Full wwPDB X-ray Structure Validation Report ⓘ

Oct 15, 2023 – 05:58 PM EDT

PDB ID	:	7TJP
Title	:	HIV-1 gp120 complex with CJF-II-195
Authors	:	Gong, Z.; Hendrickson, W.A.
Deposited on	:	2022-01-16
Resolution	:	2.77 Å(reported)

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

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

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references ⓘ) were used in the production of this report:

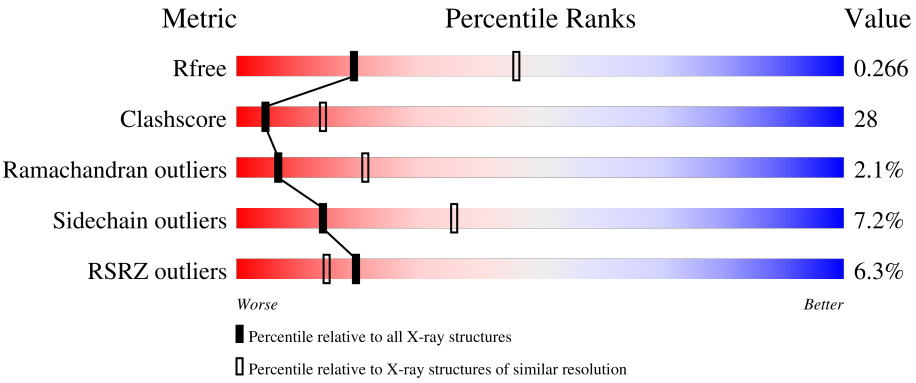
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber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

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.77 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	4107 (2.80-2.76)
Clashscore	141614	4575 (2.80-2.76)
Ramachandran outliers	138981	4487 (2.80-2.76)
Sidechain outliers	138945	4489 (2.80-2.76)
RSRZ outliers	127900	4027 (2.80-2.76)

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	358	3% 50% 37% 6% • 6%
1	B	358	8% 51% 37% • • 6%
1	C	358	5% 46% 41% 5% • 6%
1	D	358	7% 49% 38% 5% • 6%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	NAG	B	504	-	-	-	X
2	NAG	B	505	-	-	-	X
2	NAG	C	504	-	-	-	X
2	NAG	C	508	-	-	X	X
2	NAG	D	504	-	-	X	X
2	NAG	D	505	-	-	-	X
2	NAG	D	508	-	-	-	X

2 Entry composition

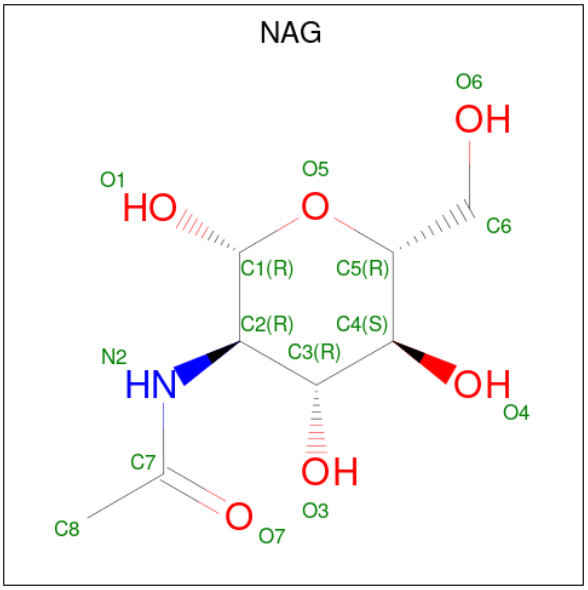
There are 5 unique types of molecules in this entry. The entry contains 11431 atoms, of which 5 are hydrogens and 0 are deuteriums.

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 Glycoprotein 120.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	335	Total	C	N	O	S	0	0	0
			2627	1642	459	506	20			
1	B	335	Total	C	N	O	S	0	0	0
			2627	1642	459	506	20			
1	D	335	Total	C	N	O	S	0	0	0
			2627	1642	459	506	20			
1	C	335	Total	C	N	O	S	0	0	0
			2627	1642	459	506	20			

- Molecule 2 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	A	1	Total	C	N	O	0	0
			14	8	1	5		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C N O 14 8 1 5	0	0
2	A	1	Total C N O 14 8 1 5	0	0
2	A	1	Total C N O 14 8 1 5	0	0
2	A	1	Total C N O 14 8 1 5	0	0
2	A	1	Total C N O 14 8 1 5	0	0
2	A	1	Total C N O 14 8 1 5	0	0
2	A	1	Total C N O 14 8 1 5	0	0
2	B	1	Total C N O 14 8 1 5	0	0
2	B	1	Total C N O 14 8 1 5	0	0
2	B	1	Total C N O 14 8 1 5	0	0
2	B	1	Total C N O 14 8 1 5	0	0
2	B	1	Total C N O 14 8 1 5	0	0
2	B	1	Total C N O 14 8 1 5	0	0
2	B	1	Total C N O 14 8 1 5	0	0
2	B	1	Total C N O 14 8 1 5	0	0
2	B	1	Total C N O 14 8 1 5	0	0
2	D	1	Total C N O 14 8 1 5	0	0
2	D	1	Total C N O 14 8 1 5	0	0
2	D	1	Total C N O 14 8 1 5	0	0
2	D	1	Total C N O 14 8 1 5	0	0
2	D	1	Total C N O 14 8 1 5	0	0

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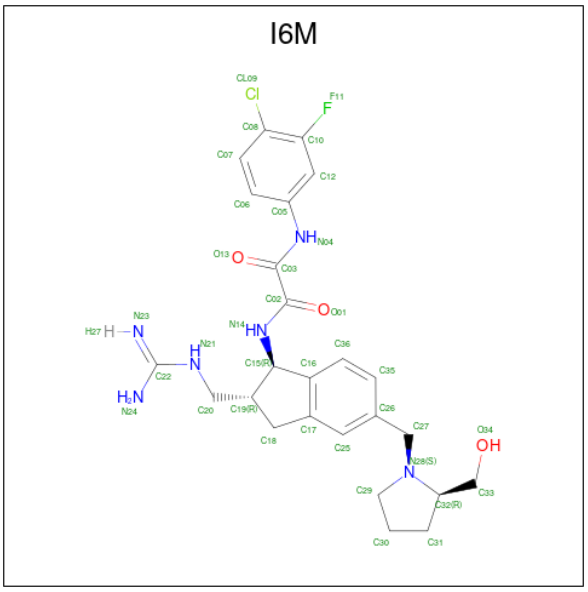
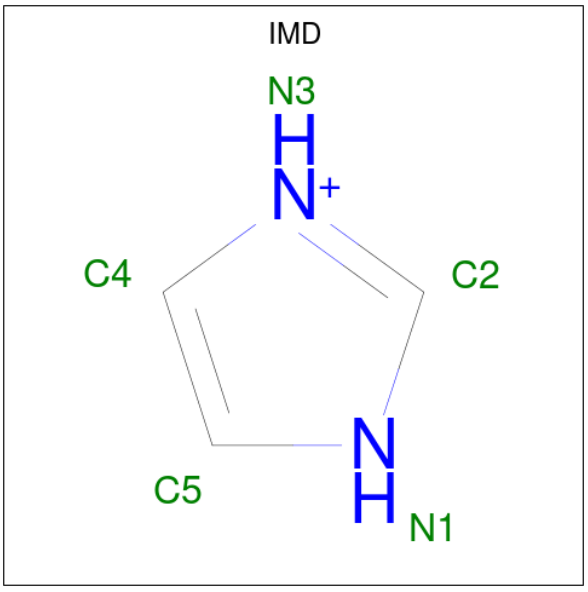
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
2	D	1	14	8	1	5	0	0
2	D	1	14	8	1	5	0	0
2	D	1	14	8	1	5	0	0
2	D	1	14	8	1	5	0	0
2	C	1	14	8	1	5	0	0
2	C	1	14	8	1	5	0	0
2	C	1	14	8	1	5	0	0
2	C	1	14	8	1	5	0	0
2	C	1	14	8	1	5	0	0
2	C	1	14	8	1	5	0	0
2	C	1	14	8	1	5	0	0
2	C	1	14	8	1	5	0	0
2	C	1	14	8	1	5	0	0

- Molecule 3 is N 1 -[(1R,2R)-2-(carbamimidamidomethyl)-5-{[(2R)-2-(hydroxymethyl)pyrrolidin-1-yl]methyl}-2,3-dihydro-1H-inden-1-yl]-N 2 -(4-chloro-3-fluorophenyl)ethanediamide (three-letter code: I6M) (formula: $C_{25}H_{30}ClFN_6O_3$).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	A	1	Total	C	Cl	F	N	O	0	1
			72	50	2	2	12	6		
3	B	1	Total	C	Cl	F	N	O	0	1
			72	50	2	2	12	6		
3	D	1	Total	C	Cl	F	N	O	0	1
			72	50	2	2	12	6		
3	C	1	Total	C	Cl	F	N	O	0	1
			72	50	2	2	12	6		

- Molecule 4 is IMIDAZOLE (three-letter code: IMD) (formula: $C_3H_5N_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C H N 10 3 5 2	0	0

- Molecule 5 is water.

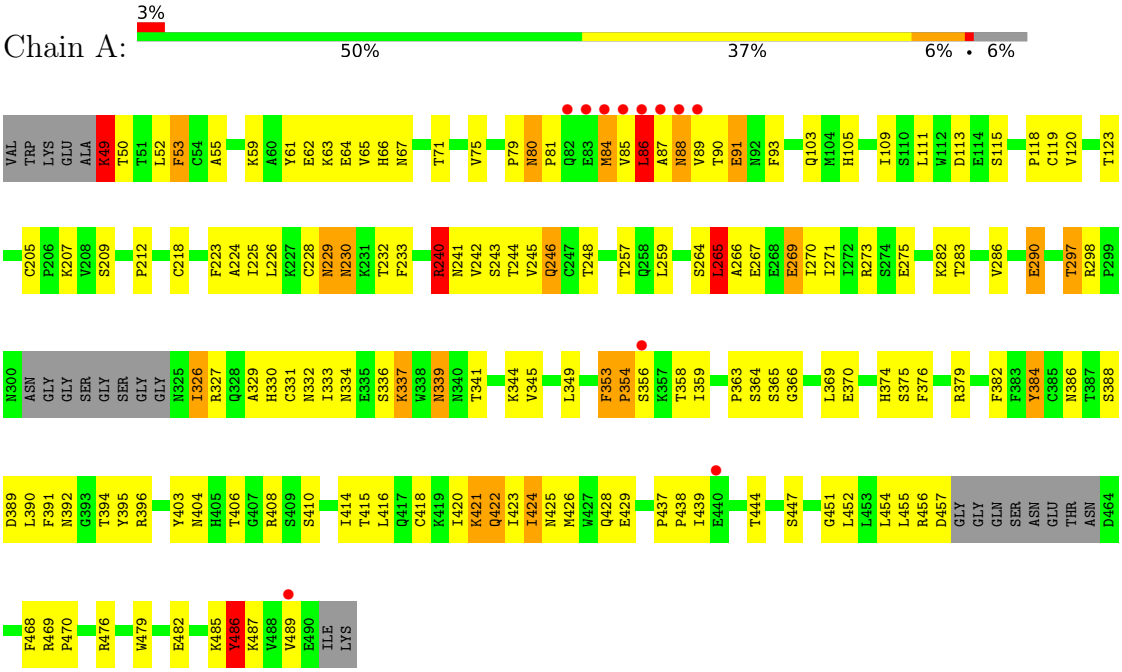
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	32	Total O 33 33	0	1
5	B	21	Total O 21 21	0	0
5	D	27	Total O 27 27	0	0
5	C	40	Total O 40 40	0	0

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.

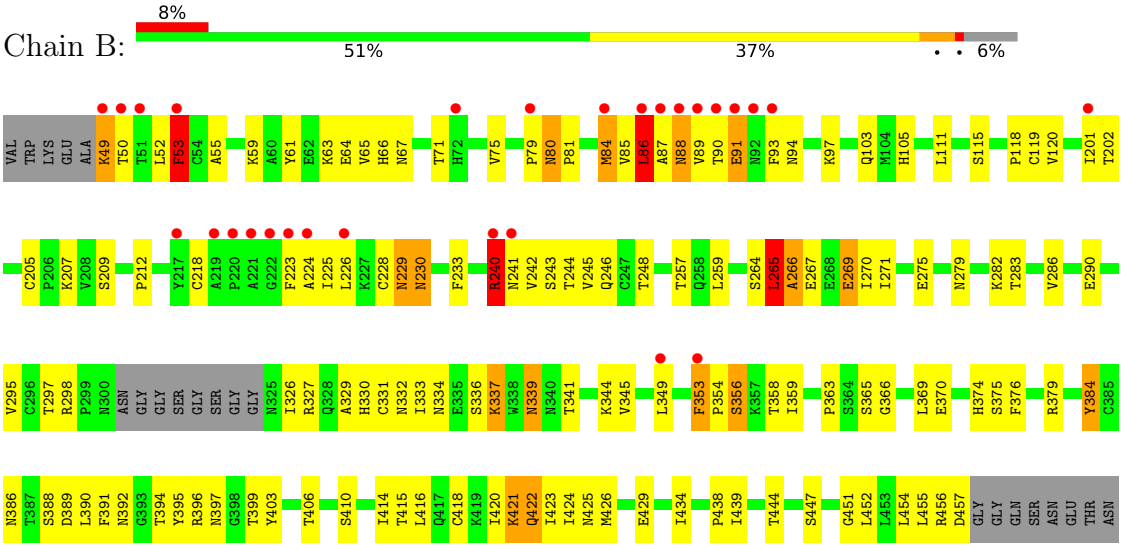
- Molecule 1: Glycoprotein 120

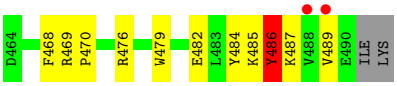
Chain A:



- Molecule 1: Glycoprotein 120

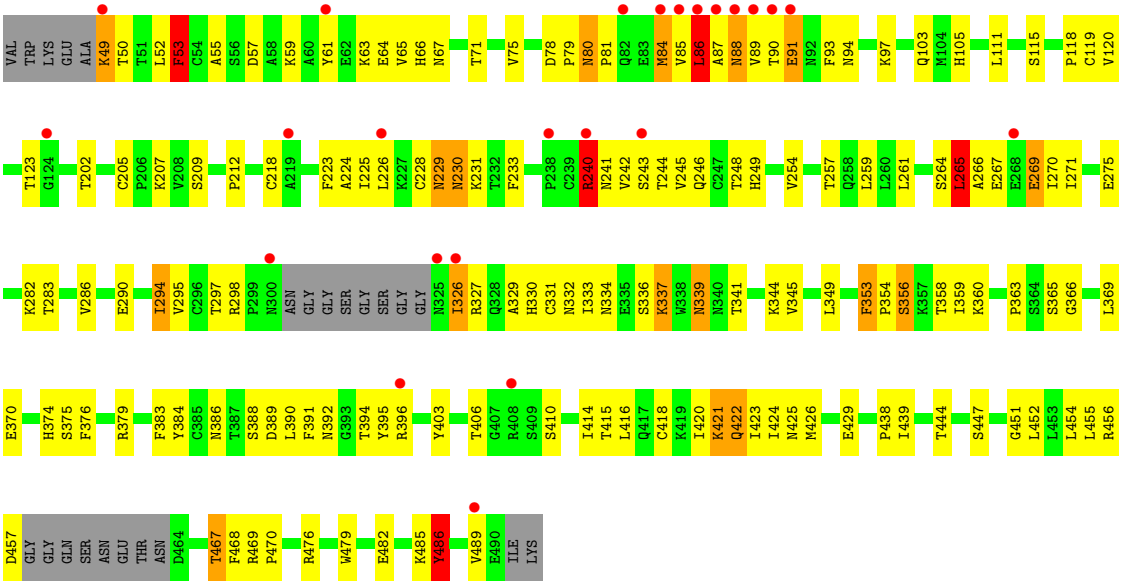
Chain B:





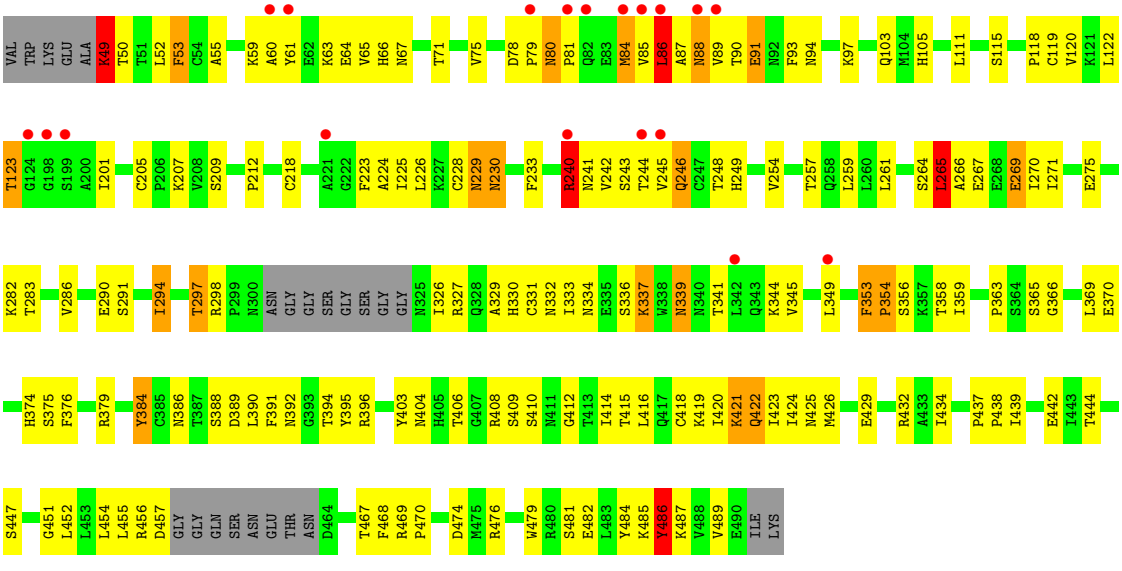
• Molecule 1: Glycoprotein 120

Chain D:



• Molecule 1: Glycoprotein 120

Chain C:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	71.21Å 121.64Å 194.97Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.74 – 2.77 48.74 – 2.77	Depositor EDS
% Data completeness (in resolution range)	72.3 (48.74-2.77) 72.3 (48.74-2.77)	Depositor EDS
R_{merge}	0.25	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.57 (at 2.77Å)	Xtriage
Refinement program	PHENIX 1.20rc3_4406, PHENIX 1.20rc3_4406	Depositor
R, R_{free}	0.224 , 0.265 0.226 , 0.266	Depositor DCC
R_{free} test set	1999 reflections (6.32%)	wwPDB-VP
Wilson B-factor (Å^2)	60.8	Xtriage
Anisotropy	0.055	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 51.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	11431	wwPDB-VP
Average B, all atoms (Å^2)	53.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 17.28% 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: I6M, IMD, NAG

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	2/2682 (0.1%)	0.93	9/3640 (0.2%)
1	B	0.64	1/2682 (0.0%)	0.93	9/3640 (0.2%)
1	C	0.64	1/2682 (0.0%)	0.93	9/3640 (0.2%)
1	D	0.64	1/2682 (0.0%)	0.93	9/3640 (0.2%)
All	All	0.64	5/10728 (0.0%)	0.93	36/14560 (0.2%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	3
1	B	0	3
1	C	0	3
1	D	0	3
All	All	0	12

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	269	GLU	CD-OE1	7.59	1.33	1.25
1	A	269	GLU	CD-OE1	7.59	1.33	1.25
1	C	269	GLU	CD-OE1	7.57	1.33	1.25
1	D	269	GLU	CD-OE1	7.56	1.33	1.25
1	A	290	GLU	CD-OE2	5.01	1.31	1.25

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	63	LYS	CD-CE-NZ	-7.71	93.96	111.70
1	C	63	LYS	CD-CE-NZ	-7.70	93.99	111.70
1	B	63	LYS	CD-CE-NZ	-7.69	94.01	111.70
1	A	63	LYS	CD-CE-NZ	-7.68	94.03	111.70
1	B	265	LEU	CB-CG-CD2	-6.93	99.22	111.00
1	A	265	LEU	CB-CG-CD2	-6.91	99.25	111.00
1	D	265	LEU	CB-CG-CD2	-6.90	99.27	111.00
1	C	265	LEU	CB-CG-CD2	-6.90	99.27	111.00
1	A	267	GLU	N-CA-CB	-6.07	99.67	110.60
1	C	267	GLU	N-CA-CB	-6.07	99.68	110.60
1	B	267	GLU	N-CA-CB	-6.05	99.72	110.60
1	D	267	GLU	N-CA-CB	-6.04	99.72	110.60
1	D	49	LYS	CA-CB-CG	-5.94	100.34	113.40
1	A	49	LYS	CA-CB-CG	-5.93	100.35	113.40
1	B	49	LYS	CA-CB-CG	-5.91	100.40	113.40
1	C	49	LYS	CA-CB-CG	-5.91	100.40	113.40
1	D	63	LYS	CB-CG-CD	-5.89	96.28	111.60
1	C	63	LYS	CB-CG-CD	-5.88	96.31	111.60
1	A	63	LYS	CB-CG-CD	-5.87	96.33	111.60
1	B	63	LYS	CB-CG-CD	-5.87	96.34	111.60
1	C	240	ARG	CG-CD-NE	5.42	123.19	111.80
1	A	240	ARG	CG-CD-NE	5.40	123.15	111.80
1	B	240	ARG	CG-CD-NE	5.39	123.13	111.80
1	D	240	ARG	CG-CD-NE	5.39	123.11	111.80
1	D	421	LYS	CD-CE-NZ	5.19	123.64	111.70
1	C	421	LYS	CD-CE-NZ	5.18	123.62	111.70
1	A	421	LYS	CD-CE-NZ	5.18	123.61	111.70
1	B	421	LYS	CD-CE-NZ	5.16	123.57	111.70
1	A	53	PHE	CB-CG-CD2	-5.14	117.20	120.80
1	C	53	PHE	CB-CG-CD2	-5.12	117.22	120.80
1	B	53	PHE	CB-CG-CD2	-5.09	117.24	120.80
1	D	53	PHE	CB-CG-CD2	-5.07	117.25	120.80
1	D	240	ARG	CB-CG-CD	-5.03	98.53	111.60
1	A	240	ARG	CB-CG-CD	-5.02	98.55	111.60
1	B	240	ARG	CB-CG-CD	-5.02	98.55	111.60
1	C	240	ARG	CB-CG-CD	-5.01	98.57	111.60

There are no chirality outliers.

All (12) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	240	ARG	Sidechain
1	A	266	ALA	Peptide

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Mol	Chain	Res	Type	Group
1	A	486	TYR	Sidechain
1	B	240	ARG	Sidechain
1	B	266	ALA	Peptide
1	B	486	TYR	Sidechain
1	C	240	ARG	Sidechain
1	C	266	ALA	Peptide
1	C	486	TYR	Sidechain
1	D	240	ARG	Sidechain
1	D	266	ALA	Peptide
1	D	486	TYR	Sidechain

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	2627	0	2539	148	1
1	B	2627	0	2539	140	2
1	C	2627	0	2539	170	1
1	D	2627	0	2539	147	2
2	A	126	0	117	8	0
2	B	126	0	117	5	1
2	C	126	0	117	18	0
2	D	126	0	117	17	1
3	A	72	0	0	0	0
3	B	72	0	0	0	0
3	C	72	0	0	0	0
3	D	72	0	0	0	0
4	A	5	5	5	0	0
5	A	33	0	0	13	0
5	B	21	0	0	3	0
5	C	40	0	0	13	0
5	D	27	0	0	3	0
All	All	11426	5	10629	611	4

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 28.

All (611) 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:248:THR:HG22	1:B:486:TYR:CD2	1.68	1.29
1:A:248:THR:HG22	1:A:486:TYR:CD2	1.68	1.28
1:A:248:THR:HG22	1:A:486:TYR:CE2	1.85	1.11
1:B:248:THR:HG22	1:B:486:TYR:CE2	1.85	1.09
1:C:123:THR:HG23	5:C:612:HOH:O	1.62	1.00
1:A:422:GLN:HE22	1:A:438:PRO:HD3	1.27	0.98
1:A:290:GLU:OE2	1:A:344:LYS:NZ	1.96	0.97
1:A:404:ASN:OD1	1:C:408:ARG:HA	1.63	0.97
1:C:290:GLU:OE2	1:C:344:LYS:NZ	1.96	0.97
1:C:422:GLN:HE22	1:C:438:PRO:HD3	1.27	0.97
1:D:290:GLU:OE2	1:D:344:LYS:NZ	1.96	0.96
1:B:248:THR:HA	1:B:486:TYR:HE2	1.31	0.96
1:B:248:THR:HG22	1:B:486:TYR:HD2	1.31	0.96
1:B:290:GLU:OE2	1:B:344:LYS:NZ	1.96	0.95
1:D:248:THR:HA	1:D:486:TYR:HE2	1.30	0.95
1:C:248:THR:HA	1:C:486:TYR:HE2	1.30	0.95
2:D:504:NAG:HN2	2:C:508:NAG:H62	1.29	0.95
1:A:248:THR:HA	1:A:486:TYR:HE2	1.31	0.95
2:D:508:NAG:C6	2:C:501:NAG:H61	1.97	0.94
2:D:503:NAG:H3	2:D:503:NAG:H83	1.49	0.94
2:B:503:NAG:H3	2:B:503:NAG:H83	1.49	0.94
2:C:503:NAG:H83	2:C:503:NAG:H3	1.49	0.93
1:A:86:LEU:HD12	1:A:89:VAL:HG21	1.52	0.92
1:D:86:LEU:HD12	1:D:89:VAL:HG21	1.52	0.92
1:D:248:THR:HG22	1:D:486:TYR:CD2	2.03	0.92
1:C:86:LEU:CD1	1:C:89:VAL:HG21	2.00	0.92
1:D:86:LEU:CD1	1:D:89:VAL:HG21	2.00	0.92
1:C:248:THR:HG22	1:C:486:TYR:CD2	2.03	0.92
1:B:86:LEU:HD12	1:B:89:VAL:HG21	1.52	0.91
2:D:504:NAG:N2	2:C:508:NAG:H62	1.84	0.91
1:A:86:LEU:CD1	1:A:89:VAL:HG21	2.00	0.91
2:A:504:NAG:H83	2:A:504:NAG:H3	1.49	0.91
1:B:86:LEU:CD1	1:B:89:VAL:HG21	2.00	0.90
2:D:508:NAG:H61	2:C:501:NAG:H61	1.52	0.90
1:C:86:LEU:HD12	1:C:89:VAL:HG21	1.52	0.90
1:A:248:THR:HG22	1:A:486:TYR:HD2	1.31	0.88
1:A:113:ASP:OD2	5:A:601:HOH:O	1.91	0.88
1:A:248:THR:HA	1:A:486:TYR:CE2	2.10	0.87
1:B:248:THR:HA	1:B:486:TYR:CE2	2.10	0.87
2:A:506:NAG:H61	2:C:505:NAG:H61	1.56	0.86
2:A:506:NAG:HO3	1:C:409:SER:HG	1.02	0.86
1:D:297:THR:O	1:D:329:ALA:HB1	1.76	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:297:THR:O	1:B:329:ALA:HB1	1.76	0.86
1:C:297:THR:O	1:C:329:ALA:HB1	1.76	0.86
1:A:297:THR:O	1:A:329:ALA:HB1	1.76	0.85
1:D:422:GLN:NE2	1:D:438:PRO:HD3	1.93	0.84
1:A:248:THR:CA	1:A:486:TYR:HE2	1.91	0.83
1:C:422:GLN:NE2	1:C:437:PRO:HA	1.93	0.83
1:A:422:GLN:NE2	1:A:437:PRO:HA	1.93	0.83
1:B:422:GLN:NE2	1:B:438:PRO:HD3	1.93	0.83
1:B:248:THR:CA	1:B:486:TYR:HE2	1.90	0.83
1:B:422:GLN:HE22	1:B:438:PRO:HD3	1.45	0.81
1:D:65:VAL:HB	1:D:115:SER:HB3	1.62	0.81
1:B:65:VAL:HB	1:B:115:SER:HB3	1.62	0.81
1:A:65:VAL:HB	1:A:115:SER:HB3	1.62	0.81
2:D:504:NAG:H83	1:C:291:SER:OG	1.80	0.81
1:C:65:VAL:HB	1:C:115:SER:HB3	1.62	0.80
1:D:422:GLN:HE22	1:D:438:PRO:HD3	1.45	0.80
1:A:248:THR:CG2	1:A:486:TYR:CE2	2.64	0.80
2:D:504:NAG:HN2	2:C:508:NAG:C6	1.94	0.80
1:C:85:VAL:O	1:C:86:LEU:HD23	1.82	0.80
1:B:248:THR:CG2	1:B:486:TYR:CE2	2.65	0.80
1:D:85:VAL:O	1:D:86:LEU:HD23	1.82	0.80
1:C:297:THR:OG1	1:C:444:THR:OG1	1.99	0.80
1:A:297:THR:OG1	1:A:444:THR:OG1	1.99	0.79
1:A:85:VAL:O	1:A:86:LEU:HD23	1.82	0.78
1:B:85:VAL:O	1:B:86:LEU:HD23	1.82	0.78
1:C:87:ALA:O	1:C:88:ASN:HB3	1.85	0.77
1:C:248:THR:HG22	1:C:486:TYR:CE2	2.20	0.77
1:A:62:GLU:OE2	5:A:602:HOH:O	2.02	0.76
1:D:248:THR:HA	1:D:486:TYR:CE2	2.19	0.76
1:C:207:LYS:HG3	1:C:439:ILE:HG22	1.67	0.76
1:B:87:ALA:O	1:B:88:ASN:HB3	1.85	0.76
1:D:248:THR:HG22	1:D:486:TYR:CE2	2.20	0.76
1:A:87:ALA:O	1:A:88:ASN:HB3	1.85	0.76
1:A:404:ASN:OD1	1:C:408:ARG:CA	2.34	0.76
1:B:207:LYS:HG3	1:B:439:ILE:HG22	1.67	0.75
1:A:81:PRO:HD2	5:A:623:HOH:O	1.86	0.75
1:D:485:LYS:C	1:D:486:TYR:HD1	1.90	0.74
1:A:207:LYS:HG3	1:A:439:ILE:HG22	1.67	0.74
1:A:248:THR:CB	1:A:486:TYR:HE2	2.00	0.74
1:D:87:ALA:O	1:D:88:ASN:HB3	1.85	0.74
1:C:331:CYS:HB2	1:C:416:LEU:HD12	1.69	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:248:THR:CB	1:B:486:TYR:HE2	2.00	0.74
1:C:336:SER:O	1:C:339:ASN:HB2	1.88	0.74
1:B:336:SER:O	1:B:339:ASN:HB2	1.88	0.74
1:C:485:LYS:C	1:C:486:TYR:HD1	1.90	0.74
1:C:474:ASP:OD1	5:C:601:HOH:O	2.05	0.74
1:D:207:LYS:HG3	1:D:439:ILE:HG22	1.67	0.73
1:A:336:SER:O	1:A:339:ASN:HB2	1.88	0.73
2:D:503:NAG:H3	2:D:503:NAG:C8	2.18	0.73
2:C:503:NAG:H3	2:C:503:NAG:C8	2.18	0.73
1:D:336:SER:O	1:D:339:ASN:HB2	1.88	0.73
2:A:504:NAG:H3	2:A:504:NAG:C8	2.18	0.73
1:D:86:LEU:O	1:D:89:VAL:HG23	1.89	0.73
1:B:331:CYS:HB2	1:B:416:LEU:HD12	1.69	0.72
1:A:331:CYS:HB2	1:A:416:LEU:HD12	1.69	0.72
1:B:485:LYS:O	1:B:486:TYR:HD1	1.72	0.72
1:C:86:LEU:O	1:C:89:VAL:HG23	1.89	0.72
1:D:59:LYS:HE2	1:C:60:ALA:O	1.88	0.72
1:B:86:LEU:O	1:B:89:VAL:HG23	1.89	0.72
2:B:503:NAG:H3	2:B:503:NAG:C8	2.18	0.72
1:A:485:LYS:O	1:A:486:TYR:HD1	1.72	0.71
1:D:331:CYS:HB2	1:D:416:LEU:HD12	1.69	0.71
1:C:248:THR:HA	1:C:486:TYR:CE2	2.19	0.71
1:A:423:ILE:C	1:A:424:ILE:HG12	2.12	0.70
1:A:86:LEU:O	1:A:89:VAL:HG23	1.89	0.70
1:A:109:ILE:HG23	5:A:601:HOH:O	1.91	0.70
1:D:59:LYS:HE2	1:C:60:ALA:C	2.12	0.69
1:B:224:ALA:O	1:B:489:VAL:HG22	1.93	0.69
1:C:224:ALA:O	1:C:489:VAL:HG22	1.93	0.69
1:D:332:ASN:OD1	1:D:415:THR:HG22	1.92	0.69
1:A:364:SER:HB3	5:A:603:HOH:O	1.92	0.69
1:B:332:ASN:OD1	1:B:415:THR:HG22	1.92	0.69
1:A:326:ILE:HD13	1:A:438:PRO:HG2	1.74	0.69
1:C:423:ILE:C	1:C:424:ILE:HG12	2.13	0.69
1:D:224:ALA:O	1:D:489:VAL:HG22	1.93	0.69
1:D:326:ILE:HD13	1:D:438:PRO:HG2	1.74	0.69
1:D:423:ILE:C	1:D:424:ILE:HG12	2.13	0.68
1:A:224:ALA:O	1:A:489:VAL:HG22	1.93	0.68
1:C:226:LEU:HD12	1:C:489:VAL:HG11	1.76	0.68
1:D:59:LYS:HB3	1:D:61:TYR:CZ	2.29	0.68
1:B:226:LEU:HD12	1:B:489:VAL:HG11	1.76	0.68
1:D:226:LEU:HD12	1:D:489:VAL:HG11	1.76	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:423:ILE:C	1:B:424:ILE:HG12	2.13	0.68
1:A:59:LYS:HB3	1:A:61:TYR:CZ	2.29	0.67
1:C:78:ASP:OD2	1:C:80:ASN:OD1	2.13	0.67
1:A:349:LEU:HD13	1:A:468:PHE:CE1	2.30	0.67
1:C:201:ILE:HD12	5:C:612:HOH:O	1.94	0.67
1:B:349:LEU:HD13	1:B:468:PHE:CE1	2.30	0.67
1:D:349:LEU:HD13	1:D:468:PHE:CE1	2.30	0.67
2:D:504:NAG:C8	2:C:508:NAG:H62	2.24	0.67
1:B:59:LYS:HB3	1:B:61:TYR:CZ	2.29	0.67
1:C:59:LYS:HB3	1:C:61:TYR:CZ	2.29	0.67
1:B:370:GLU:OE1	1:B:425:ASN:HB2	1.95	0.67
1:A:230:ASN:HB3	1:A:233:PHE:HB2	1.78	0.66
1:A:370:GLU:OE1	1:A:425:ASN:HB2	1.95	0.66
1:A:403:TYR:O	2:A:506:NAG:H81	1.96	0.66
1:C:370:GLU:OE1	1:C:425:ASN:HB2	1.95	0.66
1:A:332:ASN:OD1	1:A:415:THR:HG22	1.96	0.66
1:D:78:ASP:OD2	1:D:80:ASN:OD1	2.13	0.66
1:A:226:LEU:HD12	1:A:489:VAL:HG11	1.76	0.66
1:B:64:GLU:HG2	1:B:209:SER:O	1.96	0.66
1:C:332:ASN:OD1	1:C:415:THR:HG22	1.96	0.66
1:B:353:PHE:HE2	1:B:456:ARG:NH1	1.94	0.66
1:D:64:GLU:HG2	1:D:209:SER:O	1.96	0.66
1:C:64:GLU:HG2	1:C:209:SER:O	1.96	0.66
1:C:403:TYR:O	2:C:505:NAG:H81	1.96	0.66
1:B:230:ASN:HB3	1:B:233:PHE:HB2	1.78	0.66
1:D:230:ASN:HB3	1:D:233:PHE:HB2	1.78	0.66
1:C:349:LEU:HD13	1:C:468:PHE:CE1	2.30	0.66
1:A:353:PHE:HE2	1:A:456:ARG:NH1	1.94	0.66
1:B:403:TYR:O	2:B:505:NAG:H81	1.96	0.66
1:D:403:TYR:O	2:D:505:NAG:H81	1.96	0.66
1:D:370:GLU:OE1	1:D:425:ASN:HB2	1.95	0.65
1:C:230:ASN:HB3	1:C:233:PHE:HB2	1.78	0.65
2:D:504:NAG:H82	2:C:508:NAG:H62	1.78	0.65
1:C:422:GLN:HE22	1:C:438:PRO:CD	2.07	0.65
1:A:64:GLU:HG2	1:A:209:SER:O	1.96	0.65
1:C:353:PHE:HE2	1:C:456:ARG:HH11	1.45	0.65
1:A:353:PHE:HE2	1:A:456:ARG:HH11	1.45	0.64
1:C:353:PHE:HE2	1:C:456:ARG:NH1	1.94	0.64
1:B:353:PHE:HE2	1:B:456:ARG:HH11	1.45	0.64
1:D:353:PHE:HE2	1:D:456:ARG:HH11	1.45	0.64
1:B:341:THR:O	1:B:345:VAL:HG23	1.98	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:353:PHE:HE2	1:D:456:ARG:NH1	1.94	0.64
1:A:246:GLN:OE1	1:A:246:GLN:HA	1.98	0.63
1:D:485:LYS:HG2	1:D:486:TYR:CE1	2.33	0.63
1:C:283:THR:HA	1:C:455:LEU:CD2	2.29	0.63
1:C:341:THR:O	1:C:345:VAL:HG23	1.99	0.63
1:A:422:GLN:HE22	1:A:438:PRO:CD	2.07	0.63
1:A:283:THR:HA	1:A:455:LEU:CD2	2.29	0.63
1:D:59:LYS:NZ	1:C:61:TYR:HA	2.13	0.63
2:C:503:NAG:H83	2:C:503:NAG:C3	2.27	0.63
1:D:283:THR:HA	1:D:455:LEU:CD2	2.29	0.63
1:C:485:LYS:HG2	1:C:486:TYR:CE1	2.33	0.63
1:A:341:THR:O	1:A:345:VAL:HG23	1.99	0.63
1:C:246:GLN:HA	1:C:246:GLN:OE1	1.98	0.63
1:C:370:GLU:CD	1:C:425:ASN:HB2	2.20	0.63
1:B:370:GLU:CD	1:B:425:ASN:HB2	2.19	0.63
1:B:283:THR:HA	1:B:455:LEU:CD2	2.29	0.62
2:D:504:NAG:C7	2:C:508:NAG:H62	2.29	0.62
1:A:331:CYS:O	1:A:415:THR:HA	1.99	0.62
1:D:341:THR:O	1:D:345:VAL:HG23	1.99	0.62
2:D:503:NAG:H83	2:D:503:NAG:C3	2.27	0.62
1:C:369:LEU:HD23	1:C:421:LYS:HE3	1.81	0.62
1:A:370:GLU:CD	1:A:425:ASN:HB2	2.20	0.62
1:B:369:LEU:HD23	1:B:421:LYS:HE3	1.81	0.62
1:A:369:LEU:HD23	1:A:421:LYS:HE3	1.81	0.61
1:D:369:LEU:HD23	1:D:421:LYS:HE3	1.81	0.61
1:D:370:GLU:CD	1:D:425:ASN:HB2	2.20	0.61
1:C:201:ILE:CD1	5:C:612:HOH:O	2.47	0.61
1:B:331:CYS:O	1:B:415:THR:HA	1.99	0.61
1:B:248:THR:CB	1:B:486:TYR:CE2	2.83	0.61
1:C:331:CYS:O	1:C:415:THR:HA	1.99	0.61
1:A:93:PHE:CE2	1:A:228:CYS:HB2	2.36	0.61
1:D:93:PHE:CE2	1:D:228:CYS:HB2	2.36	0.61
1:D:331:CYS:O	1:D:415:THR:HA	1.99	0.61
1:C:326:ILE:HD11	5:C:604:HOH:O	2.00	0.61
1:C:93:PHE:CE2	1:C:228:CYS:HB2	2.36	0.61
1:A:406:THR:HG21	5:A:629:HOH:O	2.01	0.60
2:B:503:NAG:H83	2:B:503:NAG:C3	2.27	0.60
1:C:90:THR:O	1:C:90:THR:HG22	2.01	0.60
1:D:422:GLN:OE1	1:D:422:GLN:N	2.35	0.60
1:B:93:PHE:CE2	1:B:228:CYS:HB2	2.36	0.60
1:D:90:THR:HG22	1:D:90:THR:O	2.01	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:504:NAG:H83	2:A:504:NAG:C3	2.27	0.60
1:A:248:THR:CB	1:A:486:TYR:CE2	2.83	0.59
1:D:485:LYS:HG2	1:D:486:TYR:HE1	1.67	0.59
1:A:80:ASN:HA	5:A:623:HOH:O	2.01	0.59
1:B:90:THR:HG22	1:B:90:THR:O	2.01	0.59
1:A:428:GLN:HG2	5:A:601:HOH:O	2.01	0.59
1:D:363:PRO:HB3	1:D:388:SER:HA	1.85	0.59
1:B:363:PRO:HB3	1:B:388:SER:HA	1.85	0.59
1:B:422:GLN:N	1:B:422:GLN:OE1	2.35	0.59
1:D:229:ASN:N	1:D:229:ASN:HD22	2.01	0.59
1:B:229:ASN:N	1:B:229:ASN:HD22	2.01	0.59
1:C:485:LYS:HG2	1:C:486:TYR:HE1	1.67	0.59
1:A:90:THR:HG22	1:A:90:THR:O	2.01	0.59
1:C:55:ALA:HA	1:C:75:VAL:O	2.03	0.59
1:B:55:ALA:HA	1:B:75:VAL:O	2.03	0.59
1:D:246:GLN:HG2	5:D:625:HOH:O	2.01	0.59
1:C:86:LEU:HD13	1:C:89:VAL:HG21	1.84	0.59
1:C:363:PRO:HB3	1:C:388:SER:HA	1.85	0.58
1:A:408:ARG:HA	1:C:404:ASN:OD1	2.04	0.58
1:D:55:ALA:HA	1:D:75:VAL:O	2.03	0.58
1:A:363:PRO:HB3	1:A:388:SER:HA	1.85	0.58
1:B:86:LEU:HD13	1:B:89:VAL:HG21	1.84	0.58
1:A:80:ASN:OD1	1:A:80:ASN:O	2.22	0.58
1:B:421:LYS:C	1:B:422:GLN:OE1	2.42	0.58
1:A:55:ALA:HA	1:A:75:VAL:O	2.03	0.58
1:A:86:LEU:HD13	1:A:89:VAL:HG21	1.84	0.58
1:D:86:LEU:HD13	1:D:89:VAL:HG21	1.84	0.57
1:B:422:GLN:OE1	1:B:422:GLN:CA	2.52	0.57
1:D:422:GLN:OE1	1:D:422:GLN:CA	2.52	0.57
1:A:404:ASN:OD1	1:C:408:ARG:CB	2.51	0.57
1:D:59:LYS:HB3	1:D:61:TYR:CE2	2.40	0.57
1:B:59:LYS:HB3	1:B:61:TYR:CE2	2.40	0.57
1:C:369:LEU:CD2	1:C:421:LYS:HE3	2.34	0.57
1:B:80:ASN:OD1	1:B:80:ASN:O	2.22	0.57
1:A:369:LEU:CD2	1:A:421:LYS:HE3	2.34	0.57
1:A:59:LYS:HB3	1:A:61:TYR:CE2	2.40	0.57
1:C:454:LEU:O	1:C:455:LEU:HD23	2.05	0.57
1:D:369:LEU:CD2	1:D:421:LYS:HE3	2.34	0.57
1:C:84:MET:HG2	1:C:86:LEU:HD23	1.87	0.57
1:C:406:THR:CG2	5:C:633:HOH:O	2.53	0.57
1:A:382:PHE:CG	1:A:424:ILE:HD12	2.40	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:358:THR:HG22	1:C:396:ARG:HG3	1.87	0.56
1:A:454:LEU:O	1:A:455:LEU:HD23	2.04	0.56
1:B:369:LEU:CD2	1:B:421:LYS:HE3	2.34	0.56
1:D:421:LYS:C	1:D:422:GLN:OE1	2.42	0.56
1:A:86:LEU:HB2	1:A:89:VAL:CG2	2.35	0.56
1:B:454:LEU:O	1:B:455:LEU:HD23	2.05	0.56
1:D:228:CYS:C	1:D:229:ASN:HD22	2.08	0.56
1:D:240:ARG:HG2	5:D:601:HOH:O	2.04	0.56
1:C:59:LYS:HB3	1:C:61:TYR:CE2	2.40	0.56
1:C:86:LEU:HB2	1:C:89:VAL:CG2	2.36	0.56
1:A:84:MET:HG2	1:A:86:LEU:HD23	1.87	0.56
1:D:454:LEU:O	1:D:455:LEU:HD23	2.05	0.56
1:A:105:HIS:ND1	1:A:476:ARG:HG3	2.21	0.56
1:A:248:THR:CG2	1:A:486:TYR:HE2	2.13	0.56
1:B:84:MET:HG2	1:B:86:LEU:HD23	1.87	0.56
1:C:65:VAL:CB	1:C:115:SER:HB3	2.36	0.56
1:B:246:GLN:OE1	1:B:246:GLN:HA	2.06	0.56
1:D:358:THR:HG22	1:D:396:ARG:HG3	1.88	0.55
1:C:80:ASN:OD1	1:C:80:ASN:O	2.24	0.55
1:C:426:MET:CE	1:C:429:GLU:HG2	2.37	0.55
1:A:228:CYS:C	1:A:229:ASN:HD22	2.09	0.55
1:B:111:LEU:C	1:B:111:LEU:HD23	2.27	0.55
1:D:86:LEU:HB2	1:D:89:VAL:CG2	2.35	0.55
1:A:358:THR:HG22	1:A:396:ARG:HG3	1.87	0.55
1:B:228:CYS:C	1:B:229:ASN:HD22	2.08	0.55
1:C:49:LYS:HB3	5:C:634:HOH:O	2.06	0.55
1:C:105:HIS:ND1	1:C:476:ARG:HG3	2.21	0.55
1:B:86:LEU:HB2	1:B:89:VAL:CG2	2.36	0.55
1:D:84:MET:HG2	1:D:86:LEU:HD23	1.87	0.55
1:D:111:LEU:C	1:D:111:LEU:HD23	2.27	0.55
1:A:111:LEU:HD23	1:A:111:LEU:C	2.27	0.55
1:C:65:VAL:HB	1:C:115:SER:CB	2.36	0.55
1:A:119:CYS:N	1:A:205:CYS:HB3	2.22	0.55
1:D:105:HIS:ND1	1:D:476:ARG:HG3	2.21	0.55
1:B:358:THR:HG22	1:B:396:ARG:HG3	1.88	0.54
1:D:80:ASN:OD1	1:D:80:ASN:O	2.24	0.54
1:D:119:CYS:N	1:D:205:CYS:HB3	2.22	0.54
1:D:246:GLN:OE1	1:D:246:GLN:HA	2.06	0.54
1:C:228:CYS:C	1:C:229:ASN:HD22	2.09	0.54
1:B:53:PHE:H	1:B:53:PHE:HD2	1.55	0.54
1:B:105:HIS:ND1	1:B:476:ARG:HG3	2.21	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:119:CYS:N	1:B:205:CYS:HB3	2.22	0.54
1:C:119:CYS:N	1:C:205:CYS:HB3	2.22	0.54
1:A:65:VAL:CB	1:A:115:SER:HB3	2.36	0.54
1:B:226:LEU:HD22	1:B:242:VAL:CG1	2.38	0.54
1:D:383:PHE:C	1:D:384:TYR:HD2	2.10	0.54
1:D:426:MET:CE	1:D:429:GLU:HG2	2.37	0.54
1:C:294:ILE:HD12	1:C:333:ILE:HD11	1.88	0.54
1:A:50:THR:HG21	1:A:223:PHE:CD2	2.43	0.54
1:A:334:ASN:HB3	1:A:337:LYS:HB2	1.90	0.54
1:A:426:MET:CE	1:A:429:GLU:HG2	2.37	0.54
1:D:294:ILE:HD12	1:D:333:ILE:HD11	1.89	0.54
1:C:111:LEU:HD23	1:C:111:LEU:C	2.27	0.54
1:C:226:LEU:HD22	1:C:242:VAL:CG1	2.38	0.54
1:B:426:MET:CE	1:B:429:GLU:HG2	2.37	0.54
1:D:53:PHE:H	1:D:53:PHE:HD2	1.55	0.54
1:D:334:ASN:HB3	1:D:337:LYS:HB2	1.90	0.54
1:B:248:THR:CG2	1:B:486:TYR:HE2	2.13	0.54
1:D:50:THR:HG21	1:D:223:PHE:CD2	2.43	0.54
1:D:226:LEU:HD22	1:D:242:VAL:CG1	2.38	0.54
1:C:50:THR:HG21	1:C:223:PHE:CD2	2.43	0.53
1:C:354:PRO:HD2	5:C:611:HOH:O	2.07	0.53
1:A:229:ASN:HD22	1:A:229:ASN:N	2.06	0.53
1:A:358:THR:CG2	1:A:396:ARG:HG3	2.38	0.53
1:D:65:VAL:HB	1:D:115:SER:CB	2.36	0.53
1:B:358:THR:CG2	1:B:396:ARG:HG3	2.38	0.53
1:B:50:THR:HG21	1:B:223:PHE:CD2	2.43	0.53
1:B:334:ASN:HB3	1:B:337:LYS:HB2	1.91	0.53
1:B:65:VAL:CB	1:B:115:SER:HB3	2.36	0.53
1:D:358:THR:CG2	1:D:396:ARG:HG3	2.38	0.53
1:A:65:VAL:HB	1:A:115:SER:CB	2.36	0.53
1:A:226:LEU:HD22	1:A:242:VAL:CG1	2.38	0.53
1:C:229:ASN:HD22	1:C:229:ASN:N	2.06	0.53
1:A:85:VAL:HG12	1:A:86:LEU:N	2.24	0.53
1:C:422:GLN:HE21	1:C:437:PRO:HA	1.71	0.53
1:A:229:ASN:HB2	1:A:241:ASN:O	2.09	0.53
1:A:422:GLN:HE21	1:A:437:PRO:HA	1.71	0.53
1:C:358:THR:CG2	1:C:396:ARG:HG3	2.38	0.53
1:D:85:VAL:HG12	1:D:86:LEU:N	2.24	0.52
1:D:229:ASN:HB2	1:D:241:ASN:O	2.10	0.52
1:C:229:ASN:HB2	1:C:241:ASN:O	2.09	0.52
1:C:225:ILE:HG21	1:C:486:TYR:HD2	1.74	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:225:ILE:HG21	1:D:486:TYR:HD2	1.74	0.52
1:B:229:ASN:HB2	1:B:241:ASN:O	2.10	0.52
2:D:508:NAG:C5	2:C:501:NAG:H61	2.40	0.52
1:C:85:VAL:HG12	1:C:86:LEU:N	2.24	0.52
2:A:506:NAG:O4	1:C:412:GLY:HA2	2.10	0.51
1:B:85:VAL:HG12	1:B:86:LEU:N	2.24	0.51
1:B:423:ILE:HD11	1:C:423:ILE:HG21	1.92	0.51
1:C:334:ASN:HB3	1:C:337:LYS:HB2	1.90	0.51
1:A:406:THR:CG2	5:A:629:HOH:O	2.58	0.51
1:D:485:LYS:C	1:D:486:TYR:CD1	2.79	0.51
1:D:257:THR:O	1:D:259:LEU:N	2.44	0.51
2:C:503:NAG:C8	2:C:503:NAG:C3	2.83	0.51
1:A:257:THR:O	1:A:259:LEU:N	2.44	0.50
1:C:419:LYS:NZ	5:C:602:HOH:O	2.11	0.50
1:B:201:ILE:HD12	5:B:603:HOH:O	2.10	0.50
1:D:65:VAL:CB	1:D:115:SER:HB3	2.36	0.50
1:A:374:HIS:NE2	1:A:376:PHE:CD1	2.80	0.50
1:B:374:HIS:NE2	1:B:376:PHE:CD1	2.80	0.50
1:C:485:LYS:C	1:C:486:TYR:CD1	2.79	0.50
1:D:53:PHE:HD2	1:D:53:PHE:N	2.10	0.49
1:D:374:HIS:NE2	1:D:376:PHE:CD1	2.80	0.49
1:B:53:PHE:N	1:B:53:PHE:CD2	2.81	0.49
1:C:374:HIS:NE2	1:C:376:PHE:CD1	2.80	0.49
1:C:257:THR:O	1:C:259:LEU:N	2.44	0.49
1:B:257:THR:O	1:B:259:LEU:N	2.44	0.49
1:C:270:ILE:C	1:C:271:ILE:HD12	2.34	0.49
1:A:270:ILE:C	1:A:271:ILE:HD12	2.34	0.49
1:C:375:SER:O	1:C:376:PHE:HB3	2.13	0.49
1:B:53:PHE:HD2	1:B:53:PHE:N	2.11	0.48
1:B:270:ILE:C	1:B:271:ILE:HD12	2.34	0.48
1:B:279:ASN:HA	5:B:609:HOH:O	2.13	0.48
1:B:384:TYR:OH	1:B:424:ILE:HD13	2.13	0.48
1:D:53:PHE:N	1:D:53:PHE:CD2	2.81	0.48
1:D:86:LEU:HB2	1:D:89:VAL:HG21	1.95	0.48
1:D:406:THR:HG22	1:D:406:THR:O	2.14	0.48
1:D:375:SER:O	1:D:376:PHE:HB3	2.13	0.48
1:B:65:VAL:HB	1:B:115:SER:CB	2.36	0.48
1:B:264:SER:OG	1:B:482:GLU:OE2	2.31	0.48
1:B:375:SER:O	1:B:376:PHE:HB3	2.13	0.48
1:D:359:ILE:HB	1:D:395:TYR:HB3	1.96	0.48
1:D:59:LYS:CE	1:C:60:ALA:O	2.61	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:406:THR:O	1:A:406:THR:HG22	2.13	0.48
1:B:406:THR:HG22	1:B:406:THR:O	2.14	0.48
1:D:270:ILE:C	1:D:271:ILE:HD12	2.34	0.48
1:A:86:LEU:HB2	1:A:89:VAL:HG21	1.95	0.48
1:C:264:SER:OG	1:C:482:GLU:OE2	2.31	0.48
1:A:359:ILE:HB	1:A:395:TYR:HB3	1.96	0.48
1:D:327:ARG:HD2	1:D:420:ILE:O	2.14	0.48
1:D:333:ILE:HD12	1:D:390:LEU:CD1	2.44	0.48
1:B:86:LEU:HB2	1:B:89:VAL:HG21	1.95	0.48
1:C:86:LEU:HB2	1:C:89:VAL:HG21	1.95	0.48
1:C:359:ILE:HB	1:C:395:TYR:HB3	1.96	0.48
1:C:384:TYR:OH	1:C:424:ILE:HD13	2.13	0.47
1:B:333:ILE:HD12	1:B:390:LEU:CD1	2.44	0.47
1:C:353:PHE:CE2	1:C:456:ARG:NH1	2.77	0.47
1:B:327:ARG:HD2	1:B:420:ILE:O	2.14	0.47
1:C:394:THR:HG22	1:C:395:TYR:N	2.30	0.47
1:A:226:LEU:CD1	1:A:489:VAL:HG11	2.44	0.47
1:B:359:ILE:HB	1:B:395:TYR:HB3	1.96	0.47
1:C:486:TYR:CD1	1:C:486:TYR:N	2.82	0.47
1:B:422:GLN:HG2	1:C:432:ARG:HH22	1.79	0.47
1:D:337:LYS:HD3	1:D:337:LYS:HA	1.80	0.47
1:D:389:ASP:O	1:D:414:ILE:HD13	2.15	0.47
1:D:486:TYR:CD1	1:D:486:TYR:N	2.82	0.47
1:A:333:ILE:HD12	1:A:390:LEU:CD1	2.44	0.47
1:B:333:ILE:HD12	1:B:390:LEU:HD13	1.97	0.47
1:B:389:ASP:O	1:B:414:ILE:HD13	2.15	0.47
1:C:327:ARG:HD2	1:C:420:ILE:O	2.14	0.47
1:C:333:ILE:HD12	1:C:390:LEU:CD1	2.44	0.47
1:C:406:THR:HG21	5:C:633:HOH:O	2.14	0.47
1:A:375:SER:O	1:A:376:PHE:HB3	2.13	0.47
1:A:394:THR:HG22	1:A:395:TYR:N	2.30	0.47
1:B:434:ILE:CD1	1:C:434:ILE:HD11	2.45	0.47
1:C:486:TYR:HD1	1:C:486:TYR:N	2.13	0.47
1:D:249:HIS:ND1	1:D:486:TYR:OH	2.30	0.47
1:D:333:ILE:HD12	1:D:390:LEU:HD13	1.97	0.47
1:A:327:ARG:HD2	1:A:420:ILE:O	2.14	0.47
1:C:333:ILE:HD12	1:C:390:LEU:HD13	1.97	0.47
1:A:389:ASP:O	1:A:414:ILE:HD13	2.15	0.46
1:A:333:ILE:HD12	1:A:390:LEU:HD13	1.97	0.46
1:B:84:MET:HB3	1:B:244:THR:HB	1.97	0.46
1:D:59:LYS:CE	1:C:61:TYR:HA	2.45	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:486:TYR:HD1	1:D:486:TYR:N	2.13	0.46
1:A:84:MET:HB3	1:A:244:THR:HB	1.97	0.46
1:A:265:LEU:HA	1:A:265:LEU:HD23	1.54	0.46
1:C:337:LYS:HD3	1:C:337:LYS:HA	1.80	0.46
1:D:118:PRO:HB2	1:D:120:VAL:O	2.16	0.46
1:A:49:LYS:HB3	1:A:50:THR:H	1.63	0.46
1:A:485:LYS:O	1:A:486:TYR:CD1	2.61	0.46
1:D:394:THR:HG22	1:D:395:TYR:N	2.30	0.46
1:C:84:MET:HB3	1:C:244:THR:HB	1.97	0.46
1:B:118:PRO:HB2	1:B:120:VAL:O	2.16	0.46
1:B:226:LEU:CD1	1:B:489:VAL:HG11	2.44	0.46
1:B:282:LYS:HA	1:B:282:LYS:HD3	1.68	0.46
1:C:349:LEU:HD23	1:C:349:LEU:HA	1.69	0.46
1:C:422:GLN:NE2	1:C:438:PRO:HD3	2.11	0.46
1:A:422:GLN:NE2	1:A:438:PRO:HD3	2.11	0.46
1:D:84:MET:HB3	1:D:244:THR:HB	1.97	0.46
1:C:389:ASP:O	1:C:414:ILE:HD13	2.15	0.46
1:A:349:LEU:HA	1:A:349:LEU:HD23	1.69	0.46
1:D:386:ASN:O	1:D:416:LEU:HD22	2.16	0.46
1:C:269:GLU:O	1:C:271:ILE:CD1	2.64	0.46
1:A:264:SER:OG	1:A:482:GLU:OE2	2.31	0.45
1:A:353:PHE:CE2	1:A:456:ARG:NH1	2.77	0.45
1:A:269:GLU:O	1:A:271:ILE:CD1	2.64	0.45
1:D:57:ASP:HB3	1:C:61:TYR:O	2.15	0.45
1:D:485:LYS:CG	1:D:486:TYR:CE1	3.00	0.45
1:C:406:THR:O	1:C:406:THR:HG22	2.14	0.45
1:C:485:LYS:CG	1:C:486:TYR:CE1	2.99	0.45
1:A:331:CYS:CB	1:A:416:LEU:HD12	2.44	0.45
1:B:269:GLU:O	1:B:271:ILE:CD1	2.64	0.45
1:B:331:CYS:CB	1:B:416:LEU:HD12	2.44	0.45
1:D:264:SER:OG	1:D:482:GLU:OE2	2.31	0.45
1:B:290:GLU:CD	2:B:503:NAG:H81	2.37	0.45
1:D:269:GLU:O	1:D:271:ILE:CD1	2.64	0.45
1:A:386:ASN:O	1:A:416:LEU:HD22	2.16	0.45
1:D:226:LEU:CD1	1:D:489:VAL:HG11	2.44	0.45
1:D:290:GLU:CD	2:D:503:NAG:H81	2.37	0.45
1:C:67:ASN:O	1:C:71:THR:HG23	2.17	0.45
1:C:118:PRO:HB2	1:C:120:VAL:O	2.16	0.45
1:A:118:PRO:HB2	1:A:120:VAL:O	2.16	0.45
1:B:386:ASN:O	1:B:416:LEU:HD22	2.16	0.45
1:C:386:ASN:O	1:C:416:LEU:HD22	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:379:ARG:NH1	1:D:444:THR:H	2.15	0.45
1:C:249:HIS:ND1	1:C:486:TYR:OH	2.30	0.45
1:B:79:PRO:O	1:B:81:PRO:HD3	2.17	0.45
1:B:394:THR:HG22	1:B:395:TYR:N	2.30	0.45
1:C:290:GLU:CD	2:C:503:NAG:H81	2.37	0.45
1:B:379:ARG:NH1	1:B:444:THR:H	2.15	0.45
1:B:275:GLU:OE1	1:B:282:LYS:HE3	2.17	0.45
1:B:337:LYS:HD3	1:B:337:LYS:HA	1.84	0.45
1:D:67:ASN:O	1:D:71:THR:HG23	2.17	0.45
2:D:504:NAG:H82	2:C:508:NAG:C6	2.47	0.45
1:A:379:ARG:NH1	1:A:444:THR:H	2.15	0.44
1:A:476:ARG:HA	1:A:479:TRP:CD1	2.53	0.44
1:B:52:LEU:HB3	1:B:218:CYS:O	2.18	0.44
1:B:349:LEU:HD23	1:B:349:LEU:HA	1.69	0.44
1:C:79:PRO:O	1:C:81:PRO:HD3	2.17	0.44
1:C:379:ARG:NH1	1:C:444:THR:H	2.15	0.44
1:A:275:GLU:OE1	1:A:282:LYS:HE3	2.17	0.44
1:B:476:ARG:HA	1:B:479:TRP:CD1	2.52	0.44
1:D:297:THR:HG22	1:D:330:HIS:NE2	2.32	0.44
1:D:476:ARG:HA	1:D:479:TRP:CD1	2.52	0.44
1:C:275:GLU:OE1	1:C:282:LYS:HE3	2.17	0.44
1:C:330:HIS:HA	1:C:416:LEU:O	2.18	0.44
1:A:225:ILE:HB	1:A:245:VAL:HG23	2.00	0.44
1:A:286:VAL:HB	1:A:452:LEU:HB2	1.99	0.44
1:A:290:GLU:CD	2:A:504:NAG:H81	2.37	0.44
1:B:67:ASN:O	1:B:71:THR:HG23	2.17	0.44
1:A:67:ASN:O	1:A:71:THR:HG23	2.17	0.44
1:A:79:PRO:O	1:A:81:PRO:HD3	2.17	0.44
1:A:330:HIS:HA	1:A:416:LEU:O	2.18	0.44
1:A:388:SER:O	1:A:392:ASN:HB2	2.18	0.44
1:B:297:THR:HG22	1:B:330:HIS:NE2	2.32	0.44
1:B:485:LYS:O	1:B:486:TYR:CD1	2.61	0.44
1:D:388:SER:O	1:D:392:ASN:HB2	2.18	0.44
1:A:52:LEU:HB3	1:A:218:CYS:O	2.18	0.44
1:B:242:VAL:HG12	1:B:243:SER:N	2.33	0.44
1:D:330:HIS:HA	1:D:416:LEU:O	2.18	0.44
1:D:451:GLY:C	1:D:452:LEU:HD23	2.38	0.44
1:C:286:VAL:HB	1:C:452:LEU:HB2	1.99	0.44
1:C:388:SER:O	1:C:392:ASN:HB2	2.18	0.44
1:C:476:ARG:HA	1:C:479:TRP:CD1	2.53	0.44
1:D:79:PRO:O	1:D:81:PRO:HD3	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:242:VAL:HG12	1:D:243:SER:N	2.33	0.44
1:A:242:VAL:HG12	1:A:243:SER:N	2.33	0.44
1:A:365:SER:OG	1:A:366:GLY:N	2.51	0.44
1:B:265:LEU:HA	1:B:265:LEU:HD23	1.54	0.44
1:B:330:HIS:HA	1:B:416:LEU:O	2.18	0.44
1:D:265:LEU:HA	1:D:265:LEU:HD23	1.54	0.44
1:C:282:LYS:HA	1:C:282:LYS:HD3	1.68	0.44
1:A:66:HIS:CE1	1:A:212:PRO:HA	2.53	0.43
1:D:365:SER:OG	1:D:366:GLY:N	2.51	0.43
1:B:451:GLY:C	1:B:452:LEU:HD23	2.38	0.43
1:C:52:LEU:HB3	1:C:218:CYS:O	2.18	0.43
1:C:87:ALA:O	1:C:88:ASN:CB	2.62	0.43
1:C:298:ARG:NH1	1:C:326:ILE:O	2.49	0.43
1:C:331:CYS:CB	1:C:416:LEU:HD12	2.44	0.43
1:A:282:LYS:HA	1:A:282:LYS:HD3	1.68	0.43
1:B:286:VAL:HB	1:B:452:LEU:HB2	1.99	0.43
1:D:52:LEU:HB3	1:D:218:CYS:O	2.18	0.43
1:B:66:HIS:CE1	1:B:212:PRO:HA	2.53	0.43
1:B:434:ILE:HD12	1:C:434:ILE:HD11	2.00	0.43
1:D:275:GLU:OE1	1:D:282:LYS:HE3	2.17	0.43
1:C:225:ILE:HB	1:C:245:VAL:HG23	1.99	0.43
1:C:226:LEU:CD1	1:C:489:VAL:HG11	2.44	0.43
1:D:225:ILE:HB	1:D:245:VAL:HG23	2.00	0.43
1:D:286:VAL:HB	1:D:452:LEU:HB2	1.99	0.43
1:C:242:VAL:HG12	1:C:243:SER:N	2.33	0.43
1:B:225:ILE:HB	1:B:245:VAL:HG23	1.99	0.43
1:B:422:GLN:OE1	1:B:422:GLN:HA	2.19	0.43
1:D:231:LYS:NZ	1:C:442:GLU:OE1	2.51	0.43
1:D:384:TYR:HD2	1:D:384:TYR:N	2.17	0.43
1:B:365:SER:OG	1:B:366:GLY:N	2.51	0.43
1:B:388:SER:O	1:B:392:ASN:HB2	2.18	0.43
1:A:87:ALA:O	1:A:88:ASN:CB	2.62	0.43
1:A:451:GLY:C	1:A:452:LEU:HD23	2.39	0.43
1:B:384:TYR:N	1:B:384:TYR:CD2	2.87	0.43
1:D:66:HIS:CE1	1:D:212:PRO:HA	2.53	0.43
1:D:87:ALA:O	1:D:88:ASN:CB	2.62	0.43
1:C:384:TYR:O	1:C:418:CYS:HA	2.19	0.43
1:C:451:GLY:C	1:C:452:LEU:HD23	2.39	0.43
1:D:282:LYS:HA	1:D:282:LYS:HD3	1.68	0.43
1:C:365:SER:OG	1:C:366:GLY:N	2.51	0.43
1:C:384:TYR:N	1:C:384:TYR:CD2	2.87	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:384:TYR:N	1:D:384:TYR:CD2	2.87	0.43
1:C:49:LYS:HA	1:C:49:LYS:HD2	0.93	0.43
1:C:66:HIS:CE1	1:C:212:PRO:HA	2.53	0.43
1:A:404:ASN:OD1	1:C:408:ARG:HB2	2.19	0.42
1:A:364:SER:N	5:A:603:HOH:O	2.31	0.42
1:B:384:TYR:N	1:B:384:TYR:HD2	2.17	0.42
1:D:384:TYR:O	1:D:418:CYS:HA	2.19	0.42
1:D:384:TYR:OH	1:D:424:ILE:HD13	2.20	0.42
1:A:457:ASP:OD1	1:A:469:ARG:NH1	2.53	0.42
1:C:384:TYR:N	1:C:384:TYR:HD2	2.18	0.42
1:A:384:TYR:O	1:A:418:CYS:HA	2.19	0.42
1:B:384:TYR:O	1:B:418:CYS:HA	2.19	0.42
1:B:391:PHE:CE2	1:B:470:PRO:HB3	2.55	0.42
1:A:391:PHE:CE2	1:A:470:PRO:HB3	2.55	0.42
1:D:246:GLN:CG	5:D:625:HOH:O	2.65	0.42
1:D:298:ARG:C	1:D:298:ARG:HD2	2.40	0.42
1:C:426:MET:HA	5:C:616:HOH:O	2.19	0.42
1:A:298:ARG:NH1	1:A:326:ILE:O	2.49	0.42
1:A:354:PRO:HD2	5:A:614:HOH:O	2.19	0.42
1:B:119:CYS:HB3	1:C:122:LEU:HD21	2.01	0.42
1:D:391:PHE:CE2	1:D:470:PRO:HB3	2.55	0.42
1:C:422:GLN:HE22	1:C:437:PRO:HA	1.80	0.42
1:A:384:TYR:HD2	1:A:384:TYR:N	2.17	0.42
1:A:384:TYR:N	1:A:384:TYR:CD2	2.87	0.42
1:D:457:ASP:OD1	1:D:469:ARG:NH1	2.53	0.42
1:B:457:ASP:OD1	1:B:469:ARG:NH1	2.53	0.42
1:C:298:ARG:HD2	1:C:298:ARG:C	2.40	0.42
1:C:457:ASP:OD1	1:C:469:ARG:NH1	2.53	0.42
1:A:408:ARG:CA	1:C:404:ASN:OD1	2.68	0.41
1:B:451:GLY:O	1:B:452:LEU:HD23	2.21	0.41
1:C:481:SER:HB2	5:C:621:HOH:O	2.20	0.41
1:A:259:LEU:HB2	1:A:374:HIS:CE1	2.55	0.41
1:D:91:GLU:HG2	1:D:226:LEU:HD13	2.02	0.41
1:D:451:GLY:O	1:D:452:LEU:HD23	2.21	0.41
1:C:84:MET:O	1:C:243:SER:HB3	2.20	0.41
1:B:298:ARG:HD2	1:B:298:ARG:C	2.40	0.41
2:D:504:NAG:H82	2:C:508:NAG:C5	2.50	0.41
1:C:354:PRO:CD	5:C:611:HOH:O	2.67	0.41
1:C:391:PHE:CE2	1:C:470:PRO:HB3	2.55	0.41
1:B:298:ARG:NH1	1:B:326:ILE:O	2.49	0.41
1:D:84:MET:O	1:D:243:SER:HB3	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:360:LYS:HB2	1:D:467:THR:HB	2.02	0.41
1:C:91:GLU:HG2	1:C:226:LEU:HD13	2.02	0.41
1:C:265:LEU:HA	1:C:265:LEU:HD23	1.54	0.41
1:B:259:LEU:HB2	1:B:374:HIS:CE1	2.55	0.41
1:B:266:ALA:HB1	5:B:602:HOH:O	2.20	0.41
1:C:259:LEU:HB2	1:C:374:HIS:CE1	2.55	0.41
1:A:298:ARG:C	1:A:298:ARG:HD2	2.40	0.41
1:A:451:GLY:O	1:A:452:LEU:HD23	2.21	0.41
1:B:91:GLU:HG2	1:B:226:LEU:HD13	2.02	0.41
1:D:422:GLN:OE1	1:D:422:GLN:HA	2.19	0.41
1:C:86:LEU:HD12	1:C:89:VAL:CG2	2.37	0.41
1:C:451:GLY:O	1:C:452:LEU:HD23	2.21	0.41
1:A:91:GLU:HG2	1:A:226:LEU:HD13	2.02	0.41
1:B:84:MET:O	1:B:243:SER:HB3	2.20	0.41
1:D:94:ASN:ND2	1:D:97:LYS:HB2	2.36	0.41
1:D:353:PHE:CE2	1:D:456:ARG:NH1	2.77	0.41
1:C:484:TYR:CE2	1:C:485:LYS:HB3	2.56	0.41
1:A:80:ASN:HB3	5:A:617:HOH:O	2.21	0.41
1:A:426:MET:HA	5:A:611:HOH:O	2.20	0.41
1:A:422:GLN:HE22	1:A:437:PRO:HA	1.79	0.40
1:B:94:ASN:ND2	1:B:97:LYS:HB2	2.36	0.40
1:D:259:LEU:HB2	1:D:374:HIS:CE1	2.55	0.40
1:D:391:PHE:CD2	1:D:470:PRO:HG3	2.57	0.40
1:C:84:MET:CB	1:C:244:THR:HB	2.52	0.40
1:B:422:GLN:HG2	1:C:432:ARG:NH2	2.36	0.40
1:B:484:TYR:CE2	1:B:485:LYS:HB3	2.56	0.40
1:D:295:VAL:O	1:D:331:CYS:HA	2.22	0.40
1:C:94:ASN:ND2	1:C:97:LYS:HB2	2.36	0.40
1:A:84:MET:O	1:A:243:SER:HB3	2.20	0.40
1:A:298:ARG:HB2	1:A:329:ALA:HB2	2.04	0.40
1:D:254:VAL:HG11	1:D:261:LEU:HB2	2.03	0.40
1:D:298:ARG:NH1	1:D:326:ILE:O	2.49	0.40
1:C:254:VAL:HG11	1:C:261:LEU:HB2	2.03	0.40
1:A:273:ARG:HG2	1:A:273:ARG:HH11	1.86	0.40
1:B:295:VAL:O	1:B:331:CYS:HA	2.22	0.40
1:B:397:ASN:O	1:B:399:THR:HG23	2.22	0.40

All (4) 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:C:275:GLU:O	2:B:502:NAG:O3[1_655]	1.62	0.58
1:B:356:SER:OG	1:D:356:SER:OG[3_444]	2.01	0.19
1:B:202:THR:OG1	1:D:202:THR:OG1[4_455]	2.12	0.08
1:A:275:GLU:O	2:D:502:NAG:O3[3_444]	2.14	0.06

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	329/358 (92%)	299 (91%)	23 (7%)	7 (2%)	7 21
1	B	329/358 (92%)	299 (91%)	23 (7%)	7 (2%)	7 21
1	C	329/358 (92%)	299 (91%)	23 (7%)	7 (2%)	7 21
1	D	329/358 (92%)	299 (91%)	23 (7%)	7 (2%)	7 21
All	All	1316/1432 (92%)	1196 (91%)	92 (7%)	28 (2%)	7 21

All (28) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	88	ASN
1	B	88	ASN
1	D	88	ASN
1	C	88	ASN
1	A	86	LEU
1	A	339	ASN
1	B	86	LEU
1	B	339	ASN
1	D	86	LEU
1	D	339	ASN
1	C	86	LEU
1	C	339	ASN
1	A	230	ASN
1	A	240	ARG

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Mol	Chain	Res	Type
1	A	265	LEU
1	B	230	ASN
1	B	240	ARG
1	B	265	LEU
1	D	230	ASN
1	D	240	ARG
1	D	265	LEU
1	C	230	ASN
1	C	240	ARG
1	C	265	LEU
1	A	354	PRO
1	B	354	PRO
1	D	354	PRO
1	C	354	PRO

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	297/312 (95%)	273 (92%)	24 (8%)	11	30
1	B	297/312 (95%)	279 (94%)	18 (6%)	18	45
1	C	297/312 (95%)	274 (92%)	23 (8%)	13	32
1	D	297/312 (95%)	277 (93%)	20 (7%)	16	40
All	All	1188/1248 (95%)	1103 (93%)	85 (7%)	14	36

All (85) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	49	LYS
1	A	53	PHE
1	A	80	ASN
1	A	84	MET
1	A	86	LEU
1	A	91	GLU
1	A	103	GLN

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Mol	Chain	Res	Type
1	A	123	THR
1	A	229	ASN
1	A	232	THR
1	A	240	ARG
1	A	246	GLN
1	A	297	THR
1	A	326	ILE
1	A	337	LYS
1	A	353	PHE
1	A	356	SER
1	A	384	TYR
1	A	410	SER
1	A	422	GLN
1	A	424	ILE
1	A	447	SER
1	A	486	TYR
1	A	487	LYS
1	B	49	LYS
1	B	53	PHE
1	B	80	ASN
1	B	84	MET
1	B	86	LEU
1	B	91	GLU
1	B	103	GLN
1	B	229	ASN
1	B	240	ARG
1	B	337	LYS
1	B	353	PHE
1	B	356	SER
1	B	384	TYR
1	B	410	SER
1	B	422	GLN
1	B	447	SER
1	B	486	TYR
1	B	487	LYS
1	D	49	LYS
1	D	53	PHE
1	D	80	ASN
1	D	84	MET
1	D	86	LEU
1	D	91	GLU
1	D	103	GLN

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Mol	Chain	Res	Type
1	D	123	THR
1	D	229	ASN
1	D	240	ARG
1	D	294	ILE
1	D	326	ILE
1	D	337	LYS
1	D	353	PHE
1	D	356	SER
1	D	410	SER
1	D	422	GLN
1	D	447	SER
1	D	467	THR
1	D	486	TYR
1	C	49	LYS
1	C	53	PHE
1	C	80	ASN
1	C	84	MET
1	C	86	LEU
1	C	91	GLU
1	C	103	GLN
1	C	123	THR
1	C	229	ASN
1	C	240	ARG
1	C	246	GLN
1	C	294	ILE
1	C	297	THR
1	C	337	LYS
1	C	353	PHE
1	C	356	SER
1	C	384	TYR
1	C	410	SER
1	C	422	GLN
1	C	447	SER
1	C	467	THR
1	C	486	TYR
1	C	487	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	80	ASN
1	A	229	ASN

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Mol	Chain	Res	Type
1	A	411	ASN
1	B	80	ASN
1	B	229	ASN
1	B	411	ASN
1	D	229	ASN
1	D	411	ASN
1	C	229	ASN
1	C	411	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)

45 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	NAG	A	502	1	14,14,15	0.45	0	17,19,21	1.04	1 (5%)
2	NAG	B	502	1	14,14,15	0.49	0	17,19,21	0.60	0
2	NAG	B	507	1	14,14,15	0.68	1 (7%)	17,19,21	0.75	1 (5%)
3	I6M	B	509[A]	-	39,39,39	3.91	14 (35%)	48,55,55	1.89	10 (20%)
2	NAG	C	508	1	14,14,15	0.79	1 (7%)	17,19,21	0.61	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	NAG	B	508	1	14,14,15	0.79	1 (7%)	17,19,21	0.61	0
2	NAG	C	505	1	14,14,15	0.29	0	17,19,21	0.81	0
2	NAG	B	500	1	14,14,15	0.25	0	17,19,21	0.67	0
3	I6M	A	510[A]	-	39,39,39	3.74	14 (35%)	48,55,55	1.88	11 (22%)
2	NAG	D	506	1	14,14,15	0.76	1 (7%)	17,19,21	0.77	0
2	NAG	A	505	1	14,14,15	0.81	2 (14%)	17,19,21	0.86	1 (5%)
2	NAG	B	505	1	14,14,15	0.29	0	17,19,21	0.81	0
2	NAG	D	508	1	14,14,15	0.79	1 (7%)	17,19,21	0.61	0
4	IMD	A	511	-	3,5,5	0.42	0	4,5,5	0.97	0
2	NAG	A	506	1	14,14,15	0.29	0	17,19,21	0.81	0
2	NAG	A	509	1	14,14,15	0.79	1 (7%)	17,19,21	0.61	0
2	NAG	B	506	1	14,14,15	0.76	1 (7%)	17,19,21	0.77	0
2	NAG	C	504	1	14,14,15	0.81	2 (14%)	17,19,21	0.86	1 (5%)
2	NAG	C	506	1	14,14,15	0.76	1 (7%)	17,19,21	0.77	0
2	NAG	D	503	1	14,14,15	0.57	0	17,19,21	0.72	0
2	NAG	D	500	1	14,14,15	0.25	0	17,19,21	0.67	0
3	I6M	D	509[B]	-	39,39,39	3.91	15 (38%)	48,55,55	1.80	8 (16%)
2	NAG	A	504	1	14,14,15	0.57	0	17,19,21	0.72	0
2	NAG	B	501	1	14,14,15	0.45	0	17,19,21	1.04	1 (5%)
2	NAG	B	504	1	14,14,15	0.81	2 (14%)	17,19,21	0.86	1 (5%)
2	NAG	D	501	1	14,14,15	0.45	0	17,19,21	1.04	1 (5%)
2	NAG	C	503	1	14,14,15	0.57	0	17,19,21	0.72	0
2	NAG	D	507	1	14,14,15	0.68	1 (7%)	17,19,21	0.75	1 (5%)
3	I6M	C	509[B]	-	39,39,39	3.57	12 (30%)	48,55,55	2.12	15 (31%)
2	NAG	C	500	1	14,14,15	0.25	0	17,19,21	0.67	0
2	NAG	A	508	1	14,14,15	0.68	1 (7%)	17,19,21	0.75	1 (5%)
2	NAG	A	503	1	14,14,15	0.49	0	17,19,21	0.60	0
2	NAG	D	504	1	14,14,15	0.81	2 (14%)	17,19,21	0.86	1 (5%)
2	NAG	D	505	1	14,14,15	0.29	0	17,19,21	0.81	0
3	I6M	D	509[A]	-	39,39,39	3.78	15 (38%)	48,55,55	1.93	11 (22%)
2	NAG	C	501	1	14,14,15	0.45	0	17,19,21	1.04	1 (5%)
2	NAG	B	503	1	14,14,15	0.57	0	17,19,21	0.72	0
2	NAG	D	502	1	14,14,15	0.49	0	17,19,21	0.60	0
3	I6M	B	509[B]	-	39,39,39	3.81	14 (35%)	48,55,55	1.64	7 (14%)
2	NAG	A	507	1	14,14,15	0.76	1 (7%)	17,19,21	0.77	0
2	NAG	C	507	1	14,14,15	0.69	1 (7%)	17,19,21	0.75	1 (5%)
2	NAG	A	501	1	14,14,15	0.25	0	17,19,21	0.67	0
2	NAG	C	502	1	14,14,15	0.50	0	17,19,21	0.60	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	I6M	C	509[A]	-	39,39,39	3.69	14 (35%)	48,55,55	1.71	8 (16%)
3	I6M	A	510[B]	-	39,39,39	3.79	14 (35%)	48,55,55	2.28	13 (27%)

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	NAG	A	502	1	-	0/6/23/26	0/1/1/1
2	NAG	B	502	1	-	0/6/23/26	0/1/1/1
2	NAG	B	507	1	-	2/6/23/26	0/1/1/1
3	I6M	B	509[A]	-	-	6/23/45/45	0/4/4/4
2	NAG	C	508	1	-	3/6/23/26	0/1/1/1
2	NAG	B	508	1	-	3/6/23/26	0/1/1/1
2	NAG	C	505	1	-	2/6/23/26	0/1/1/1
2	NAG	B	500	1	-	0/6/23/26	0/1/1/1
3	I6M	A	510[A]	-	-	6/23/45/45	0/4/4/4
2	NAG	D	506	1	-	2/6/23/26	0/1/1/1
2	NAG	A	505	1	-	2/6/23/26	0/1/1/1
2	NAG	B	505	1	-	2/6/23/26	0/1/1/1
2	NAG	D	508	1	-	3/6/23/26	0/1/1/1
4	IMD	A	511	-	-	-	0/1/1/1
2	NAG	A	506	1	-	2/6/23/26	0/1/1/1
2	NAG	A	509	1	-	3/6/23/26	0/1/1/1
2	NAG	B	506	1	-	2/6/23/26	0/1/1/1
2	NAG	C	504	1	-	2/6/23/26	0/1/1/1
2	NAG	C	506	1	-	2/6/23/26	0/1/1/1
2	NAG	D	503	1	-	5/6/23/26	0/1/1/1
2	NAG	D	500	1	-	0/6/23/26	0/1/1/1
3	I6M	D	509[B]	-	-	3/23/45/45	0/4/4/4
2	NAG	A	504	1	-	5/6/23/26	0/1/1/1
2	NAG	B	501	1	-	0/6/23/26	0/1/1/1
2	NAG	B	504	1	-	2/6/23/26	0/1/1/1
2	NAG	D	501	1	-	0/6/23/26	0/1/1/1
2	NAG	C	503	1	-	5/6/23/26	0/1/1/1
2	NAG	D	507	1	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	I6M	C	509[B]	-	-	4/23/45/45	0/4/4/4
2	NAG	C	500	1	-	0/6/23/26	0/1/1/1
2	NAG	A	508	1	-	2/6/23/26	0/1/1/1
2	NAG	A	503	1	-	0/6/23/26	0/1/1/1
2	NAG	D	504	1	-	2/6/23/26	0/1/1/1
2	NAG	D	505	1	-	2/6/23/26	0/1/1/1
3	I6M	D	509[A]	-	-	6/23/45/45	0/4/4/4
2	NAG	C	501	1	-	0/6/23/26	0/1/1/1
2	NAG	B	503	1	-	5/6/23/26	0/1/1/1
2	NAG	D	502	1	-	0/6/23/26	0/1/1/1
3	I6M	B	509[B]	-	-	2/23/45/45	0/4/4/4
2	NAG	A	507	1	-	2/6/23/26	0/1/1/1
2	NAG	C	507	1	-	2/6/23/26	0/1/1/1
2	NAG	A	501	1	-	0/6/23/26	0/1/1/1
2	NAG	C	502	1	-	0/6/23/26	0/1/1/1
3	I6M	C	509[A]	-	-	8/23/45/45	0/4/4/4
3	I6M	A	510[B]	-	-	2/23/45/45	0/4/4/4

All (132) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	509[A]	I6M	C27-N28	-17.27	1.18	1.47
3	D	509[B]	I6M	C27-N28	-17.24	1.18	1.47
3	B	509[B]	I6M	C27-N28	-16.65	1.19	1.47
3	A	510[B]	I6M	C27-N28	-16.62	1.19	1.47
3	C	509[A]	I6M	C27-N28	-16.34	1.19	1.47
3	C	509[B]	I6M	C27-N28	-16.04	1.20	1.47
3	A	510[A]	I6M	C27-N28	-15.99	1.20	1.47
3	D	509[A]	I6M	C27-N28	-15.90	1.20	1.47
3	D	509[A]	I6M	C22-N21	7.42	1.47	1.33
3	D	509[B]	I6M	C32-N28	-7.13	1.29	1.47
3	D	509[B]	I6M	C22-N21	7.12	1.47	1.33
3	B	509[A]	I6M	C32-N28	-7.05	1.29	1.47
3	B	509[A]	I6M	C22-N21	7.05	1.47	1.33
3	C	509[A]	I6M	C32-N28	-6.99	1.29	1.47
3	B	509[B]	I6M	C32-N28	-6.96	1.29	1.47
3	A	510[A]	I6M	C32-N28	-6.78	1.30	1.47
3	B	509[B]	I6M	C22-N21	6.76	1.46	1.33
3	A	510[B]	I6M	C32-N28	-6.74	1.30	1.47
3	C	509[B]	I6M	C32-N28	-6.70	1.30	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	510[A]	I6M	C22-N21	6.62	1.46	1.33
3	D	509[A]	I6M	C02-N14	6.60	1.47	1.34
3	D	509[B]	I6M	C02-N14	6.47	1.47	1.34
3	A	510[B]	I6M	C22-N21	6.46	1.46	1.33
3	B	509[A]	I6M	C02-N14	6.35	1.46	1.34
3	D	509[A]	I6M	C32-N28	-6.31	1.31	1.47
3	B	509[B]	I6M	C02-N14	6.28	1.46	1.34
3	C	509[A]	I6M	C22-N21	6.21	1.45	1.33
3	B	509[B]	I6M	C30-C31	-6.20	1.25	1.51
3	D	509[B]	I6M	C30-C31	-6.06	1.26	1.51
3	C	509[B]	I6M	C30-C31	-6.03	1.26	1.51
3	A	510[B]	I6M	C03-N04	6.03	1.48	1.35
3	C	509[A]	I6M	C30-C31	-6.03	1.26	1.51
3	A	510[A]	I6M	C30-C31	-6.03	1.26	1.51
3	C	509[A]	I6M	C02-N14	6.00	1.46	1.34
3	D	509[A]	I6M	C30-C31	-5.91	1.27	1.51
3	A	510[B]	I6M	C30-C31	-5.90	1.27	1.51
3	B	509[A]	I6M	C30-C31	-5.85	1.27	1.51
3	A	510[A]	I6M	C02-N14	5.74	1.45	1.34
3	C	509[B]	I6M	C02-N14	5.67	1.45	1.34
3	A	510[A]	I6M	C03-N04	5.66	1.47	1.35
3	C	509[B]	I6M	C22-N21	5.51	1.44	1.33
3	A	510[B]	I6M	C02-N14	5.31	1.44	1.34
3	B	509[B]	I6M	C03-N04	4.54	1.45	1.35
3	C	509[A]	I6M	C03-N04	4.49	1.45	1.35
3	B	509[A]	I6M	C03-N04	4.39	1.45	1.35
3	D	509[B]	I6M	C03-N04	4.37	1.45	1.35
3	D	509[A]	I6M	C03-N04	4.26	1.44	1.35
3	D	509[A]	I6M	C31-C32	4.18	1.64	1.53
3	A	510[B]	I6M	C31-C32	4.14	1.64	1.53
3	B	509[A]	I6M	C31-C32	4.05	1.63	1.53
3	A	510[B]	I6M	C22-N23	4.03	1.48	1.32
3	C	509[B]	I6M	C03-N04	3.95	1.44	1.35
3	A	510[A]	I6M	C31-C32	3.94	1.63	1.53
3	D	509[A]	I6M	C22-N23	3.91	1.47	1.32
3	C	509[B]	I6M	C31-C32	3.91	1.63	1.53
3	A	510[A]	I6M	C22-N23	3.82	1.47	1.32
3	D	509[B]	I6M	C22-N23	3.82	1.47	1.32
3	B	509[A]	I6M	C19-C15	-3.80	1.49	1.54
3	D	509[B]	I6M	C31-C32	3.78	1.63	1.53
3	A	510[B]	I6M	C19-C15	-3.77	1.49	1.54
3	C	509[A]	I6M	C31-C32	3.76	1.63	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	509[B]	I6M	C31-C32	3.70	1.62	1.53
3	B	509[A]	I6M	C22-N23	3.65	1.46	1.32
3	A	510[A]	I6M	C19-C15	-3.62	1.49	1.54
3	B	509[B]	I6M	C19-C15	-3.61	1.49	1.54
3	B	509[B]	I6M	C22-N23	3.61	1.46	1.32
3	C	509[A]	I6M	C22-N23	3.60	1.46	1.32
3	D	509[A]	I6M	C19-C15	-3.57	1.49	1.54
3	C	509[B]	I6M	C22-N23	3.53	1.46	1.32
3	D	509[B]	I6M	C19-C15	-3.50	1.49	1.54
3	B	509[A]	I6M	C16-C15	3.31	1.54	1.51
3	B	509[B]	I6M	C16-C15	3.04	1.54	1.51
3	B	509[B]	I6M	C18-C17	2.94	1.55	1.50
3	D	509[A]	I6M	C18-C17	2.93	1.55	1.50
3	B	509[A]	I6M	C18-C17	2.92	1.55	1.50
3	D	509[A]	I6M	O01-C02	-2.90	1.18	1.23
3	D	509[B]	I6M	O01-C02	-2.86	1.18	1.23
3	D	509[A]	I6M	O13-C03	-2.80	1.18	1.23
3	D	509[B]	I6M	C18-C17	2.79	1.55	1.50
3	D	509[B]	I6M	O13-C03	-2.74	1.18	1.23
3	B	509[A]	I6M	O01-C02	-2.73	1.18	1.23
3	B	509[A]	I6M	C36-C16	2.73	1.43	1.39
3	C	509[B]	I6M	O13-C03	-2.68	1.18	1.23
3	B	509[B]	I6M	O01-C02	-2.68	1.18	1.23
2	B	508	NAG	C1-C2	2.66	1.56	1.52
2	C	508	NAG	C1-C2	2.66	1.56	1.52
2	D	508	NAG	C1-C2	2.66	1.56	1.52
2	A	509	NAG	C1-C2	2.65	1.56	1.52
3	A	510[A]	I6M	O01-C02	-2.58	1.18	1.23
3	C	509[A]	I6M	O13-C03	-2.56	1.18	1.23
3	C	509[A]	I6M	O01-C02	-2.53	1.18	1.23
3	C	509[A]	I6M	C18-C17	2.53	1.55	1.50
3	A	510[B]	I6M	C08-CL09	2.53	1.79	1.73
2	D	506	NAG	O5-C1	2.49	1.47	1.43
2	B	506	NAG	O5-C1	2.49	1.47	1.43
3	D	509[A]	I6M	C16-C15	2.48	1.53	1.51
2	A	507	NAG	O5-C1	2.48	1.47	1.43
2	C	506	NAG	O5-C1	2.48	1.47	1.43
3	A	510[A]	I6M	C08-CL09	2.46	1.79	1.73
3	D	509[A]	I6M	C05-N04	2.45	1.46	1.41
2	C	507	NAG	O5-C1	2.42	1.47	1.43
3	A	510[B]	I6M	O01-C02	-2.42	1.19	1.23
2	A	508	NAG	O5-C1	2.42	1.47	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	507	NAG	O5-C1	2.42	1.47	1.43
2	B	507	NAG	O5-C1	2.42	1.47	1.43
3	C	509[A]	I6M	C19-C15	-2.38	1.51	1.54
3	D	509[B]	I6M	C05-N04	2.37	1.46	1.41
3	C	509[B]	I6M	O01-C02	-2.33	1.19	1.23
3	C	509[B]	I6M	C18-C17	2.32	1.54	1.50
3	A	510[A]	I6M	C18-C17	2.27	1.54	1.50
3	D	509[B]	I6M	C08-CL09	2.25	1.79	1.73
3	A	510[B]	I6M	C05-N04	2.25	1.46	1.41
3	D	509[A]	I6M	C08-CL09	2.24	1.79	1.73
3	A	510[A]	I6M	C05-N04	2.23	1.46	1.41
3	C	509[A]	I6M	C08-CL09	2.18	1.78	1.73
3	A	510[A]	I6M	C27-C26	2.15	1.55	1.51
3	A	510[B]	I6M	C36-C16	2.15	1.42	1.39
3	B	509[B]	I6M	O13-C03	-2.13	1.19	1.23
3	C	509[B]	I6M	C12-C05	-2.12	1.36	1.39
2	A	505	NAG	O5-C1	2.10	1.47	1.43
2	D	504	NAG	O5-C1	2.10	1.47	1.43
2	C	504	NAG	O5-C1	2.10	1.47	1.43
2	B	504	NAG	O5-C1	2.10	1.47	1.43
3	B	509[B]	I6M	C36-C16	2.10	1.42	1.39
3	D	509[B]	I6M	C16-C15	2.10	1.53	1.51
3	A	510[B]	I6M	C29-N28	2.07	1.52	1.47
2	B	504	NAG	C1-C2	2.07	1.55	1.52
3	B	509[A]	I6M	O13-C03	-2.07	1.19	1.23
2	A	505	NAG	C1-C2	2.07	1.55	1.52
2	C	504	NAG	C1-C2	2.07	1.55	1.52
2	D	504	NAG	C1-C2	2.06	1.55	1.52
3	C	509[A]	I6M	C22-N24	-2.02	1.26	1.34

All (95) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	510[B]	I6M	C05-N04-C03	-6.39	116.44	127.53
3	A	510[B]	I6M	C15-N14-C02	-6.02	112.61	122.32
3	D	509[A]	I6M	C05-N04-C03	-5.98	117.16	127.53
3	D	509[B]	I6M	C05-N04-C03	-5.98	117.16	127.53
3	A	510[A]	I6M	C05-N04-C03	-5.76	117.53	127.53
3	A	510[B]	I6M	C16-C15-N14	-5.17	106.31	114.61
3	A	510[B]	I6M	C02-C03-N04	5.01	120.22	112.31
3	B	509[A]	I6M	C05-N04-C03	-4.99	118.87	127.53
3	B	509[B]	I6M	C05-N04-C03	-4.99	118.87	127.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	510[A]	I6M	C16-C15-N14	-4.96	106.64	114.61
3	A	510[A]	I6M	C02-C03-N04	4.94	120.12	112.31
3	C	509[A]	I6M	C02-C03-N04	4.82	119.93	112.31
3	D	509[A]	I6M	C16-C15-C19	4.80	108.91	104.38
3	C	509[B]	I6M	C16-C15-N14	-4.71	107.04	114.61
3	D	509[B]	I6M	C02-C03-N04	4.66	119.68	112.31
3	C	509[A]	I6M	C05-N04-C03	-4.65	119.46	127.53
3	D	509[B]	I6M	C16-C15-C19	4.63	108.75	104.38
3	C	509[B]	I6M	C05-C12-C10	-4.63	114.97	118.76
3	D	509[A]	I6M	C02-C03-N04	4.46	119.36	112.31
3	C	509[A]	I6M	C16-C15-N14	-4.44	107.49	114.61
3	C	509[B]	I6M	C02-C03-N04	4.43	119.32	112.31
3	C	509[B]	I6M	C06-C07-C08	-4.37	113.69	120.00
3	D	509[A]	I6M	C27-N28-C29	-4.37	106.58	113.25
3	A	510[B]	I6M	C16-C15-C19	4.37	108.50	104.38
3	C	509[B]	I6M	C05-N04-C03	-4.33	120.01	127.53
3	C	509[B]	I6M	C07-C08-C10	4.32	122.40	118.94
3	B	509[A]	I6M	C16-C15-C19	4.30	108.44	104.38
3	B	509[A]	I6M	C27-N28-C29	-4.19	106.86	113.25
3	B	509[A]	I6M	C16-C15-N14	-4.12	108.00	114.61
3	A	510[B]	I6M	O13-C03-C02	-4.07	116.33	121.30
3	B	509[B]	I6M	C16-C15-C19	3.99	108.14	104.38
3	B	509[B]	I6M	C16-C15-N14	-3.86	108.42	114.61
3	A	510[A]	I6M	C15-N14-C02	-3.81	116.18	122.32
3	B	509[B]	I6M	C02-C03-N04	3.62	118.04	112.31
3	A	510[A]	I6M	C16-C15-C19	3.61	107.78	104.38
3	C	509[B]	I6M	C07-C06-C05	3.56	124.41	120.30
3	A	510[B]	I6M	C19-C20-N21	-3.52	106.27	112.11
2	B	501	NAG	C1-O5-C5	3.47	116.90	112.19
2	C	501	NAG	C1-O5-C5	3.47	116.90	112.19
2	A	502	NAG	C1-O5-C5	3.47	116.89	112.19
2	D	501	NAG	C1-O5-C5	3.47	116.89	112.19
3	C	509[B]	I6M	C25-C17-C16	-3.45	117.26	120.80
3	A	510[B]	I6M	C27-N28-C29	-3.24	108.31	113.25
3	B	509[A]	I6M	C07-C08-C10	3.22	121.52	118.94
3	B	509[A]	I6M	C25-C17-C16	-3.17	117.55	120.80
3	B	509[A]	I6M	C02-C03-N04	3.13	117.25	112.31
2	D	504	NAG	C1-O5-C5	3.05	116.33	112.19
2	C	504	NAG	C1-O5-C5	3.05	116.33	112.19
2	A	505	NAG	C1-O5-C5	3.05	116.33	112.19
2	B	504	NAG	C1-O5-C5	3.05	116.33	112.19
3	A	510[A]	I6M	O13-C03-C02	-2.96	117.68	121.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	510[B]	I6M	O01-C02-N14	-2.95	117.91	123.08
3	C	509[B]	I6M	C16-C15-C19	2.93	107.14	104.38
3	D	509[B]	I6M	C16-C15-N14	-2.93	109.92	114.61
3	A	510[B]	I6M	C25-C17-C16	-2.91	117.81	120.80
3	C	509[B]	I6M	C15-N14-C02	-2.87	117.69	122.32
3	D	509[A]	I6M	C16-C15-N14	-2.87	110.00	114.61
3	C	509[A]	I6M	C16-C15-C19	2.81	107.04	104.38
3	C	509[A]	I6M	C07-C08-C10	2.79	121.18	118.94
3	C	509[A]	I6M	C27-N28-C29	-2.74	109.06	113.25
3	B	509[B]	I6M	C07-C08-C10	2.74	121.14	118.94
3	B	509[A]	I6M	C17-C16-C15	-2.69	107.97	110.22
3	D	509[A]	I6M	C07-C08-C10	2.69	121.10	118.94
2	D	507	NAG	C1-O5-C5	2.62	115.74	112.19
2	C	507	NAG	C1-O5-C5	2.62	115.74	112.19
2	A	508	NAG	C1-O5-C5	2.62	115.74	112.19
2	B	507	NAG	C1-O5-C5	2.62	115.74	112.19
3	D	509[A]	I6M	O01-C02-C03	-2.60	118.12	121.30
3	A	510[A]	I6M	C19-C20-N21	-2.58	107.83	112.11
3	D	509[B]	I6M	C07-C08-C10	2.50	120.94	118.94
3	B	509[B]	I6M	C25-C17-C16	-2.48	118.25	120.80
3	A	510[A]	I6M	C27-N28-C29	-2.48	109.47	113.25
3	B	509[A]	I6M	C36-C35-C26	-2.47	117.62	121.03
3	A	510[B]	I6M	C17-C16-C15	-2.45	108.17	110.22
3	B	509[A]	I6M	C19-C20-N21	-2.43	108.07	112.11
3	A	510[A]	I6M	O01-C02-N14	-2.37	118.93	123.08
3	D	509[A]	I6M	C25-C17-C16	-2.34	118.40	120.80
3	C	509[A]	I6M	C25-C17-C16	-2.33	118.41	120.80
3	D	509[B]	I6M	C27-N28-C29	-2.31	109.72	113.25
3	D	509[A]	I6M	C17-C18-C19	2.26	107.26	104.06
3	A	510[B]	I6M	O01-C02-C03	2.26	124.06	121.30
3	C	509[B]	I6M	C27-N28-C29	-2.25	109.82	113.25
3	C	509[A]	I6M	C06-C07-C08	-2.24	116.76	120.00
3	A	510[A]	I6M	C25-C17-C16	-2.22	118.52	120.80
3	A	510[B]	I6M	C36-C35-C26	-2.22	117.97	121.03
3	D	509[A]	I6M	C03-C02-N14	2.21	119.03	113.73
3	C	509[B]	I6M	C36-C35-C26	-2.20	118.00	121.03
3	D	509[B]	I6M	C25-C17-C16	-2.18	118.56	120.80
3	C	509[B]	I6M	O13-C03-C02	-2.17	118.65	121.30
3	D	509[A]	I6M	F11-C10-C08	-2.14	117.01	118.98
3	C	509[B]	I6M	F11-C10-C08	-2.07	117.07	118.98
3	A	510[A]	I6M	C03-C02-N14	2.07	118.69	113.73
3	D	509[B]	I6M	C03-C02-N14	2.06	118.67	113.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	509[B]	I6M	C12-C10-C08	2.05	123.69	121.72
3	B	509[B]	I6M	C19-C20-N21	-2.03	108.74	112.11

There are no chirality outliers.

All (101) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	510[A]	I6M	C15-C19-C20-N21
3	A	510[A]	I6M	C26-C27-N28-C29
3	A	510[A]	I6M	C26-C27-N28-C32
3	A	510[A]	I6M	N28-C32-C33-O34
3	B	509[A]	I6M	C15-C19-C20-N21
3	B	509[A]	I6M	C26-C27-N28-C29
3	B	509[A]	I6M	C26-C27-N28-C32
3	B	509[A]	I6M	N28-C32-C33-O34
3	B	509[B]	I6M	C15-C19-C20-N21
3	D	509[A]	I6M	C15-C19-C20-N21
3	D	509[A]	I6M	C26-C27-N28-C29
3	D	509[A]	I6M	C26-C27-N28-C32
3	C	509[A]	I6M	C15-C19-C20-N21
3	C	509[A]	I6M	C26-C27-N28-C29
3	C	509[A]	I6M	C26-C27-N28-C32
3	C	509[A]	I6M	N28-C32-C33-O34
3	C	509[B]	I6M	C15-C19-C20-N21
2	A	506	NAG	O5-C5-C6-O6
2	A	508	NAG	O5-C5-C6-O6
2	B	505	NAG	O5-C5-C6-O6
2	B	507	NAG	O5-C5-C6-O6
2	D	505	NAG	O5-C5-C6-O6
2	D	507	NAG	O5-C5-C6-O6
2	C	505	NAG	O5-C5-C6-O6
2	C	507	NAG	O5-C5-C6-O6
2	A	504	NAG	O5-C5-C6-O6
2	A	505	NAG	O5-C5-C6-O6
2	A	507	NAG	O5-C5-C6-O6
2	B	503	NAG	O5-C5-C6-O6
2	B	504	NAG	O5-C5-C6-O6
2	B	506	NAG	O5-C5-C6-O6
2	D	503	NAG	O5-C5-C6-O6
2	D	504	NAG	O5-C5-C6-O6
2	D	506	NAG	O5-C5-C6-O6
2	C	503	NAG	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
2	C	504	NAG	O5-C5-C6-O6
2	C	506	NAG	O5-C5-C6-O6
2	A	505	NAG	C4-C5-C6-O6
2	A	508	NAG	C4-C5-C6-O6
2	B	504	NAG	C4-C5-C6-O6
2	B	507	NAG	C4-C5-C6-O6
2	D	504	NAG	C4-C5-C6-O6
2	D	507	NAG	C4-C5-C6-O6
2	C	504	NAG	C4-C5-C6-O6
2	C	507	NAG	C4-C5-C6-O6
2	A	506	NAG	C4-C5-C6-O6
2	B	505	NAG	C4-C5-C6-O6
2	D	505	NAG	C4-C5-C6-O6
2	C	505	NAG	C4-C5-C6-O6
2	A	504	NAG	C8-C7-N2-C2
2	A	504	NAG	O7-C7-N2-C2
2	B	503	NAG	C8-C7-N2-C2
2	B	503	NAG	O7-C7-N2-C2
2	D	503	NAG	C8-C7-N2-C2
2	D	503	NAG	O7-C7-N2-C2
2	C	503	NAG	C8-C7-N2-C2
2	C	503	NAG	O7-C7-N2-C2
2	A	504	NAG	C4-C5-C6-O6
2	B	503	NAG	C4-C5-C6-O6
2	D	503	NAG	C4-C5-C6-O6
2	C	503	NAG	C4-C5-C6-O6
2	A	507	NAG	C4-C5-C6-O6
2	B	506	NAG	C4-C5-C6-O6
2	D	506	NAG	C4-C5-C6-O6
2	C	506	NAG	C4-C5-C6-O6
2	A	509	NAG	C1-C2-N2-C7
2	B	508	NAG	C1-C2-N2-C7
2	D	508	NAG	C1-C2-N2-C7
2	C	508	NAG	C1-C2-N2-C7
3	A	510[A]	I6M	C31-C32-C33-O34
3	B	509[A]	I6M	C31-C32-C33-O34
3	D	509[A]	I6M	N28-C32-C33-O34
3	C	509[A]	I6M	C31-C32-C33-O34
3	C	509[B]	I6M	N28-C32-C33-O34
3	D	509[B]	I6M	N28-C32-C33-O34
3	A	510[A]	I6M	C18-C19-C20-N21
3	B	509[A]	I6M	C18-C19-C20-N21

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Mol	Chain	Res	Type	Atoms
3	B	509[B]	I6M	C18-C19-C20-N21
3	D	509[A]	I6M	C18-C19-C20-N21
3	C	509[A]	I6M	C18-C19-C20-N21
3	C	509[B]	I6M	C18-C19-C20-N21
3	A	510[B]	I6M	C15-C19-C20-N21
3	D	509[B]	I6M	C15-C19-C20-N21
2	A	509	NAG	C4-C5-C6-O6
2	B	508	NAG	C4-C5-C6-O6
2	D	508	NAG	C4-C5-C6-O6
2	C	508	NAG	C4-C5-C6-O6
2	A	509	NAG	O5-C5-C6-O6
2	B	508	NAG	O5-C5-C6-O6
2	D	508	NAG	O5-C5-C6-O6
2	C	508	NAG	O5-C5-C6-O6
2	A	504	NAG	C3-C2-N2-C7
2	B	503	NAG	C3-C2-N2-C7
2	D	503	NAG	C3-C2-N2-C7
2	C	503	NAG	C3-C2-N2-C7
3	A	510[B]	I6M	N28-C32-C33-O34
3	D	509[A]	I6M	C31-C32-C33-O34
3	D	509[B]	I6M	C31-C32-C33-O34
3	C	509[B]	I6M	C31-C32-C33-O34
3	C	509[A]	I6M	C35-C26-C27-N28
3	C	509[A]	I6M	C25-C26-C27-N28

There are no ring outliers.

14 monomers are involved in 38 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	502	NAG	0	1
2	C	508	NAG	8	0
2	C	505	NAG	2	0
2	B	505	NAG	1	0
2	D	508	NAG	3	0
2	A	506	NAG	4	0
2	D	503	NAG	4	0
2	A	504	NAG	4	0
2	C	503	NAG	5	0
2	D	504	NAG	9	0
2	D	505	NAG	1	0
2	C	501	NAG	3	0
2	B	503	NAG	4	0

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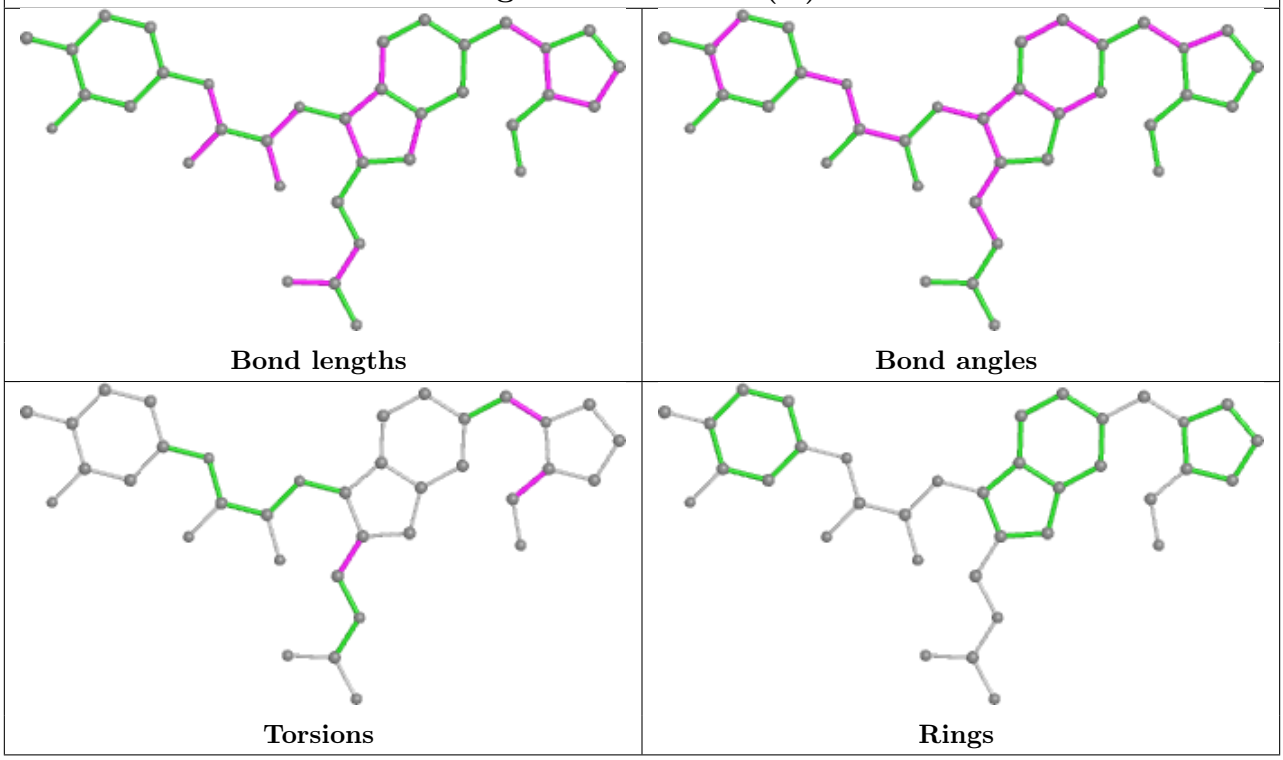
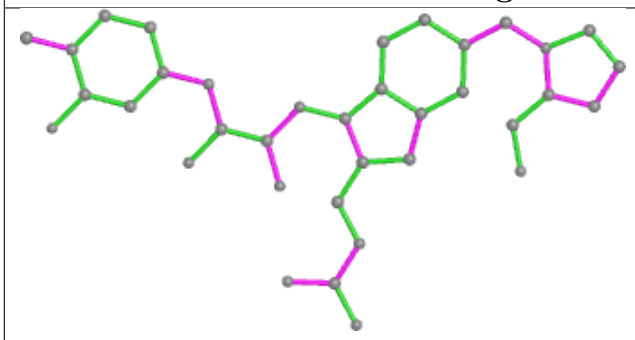
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	502	NAG	0	1

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.

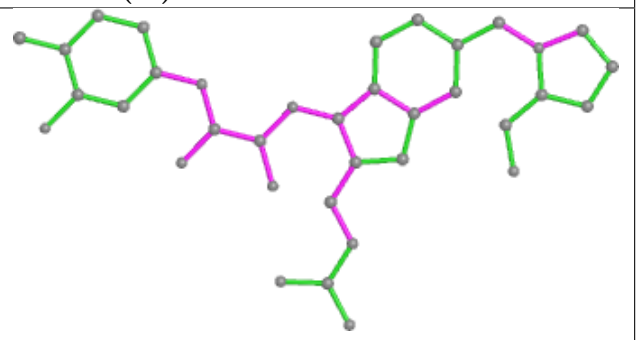
Ligand I6M B 509 (A)



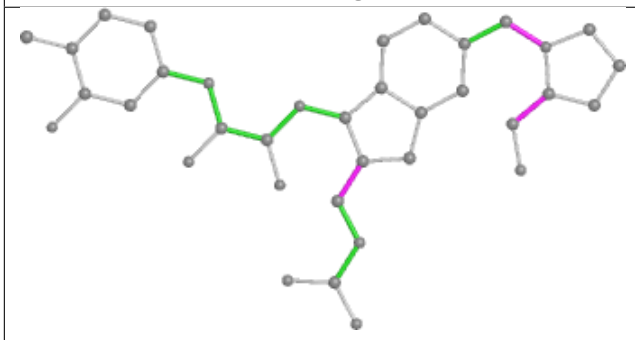
Ligand I6M A 510 (A)



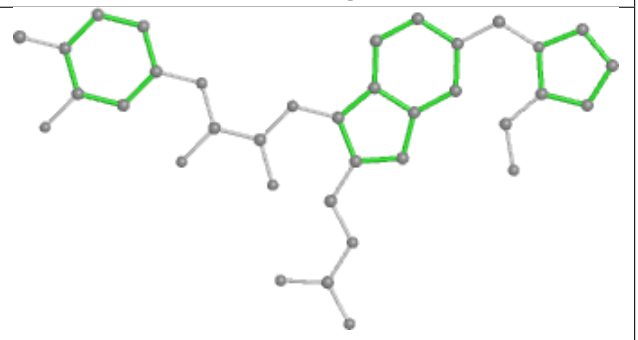
Bond lengths



Bond angles

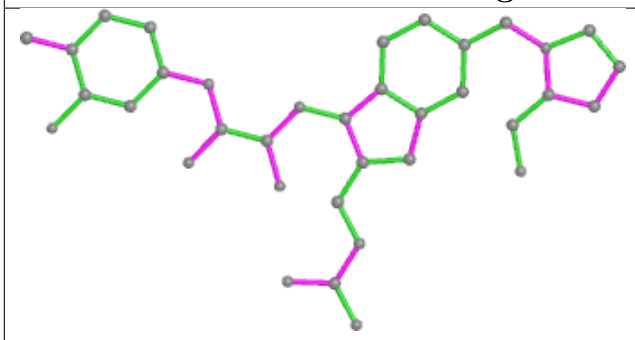


Torsions

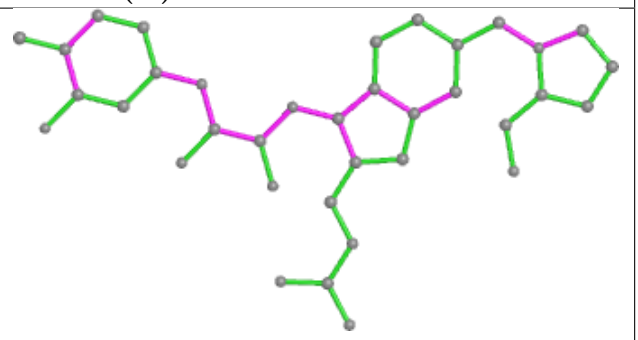


Rings

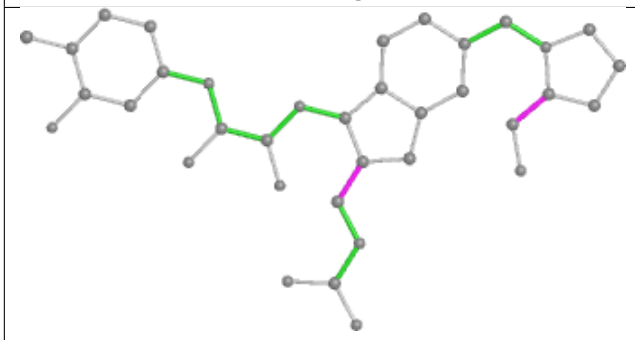
Ligand I6M D 509 (B)



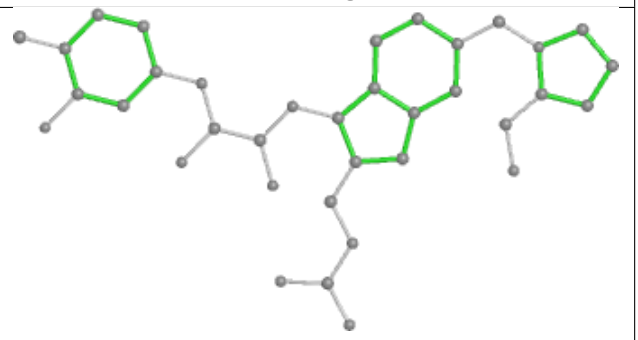
Bond lengths



Bond angles

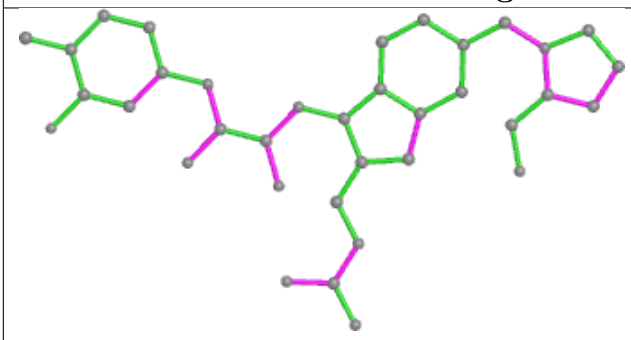


Torsions

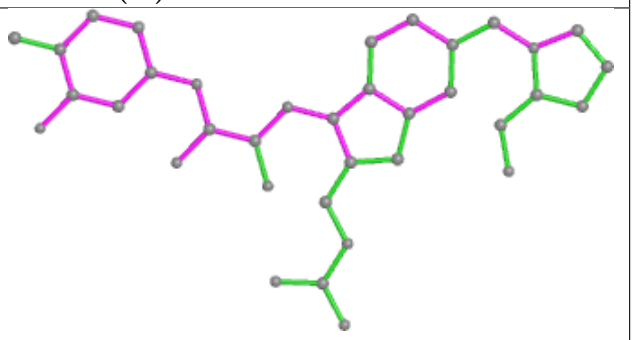


Rings

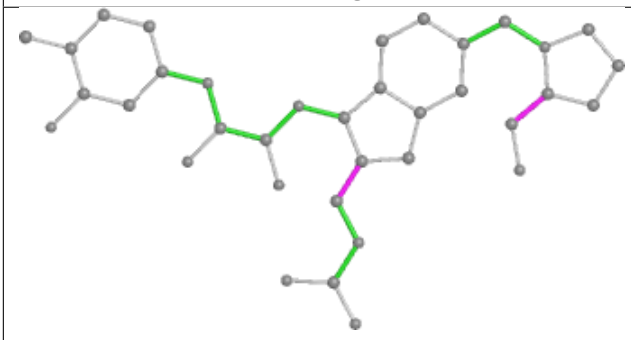
Ligand I6M C 509 (B)



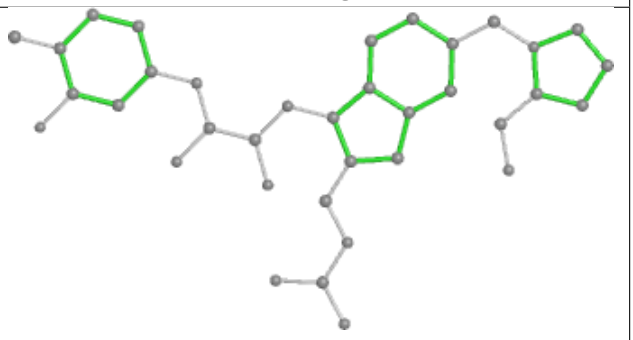
Bond lengths



Bond angles

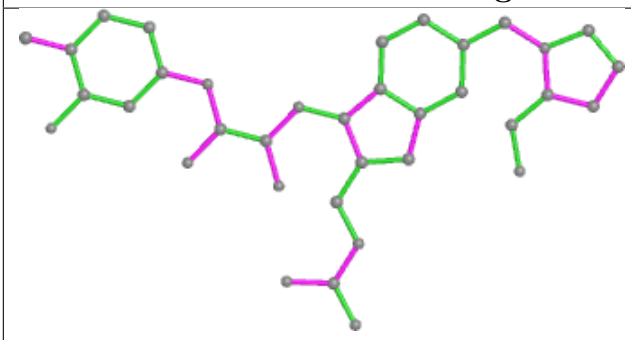


Torsions

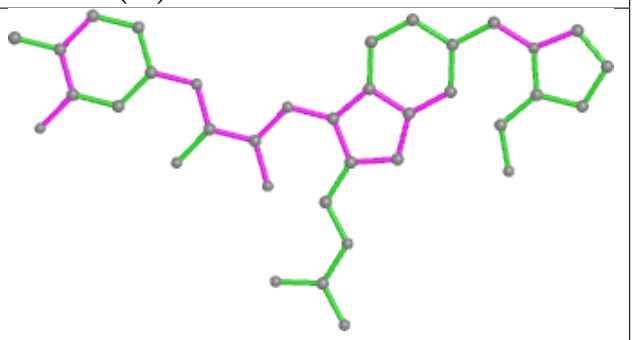


Rings

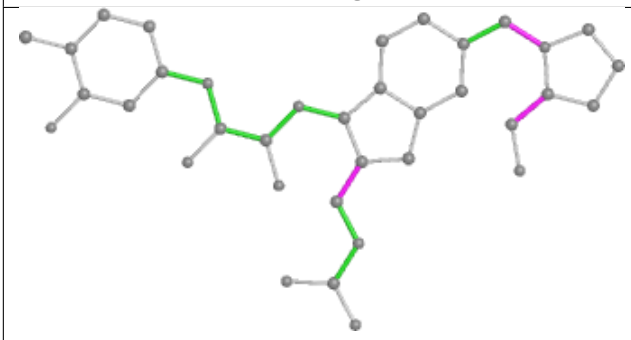
Ligand I6M D 509 (A)



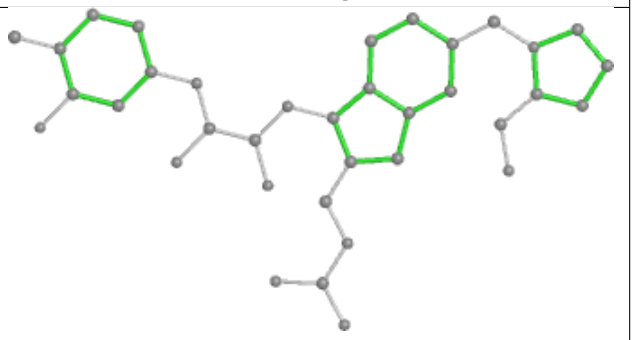
Bond lengths



Bond angles

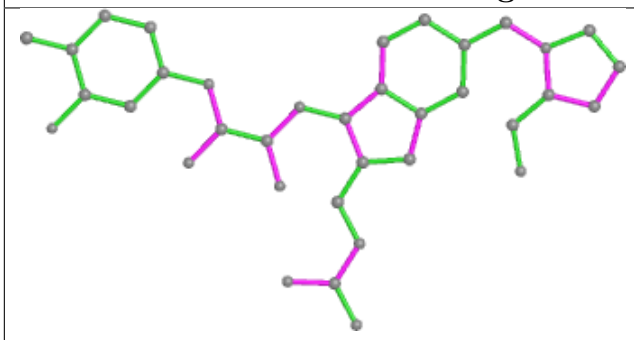


Torsions

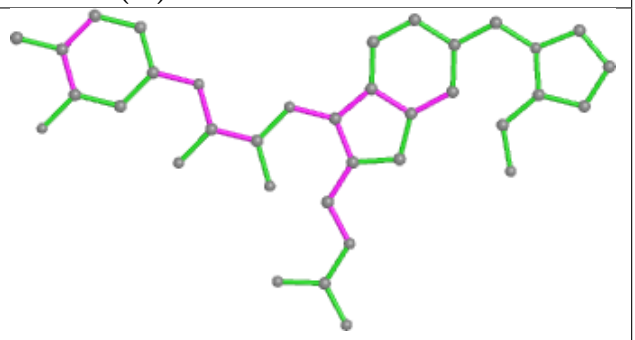


Rings

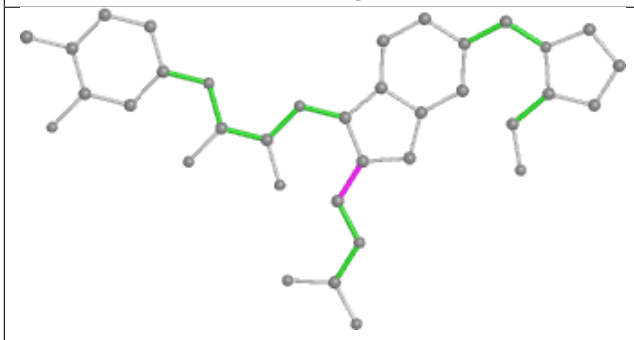
Ligand I6M B 509 (B)



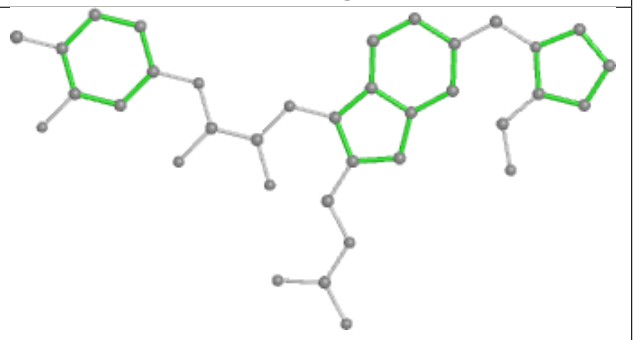
Bond lengths



Bond angles

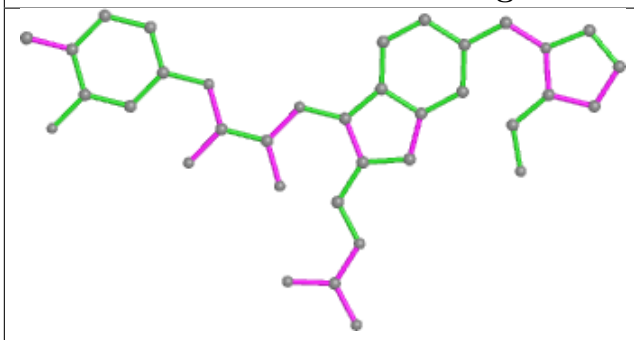


Torsions

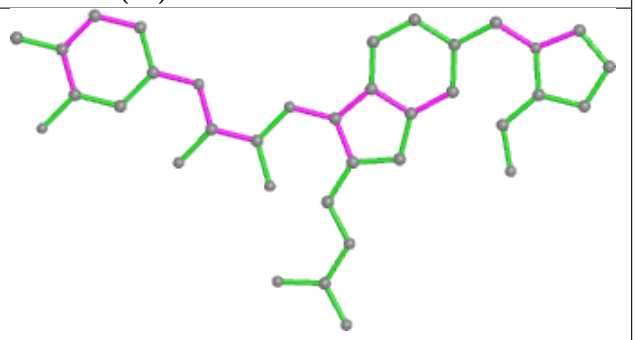


Rings

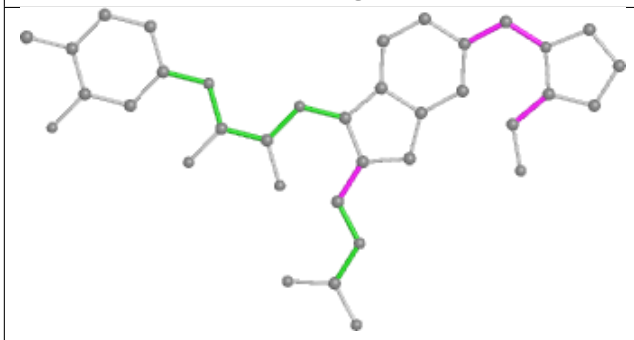
Ligand I6M C 509 (A)



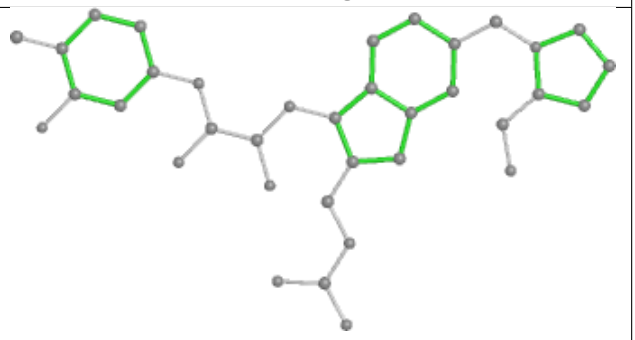
Bond lengths



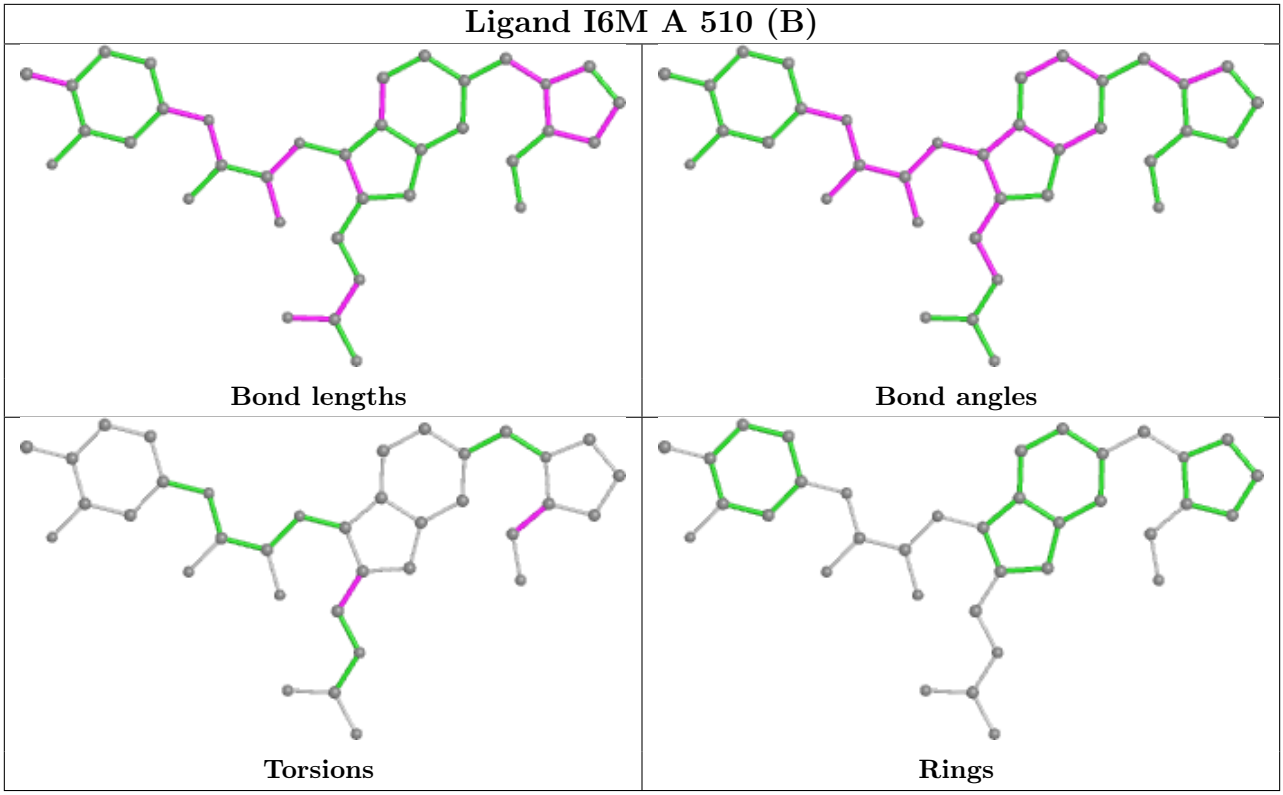
Bond angles



Torsions



Rings



5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	335/358 (93%)	0.05	11 (3%) 46 41	23, 47, 75, 90	0
1	B	335/358 (93%)	0.37	30 (8%) 9 6	25, 57, 93, 112	0
1	C	335/358 (93%)	0.14	19 (5%) 23 18	22, 44, 79, 105	0
1	D	335/358 (93%)	0.30	24 (7%) 15 11	28, 55, 87, 110	0
All	All	1340/1432 (93%)	0.22	84 (6%) 20 15	22, 50, 85, 112	0

All (84) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	91	GLU	6.0
1	D	89	VAL	5.9
1	B	240	ARG	5.8
1	D	240	ARG	5.6
1	C	88	ASN	5.4
1	D	87	ALA	5.1
1	B	226	LEU	5.1
1	C	61	TYR	4.9
1	B	87	ALA	4.8
1	B	50	THR	4.5
1	B	488	VAL	4.4
1	C	85	VAL	4.3
1	C	86	LEU	4.2
1	D	326	ILE	4.1
1	C	81	PRO	4.1
1	C	84	MET	4.0
1	C	240	ARG	4.0
1	C	89	VAL	3.9
1	D	219	ALA	3.8
1	B	221	ALA	3.8
1	C	60	ALA	3.8

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Mol	Chain	Res	Type	RSRZ
1	D	90	THR	3.8
1	A	85	VAL	3.7
1	A	86	LEU	3.6
1	D	84	MET	3.5
1	B	224	ALA	3.5
1	A	87	ALA	3.4
1	C	124	GLY	3.4
1	D	85	VAL	3.4
1	C	82	GLN	3.4
1	D	86	LEU	3.4
1	D	88	ASN	3.1
1	D	226	LEU	3.1
1	D	91	GLU	3.1
1	B	53	PHE	3.0
1	B	93	PHE	3.0
1	B	220	PRO	3.0
1	D	300	ASN	3.0
1	D	238	PRO	3.0
1	D	489	VAL	2.9
1	B	88	ASN	2.9
1	B	51	THR	2.8
1	B	489	VAL	2.8
1	B	72	HIS	2.8
1	B	49	LYS	2.8
1	C	221	ALA	2.8
1	C	244	THR	2.7
1	B	84	MET	2.7
1	B	219	ALA	2.7
1	D	243	SER	2.7
1	B	90	THR	2.7
1	A	88	ASN	2.7
1	B	86	LEU	2.7
1	B	353	PHE	2.7
1	B	89	VAL	2.6
1	C	198	GLY	2.6
1	B	201	ILE	2.5
1	A	89	VAL	2.4
1	B	223	PHE	2.4
1	D	124	GLY	2.4
1	C	79	PRO	2.4
1	B	349	LEU	2.3
1	C	349	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
1	D	268	GLU	2.2
1	B	217	TYR	2.2
1	A	84	MET	2.2
1	A	82	GLN	2.2
1	D	82	GLN	2.1
1	C	342	LEU	2.1
1	D	408	ARG	2.1
1	D	325	ASN	2.1
1	C	199	SER	2.1
1	B	222	GLY	2.1
1	D	396	ARG	2.1
1	B	92	ASN	2.1
1	B	241	ASN	2.1
1	B	79	PRO	2.1
1	D	61	TYR	2.1
1	A	356	SER	2.1
1	D	49	LYS	2.0
1	A	83	GLU	2.0
1	A	440	GLU	2.0
1	A	489	VAL	2.0
1	C	245	VAL	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	NAG	B	505	14/15	0.37	0.64	104,124,135,136	0
2	NAG	D	504	14/15	0.55	0.71	86,116,123,124	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	NAG	D	508	14/15	0.56	0.49	56,98,105,108	0
2	NAG	D	505	14/15	0.57	0.54	75,111,120,123	0
2	NAG	C	508	14/15	0.62	0.50	58,104,115,116	0
2	NAG	B	504	14/15	0.63	0.75	95,113,122,131	0
2	NAG	C	504	14/15	0.67	0.53	90,106,118,137	0
2	NAG	B	508	14/15	0.68	0.36	59,103,115,121	0
2	NAG	A	503	14/15	0.73	0.31	82,94,112,113	0
2	NAG	D	502	14/15	0.79	0.23	61,72,78,79	0
2	NAG	B	502	14/15	0.80	0.21	59,75,88,93	0
2	NAG	A	509	14/15	0.80	0.27	56,84,95,97	0
2	NAG	C	502	14/15	0.82	0.34	55,85,97,117	0
2	NAG	A	505	14/15	0.85	0.39	76,85,102,108	0
2	NAG	D	503	14/15	0.85	0.21	59,77,88,95	0
2	NAG	D	507	14/15	0.87	0.23	38,72,82,85	0
2	NAG	D	506	14/15	0.88	0.22	51,62,72,75	0
2	NAG	B	503	14/15	0.88	0.20	49,72,85,95	0
2	NAG	B	500	14/15	0.88	0.20	56,73,87,93	0
2	NAG	A	506	14/15	0.90	0.25	50,61,77,80	0
2	NAG	D	500	14/15	0.90	0.22	52,61,69,73	0
2	NAG	C	505	14/15	0.90	0.19	54,67,73,89	0
2	NAG	B	506	14/15	0.90	0.15	40,56,65,68	0
2	NAG	C	506	14/15	0.92	0.16	31,51,61,73	0
2	NAG	A	504	14/15	0.92	0.20	45,59,65,86	0
3	I6M	A	510[A]	36/36	0.92	0.24	29,38,52,56	36
3	I6M	A	510[B]	36/36	0.92	0.24	29,38,55,59	36
2	NAG	A	507	14/15	0.93	0.18	39,49,63,65	0
2	NAG	C	503	14/15	0.93	0.14	52,62,73,87	0
2	NAG	A	501	14/15	0.93	0.17	43,67,77,84	0
2	NAG	B	507	14/15	0.93	0.21	62,69,72,77	0
3	I6M	D	509[A]	36/36	0.93	0.20	30,38,52,55	36
3	I6M	D	509[B]	36/36	0.93	0.20	30,38,50,55	36
4	IMD	A	511	5/5	0.93	0.22	40,58,71,71	0
2	NAG	C	500	14/15	0.94	0.17	50,60,74,76	0
3	I6M	C	509[A]	36/36	0.94	0.20	23,32,47,51	36
3	I6M	C	509[B]	36/36	0.94	0.20	23,31,49,53	36
2	NAG	D	501	14/15	0.94	0.24	39,49,66,67	0
2	NAG	A	502	14/15	0.95	0.21	30,37,45,45	0
2	NAG	A	508	14/15	0.95	0.15	21,34,60,65	0
2	NAG	C	507	14/15	0.95	0.14	31,42,56,56	0
3	I6M	B	509[A]	36/36	0.95	0.17	32,39,44,47	36
3	I6M	B	509[B]	36/36	0.95	0.17	31,38,45,46	36
2	NAG	B	501	14/15	0.96	0.19	45,54,65,68	0

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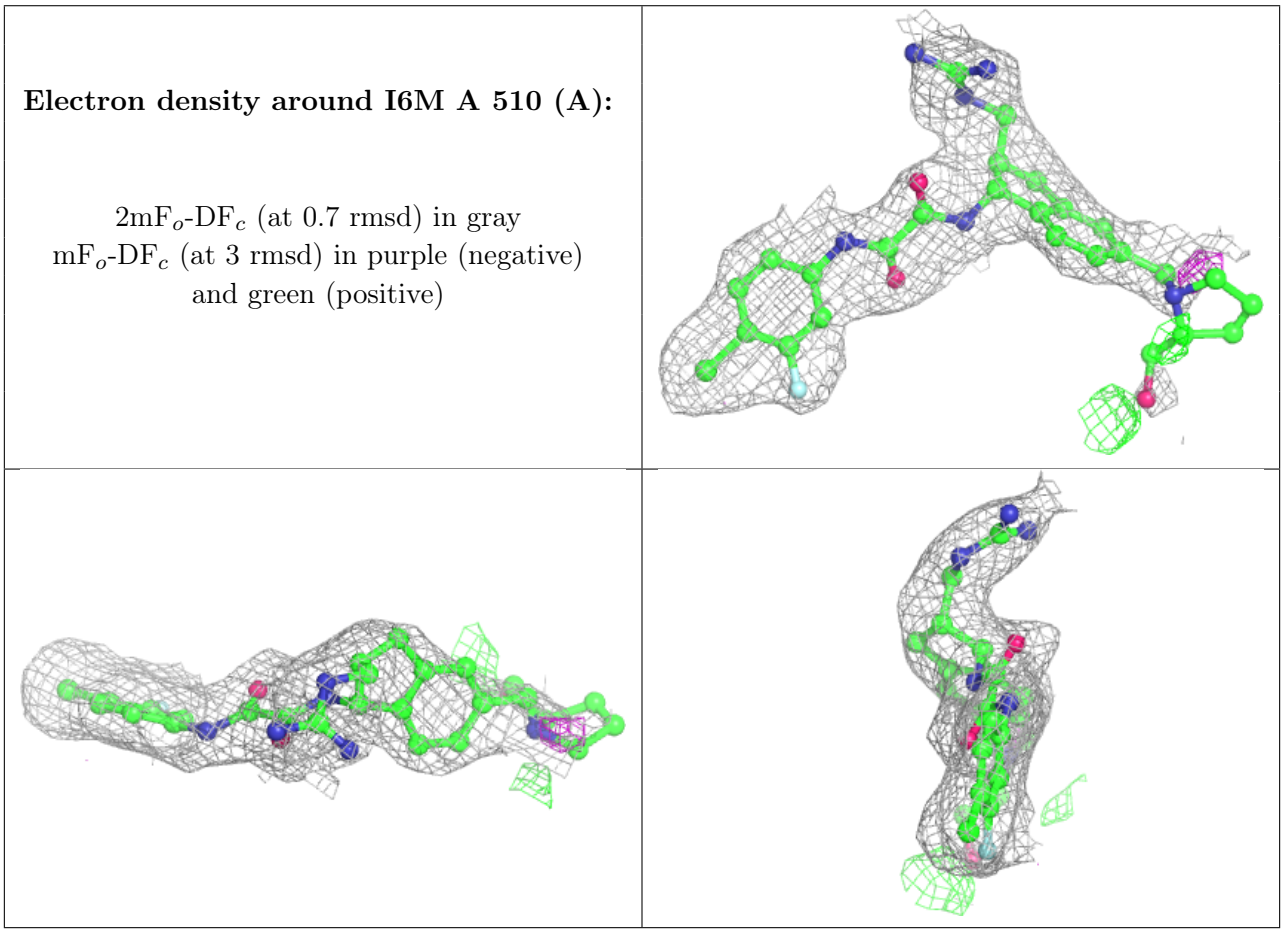
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	NAG	C	501	14/15	0.96	0.24	31,44,57,62	0

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.

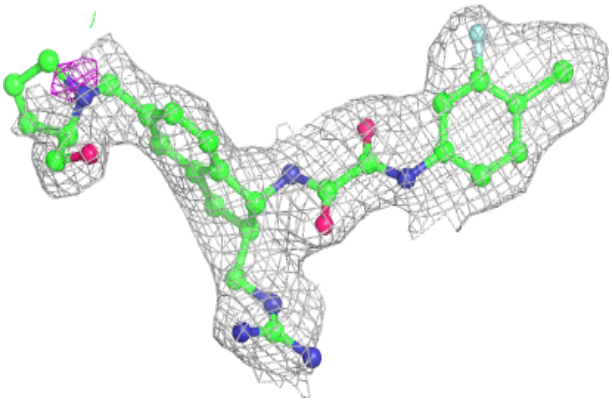
Electron density around I6M A 510 (A):

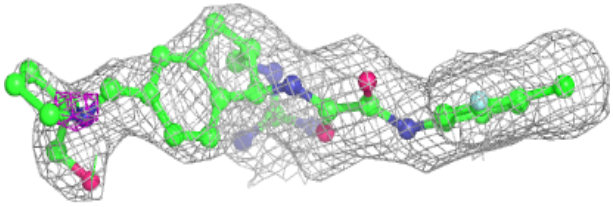
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

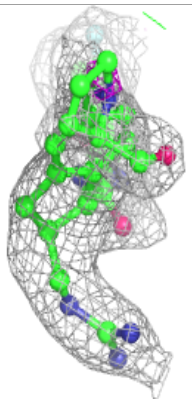


Electron density around I6M A 510 (B):

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

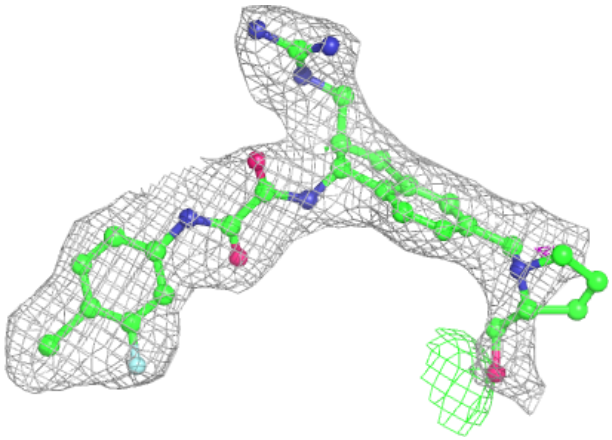


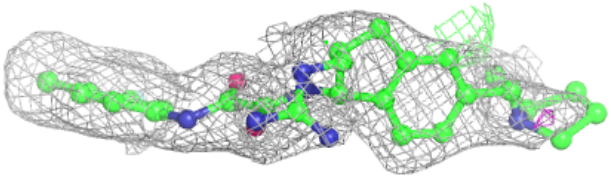


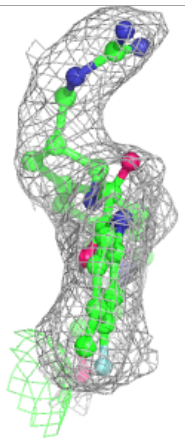


Electron density around I6M D 509 (A):

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

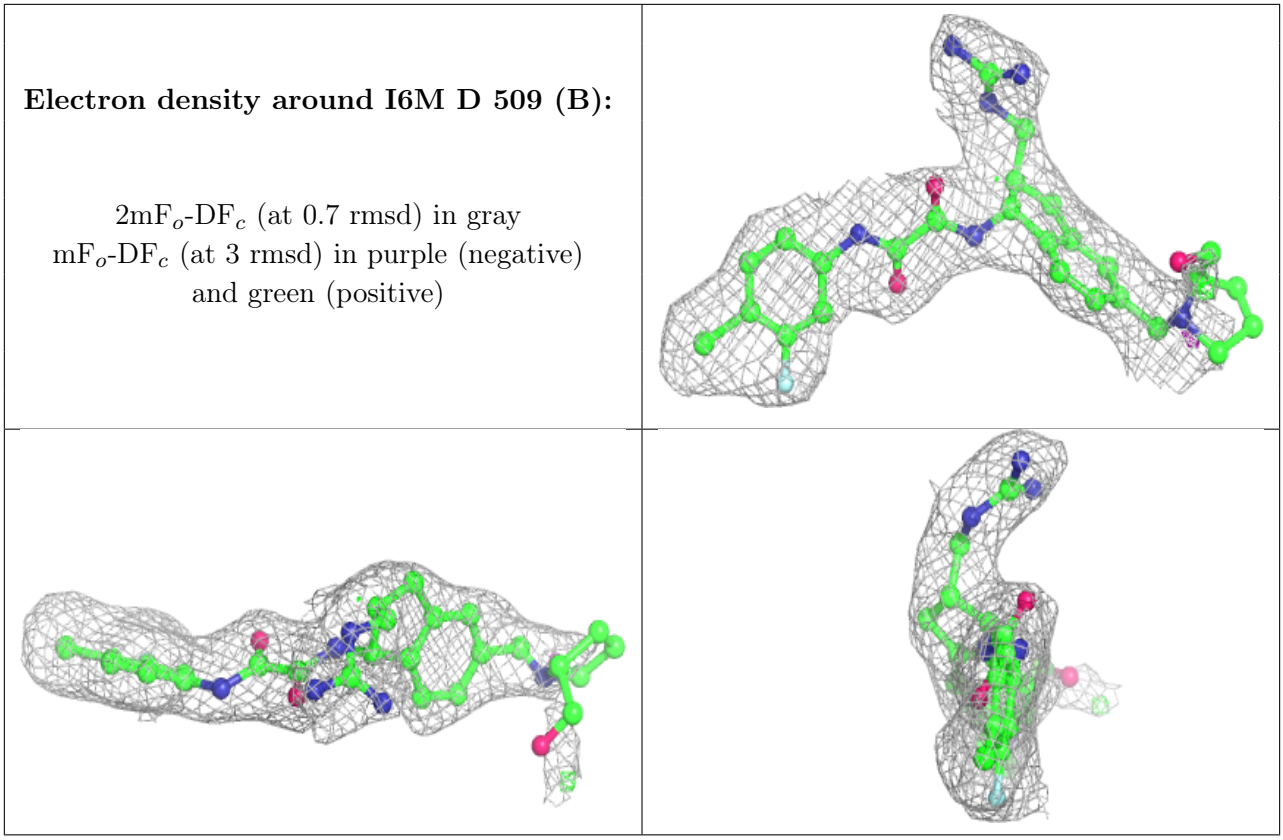






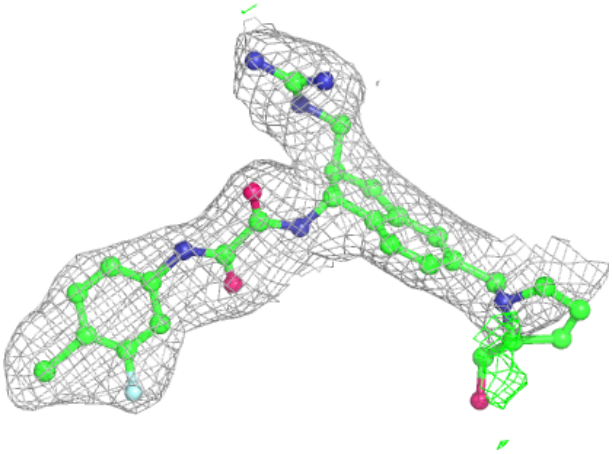
Electron density around I6M D 509 (B):

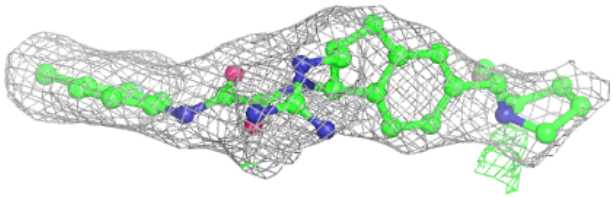
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

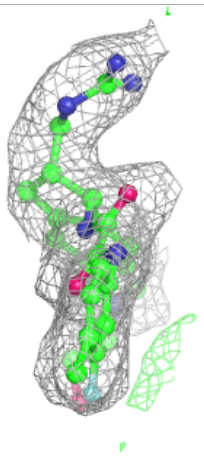


Electron density around I6M C 509 (A):

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

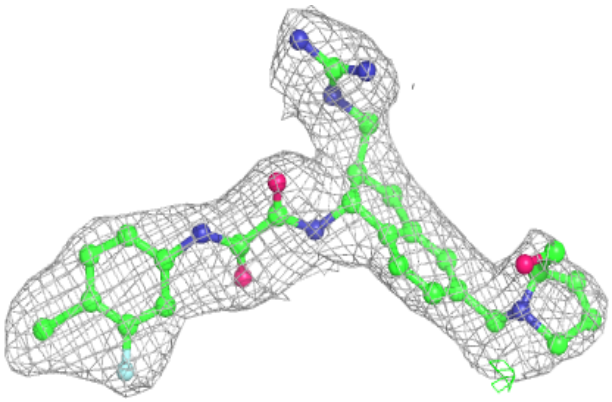


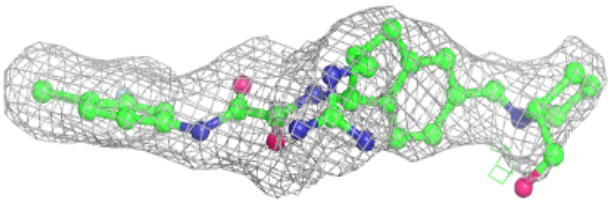


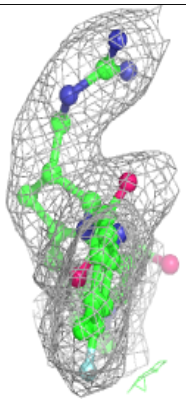


Electron density around I6M C 509 (B):

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

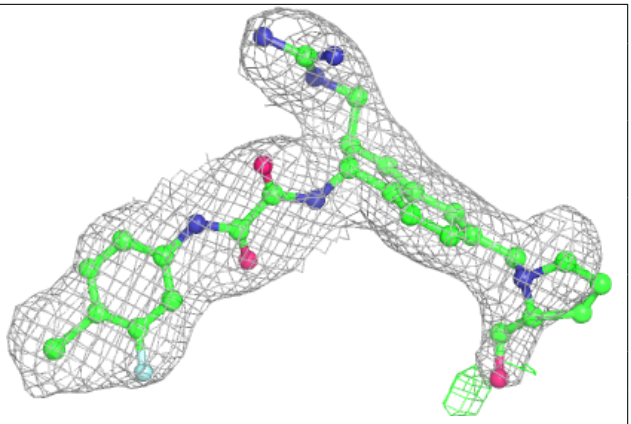


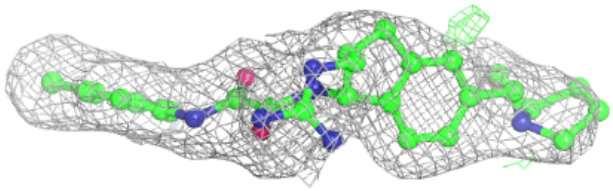


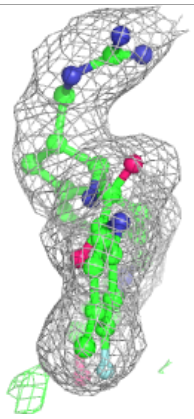


Electron density around I6M B 509 (A):

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

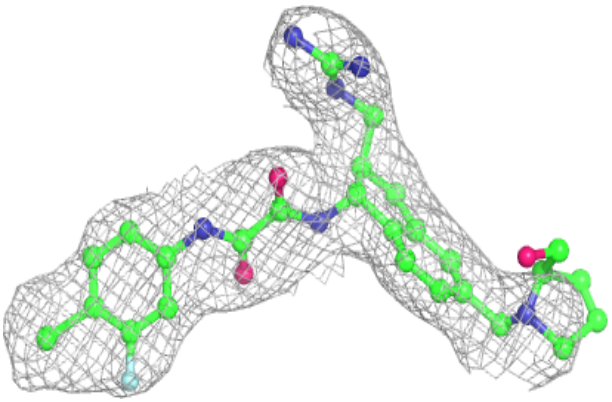


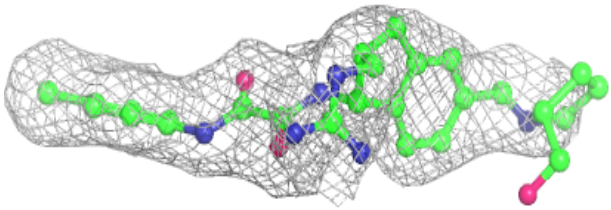


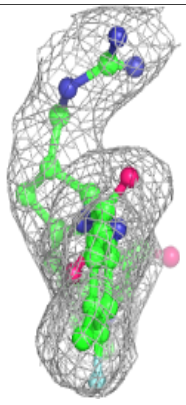


Electron density around I6M B 509 (B):

$2mF_o$-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.