 , 0.222 0.208 , 0.224	Depositor DCC
R_{free} test set	6840 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å^2)	20.2	Xtriage
Anisotropy	0.129	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.39 , 41.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.021 for h,-k,-l 0.019 for -h,k,-l 0.478 for -h,-k,l	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	12391	wwPDB-VP
Average B, all atoms (Å^2)	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 34.48 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 6.7811e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[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: AG7

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\|>5$	RMSZ	$\#\|Z\|>5$
1	A	0.49	0/1417	0.58	0/1918
1	B	0.50	3/1417 (0.2%)	0.58	0/1918
1	C	0.48	0/1417	0.58	0/1918
1	D	0.35	0/1417	0.55	0/1918
1	E	0.31	0/1417	0.53	0/1918
1	F	0.34	0/1417	0.54	0/1918
1	G	0.36	0/1417	0.51	0/1918
1	H	0.32	0/1417	0.52	0/1918
All	All	0.40	3/11336 (0.0%)	0.55	0/15344

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	92	GLU	CB-CG	-6.18	1.40	1.52
1	B	100	ALA	N-CA	-5.12	1.36	1.46
1	B	100	ALA	CA-CB	-5.06	1.41	1.52

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	1391	0	1404	33	0
1	B	1391	0	1404	90	0
1	C	1391	0	1404	37	0
1	D	1391	0	1404	32	0
1	E	1391	0	1404	54	0
1	F	1391	0	1404	81	1
1	G	1391	0	1404	70	0
1	H	1391	0	1404	68	0
2	A	43	0	40	0	0
2	B	43	0	40	7	0
2	C	43	0	40	2	0
2	D	43	0	40	0	0
2	E	43	0	40	0	0
2	F	43	0	40	3	0
2	G	43	0	40	2	0
2	H	43	0	40	1	0
3	A	124	0	0	21	0
3	B	97	0	0	79	0
3	C	144	0	0	25	0
3	D	137	0	0	22	1
3	E	146	0	0	37	0
3	F	106	0	0	66	1
3	G	73	0	0	49	0
3	H	92	0	0	48	2
All	All	12391	0	11552	473	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 21.

All (473) 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:B:145:GLY:HA2	3:B:481:HOH:O	1.20	1.34
1:B:103:VAL:HG23	3:B:736:HOH:O	1.10	1.28
1:H:101:THR:HA	3:H:502:HOH:O	1.13	1.26
1:G:11:LEU:HD21	3:G:440:HOH:O	1.14	1.25
1:H:14:ASN:HB3	3:H:831:HOH:O	1.14	1.25
1:B:106:THR:HG23	3:B:664:HOH:O	1.10	1.24
1:B:140:PHE:HD2	3:B:292:HOH:O	1.20	1.23
1:B:109:MET:SD	3:B:195:HOH:O	1.94	1.22
1:C:112:MET:SD	3:C:857:HOH:O	1.95	1.21
1:H:17:GLN:HB3	3:H:612:HOH:O	1.39	1.21

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:111:SER:CB	3:G:440:HOH:O	1.85	1.19
1:H:96:THR:HG23	3:H:695:HOH:O	1.42	1.19
1:G:111:SER:HB3	3:G:440:HOH:O	1.40	1.18
1:D:176:ARG:CZ	3:D:855:HOH:O	1.92	1.17
1:B:114:VAL:HG21	3:B:842:HOH:O	1.42	1.16
1:F:151:VAL:C	3:F:309:HOH:O	1.87	1.13
1:F:13:ARG:NH1	3:F:765:HOH:O	1.80	1.12
1:B:103:VAL:N	3:B:736:HOH:O	1.80	1.11
1:B:139:ASN:HB3	3:B:341:HOH:O	1.51	1.11
1:B:106:THR:N	3:B:664:HOH:O	1.84	1.10
1:A:81:GLU:C	3:A:786:HOH:O	1.90	1.10
1:H:110:PRO:HG3	3:H:749:HOH:O	1.50	1.10
1:F:151:VAL:N	3:F:309:HOH:O	1.83	1.08
1:F:108:HIS:ND1	3:F:624:HOH:O	1.86	1.08
1:H:96:THR:N	3:H:695:HOH:O	1.86	1.06
1:D:176:ARG:NE	3:D:855:HOH:O	1.88	1.06
1:B:145:GLY:N	3:B:527:HOH:O	1.86	1.05
1:F:100:ALA:N	3:F:707:HOH:O	1.84	1.05
1:B:25:PHE:CE1	3:B:222:HOH:O	2.08	1.05
1:H:161:HIS:HB2	3:H:479:HOH:O	1.56	1.04
1:F:170:PHE:HB3	3:F:754:HOH:O	1.55	1.03
1:B:139:ASN:ND2	3:B:341:HOH:O	1.88	1.03
1:E:120:VAL:HB	3:E:911:HOH:O	1.56	1.02
1:C:66:GLN:HG3	3:C:688:HOH:O	1.60	1.02
1:F:150:VAL:C	3:F:309:HOH:O	1.97	1.02
1:F:170:PHE:CB	3:F:754:HOH:O	2.04	1.01
1:H:106:THR:HA	3:H:612:HOH:O	1.60	1.01
1:F:133:HIS:ND1	3:F:883:HOH:O	1.90	1.00
1:G:119:VAL:HA	3:G:808:HOH:O	1.60	0.99
1:G:138:TYR:HB3	3:G:808:HOH:O	1.62	0.99
1:E:16:ARG:NE	3:E:633:HOH:O	1.96	0.98
1:H:96:THR:CG2	3:H:695:HOH:O	2.02	0.98
1:H:114:VAL:O	3:H:502:HOH:O	1.80	0.98
1:B:139:ASN:CB	3:B:341:HOH:O	2.06	0.97
1:B:112:MET:CE	3:B:195:HOH:O	2.10	0.97
1:A:93:ASN:OD1	3:A:835:HOH:O	1.83	0.96
1:G:167:ARG:NH1	3:G:558:HOH:O	1.98	0.96
1:A:81:GLU:CB	3:A:786:HOH:O	2.12	0.96
1:F:167:ARG:NE	3:F:379:HOH:O	1.98	0.96
1:A:143:LYS:HE2	3:A:801:HOH:O	1.64	0.96
1:H:94:ILE:O	3:H:740:HOH:O	1.84	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:67:GLY:O	3:B:814:HOH:O	1.82	0.95
1:B:142:THR:HG23	3:B:292:HOH:O	1.65	0.95
2:B:501:AG7:N12	3:B:681:HOH:O	1.99	0.95
1:G:169:GLY:O	3:G:778:HOH:O	1.84	0.94
1:B:167:ARG:O	3:B:556:HOH:O	1.86	0.94
1:G:68:VAL:O	3:G:532:HOH:O	1.85	0.93
1:A:182:GLU:OE2	3:A:737:HOH:O	1.85	0.92
1:H:80:ASN:OD1	3:H:273:HOH:O	1.85	0.92
1:G:63:VAL:CA	3:G:532:HOH:O	2.17	0.92
1:A:81:GLU:HB3	3:A:786:HOH:O	1.69	0.92
1:D:16:ARG:NH2	3:D:631:HOH:O	2.03	0.91
1:G:116:VAL:HA	3:G:594:HOH:O	1.68	0.91
1:A:81:GLU:O	3:A:786:HOH:O	1.86	0.91
1:H:17:GLN:OE1	3:H:365:HOH:O	1.88	0.91
1:F:146:GLN:HG3	3:F:201:HOH:O	1.69	0.91
2:F:501:AG7:H192	3:F:529:HOH:O	1.69	0.91
1:D:16:ARG:NE	3:D:631:HOH:O	2.03	0.91
1:A:121:GLN:NE2	3:A:760:HOH:O	2.02	0.91
1:B:65:GLU:OE2	3:B:877:HOH:O	1.88	0.90
1:F:64:ASP:OD1	3:F:883:HOH:O	1.88	0.90
2:F:501:AG7:O23	3:F:529:HOH:O	1.89	0.90
1:H:42:GLN:NE2	3:H:720:HOH:O	2.02	0.90
1:G:140:PHE:CD1	3:G:594:HOH:O	2.22	0.90
1:F:21:ASP:N	3:F:636:HOH:O	2.06	0.89
1:G:63:VAL:HB	3:G:532:HOH:O	1.71	0.89
1:F:104:ILE:O	3:F:243:HOH:O	1.89	0.89
1:H:107:GLU:O	3:H:749:HOH:O	1.91	0.89
1:B:142:THR:N	3:B:292:HOH:O	2.05	0.89
1:F:100:ALA:HA	3:F:707:HOH:O	1.72	0.89
1:G:58:ASP:OD2	3:G:818:HOH:O	1.91	0.88
1:F:168:GLN:C	3:F:277:HOH:O	2.11	0.87
1:D:139:ASN:OD1	3:D:802:HOH:O	1.91	0.87
1:F:136:MET:O	3:F:754:HOH:O	1.92	0.87
1:G:64:ASP:N	3:G:532:HOH:O	1.85	0.87
1:H:14:ASN:O	3:H:831:HOH:O	1.92	0.87
1:G:11:LEU:CD2	3:G:440:HOH:O	1.87	0.86
1:F:150:VAL:HG12	3:F:309:HOH:O	1.73	0.86
1:E:55:ASN:CB	3:E:592:HOH:O	2.22	0.86
1:F:21:ASP:OD1	3:F:636:HOH:O	1.92	0.86
1:B:113:PHE:CE2	3:B:860:HOH:O	2.27	0.86
1:E:55:ASN:CG	3:E:592:HOH:O	2.13	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:115:PRO:C	3:B:201:HOH:O	2.15	0.85
1:E:51:HIS:CD2	3:E:698:HOH:O	2.30	0.85
1:B:168:GLN:HA	3:B:556:HOH:O	1.76	0.84
2:B:501:AG7:H28	3:B:681:HOH:O	1.75	0.84
1:C:55:ASN:HB2	3:C:796:HOH:O	1.76	0.84
1:A:13:ARG:HG2	3:A:810:HOH:O	1.77	0.84
2:C:501:AG7:H77	3:C:770:HOH:O	1.77	0.84
1:G:115:PRO:O	3:G:594:HOH:O	1.96	0.83
1:C:66:GLN:OE1	3:C:688:HOH:O	1.97	0.83
1:F:152:THR:O	3:F:526:HOH:O	1.97	0.83
1:C:143:LYS:HE2	3:C:367:HOH:O	1.79	0.83
1:B:106:THR:HA	3:B:756:HOH:O	1.79	0.82
1:H:182:GLU:O	3:H:641:HOH:O	1.96	0.82
1:B:25:PHE:HE1	3:B:222:HOH:O	1.52	0.81
1:H:93:ASN:HB3	3:H:397:HOH:O	1.80	0.81
1:H:42:GLN:NE2	3:H:675:HOH:O	2.13	0.81
1:H:94:ILE:C	3:H:740:HOH:O	2.15	0.81
2:B:501:AG7:H192	3:B:527:HOH:O	1.78	0.81
1:B:106:THR:CG2	3:B:664:HOH:O	1.85	0.81
1:B:144:ALA:HA	3:B:527:HOH:O	1.79	0.81
1:H:65:GLU:OE2	3:H:659:HOH:O	1.98	0.80
1:F:170:PHE:CD2	3:F:754:HOH:O	2.33	0.80
1:D:16:ARG:CZ	3:D:631:HOH:O	2.25	0.80
1:F:21:ASP:CG	3:F:636:HOH:O	2.20	0.80
1:G:133:HIS:ND1	3:G:893:HOH:O	2.13	0.80
1:B:25:PHE:O	3:B:745:HOH:O	1.97	0.80
1:F:21:ASP:CA	3:F:636:HOH:O	2.31	0.79
1:F:145:GLY:N	3:F:529:HOH:O	2.01	0.79
2:B:501:AG7:C47	3:B:681:HOH:O	2.29	0.79
1:B:8:LEU:N	3:B:860:HOH:O	2.16	0.78
1:E:12:ARG:CD	3:E:258:HOH:O	2.31	0.78
1:G:21:ASP:OD2	3:G:572:HOH:O	2.00	0.78
1:G:138:TYR:CD1	3:G:778:HOH:O	2.36	0.78
1:C:81:GLU:HB2	3:C:671:HOH:O	1.83	0.77
1:B:115:PRO:CB	3:B:201:HOH:O	2.31	0.77
1:G:58:ASP:CB	3:G:818:HOH:O	2.31	0.77
1:H:93:ASN:CB	3:H:397:HOH:O	2.32	0.77
1:G:111:SER:OG	3:G:440:HOH:O	1.85	0.76
1:A:121:GLN:CD	3:A:760:HOH:O	2.23	0.76
1:E:4:LEU:HA	3:E:489:HOH:O	1.84	0.76
1:F:151:VAL:CA	3:F:309:HOH:O	2.14	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:182:GLU:HB3	3:F:727:HOH:O	1.86	0.76
1:F:17:GLN:NE2	3:F:649:HOH:O	2.17	0.76
1:B:140:PHE:CD2	3:B:292:HOH:O	2.07	0.76
1:B:50:GLU:OE2	3:B:362:HOH:O	2.04	0.75
1:E:16:ARG:HG3	3:E:633:HOH:O	1.86	0.75
1:G:84:ARG:CZ	3:G:660:HOH:O	2.35	0.75
1:C:66:GLN:CG	3:C:688:HOH:O	2.24	0.75
1:C:94:ILE:HG13	1:C:175:LYS:HG3	1.69	0.75
1:F:168:GLN:O	3:F:277:HOH:O	2.05	0.74
1:E:137:MET:O	3:E:911:HOH:O	2.05	0.74
1:G:138:TYR:CG	3:G:778:HOH:O	2.38	0.74
1:B:142:THR:CG2	3:B:292:HOH:O	2.26	0.74
1:B:100:ALA:HA	1:B:152:THR:O	1.87	0.74
1:D:176:ARG:CD	3:D:855:HOH:O	2.33	0.74
1:E:12:ARG:NE	3:E:258:HOH:O	2.21	0.73
1:E:4:LEU:N	3:E:585:HOH:O	2.19	0.73
1:B:95:SER:C	3:B:919:HOH:O	2.27	0.73
1:D:19:GLN:HB3	3:D:838:HOH:O	1.88	0.73
1:G:17:GLN:NE2	3:G:758:HOH:O	2.09	0.73
1:B:25:PHE:CD1	3:B:222:HOH:O	2.33	0.73
1:B:94:ILE:HD13	1:B:173:GLY:HA3	1.70	0.73
1:C:128:SER:CA	3:C:770:HOH:O	2.36	0.73
2:C:501:AG7:O60	3:C:770:HOH:O	2.05	0.73
1:B:115:PRO:CA	3:B:201:HOH:O	2.36	0.73
1:C:139:ASN:OD1	3:C:500:HOH:O	2.06	0.73
1:F:62:LEU:HD21	1:F:74:LEU:HD22	1.71	0.73
1:C:128:SER:N	3:C:770:HOH:O	2.21	0.72
1:G:38:PRO:HD3	3:G:769:HOH:O	1.87	0.72
1:G:89:PHE:HE2	3:G:660:HOH:O	1.73	0.72
1:B:99:ASP:O	1:B:100:ALA:HB3	1.89	0.72
1:F:144:ALA:HA	3:F:529:HOH:O	1.90	0.72
1:G:126:ASN:O	3:G:680:HOH:O	2.07	0.72
1:H:155:GLY:O	3:H:711:HOH:O	2.07	0.72
2:B:501:AG7:O23	3:B:527:HOH:O	2.07	0.72
1:E:55:ASN:HB3	3:E:592:HOH:O	1.86	0.72
1:A:81:GLU:O	3:A:431:HOH:O	2.08	0.71
1:D:8:LEU:HD21	1:H:131:PRO:HG3	1.70	0.71
1:A:181:SER:O	1:A:182:GLU:HG2	1.92	0.70
1:F:140:PHE:O	3:F:277:HOH:O	2.08	0.70
1:H:96:THR:CA	3:H:695:HOH:O	2.30	0.70
1:G:58:ASP:HB3	3:G:818:HOH:O	1.89	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:501:AG7:C04	3:B:681:HOH:O	2.40	0.70
1:C:52:LYS:NZ	3:C:805:HOH:O	2.25	0.69
1:E:16:ARG:CG	3:E:633:HOH:O	2.39	0.69
1:H:24:HIS:HD2	3:H:528:HOH:O	1.74	0.69
1:B:24:HIS:CG	3:B:647:HOH:O	2.46	0.68
1:B:105:ASN:C	3:B:664:HOH:O	2.20	0.68
1:F:22:GLN:NE2	3:F:917:HOH:O	2.12	0.68
1:E:52:LYS:HD3	3:E:759:HOH:O	1.92	0.68
1:F:100:ALA:CA	3:F:707:HOH:O	2.21	0.68
1:F:65:GLU:OE1	3:F:812:HOH:O	2.11	0.68
1:H:4:LEU:HD22	3:H:598:HOH:O	1.94	0.68
1:F:170:PHE:CA	3:F:754:HOH:O	2.32	0.68
1:H:138:TYR:OH	3:H:479:HOH:O	2.07	0.67
1:G:138:TYR:CB	3:G:808:HOH:O	2.31	0.67
1:F:170:PHE:HD2	3:F:754:HOH:O	1.72	0.66
1:B:108:HIS:ND1	3:B:647:HOH:O	2.28	0.66
1:E:52:LYS:HE2	3:E:525:HOH:O	1.95	0.66
1:B:116:VAL:N	3:B:400:HOH:O	2.29	0.66
1:E:51:HIS:NE2	3:E:698:HOH:O	2.28	0.66
1:E:139:ASN:OD1	3:E:345:HOH:O	2.14	0.66
1:C:55:ASN:CB	3:C:796:HOH:O	2.35	0.66
1:F:170:PHE:HA	3:F:754:HOH:O	1.96	0.65
1:C:55:ASN:OD1	3:C:796:HOH:O	2.14	0.65
1:B:112:MET:HE1	3:B:195:HOH:O	1.82	0.65
1:F:81:GLU:C	3:F:792:HOH:O	2.35	0.65
1:D:167:ARG:NH1	3:D:904:HOH:O	2.26	0.65
1:E:5:ASP:N	3:E:302:HOH:O	2.29	0.65
1:F:101:THR:O	3:F:526:HOH:O	2.15	0.65
1:A:16:ARG:CZ	3:A:584:HOH:O	2.45	0.65
1:E:62:LEU:HD21	1:E:74:LEU:HD22	1.79	0.64
1:F:128:SER:CA	3:F:871:HOH:O	2.45	0.64
1:H:155:GLY:HA3	3:H:711:HOH:O	1.97	0.64
1:B:81:GLU:OE1	3:B:888:HOH:O	2.15	0.64
1:B:18:VAL:N	3:B:745:HOH:O	2.04	0.64
1:C:78:ASP:OD2	3:C:796:HOH:O	2.15	0.64
1:E:112:MET:HE1	3:E:859:HOH:O	1.96	0.64
1:B:113:PHE:CZ	3:B:860:HOH:O	2.49	0.64
1:C:40:HIS:HB3	3:C:392:HOH:O	1.98	0.64
1:F:146:GLN:NE2	3:F:709:HOH:O	2.30	0.63
1:B:18:VAL:O	3:B:745:HOH:O	2.15	0.63
1:F:128:SER:HA	3:F:871:HOH:O	1.99	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:13:ARG:C	3:A:584:HOH:O	2.37	0.63
1:E:112:MET:CE	3:E:859:HOH:O	2.45	0.63
1:E:143:LYS:HE2	3:E:260:HOH:O	1.99	0.62
1:G:138:TYR:CA	3:G:808:HOH:O	2.47	0.62
1:B:9:SER:CB	3:B:785:HOH:O	2.48	0.61
1:G:138:TYR:HA	3:G:808:HOH:O	2.00	0.61
1:D:154:VAL:HG13	3:D:715:HOH:O	2.00	0.61
1:G:153:SER:O	1:G:155:GLY:N	2.34	0.61
1:D:182:GLU:N	3:D:233:HOH:O	2.33	0.61
1:A:14:ASN:CA	3:A:584:HOH:O	2.48	0.61
1:D:176:ARG:HD3	3:D:855:HOH:O	1.98	0.61
1:A:14:ASN:HA	3:A:584:HOH:O	2.00	0.61
1:F:94:ILE:CD1	1:F:134:ARG:HB3	2.31	0.61
1:F:152:THR:HG23	3:F:309:HOH:O	2.00	0.61
1:H:63:VAL:O	3:H:457:HOH:O	2.16	0.61
1:A:13:ARG:CG	3:A:810:HOH:O	2.42	0.60
1:G:68:VAL:HG11	1:G:133:HIS:CD2	2.36	0.60
1:E:57:LEU:O	1:G:167:ARG:HG2	2.01	0.60
1:F:108:HIS:CG	3:F:624:HOH:O	2.44	0.60
1:F:146:GLN:CD	3:F:709:HOH:O	2.38	0.60
1:G:84:ARG:NH1	3:G:660:HOH:O	2.32	0.60
1:B:112:MET:HE2	3:B:195:HOH:O	1.86	0.60
1:F:17:GLN:HB3	1:F:106:THR:O	2.01	0.60
1:H:153:SER:O	1:H:155:GLY:N	2.35	0.60
1:B:65:GLU:HB3	3:B:518:HOH:O	2.01	0.60
1:G:90:ILE:HG12	1:G:157:VAL:HG13	1.83	0.60
1:H:101:THR:CA	3:H:502:HOH:O	1.98	0.60
1:B:24:HIS:CD2	3:B:647:HOH:O	2.54	0.59
1:B:68:VAL:HA	3:B:814:HOH:O	2.00	0.59
1:B:96:THR:N	3:B:919:HOH:O	2.35	0.59
1:G:133:HIS:ND1	3:G:395:HOH:O	2.21	0.59
1:D:182:GLU:HG2	3:D:233:HOH:O	2.02	0.59
1:G:133:HIS:CG	3:G:893:HOH:O	2.55	0.59
1:A:13:ARG:O	3:A:584:HOH:O	2.17	0.58
1:A:81:GLU:CG	3:A:786:HOH:O	2.47	0.58
1:E:4:LEU:C	3:E:302:HOH:O	2.42	0.58
1:F:128:SER:N	3:F:871:HOH:O	2.36	0.58
1:E:16:ARG:CD	3:E:633:HOH:O	2.41	0.57
1:A:82:LYS:NZ	3:A:298:HOH:O	2.29	0.57
1:G:63:VAL:HA	3:G:532:HOH:O	1.94	0.57
1:D:4:LEU:HD23	1:H:133:HIS:NE2	2.20	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:161:HIS:CB	3:H:479:HOH:O	2.32	0.57
1:E:126:ASN:HD21	1:E:129:GLY:HA2	1.70	0.57
1:G:138:TYR:CD2	3:G:778:HOH:O	2.58	0.57
1:B:117:GLY:N	3:B:400:HOH:O	1.84	0.57
1:D:33:ARG:NH2	3:D:294:HOH:O	2.37	0.57
1:E:55:ASN:ND2	3:E:592:HOH:O	2.32	0.57
1:F:112:MET:CE	3:F:197:HOH:O	2.53	0.57
1:D:19:GLN:CB	3:D:838:HOH:O	2.49	0.56
1:G:138:TYR:CE1	3:G:778:HOH:O	2.56	0.56
1:H:95:SER:C	3:H:695:HOH:O	2.30	0.56
1:B:103:VAL:CG2	3:B:736:HOH:O	1.89	0.56
1:H:167:ARG:HD3	3:H:464:HOH:O	2.05	0.56
1:D:24:HIS:HD2	3:D:195:HOH:O	1.87	0.56
1:B:100:ALA:O	3:B:400:HOH:O	2.18	0.55
1:C:94:ILE:HG13	1:C:175:LYS:CG	2.35	0.55
1:C:4:LEU:HD21	1:C:113:PHE:HD2	1.72	0.55
1:H:81:GLU:HB2	3:H:406:HOH:O	2.06	0.55
1:B:139:ASN:HA	3:B:556:HOH:O	2.06	0.55
1:E:4:LEU:CA	3:E:489:HOH:O	2.48	0.55
1:E:4:LEU:HD21	1:E:113:PHE:HD2	1.73	0.54
1:C:128:SER:HA	3:C:770:HOH:O	2.06	0.54
1:D:19:GLN:CG	3:D:838:HOH:O	2.55	0.54
1:D:108:HIS:HE1	3:D:304:HOH:O	1.90	0.54
1:F:133:HIS:CG	3:F:883:HOH:O	2.51	0.54
1:B:62:LEU:HD21	1:B:74:LEU:HD22	1.89	0.54
1:G:4:LEU:HD13	1:G:7:ALA:HB3	1.88	0.54
1:D:4:LEU:N	3:D:310:HOH:O	2.41	0.54
1:B:106:THR:CA	3:B:756:HOH:O	2.47	0.53
1:B:141:PRO:HA	3:B:275:HOH:O	2.08	0.53
1:C:57:LEU:O	1:H:167:ARG:HG2	2.09	0.53
1:B:65:GLU:CB	3:B:518:HOH:O	2.57	0.53
1:G:104:ILE:HD13	1:G:146:GLN:HG2	1.89	0.53
1:D:46:THR:HG22	1:D:55:ASN:HD22	1.74	0.53
1:G:8:LEU:O	1:G:12:ARG:HG3	2.09	0.53
1:C:8:LEU:O	1:C:12:ARG:HG3	2.09	0.53
1:C:165:ASN:ND2	3:C:775:HOH:O	2.41	0.53
1:D:8:LEU:O	1:D:12:ARG:HG2	2.08	0.53
1:A:14:ASN:N	3:A:584:HOH:O	2.41	0.52
1:H:4:LEU:CD2	3:H:598:HOH:O	2.53	0.52
1:B:142:THR:CA	3:B:292:HOH:O	2.52	0.52
1:E:11:LEU:HD22	1:E:113:PHE:CE1	2.44	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:94:ILE:CD1	1:H:134:ARG:HB3	2.39	0.52
1:H:115:PRO:HA	3:H:502:HOH:O	2.10	0.52
1:H:104:ILE:HD13	1:H:146:GLN:HG2	1.91	0.52
1:E:120:VAL:HG22	1:F:81:GLU:HG2	1.91	0.52
1:G:46:THR:HG22	1:G:55:ASN:HD22	1.73	0.52
1:G:94:ILE:HG13	1:G:175:LYS:HG3	1.91	0.52
1:E:4:LEU:N	3:E:489:HOH:O	2.42	0.51
1:E:5:ASP:CA	3:E:302:HOH:O	2.58	0.51
1:G:55:ASN:HB2	1:G:78:ASP:HB3	1.93	0.51
1:B:46:THR:HG22	1:B:55:ASN:HD22	1.76	0.51
1:F:143:LYS:HB2	3:F:201:HOH:O	2.11	0.51
1:H:55:ASN:HB2	1:H:78:ASP:HB3	1.93	0.51
1:C:98:SER:OG	3:C:656:HOH:O	1.91	0.51
1:E:112:MET:HG3	3:E:546:HOH:O	2.11	0.51
1:E:8:LEU:O	1:E:12:ARG:HG3	2.11	0.50
1:B:21:ASP:HB2	3:B:619:HOH:O	2.10	0.50
1:B:4:LEU:C	1:B:6:PHE:H	2.14	0.50
1:F:103:VAL:CG1	3:F:243:HOH:O	2.60	0.50
1:F:24:HIS:CG	3:F:624:HOH:O	2.64	0.50
1:F:47:ILE:HG22	3:F:405:HOH:O	2.11	0.50
1:G:138:TYR:N	3:G:778:HOH:O	2.37	0.50
1:E:167:ARG:HG3	1:E:168:GLN:HG3	1.94	0.49
1:E:5:ASP:HA	3:E:302:HOH:O	2.11	0.49
1:E:65:GLU:CG	3:E:402:HOH:O	2.60	0.49
2:G:501:AG7:C2	3:G:680:HOH:O	2.61	0.49
1:H:4:LEU:CD1	1:H:7:ALA:HB3	2.42	0.49
1:E:12:ARG:HD2	3:E:258:HOH:O	2.04	0.49
1:E:181:SER:O	1:E:182:GLU:C	2.50	0.49
1:G:4:LEU:O	3:G:223:HOH:O	2.20	0.49
1:G:30:VAL:HG21	1:G:179:PHE:CE1	2.48	0.49
1:H:19:GLN:HG2	1:H:24:HIS:CD2	2.48	0.49
1:B:99:ASP:O	1:B:100:ALA:O	2.29	0.49
1:D:40:HIS:HD2	3:D:216:HOH:O	1.95	0.49
1:A:88:LYS:HE3	1:A:89:PHE:CZ	2.47	0.49
1:B:94:ILE:HD12	1:B:134:ARG:HB3	1.95	0.49
1:G:69:ASN:ND2	1:G:71:GLU:H	2.10	0.49
1:C:181:SER:O	1:C:182:GLU:C	2.51	0.49
1:E:104:ILE:HD13	1:E:146:GLN:HG2	1.95	0.49
1:G:63:VAL:CB	3:G:532:HOH:O	2.28	0.49
1:H:14:ASN:C	3:H:831:HOH:O	2.37	0.48
1:C:30:VAL:HG21	1:C:179:PHE:CE1	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:141:PRO:HB2	3:C:701:HOH:O	2.13	0.48
1:B:116:VAL:N	3:B:201:HOH:O	2.41	0.48
1:F:82:LYS:N	3:F:792:HOH:O	2.46	0.48
1:F:99:ASP:HB3	3:F:707:HOH:O	2.14	0.48
1:G:160:ILE:HD12	3:G:811:HOH:O	2.13	0.48
1:G:140:PHE:CE1	3:G:594:HOH:O	2.59	0.48
1:A:13:ARG:CB	3:A:810:HOH:O	2.61	0.48
1:B:94:ILE:CD1	1:B:134:ARG:HB3	2.43	0.48
1:H:161:HIS:CG	3:H:479:HOH:O	2.64	0.48
1:B:9:SER:HB3	3:B:785:HOH:O	2.09	0.48
1:B:113:PHE:HE2	3:B:860:HOH:O	1.79	0.48
1:F:7:ALA:HB3	1:F:113:PHE:HE2	1.77	0.48
1:F:38:PRO:HB2	1:F:40:HIS:CE1	2.49	0.48
1:G:94:ILE:CD1	1:G:134:ARG:HB3	2.43	0.48
1:A:8:LEU:O	1:A:12:ARG:HG2	2.14	0.48
1:D:115:PRO:HD2	3:D:863:HOH:O	2.13	0.48
1:F:24:HIS:CD2	3:F:301:HOH:O	2.66	0.48
1:H:28:LEU:HD12	3:H:831:HOH:O	2.13	0.48
1:G:71:GLU:HG3	1:G:71:GLU:O	2.13	0.47
1:H:14:ASN:CB	3:H:831:HOH:O	1.99	0.47
1:H:153:SER:O	1:H:154:VAL:C	2.51	0.47
1:G:140:PHE:CG	3:G:594:HOH:O	2.62	0.47
1:B:144:ALA:CA	3:B:527:HOH:O	2.43	0.47
1:F:46:THR:HG22	1:F:55:ASN:HD22	1.80	0.47
1:B:7:ALA:HB3	3:B:311:HOH:O	2.15	0.47
1:C:140:PHE:CD2	1:C:141:PRO:HD2	2.50	0.47
1:D:19:GLN:HG2	3:D:838:HOH:O	2.14	0.47
1:B:153:SER:OG	1:B:154:VAL:N	2.48	0.47
1:E:69:ASN:ND2	1:E:71:GLU:H	2.12	0.47
2:F:501:AG7:C19	3:F:529:HOH:O	2.45	0.47
1:H:34:LEU:HD11	1:H:74:LEU:HG	1.97	0.47
1:B:102:LEU:HG	1:B:104:ILE:HD11	1.97	0.46
1:H:69:ASN:ND2	1:H:71:GLU:H	2.12	0.46
1:B:66:GLN:OE1	3:B:518:HOH:O	2.20	0.46
1:G:55:ASN:HB2	1:G:78:ASP:CB	2.45	0.46
1:G:139:ASN:ND2	1:G:168:GLN:HG2	2.30	0.46
1:G:181:SER:O	1:G:182:GLU:C	2.53	0.46
1:H:101:THR:HG23	3:H:502:HOH:O	2.15	0.46
1:D:140:PHE:CG	1:D:141:PRO:HD2	2.51	0.46
1:H:17:GLN:HA	1:H:105:ASN:O	2.16	0.46
1:B:8:LEU:HB2	3:B:860:HOH:O	2.14	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:8:LEU:O	1:D:12:ARG:CG	2.64	0.46
1:F:24:HIS:CD2	3:F:624:HOH:O	2.67	0.46
1:F:103:VAL:HG13	3:F:243:HOH:O	2.16	0.46
1:A:69:ASN:ND2	1:A:71:GLU:H	2.14	0.46
1:H:55:ASN:HB2	1:H:78:ASP:CB	2.46	0.46
1:A:62:LEU:HD21	1:A:74:LEU:HG	1.97	0.46
1:F:104:ILE:N	3:F:243:HOH:O	2.48	0.46
1:H:106:THR:CA	3:H:612:HOH:O	2.39	0.46
1:C:94:ILE:CG1	1:C:175:LYS:HG3	2.43	0.45
1:F:30:VAL:HG21	1:F:179:PHE:CE1	2.51	0.45
1:H:30:VAL:HG21	1:H:179:PHE:CE1	2.51	0.45
1:A:8:LEU:O	1:A:12:ARG:CG	2.64	0.45
1:B:7:ALA:HB3	1:B:113:PHE:HE2	1.82	0.45
1:H:17:GLN:CB	3:H:612:HOH:O	2.23	0.45
1:C:69:ASN:ND2	1:C:71:GLU:H	2.14	0.45
1:E:112:MET:HB3	1:E:112:MET:HE2	1.72	0.45
1:F:153:SER:HA	3:F:707:HOH:O	2.16	0.45
1:F:101:THR:HB	3:F:526:HOH:O	2.17	0.45
1:G:154:VAL:HG23	1:G:154:VAL:O	2.15	0.45
1:B:4:LEU:CD1	3:B:311:HOH:O	2.65	0.45
1:C:8:LEU:O	1:C:8:LEU:HD12	2.17	0.45
1:G:125:LEU:CD1	3:G:680:HOH:O	2.66	0.44
1:E:46:THR:O	3:E:217:HOH:O	2.21	0.44
1:H:92:GLU:O	1:H:175:LYS:HG2	2.17	0.44
1:F:106:THR:O	1:F:107:GLU:HB2	2.17	0.44
1:H:69:ASN:HB2	3:H:672:HOH:O	2.18	0.44
1:H:154:VAL:O	1:H:154:VAL:HG23	2.17	0.44
1:B:10:LEU:N	3:B:785:HOH:O	2.50	0.44
1:A:112:MET:HE3	1:A:112:MET:HB3	1.56	0.44
1:A:153:SER:O	1:A:155:GLY:N	2.51	0.44
2:B:501:AG7:H41	3:B:681:HOH:O	2.18	0.44
1:C:81:GLU:CB	3:C:671:HOH:O	2.55	0.44
1:F:102:LEU:HG	1:F:104:ILE:HD11	2.00	0.44
1:F:21:ASP:HA	3:F:636:HOH:O	2.07	0.43
1:F:153:SER:OG	1:F:154:VAL:N	2.49	0.43
1:D:39:ARG:HD3	1:D:69:ASN:ND2	2.33	0.43
1:F:81:GLU:CB	3:F:792:HOH:O	2.65	0.43
1:F:38:PRO:HD3	1:F:148:GLY:HA2	1.99	0.43
1:G:133:HIS:CE1	3:G:893:HOH:O	2.62	0.43
1:E:52:LYS:CE	3:E:525:HOH:O	2.60	0.43
1:G:11:LEU:HD21	1:G:111:SER:OG	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:71:GLU:HG3	1:B:71:GLU:O	2.19	0.43
1:E:120:VAL:HG12	1:E:121:GLN:O	2.19	0.43
1:G:4:LEU:CD1	1:G:7:ALA:HB3	2.47	0.43
1:C:126:ASN:HD21	1:C:129:GLY:HA2	1.83	0.43
1:G:126:ASN:C	3:G:680:HOH:O	2.54	0.43
1:B:82:LYS:HD3	3:B:438:HOH:O	2.19	0.43
1:H:107:GLU:C	3:H:749:HOH:O	2.47	0.43
1:H:114:VAL:C	3:H:502:HOH:O	2.45	0.43
1:A:10:LEU:HD11	1:A:157:VAL:HG22	2.00	0.42
1:B:104:ILE:N	1:B:104:ILE:HD12	2.34	0.42
1:A:140:PHE:CG	1:A:141:PRO:HD2	2.54	0.42
1:B:40:HIS:CE1	3:B:681:HOH:O	2.71	0.42
1:B:63:VAL:HB	1:B:67:GLY:HA2	2.00	0.42
1:B:110:PRO:O	1:B:111:SER:C	2.56	0.42
1:E:10:LEU:HD11	1:E:157:VAL:HG22	2.01	0.42
1:F:109:MET:N	1:F:110:PRO:HD3	2.35	0.42
1:H:139:ASN:ND2	3:H:198:HOH:O	2.52	0.42
1:A:39:ARG:HD3	1:A:69:ASN:ND2	2.34	0.42
1:E:46:THR:HG22	1:E:55:ASN:HD22	1.83	0.42
1:F:4:LEU:O	1:F:4:LEU:HG	2.20	0.42
1:H:93:ASN:OD1	3:H:397:HOH:O	2.21	0.42
1:B:108:HIS:CG	3:B:647:HOH:O	2.72	0.42
1:G:66:GLN:HB2	1:G:68:VAL:HG23	2.01	0.42
1:G:120:VAL:HG22	3:G:474:HOH:O	2.18	0.42
1:A:109:MET:HE1	1:A:146:GLN:HE21	1.85	0.41
1:B:115:PRO:HB3	3:B:201:HOH:O	2.12	0.41
1:E:153:SER:O	1:E:155:GLY:N	2.54	0.41
1:C:24:HIS:HD2	3:C:193:HOH:O	2.02	0.41
1:E:65:GLU:HG3	3:E:402:HOH:O	2.21	0.41
1:F:39:ARG:NH2	3:F:601:HOH:O	2.37	0.41
1:F:7:ALA:CB	1:F:113:PHE:CE2	3.04	0.41
1:F:71:GLU:O	1:F:71:GLU:HG3	2.20	0.41
1:F:100:ALA:HB3	1:F:117:GLY:O	2.21	0.41
1:G:153:SER:O	1:G:154:VAL:C	2.59	0.41
1:C:40:HIS:HD2	3:C:226:HOH:O	2.04	0.41
1:G:40:HIS:ND1	1:G:71:GLU:OE2	2.52	0.41
1:B:126:ASN:HD21	1:B:129:GLY:HA2	1.85	0.41
1:D:8:LEU:HD21	1:H:131:PRO:CG	2.44	0.41
1:D:39:ARG:HD3	1:D:69:ASN:HD21	1.86	0.41
1:E:112:MET:HE3	3:E:859:HOH:O	2.14	0.41
1:C:139:ASN:ND2	1:C:168:GLN:HG2	2.36	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:8:LEU:HD12	1:D:8:LEU:HA	1.94	0.40
1:E:30:VAL:HG21	1:E:179:PHE:CE1	2.56	0.40
1:E:137:MET:HB3	3:E:911:HOH:O	2.21	0.40
1:F:96:THR:CG2	1:F:121:GLN:HG2	2.51	0.40
1:H:104:ILE:HB	1:H:112:MET:HB3	2.04	0.40
1:C:46:THR:HG22	1:C:55:ASN:HD22	1.85	0.40
1:E:52:LYS:NZ	3:E:303:HOH:O	2.22	0.40
1:F:133:HIS:CB	3:F:883:HOH:O	2.69	0.40
1:B:30:VAL:HG21	1:B:179:PHE:CE1	2.56	0.40
1:C:128:SER:OG	3:C:770:HOH:O	2.19	0.40
2:G:501:AG7:H8	3:G:680:HOH:O	2.20	0.40
1:H:40:HIS:HD1	2:H:501:AG7:H30	1.87	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:F:182:GLU:OE1	3:H:273:HOH:O[1_556]	1.95	0.25
3:D:550:HOH:O	3:D:634:HOH:O[1_455]	2.08	0.12
3:F:884:HOH:O	3:H:776:HOH:O[1_556]	2.18	0.02

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	177/190 (93%)	170 (96%)	6 (3%)	1 (1%)	25 11
1	B	177/190 (93%)	163 (92%)	13 (7%)	1 (1%)	25 11
1	C	177/190 (93%)	171 (97%)	5 (3%)	1 (1%)	25 11
1	D	177/190 (93%)	172 (97%)	4 (2%)	1 (1%)	25 11
1	E	177/190 (93%)	171 (97%)	5 (3%)	1 (1%)	25 11

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	F	177/190 (93%)	166 (94%)	10 (6%)	1 (1%)	25	11
1	G	177/190 (93%)	171 (97%)	5 (3%)	1 (1%)	25	11
1	H	177/190 (93%)	170 (96%)	6 (3%)	1 (1%)	25	11
All	All	1416/1520 (93%)	1354 (96%)	54 (4%)	8 (1%)	25	11

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	154	VAL
1	D	154	VAL
1	E	154	VAL
1	F	107	GLU
1	G	154	VAL
1	H	154	VAL
1	C	154	VAL
1	B	100	ALA

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	154/164 (94%)	150 (97%)	4 (3%)	46	28
1	B	154/164 (94%)	147 (96%)	7 (4%)	27	10
1	C	154/164 (94%)	148 (96%)	6 (4%)	32	13
1	D	154/164 (94%)	147 (96%)	7 (4%)	27	10
1	E	154/164 (94%)	149 (97%)	5 (3%)	39	20
1	F	154/164 (94%)	149 (97%)	5 (3%)	39	20
1	G	154/164 (94%)	147 (96%)	7 (4%)	27	10
1	H	154/164 (94%)	149 (97%)	5 (3%)	39	20
All	All	1232/1312 (94%)	1186 (96%)	46 (4%)	34	15

All (46) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	12	ARG
1	A	66	GLN
1	A	80	ASN
1	A	138	TYR
1	B	39	ARG
1	B	66	GLN
1	B	80	ASN
1	B	99	ASP
1	B	126	ASN
1	B	138	TYR
1	B	175	LYS
1	C	12	ARG
1	C	66	GLN
1	C	138	TYR
1	C	139	ASN
1	C	154	VAL
1	C	182	GLU
1	D	12	ARG
1	D	50	GLU
1	D	80	ASN
1	D	138	TYR
1	D	139	ASN
1	D	167	ARG
1	D	175	LYS
1	E	39	ARG
1	E	66	GLN
1	E	74	LEU
1	E	138	TYR
1	E	182	GLU
1	F	39	ARG
1	F	66	GLN
1	F	80	ASN
1	F	138	TYR
1	F	167	ARG
1	G	4	LEU
1	G	12	ARG
1	G	80	ASN
1	G	84	ARG
1	G	138	TYR
1	G	157	VAL
1	G	182	GLU
1	H	18	VAL
1	H	39	ARG

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Mol	Chain	Res	Type
1	H	74	LEU
1	H	138	TYR
1	H	175	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (47) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	22	GLN
1	A	69	ASN
1	A	93	ASN
1	A	126	ASN
1	A	139	ASN
1	A	146	GLN
1	B	55	ASN
1	B	66	GLN
1	B	69	ASN
1	B	121	GLN
1	B	126	ASN
1	B	168	GLN
1	C	22	GLN
1	C	24	HIS
1	C	55	ASN
1	C	66	GLN
1	C	69	ASN
1	C	93	ASN
1	C	126	ASN
1	C	139	ASN
1	D	24	HIS
1	D	40	HIS
1	D	55	ASN
1	D	66	GLN
1	D	69	ASN
1	D	108	HIS
1	D	126	ASN
1	E	22	GLN
1	E	55	ASN
1	E	69	ASN
1	E	126	ASN
1	F	24	HIS
1	F	55	ASN
1	F	69	ASN
1	F	126	ASN

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Mol	Chain	Res	Type
1	F	139	ASN
1	G	19	GLN
1	G	51	HIS
1	G	55	ASN
1	G	69	ASN
1	G	139	ASN
1	H	22	GLN
1	H	24	HIS
1	H	55	ASN
1	H	69	ASN
1	H	93	ASN
1	H	126	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

8 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	AG7	D	501	1	42,45,45	3.93	12 (28%)	49,61,61	1.80	11 (22%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	AG7	F	501	1	42,45,45	3.97	13 (30%)	49,61,61	1.88	10 (20%)
2	AG7	A	501	1	42,45,45	3.92	12 (28%)	49,61,61	1.83	10 (20%)
2	AG7	G	501	1	42,45,45	3.99	13 (30%)	49,61,61	1.77	12 (24%)
2	AG7	B	501	1	42,45,45	3.96	13 (30%)	49,61,61	1.84	11 (22%)
2	AG7	H	501	1	42,45,45	3.95	13 (30%)	49,61,61	1.84	12 (24%)
2	AG7	E	501	1	42,45,45	3.90	11 (26%)	49,61,61	1.92	15 (30%)
2	AG7	C	501	1	42,45,45	3.94	12 (28%)	49,61,61	1.88	13 (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	AG7	D	501	1	-	2/40/54/54	0/3/3/3
2	AG7	F	501	1	-	4/40/54/54	0/3/3/3
2	AG7	A	501	1	-	2/40/54/54	0/3/3/3
2	AG7	G	501	1	-	2/40/54/54	0/3/3/3
2	AG7	B	501	1	-	1/40/54/54	0/3/3/3
2	AG7	H	501	1	-	3/40/54/54	0/3/3/3
2	AG7	E	501	1	-	5/40/54/54	0/3/3/3
2	AG7	C	501	1	-	4/40/54/54	0/3/3/3

All (99) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	501	AG7	C16-N17	17.35	1.52	1.33
2	C	501	AG7	C16-N17	17.24	1.52	1.33
2	B	501	AG7	C16-N17	17.21	1.52	1.33
2	F	501	AG7	C16-N17	17.18	1.51	1.33
2	A	501	AG7	C16-N17	17.16	1.51	1.33
2	G	501	AG7	C16-N17	17.11	1.51	1.33
2	E	501	AG7	C16-N17	17.02	1.51	1.33
2	H	501	AG7	C16-N17	16.97	1.51	1.33
2	B	501	AG7	C2-C1	8.88	1.55	1.39
2	F	501	AG7	C2-C1	8.87	1.55	1.39
2	H	501	AG7	C2-C1	8.77	1.55	1.39
2	G	501	AG7	C2-C1	8.70	1.55	1.39
2	A	501	AG7	C2-C1	8.70	1.55	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	501	AG7	C2-C1	8.67	1.55	1.39
2	C	501	AG7	C2-C1	8.65	1.55	1.39
2	E	501	AG7	C2-C1	8.47	1.55	1.39
2	G	501	AG7	O18-C16	7.32	1.38	1.23
2	C	501	AG7	O18-C16	7.17	1.37	1.23
2	H	501	AG7	O18-C16	7.09	1.37	1.23
2	E	501	AG7	O18-C16	6.98	1.37	1.23
2	G	501	AG7	C10-C09	6.97	1.50	1.37
2	F	501	AG7	C10-C09	6.96	1.50	1.37
2	D	501	AG7	O18-C16	6.92	1.37	1.23
2	D	501	AG7	C10-C09	6.90	1.50	1.37
2	H	501	AG7	C10-C09	6.88	1.50	1.37
2	B	501	AG7	C10-C09	6.87	1.50	1.37
2	C	501	AG7	C10-C09	6.84	1.50	1.37
2	E	501	AG7	C10-C09	6.82	1.50	1.37
2	A	501	AG7	C10-C09	6.78	1.50	1.37
2	F	501	AG7	O18-C16	6.77	1.36	1.23
2	A	501	AG7	O18-C16	6.72	1.36	1.23
2	B	501	AG7	O18-C16	6.66	1.36	1.23
2	H	501	AG7	C47-N12	5.96	1.47	1.34
2	G	501	AG7	C47-N12	5.94	1.47	1.34
2	G	501	AG7	C08-C07	5.93	1.49	1.38
2	F	501	AG7	C08-C07	5.91	1.49	1.38
2	B	501	AG7	C47-N12	5.85	1.46	1.34
2	F	501	AG7	C47-N12	5.85	1.46	1.34
2	C	501	AG7	C08-C07	5.83	1.49	1.38
2	E	501	AG7	C08-C07	5.82	1.49	1.38
2	B	501	AG7	C08-C07	5.81	1.49	1.38
2	H	501	AG7	C08-C07	5.76	1.49	1.38
2	A	501	AG7	C47-N12	5.69	1.46	1.34
2	C	501	AG7	C47-N12	5.61	1.46	1.34
2	E	501	AG7	C47-N12	5.59	1.46	1.34
2	D	501	AG7	C47-N12	5.53	1.46	1.34
2	A	501	AG7	C08-C07	5.49	1.48	1.38
2	D	501	AG7	C08-C07	5.36	1.48	1.38
2	B	501	AG7	C59-N58	5.23	1.45	1.34
2	F	501	AG7	C59-N58	5.16	1.45	1.34
2	E	501	AG7	C59-N58	5.15	1.45	1.34
2	A	501	AG7	C59-N58	5.06	1.45	1.34
2	H	501	AG7	C59-N58	5.05	1.45	1.34
2	G	501	AG7	C59-N58	5.02	1.45	1.34
2	C	501	AG7	C59-N58	4.96	1.45	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	501	AG7	C59-N58	4.95	1.44	1.34
2	G	501	AG7	C11-C10	4.89	1.47	1.38
2	F	501	AG7	C11-C10	4.83	1.47	1.38
2	B	501	AG7	C11-C10	4.74	1.47	1.38
2	H	501	AG7	C11-C10	4.71	1.47	1.38
2	D	501	AG7	C11-C10	4.63	1.47	1.38
2	A	501	AG7	C11-C10	4.61	1.47	1.38
2	C	501	AG7	C11-C10	4.59	1.47	1.38
2	E	501	AG7	C11-C10	4.54	1.47	1.38
2	G	501	AG7	C07-C06	4.43	1.48	1.38
2	F	501	AG7	C2-C3	4.42	1.45	1.39
2	A	501	AG7	C07-C06	4.41	1.48	1.38
2	B	501	AG7	C07-C06	4.38	1.48	1.38
2	B	501	AG7	C2-C3	4.36	1.45	1.39
2	H	501	AG7	C07-C06	4.36	1.48	1.38
2	C	501	AG7	C07-C06	4.33	1.48	1.38
2	D	501	AG7	C07-C06	4.33	1.48	1.38
2	F	501	AG7	C07-C06	4.32	1.48	1.38
2	A	501	AG7	C2-C3	4.31	1.45	1.39
2	G	501	AG7	C2-C3	4.26	1.45	1.39
2	D	501	AG7	C2-C3	4.23	1.45	1.39
2	H	501	AG7	C2-C3	4.19	1.45	1.39
2	E	501	AG7	C07-C06	4.16	1.47	1.38
2	E	501	AG7	C2-C3	4.10	1.45	1.39
2	C	501	AG7	C2-C3	4.06	1.45	1.39
2	H	501	AG7	C1-N5	2.62	1.38	1.33
2	C	501	AG7	C1-N5	2.53	1.37	1.33
2	G	501	AG7	C1-N5	2.49	1.37	1.33
2	E	501	AG7	C1-N5	2.44	1.37	1.33
2	H	501	AG7	C83-N17	2.37	1.51	1.46
2	A	501	AG7	C1-N5	2.33	1.37	1.33
2	G	501	AG7	C83-N17	2.31	1.51	1.46
2	D	501	AG7	C1-N5	2.29	1.37	1.33
2	F	501	AG7	C83-N17	2.29	1.51	1.46
2	A	501	AG7	C83-N17	2.28	1.51	1.46
2	B	501	AG7	C83-N17	2.28	1.51	1.46
2	B	501	AG7	C1-N5	2.26	1.37	1.33
2	D	501	AG7	C83-N17	2.20	1.50	1.46
2	H	501	AG7	C4-C3	2.16	1.51	1.48
2	F	501	AG7	C1-N5	2.15	1.37	1.33
2	G	501	AG7	C4-C3	2.06	1.51	1.48
2	B	501	AG7	C15-C16	2.05	1.54	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	501	AG7	C83-N17	2.04	1.50	1.46
2	F	501	AG7	C4-C3	2.00	1.50	1.48

All (94) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	F	501	AG7	O18-C16-C15	-5.76	119.46	126.23
2	H	501	AG7	O18-C16-C15	-5.37	119.92	126.23
2	C	501	AG7	O18-C16-C15	-5.32	119.98	126.23
2	B	501	AG7	O18-C16-C15	-5.25	120.06	126.23
2	E	501	AG7	O18-C16-C15	-5.23	120.09	126.23
2	A	501	AG7	O18-C16-C15	-5.11	120.22	126.23
2	D	501	AG7	O18-C16-C15	-5.02	120.33	126.23
2	G	501	AG7	O18-C16-C15	-4.88	120.50	126.23
2	A	501	AG7	O18-C16-N17	-4.60	119.16	125.54
2	A	501	AG7	C83-N17-C16	-4.34	105.32	113.84
2	D	501	AG7	C83-N17-C16	-4.25	105.49	113.84
2	H	501	AG7	C83-N17-C16	-4.24	105.52	113.84
2	E	501	AG7	O18-C16-N17	-4.21	119.70	125.54
2	D	501	AG7	O18-C16-N17	-4.18	119.74	125.54
2	G	501	AG7	C83-N17-C16	-4.18	105.64	113.84
2	F	501	AG7	O18-C16-N17	-4.09	119.86	125.54
2	B	501	AG7	O18-C16-N17	-4.07	119.90	125.54
2	A	501	AG7	C78-C57-C01	3.77	115.85	110.89
2	C	501	AG7	O18-C16-N17	-3.75	120.34	125.54
2	F	501	AG7	C84-C15-C16	3.69	107.68	102.88
2	C	501	AG7	C84-C15-C16	3.63	107.60	102.88
2	B	501	AG7	C83-N17-C16	-3.59	106.79	113.84
2	C	501	AG7	C83-N17-C16	-3.55	106.87	113.84
2	B	501	AG7	C84-C15-C16	3.52	107.46	102.88
2	E	501	AG7	C83-N17-C16	-3.52	106.93	113.84
2	F	501	AG7	C02-C04-C47	3.49	114.83	109.77
2	C	501	AG7	C78-C57-C01	3.45	115.42	110.89
2	F	501	AG7	C83-N17-C16	-3.41	107.14	113.84
2	F	501	AG7	C84-C83-N17	3.40	108.42	103.43
2	D	501	AG7	C78-C57-C01	3.33	115.27	110.89
2	E	501	AG7	C84-C15-C16	3.26	107.12	102.88
2	H	501	AG7	C02-C04-C47	3.26	114.49	109.77
2	D	501	AG7	C84-C15-C16	3.25	107.11	102.88
2	E	501	AG7	C78-C57-C01	3.24	115.15	110.89
2	D	501	AG7	C14-C15-C16	3.07	119.64	112.89
2	A	501	AG7	C84-C15-C16	3.04	106.83	102.88

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	501	AG7	C14-C15-C16	3.04	119.57	112.89
2	G	501	AG7	C84-C83-N17	3.03	107.86	103.43
2	E	501	AG7	O22-C21-C20	2.99	121.28	111.91
2	B	501	AG7	C19-C13-N12	2.96	114.71	110.54
2	B	501	AG7	C84-C83-N17	2.95	107.75	103.43
2	G	501	AG7	C02-C04-C47	2.95	114.03	109.77
2	H	501	AG7	C84-C83-N17	2.93	107.73	103.43
2	C	501	AG7	O22-C21-C20	2.90	121.02	111.91
2	C	501	AG7	C14-C15-C16	2.87	119.19	112.89
2	E	501	AG7	C14-C15-C16	2.85	119.15	112.89
2	B	501	AG7	C02-C04-C47	2.84	113.89	109.77
2	G	501	AG7	O18-C16-N17	-2.83	121.61	125.54
2	H	501	AG7	C1-C59-N58	2.80	120.40	115.20
2	F	501	AG7	C19-C13-N12	2.77	114.45	110.54
2	H	501	AG7	O22-C21-C20	2.76	120.56	111.91
2	F	501	AG7	C14-C15-C16	2.75	118.93	112.89
2	E	501	AG7	O22-C50-C53	2.74	118.49	108.42
2	C	501	AG7	O22-C50-C53	2.74	118.47	108.42
2	A	501	AG7	C02-C04-C47	2.73	113.73	109.77
2	E	501	AG7	C13-N12-C47	-2.72	118.86	123.20
2	D	501	AG7	O22-C21-C20	2.69	120.35	111.91
2	B	501	AG7	C78-C57-C01	2.68	114.41	110.89
2	G	501	AG7	C14-C15-C16	2.65	118.71	112.89
2	G	501	AG7	O22-C21-C20	2.63	120.17	111.91
2	H	501	AG7	O48-C47-C04	-2.63	118.70	122.12
2	A	501	AG7	O22-C21-C20	2.61	120.10	111.91
2	C	501	AG7	C05-C04-C02	2.61	116.83	111.10
2	E	501	AG7	C1-C59-N58	2.57	119.97	115.20
2	H	501	AG7	O22-C50-C53	2.54	117.76	108.42
2	H	501	AG7	O18-C16-N17	-2.53	122.03	125.54
2	D	501	AG7	C1-C59-N58	2.52	119.88	115.20
2	E	501	AG7	C02-C04-C47	2.51	113.40	109.77
2	G	501	AG7	O22-C50-C53	2.48	117.51	108.42
2	B	501	AG7	O22-C21-C20	2.45	119.58	111.91
2	A	501	AG7	C84-C83-N17	2.44	107.00	103.43
2	G	501	AG7	O48-C47-C04	-2.42	118.97	122.12
2	H	501	AG7	C14-C15-C16	2.41	118.19	112.89
2	D	501	AG7	C02-C04-C47	2.39	113.24	109.77
2	B	501	AG7	O22-C50-C53	2.39	117.19	108.42
2	A	501	AG7	O22-C50-C53	2.37	117.14	108.42
2	C	501	AG7	C84-C83-N17	2.35	106.87	103.43
2	E	501	AG7	C05-C04-C02	2.34	116.25	111.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	501	AG7	C84-C83-N17	2.32	106.83	103.43
2	G	501	AG7	C1-C59-N58	2.30	119.47	115.20
2	D	501	AG7	O22-C50-C53	2.28	116.80	108.42
2	H	501	AG7	C78-C57-C01	2.28	113.88	110.89
2	A	501	AG7	C14-C15-C16	2.26	117.87	112.89
2	E	501	AG7	C11-C06-C07	2.25	121.70	118.17
2	C	501	AG7	C02-C04-C47	2.23	113.00	109.77
2	F	501	AG7	O22-C21-C20	2.20	118.80	111.91
2	G	501	AG7	C78-C57-C01	2.17	113.75	110.89
2	F	501	AG7	O22-C50-C53	2.17	116.39	108.42
2	H	501	AG7	C11-C06-C07	2.16	121.56	118.17
2	C	501	AG7	O48-C47-C04	-2.16	119.31	122.12
2	C	501	AG7	C11-C06-C07	2.11	121.49	118.17
2	E	501	AG7	O48-C47-C04	-2.11	119.38	122.12
2	E	501	AG7	C84-C83-N17	2.11	106.51	103.43
2	G	501	AG7	C05-C04-C02	2.00	115.50	111.10

There are no chirality outliers.

All (23) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	501	AG7	C01-C02-C04-C47
2	F	501	AG7	C01-C02-C04-C47
2	E	501	AG7	N58-C57-C78-C82
2	C	501	AG7	N58-C57-C78-C81
2	F	501	AG7	C01-C57-C78-C82
2	E	501	AG7	N58-C57-C78-C81
2	C	501	AG7	C14-C13-C19-C20
2	C	501	AG7	N58-C57-C78-C82
2	B	501	AG7	C01-C02-C04-C47
2	E	501	AG7	C14-C13-C19-C20
2	E	501	AG7	C01-C57-C78-C82
2	A	501	AG7	C2-C1-C59-O60
2	D	501	AG7	C01-C02-C04-C47
2	D	501	AG7	C2-C1-C59-O60
2	E	501	AG7	C2-C1-C59-O60
2	G	501	AG7	C2-C1-C59-O60
2	H	501	AG7	C2-C1-C59-O60
2	F	501	AG7	C02-C04-C05-C06
2	G	501	AG7	C02-C04-C05-C06
2	H	501	AG7	C02-C04-C05-C06
2	F	501	AG7	N58-C57-C78-C82

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Mol	Chain	Res	Type	Atoms
2	C	501	AG7	C53-C50-O22-C21
2	H	501	AG7	C05-C04-C47-N12

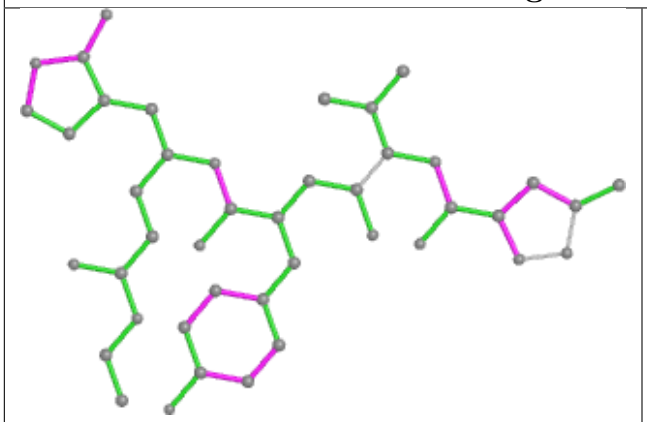
There are no ring outliers.

5 monomers are involved in 15 short contacts:

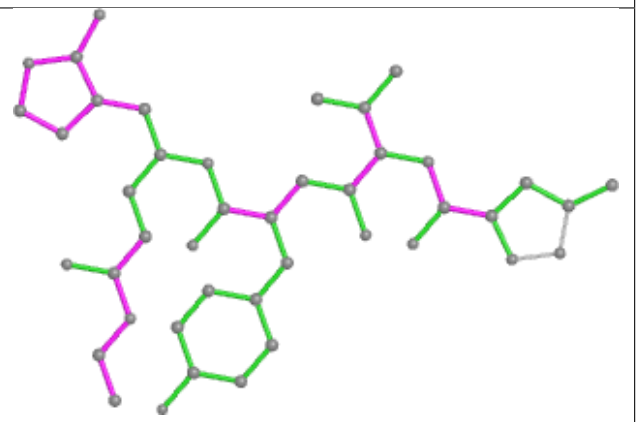
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	F	501	AG7	3	0
2	G	501	AG7	2	0
2	B	501	AG7	7	0
2	H	501	AG7	1	0
2	C	501	AG7	2	0

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.

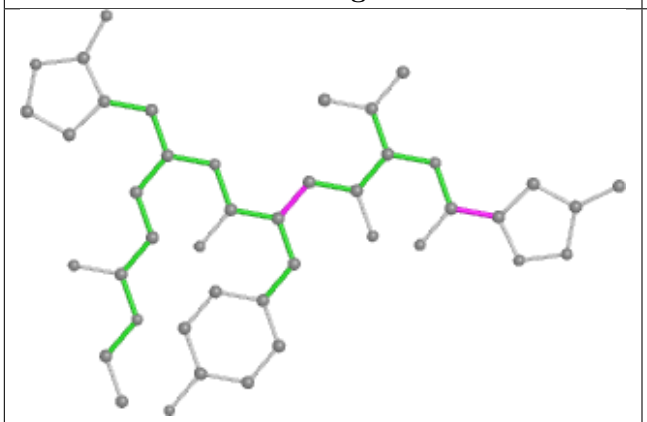
Ligand AG7 D 501



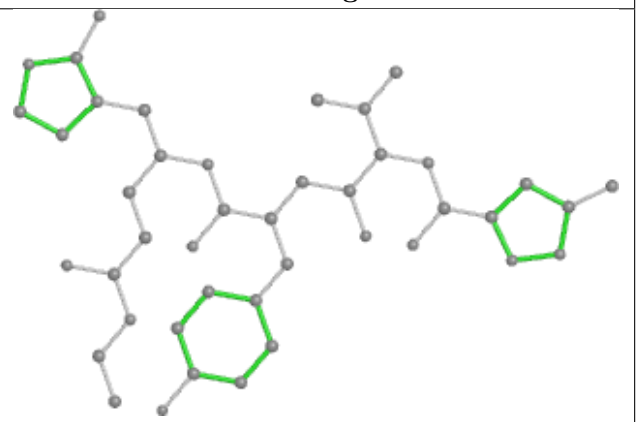
Bond lengths



Bond angles

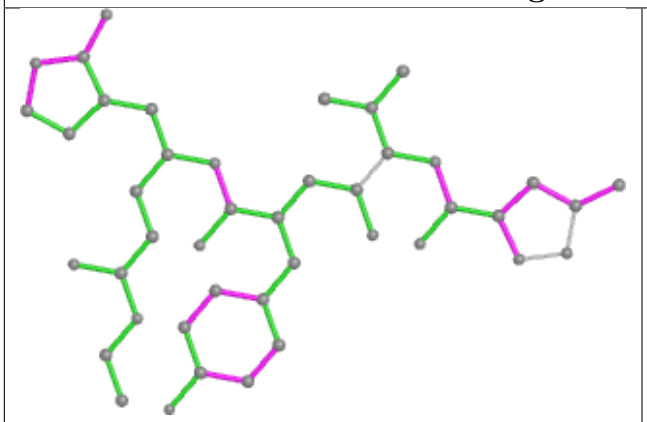


Torsions

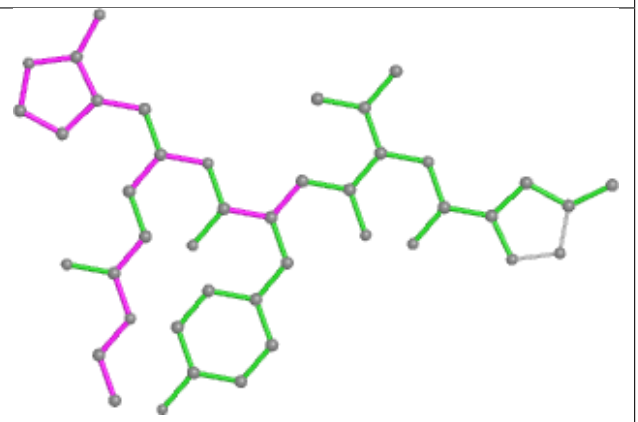


Rings

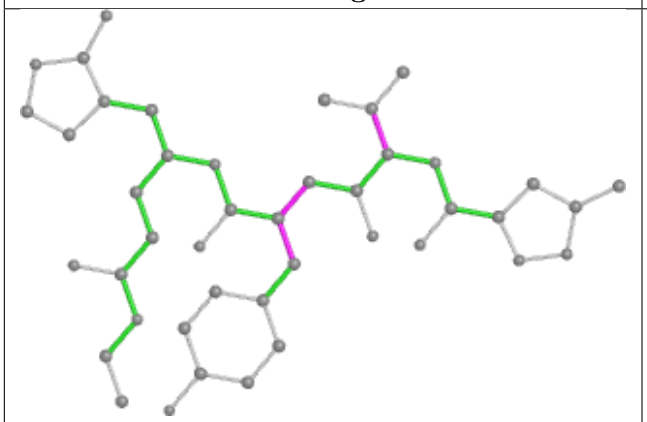
Ligand AG7 F 501



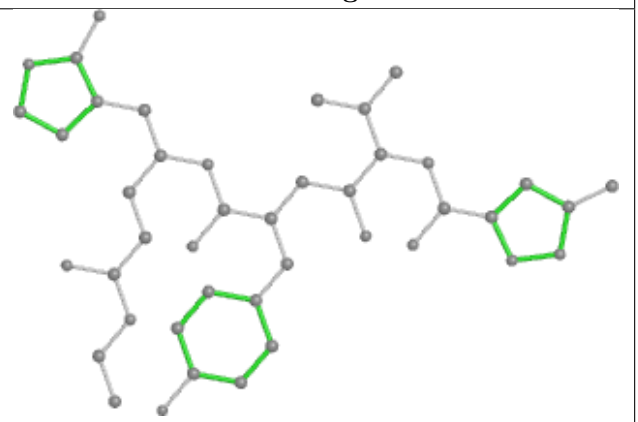
Bond lengths



Bond angles

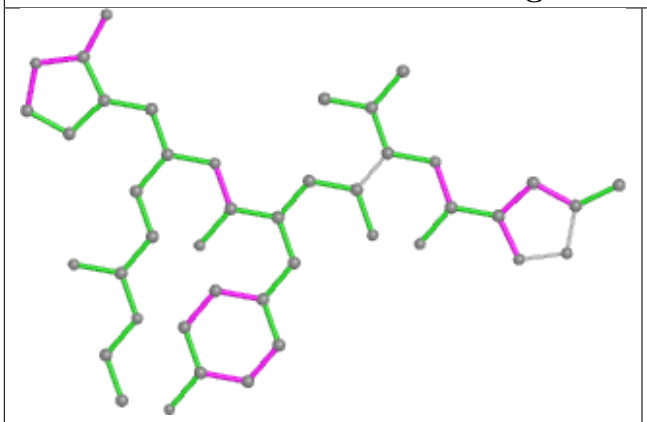


Torsions

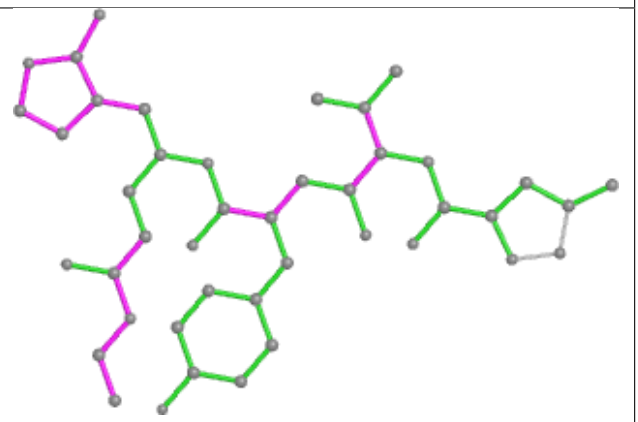


Rings

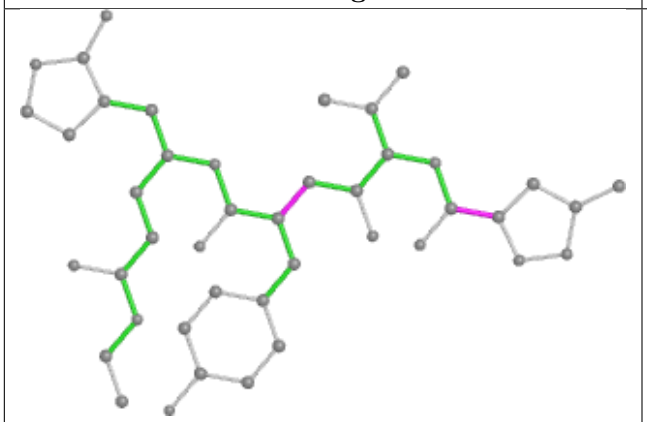
Ligand AG7 A 501



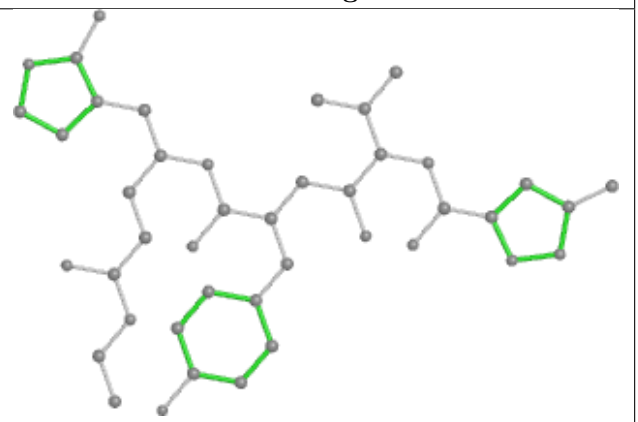
Bond lengths



Bond angles

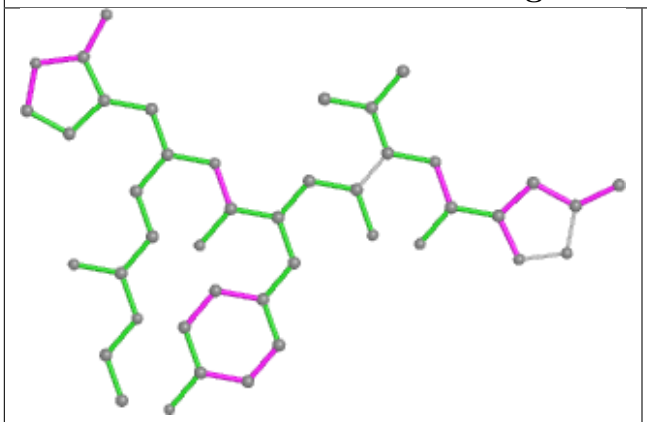


Torsions

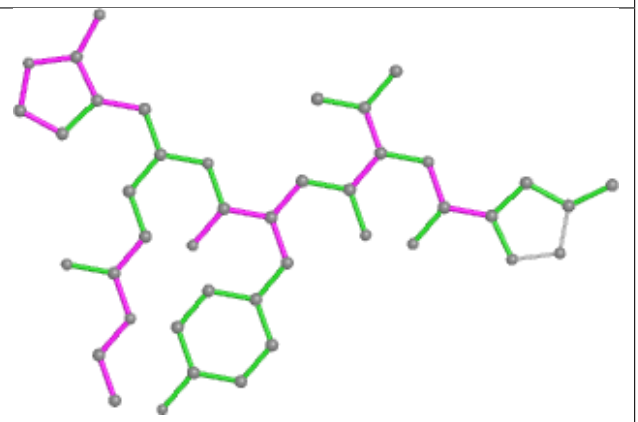


Rings

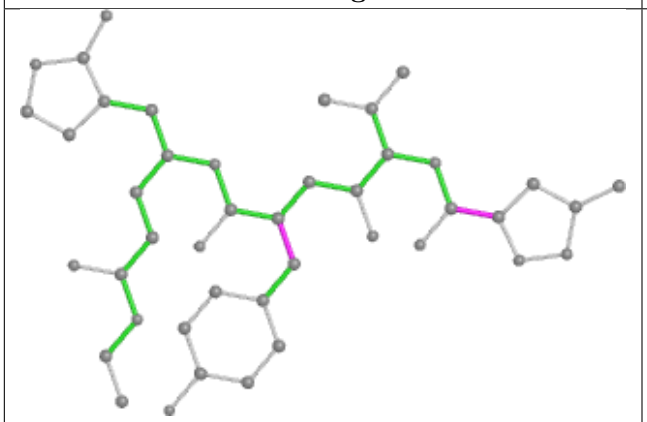
Ligand AG7 G 501



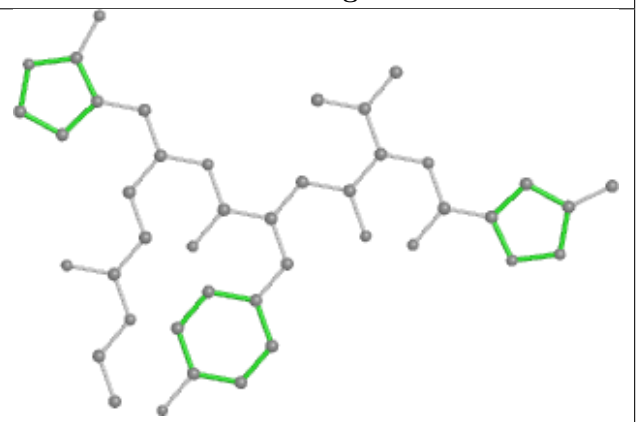
Bond lengths



Bond angles

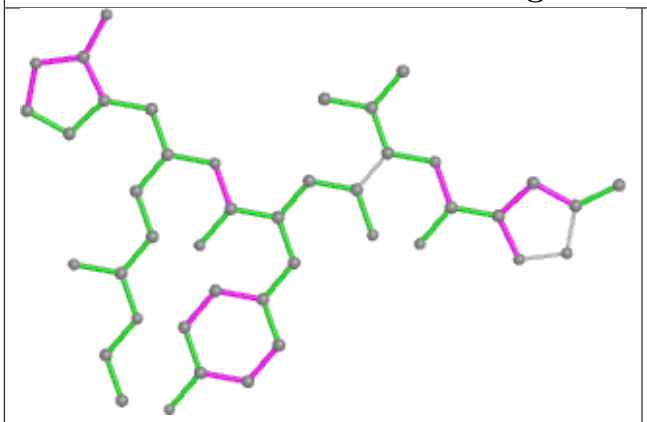


Torsions



Rings

Ligand AG7 B 501



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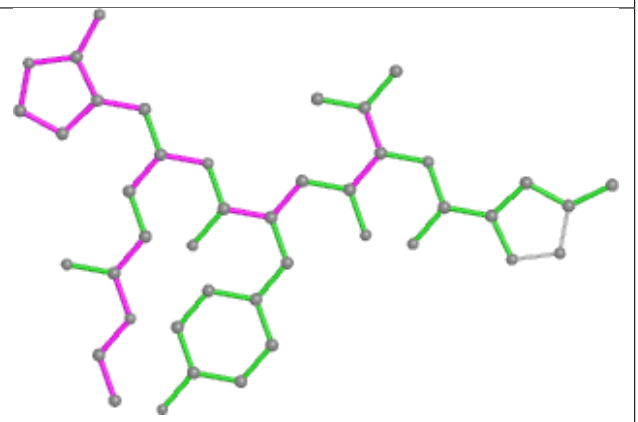
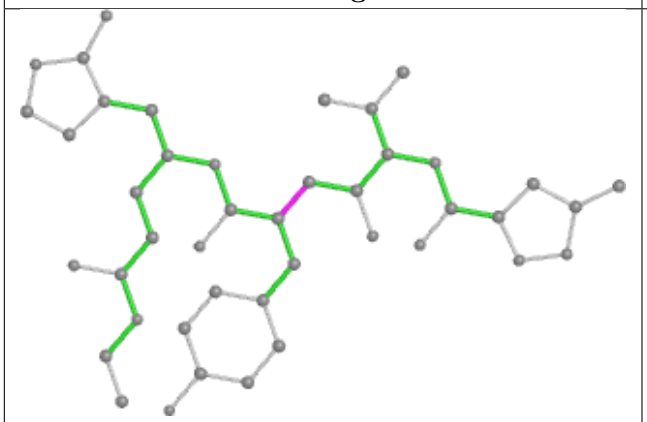
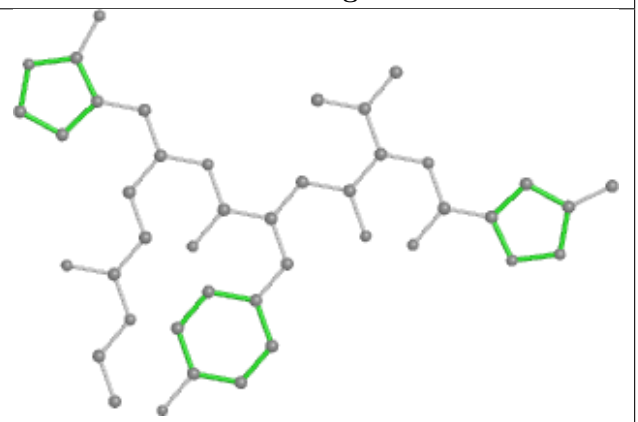


Bond angles

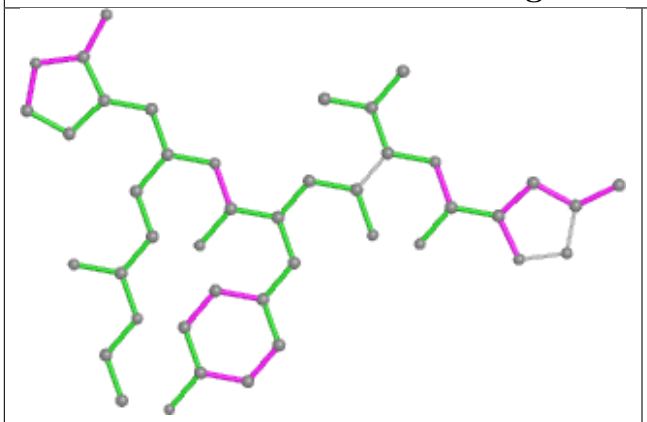


Torsions

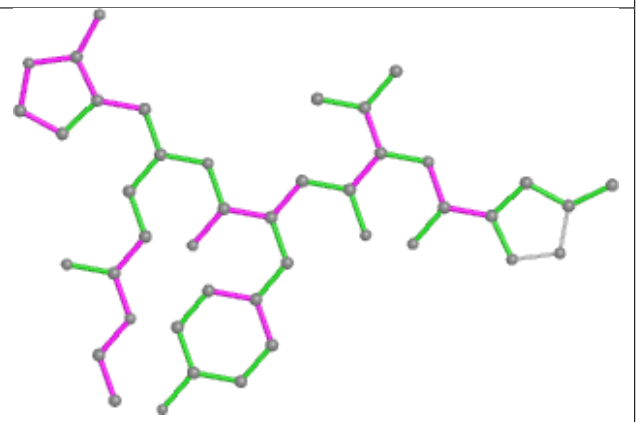


Rings

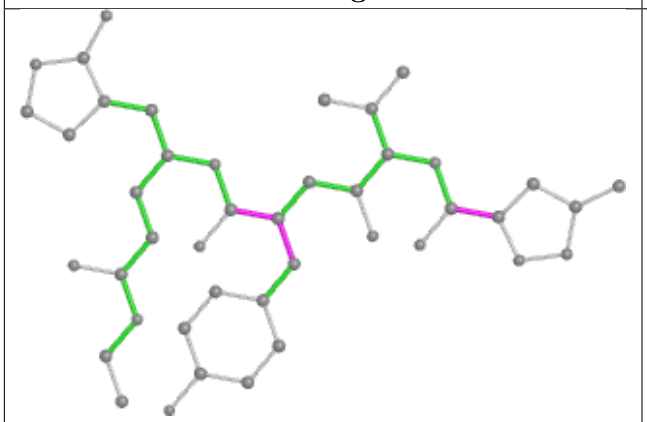
Ligand AG7 H 501



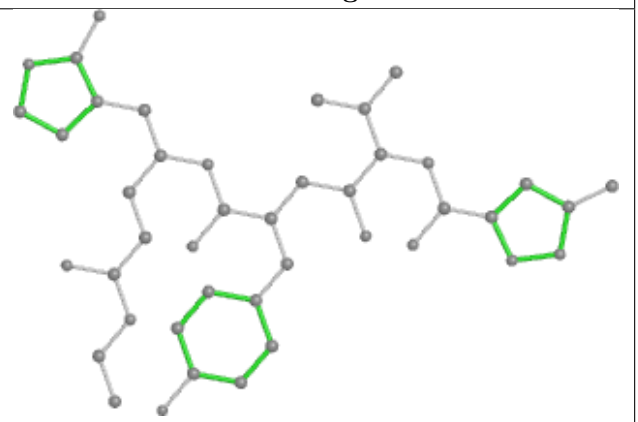
Bond lengths



Bond angles

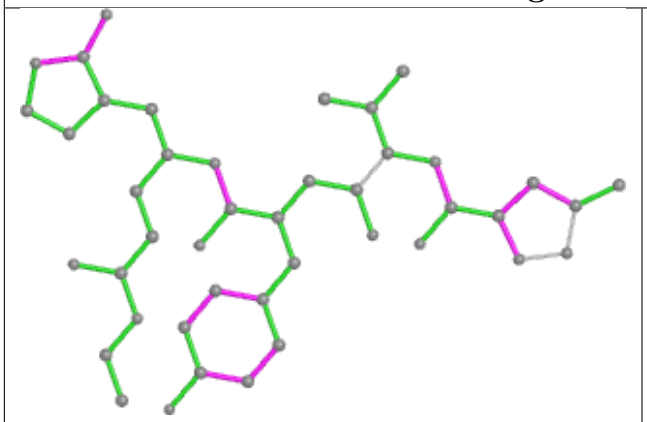


Torsions

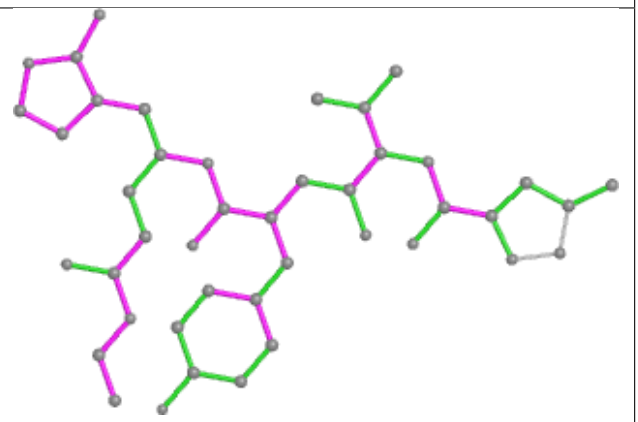


Rings

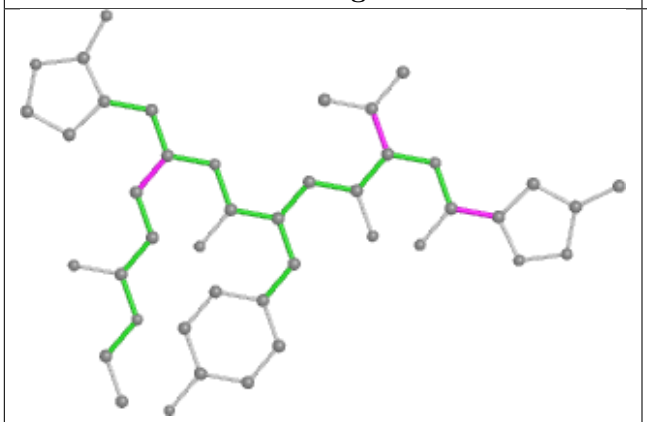
Ligand AG7 E 501



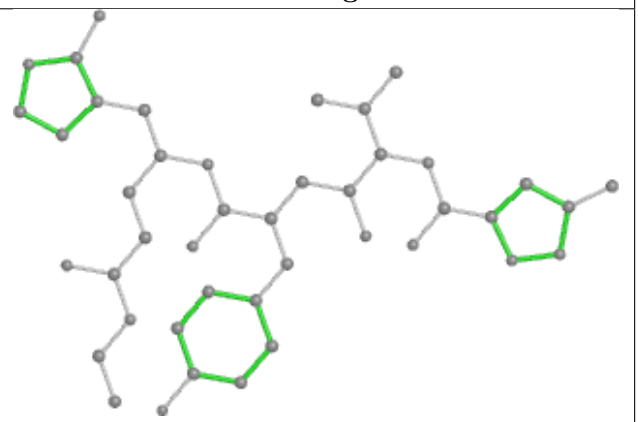
Bond lengths



Bond angles

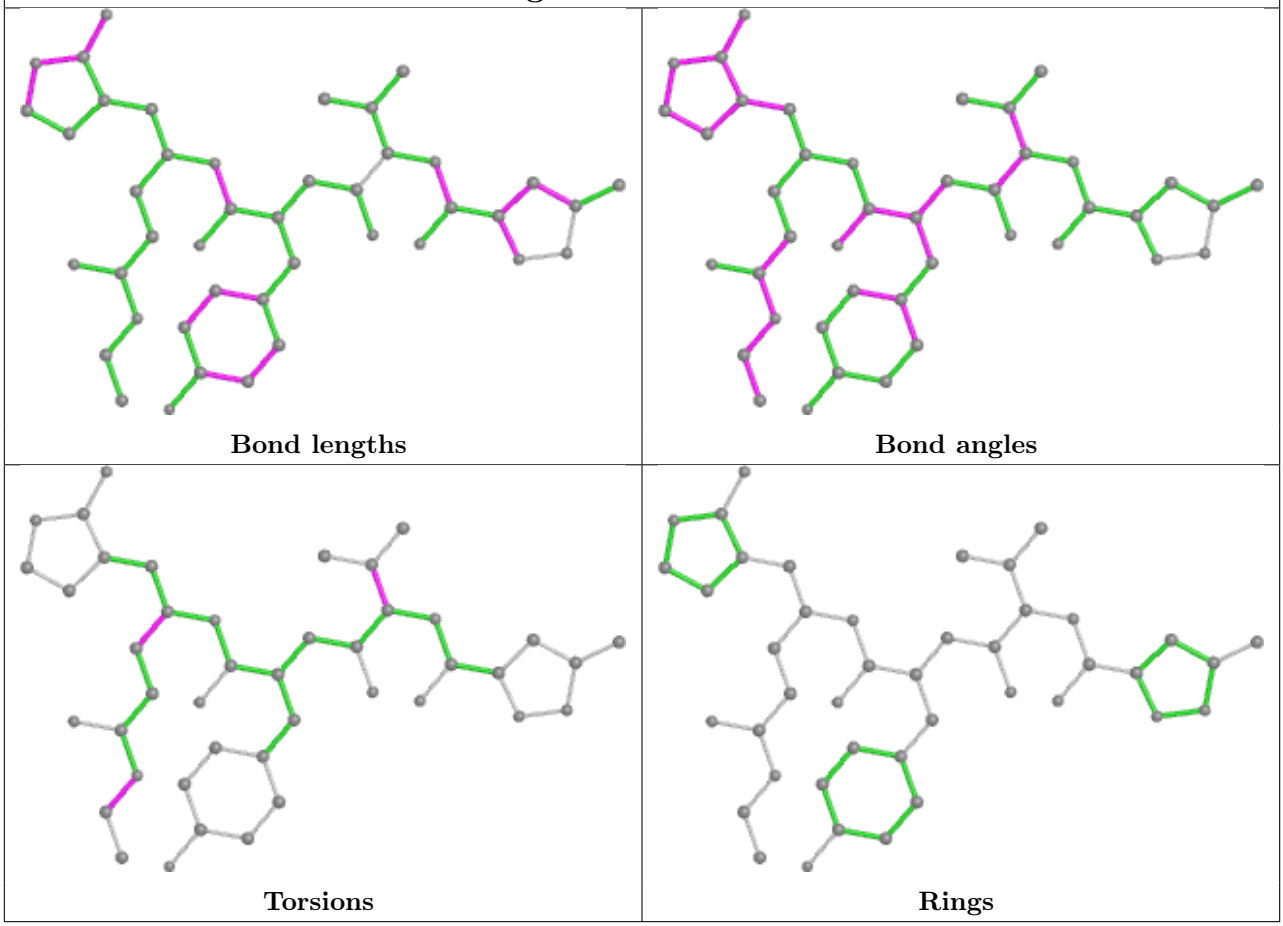


Torsions



Rings

Ligand AG7 C 501



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 (i)

6.1 Protein, DNA and RNA chains (i)

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	179/190 (94%)	-0.11	5 (2%) 53 57	11, 19, 33, 252	0
1	B	179/190 (94%)	0.85	32 (17%) 1 1	14, 27, 105, 176	0
1	C	179/190 (94%)	0.07	3 (1%) 70 74	10, 21, 41, 204	0
1	D	179/190 (94%)	-0.07	6 (3%) 45 50	10, 19, 35, 132	0
1	E	179/190 (94%)	0.13	9 (5%) 28 32	11, 20, 48, 205	0
1	F	179/190 (94%)	0.98	26 (14%) 2 2	14, 25, 128, 215	0
1	G	179/190 (94%)	0.75	25 (13%) 2 3	14, 27, 108, 176	0
1	H	179/190 (94%)	0.58	15 (8%) 11 12	15, 26, 85, 290	0
All	All	1432/1520 (94%)	0.40	121 (8%) 11 12	10, 23, 87, 290	0

All (121) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	145	GLY	15.0
1	E	4	LEU	14.8
1	H	182	GLU	10.8
1	H	4	LEU	10.6
1	F	4	LEU	10.3
1	B	116	VAL	10.2
1	H	81	GLU	10.0
1	C	65	GLU	9.6
1	C	182	GLU	9.3
1	G	113	PHE	9.1
1	H	108	HIS	8.9
1	D	4	LEU	8.7
1	G	5	ASP	8.7
1	F	42	GLN	8.6
1	D	80	ASN	8.6
1	G	116	VAL	8.3

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Mol	Chain	Res	Type	RSRZ
1	F	182	GLU	8.2
1	G	80	ASN	8.2
1	E	139	ASN	8.1
1	H	65	GLU	8.1
1	A	81	GLU	7.5
1	F	101	THR	7.5
1	F	139	ASN	7.2
1	G	107	GLU	7.1
1	F	8	LEU	7.0
1	B	6	PHE	6.7
1	B	113	PHE	6.7
1	D	182	GLU	6.6
1	B	65	GLU	6.4
1	G	128	SER	6.3
1	F	112	MET	6.3
1	G	100	ALA	6.2
1	E	99	ASP	6.2
1	F	108	HIS	6.0
1	F	109	MET	5.9
1	F	152	THR	5.9
1	B	5	ASP	5.8
1	E	5	ASP	5.7
1	G	40	HIS	5.7
1	G	82	LYS	5.6
1	F	115	PRO	5.5
1	B	155	GLY	5.5
1	F	40	HIS	5.5
1	G	117	GLY	5.1
1	B	167	ARG	5.1
1	C	154	VAL	5.1
1	F	111	SER	5.0
1	A	82	LYS	4.9
1	F	98	SER	4.8
1	B	80	ASN	4.8
1	B	4	LEU	4.7
1	B	143	LYS	4.7
1	F	118	ASP	4.7
1	D	181	SER	4.7
1	G	8	LEU	4.5
1	H	154	VAL	4.5
1	B	141	PRO	4.5
1	H	21	ASP	4.4

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Mol	Chain	Res	Type	RSRZ
1	B	154	VAL	4.3
1	D	79	THR	4.2
1	B	7	ALA	4.0
1	H	181	SER	4.0
1	H	44	GLY	3.9
1	G	119	VAL	3.8
1	B	21	ASP	3.8
1	B	168	GLN	3.6
1	B	153	SER	3.6
1	G	111	SER	3.6
1	G	182	GLU	3.6
1	B	165	ASN	3.4
1	A	98	SER	3.4
1	G	68	VAL	3.4
1	E	82	LYS	3.3
1	F	65	GLU	3.3
1	F	107	GLU	3.3
1	F	166	GLY	3.3
1	H	139	ASN	3.1
1	G	42	GLN	3.1
1	G	10	LEU	3.1
1	B	156	LYS	3.1
1	F	51	HIS	3.1
1	B	99	ASP	3.1
1	B	140	PHE	3.1
1	H	98	SER	3.1
1	F	88	LYS	3.1
1	G	6	PHE	3.0
1	A	78	ASP	3.0
1	B	12	ARG	2.9
1	B	43	PRO	2.9
1	H	121	GLN	2.9
1	H	164	GLY	2.8
1	G	12	ARG	2.8
1	F	154	VAL	2.7
1	B	164	GLY	2.7
1	B	100	ALA	2.6
1	E	80	ASN	2.6
1	F	96	THR	2.6
1	B	11	LEU	2.5
1	G	99	ASP	2.5
1	A	4	LEU	2.5

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Mol	Chain	Res	Type	RSRZ
1	F	5	ASP	2.4
1	B	10	LEU	2.4
1	H	84	ARG	2.4
1	B	138	TYR	2.3
1	B	114	VAL	2.3
1	B	142	THR	2.3
1	D	154	VAL	2.3
1	F	106	THR	2.3
1	F	20	THR	2.2
1	B	122	TYR	2.2
1	B	106	THR	2.2
1	G	153	SER	2.2
1	G	96	THR	2.1
1	E	153	SER	2.1
1	B	67	GLY	2.1
1	E	8	LEU	2.1
1	E	126	ASN	2.0
1	H	113	PHE	2.0
1	G	167	ARG	2.0
1	G	43	PRO	2.0
1	G	126	ASN	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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	AG7	F	501	43/43	0.85	0.14	21,29,37,37	0
2	AG7	B	501	43/43	0.87	0.16	23,30,39,41	0

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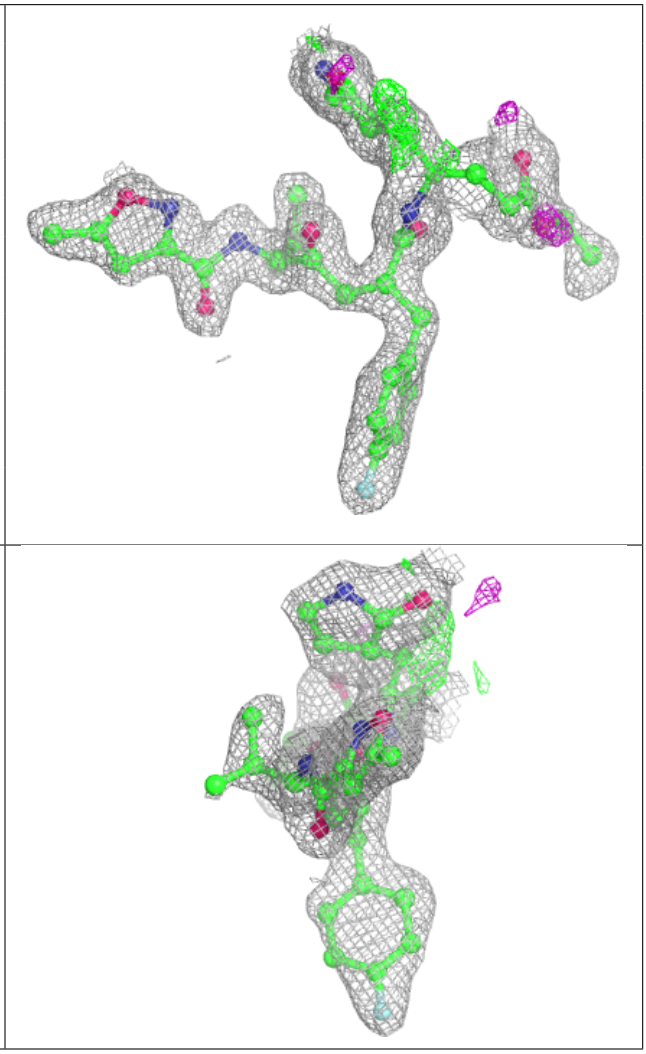
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	AG7	G	501	43/43	0.89	0.12	19,27,35,38	0
2	AG7	H	501	43/43	0.90	0.13	20,27,34,37	0
2	AG7	E	501	43/43	0.91	0.12	17,24,32,39	0
2	AG7	A	501	43/43	0.92	0.10	14,21,29,36	0
2	AG7	C	501	43/43	0.93	0.10	16,24,29,33	0
2	AG7	D	501	43/43	0.93	0.10	12,17,24,30	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.

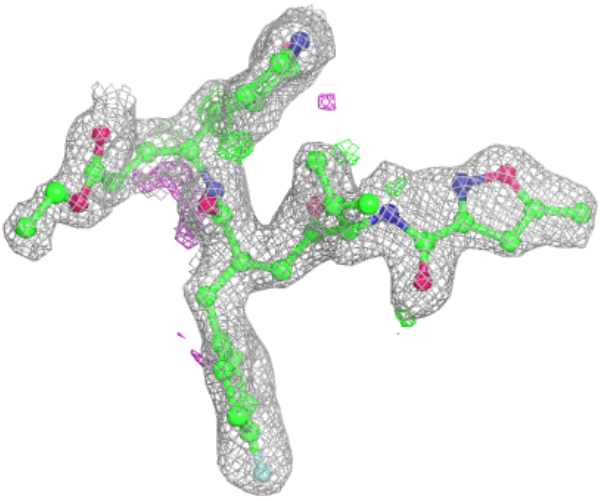
Electron density around AG7 F 501:

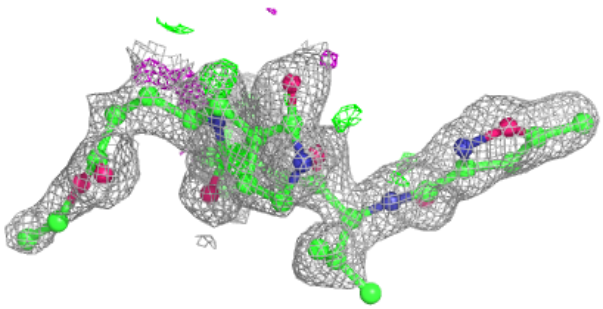
2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)

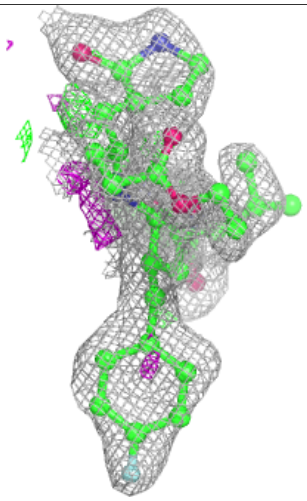


Electron density around AG7 B 501:

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

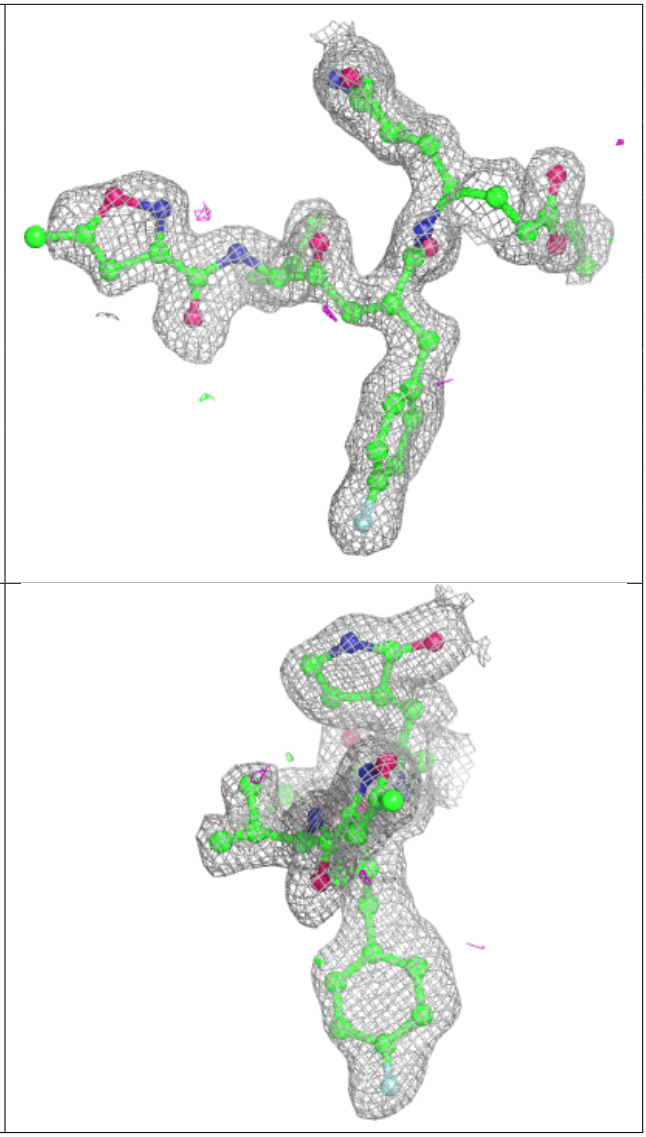






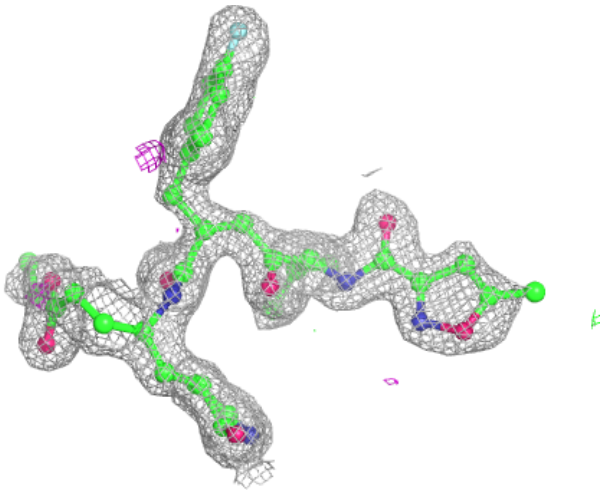
Electron density around AG7 G 501:

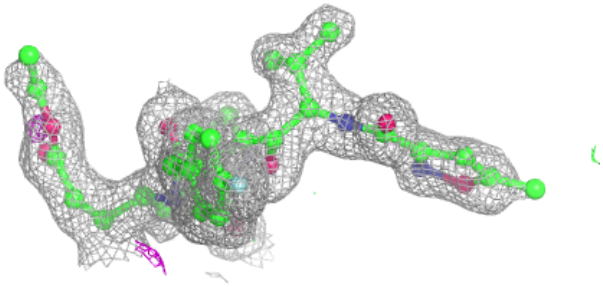
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

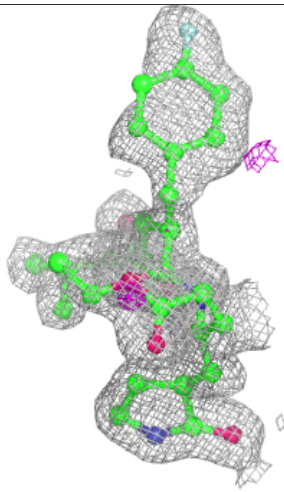


Electron density around AG7 H 501:

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

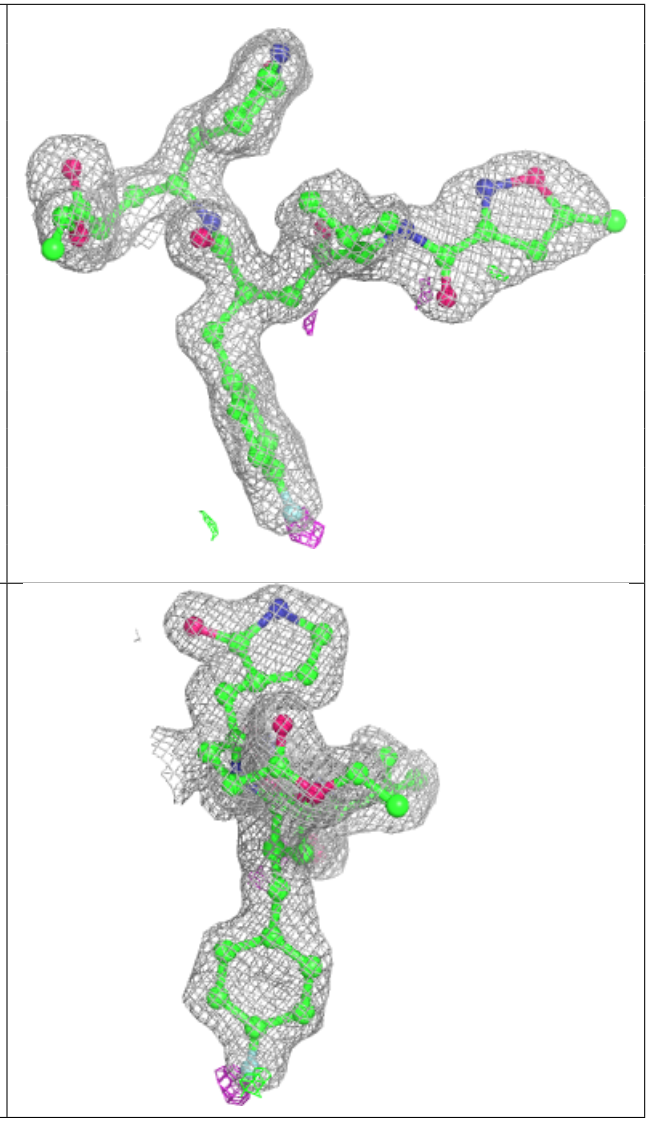






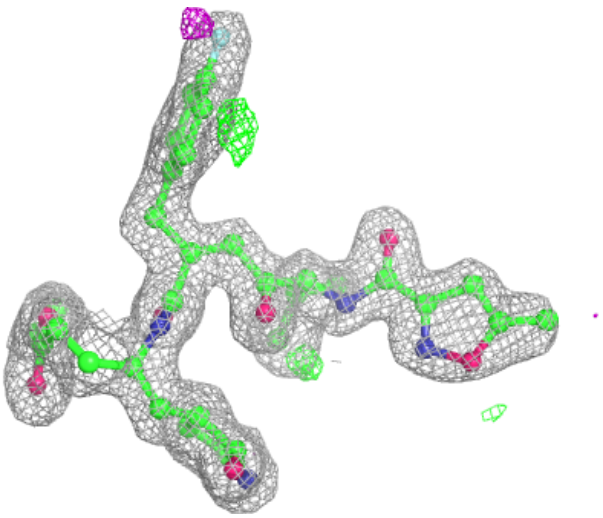
Electron density around AG7 E 501:

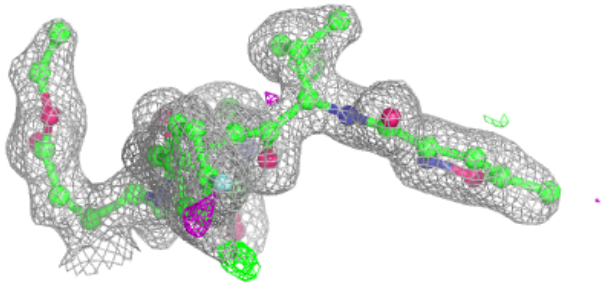
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

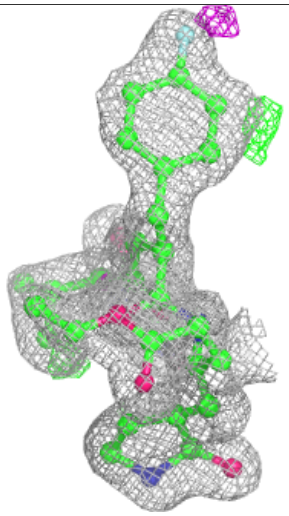


Electron density around AG7 A 501:

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

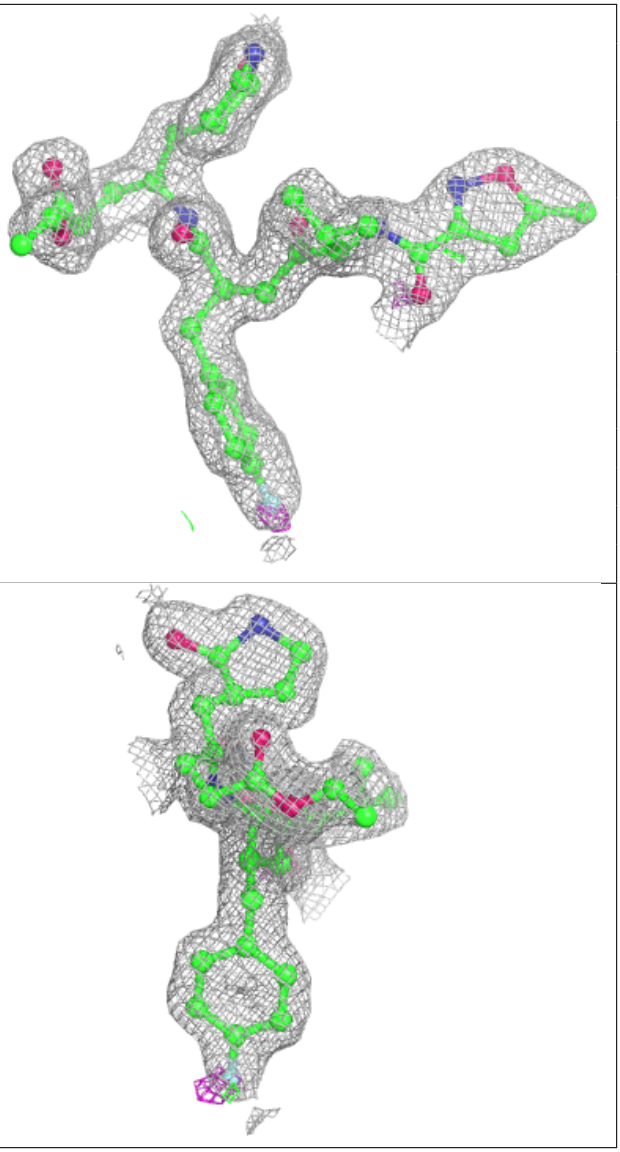


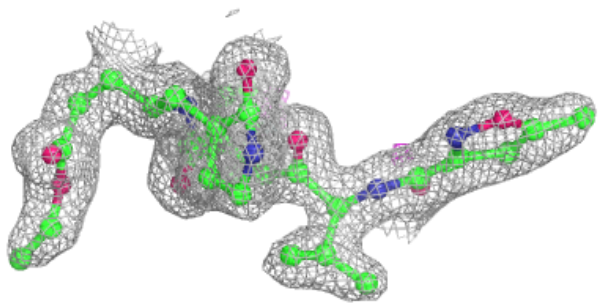




Electron density around AG7 C 501:

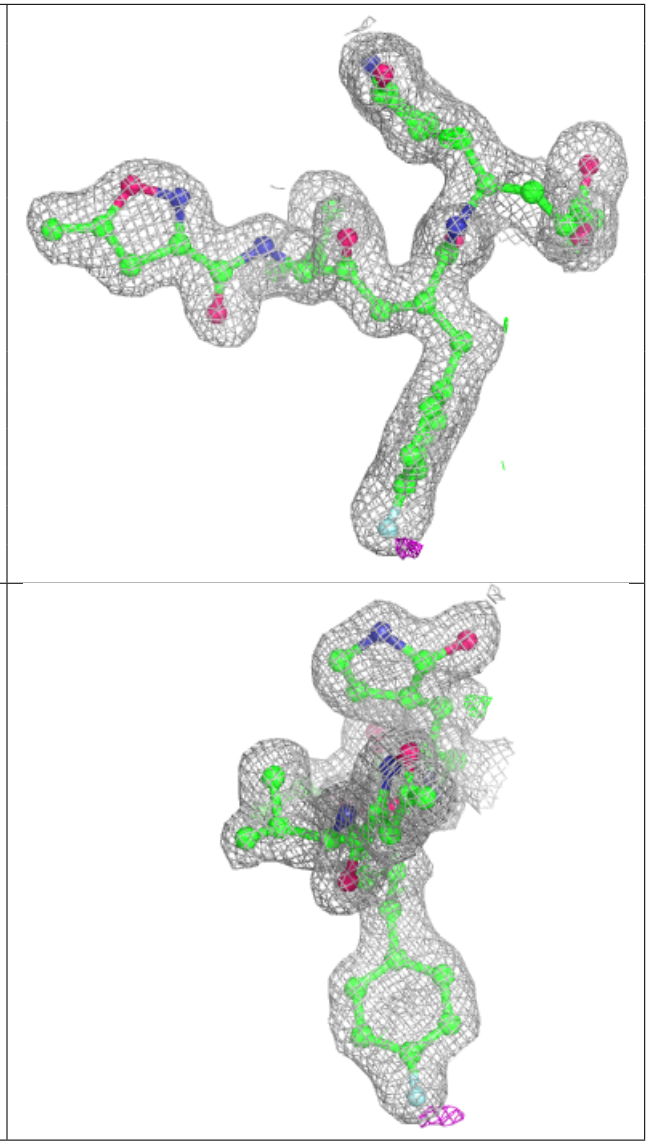
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





Electron density around AG7 D 501:

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



6.5 Other polymers (i)

There are no such residues in this entry.