



# Full wwPDB X-ray Structure Validation Report ⓘ

Jun 1, 2022 – 10:07 AM EDT

PDB ID : 7RSY  
Title : HIV-1 gp120 complex with CJF-III-049-R  
Authors : Liang, S.; Hendrickson, W.A.  
Deposited on : 2021-08-12  
Resolution : 2.70 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](mailto: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.

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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 : 2.28.1  
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) : 2.28.1

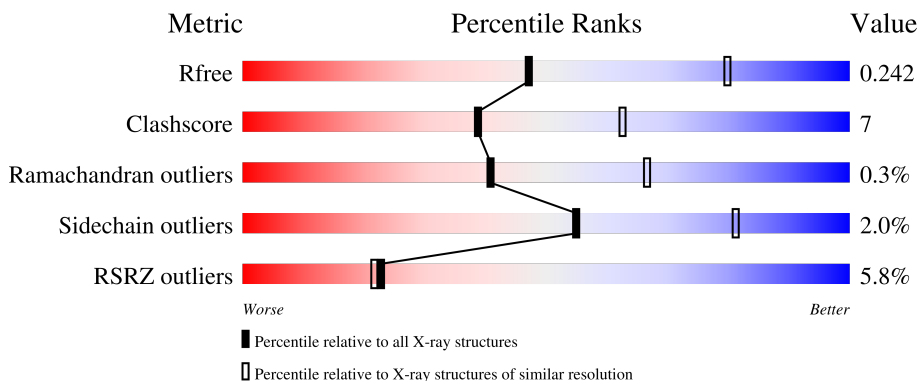
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.70 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	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (2.70-2.70)

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  $\geq 3$ , 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  $\leq 5\%$ . 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	362	<div> <div>4%</div> <div>73%</div> <div>20%</div> <div>7%</div> </div>
1	B	362	<div> <div>3%</div> <div>80%</div> <div>12%</div> <div>7%</div> </div>
1	C	362	<div> <div>8%</div> <div>77%</div> <div>14%</div> <div>7%</div> </div>
1	D	362	<div> <div>6%</div> <div>77%</div> <div>14%</div> <div>7%</div> </div>

## 2 Entry composition [i](#)

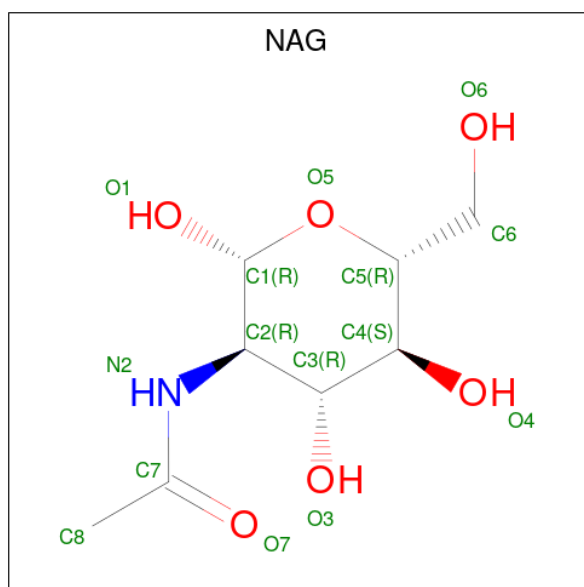
There are 4 unique types of molecules in this entry. The entry contains 11028 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 HIV-1 gp120 Clade C1086.

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	C	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			

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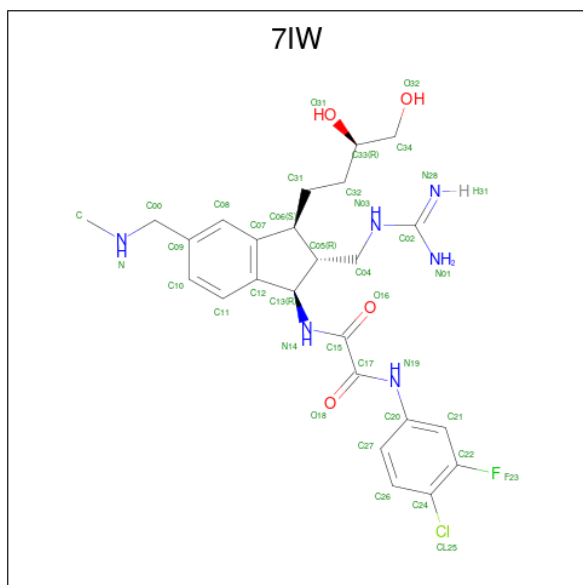
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	B	1	Total	C	N	O	0	0
			14	8	1	5		
2	B	1	Total	C	N	O	0	0
			14	8	1	5		
2	B	1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

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

- Molecule 3 is N 1 -{(1R,2R,3S)-2-(carbamimidamidomethyl)-3-[(3R)-3,4-dihydroxybutyl]-5-[(methylamino)methyl]-2,3-dihydro-1H-inden-1-yl}-N 2 -(4-chloro-3-fluorophenyl)ethanedi amide (three-letter code: 7IW) (formula: C<sub>25</sub>H<sub>32</sub>ClFN<sub>6</sub>O<sub>4</sub>) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	A	1	Total	C	Cl	F	N	O	0	0
			37	25	1	1	6	4		
3	B	1	Total	C	Cl	F	N	O	0	0
			37	25	1	1	6	4		
3	C	1	Total	C	Cl	F	N	O	0	0
			37	25	1	1	6	4		
3	D	1	Total	C	Cl	F	N	O	0	0
			37	25	1	1	6	4		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	5	Total	O	0	0
			5	5		
4	B	10	Total	O	0	0
			10	10		
4	C	15	Total	O	0	0
			15	15		

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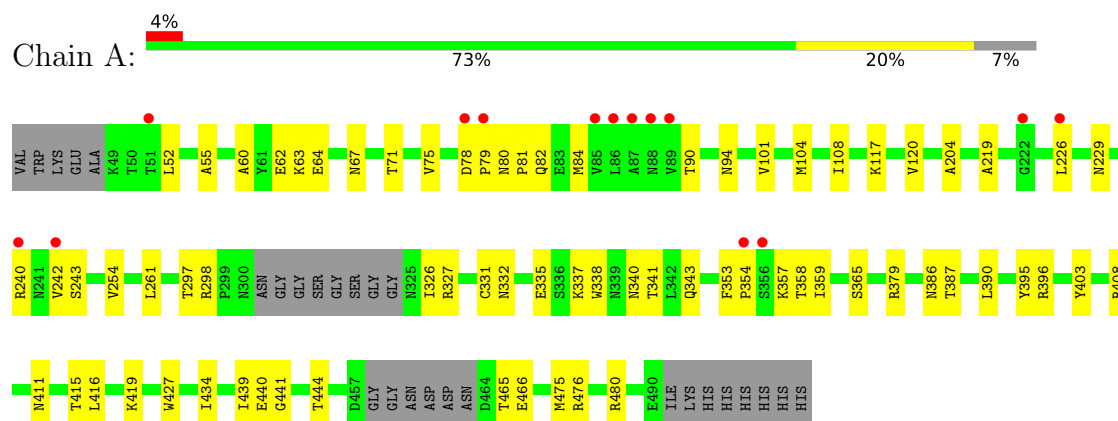
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	D	6	Total	O	0	0
			6	6		

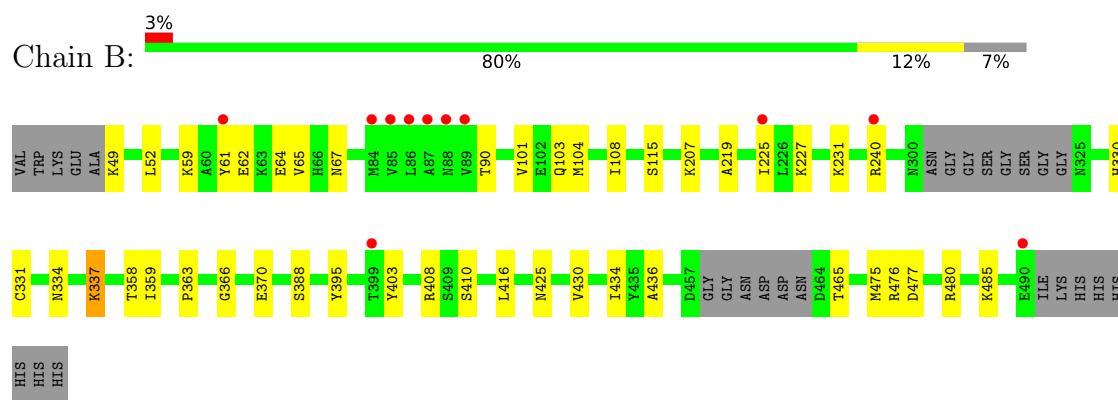
### 3 Residue-property plots [i](#)

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.

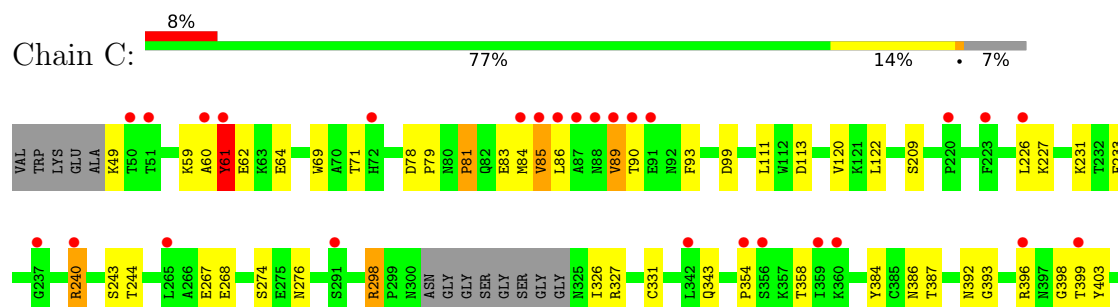
#### • Molecule 1: HIV-1 gp120 Clade C1086

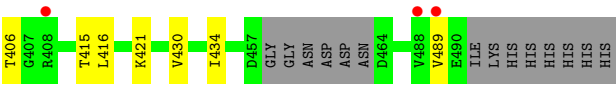


#### • Molecule 1: HIV-1 gp120 Clade C1086

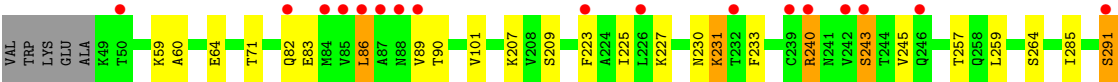
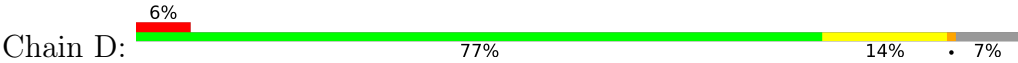


#### • Molecule 1: HIV-1 gp120 Clade C1086





● Molecule 1: HIV-1 gp120 Clade C1086





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	71.58Å 120.75Å 195.28Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.16 – 2.70 48.16 – 2.70	Depositor EDS
% Data completeness (in resolution range)	99.8 (48.16-2.70) 99.9 (48.16-2.70)	Depositor EDS
$R_{merge}$	0.11	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.91 (at 2.69Å)	Xtriage
Refinement program	PHENIX 1.14_3260	Depositor
R, $R_{free}$	0.235 , 0.279 0.239 , 0.242	Depositor DCC
$R_{free}$ test set	2000 reflections (4.23%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	64.1	Xtriage
Anisotropy	0.582	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 42.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	11028	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	66.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 15.96% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  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: 7IW, 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	0.30	0/2681	0.50	0/3637
1	B	0.29	0/2680	0.49	0/3634
1	C	0.53	7/2681 (0.3%)	0.68	4/3637 (0.1%)
1	D	0.29	0/2680	0.49	1/3634 (0.0%)
All	All	0.37	7/10722 (0.1%)	0.54	5/14542 (0.0%)

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	C	0	2

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	61	TYR	CB-CG	-11.08	1.35	1.51
1	C	61	TYR	CD2-CE2	-10.86	1.23	1.39
1	C	61	TYR	CG-CD2	-7.44	1.29	1.39
1	C	61	TYR	CZ-OH	6.91	1.49	1.37
1	C	61	TYR	CE1-CZ	6.31	1.46	1.38
1	C	61	TYR	CE2-CZ	-5.76	1.31	1.38
1	C	85	VAL	CB-CG2	-5.43	1.41	1.52

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	61	TYR	CB-CG-CD2	-18.94	109.64	121.00
1	C	61	TYR	CA-CB-CG	-13.12	88.48	113.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	61	TYR	CD1-CE1-CZ	-6.15	114.26	119.80
1	D	86	LEU	CA-CB-CG	5.37	127.65	115.30
1	C	86	LEU	CA-CB-CG	5.04	126.89	115.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	61	TYR	Sidechain
1	C	89	VAL	Peptide

## 5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2627	0	2540	45	0
1	B	2627	0	2540	29	0
1	C	2627	0	2542	49	0
1	D	2627	0	2540	38	0
2	A	98	0	91	2	0
2	B	84	0	78	2	0
2	C	70	0	65	2	0
2	D	84	0	78	1	0
3	A	37	0	0	1	0
3	B	37	0	0	1	0
3	C	37	0	0	1	0
3	D	37	0	0	1	0
4	A	5	0	0	2	0
4	B	10	0	0	3	0
4	C	15	0	0	3	0
4	D	6	0	0	2	0
All	All	11028	0	10474	160	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 7.

All (160) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:353:PHE:C	1:A:357:LYS:HE3	1.91	0.90
1:A:353:PHE:HB3	1:A:357:LYS:HG2	1.57	0.85
1:C:421:LYS:NZ	4:C:601:HOH:O	2.09	0.84
1:D:331:CYS:O	1:D:415:THR:HA	1.83	0.78
1:A:298:ARG:NH2	1:A:441:GLY:O	2.17	0.77
1:A:387:THR:OG1	4:A:601:HOH:O	2.03	0.76
1:A:358:THR:O	1:A:465:THR:OG1	2.03	0.76
1:C:343:GLN:OE1	1:C:403:TYR:N	2.19	0.76
1:A:62:GLU:HG3	1:A:64:GLU:H	1.52	0.74
1:C:399:THR:HG1	1:C:403:TYR:N	1.86	0.72
1:C:83:GLU:OE2	1:C:227:LYS:NZ	2.23	0.71
1:D:86:LEU:HB3	1:D:89:VAL:HB	1.73	0.71
1:C:59:LYS:C	1:C:61:TYR:H	1.93	0.71
1:D:227:LYS:NZ	4:D:602:HOH:O	2.18	0.70
1:A:353:PHE:CA	1:A:357:LYS:HE3	2.21	0.69
1:D:358:THR:O	1:D:465:THR:OG1	2.12	0.68
1:C:387:THR:HA	1:C:416:LEU:HD23	1.77	0.67
1:D:343:GLN:OE1	1:D:403:TYR:N	2.28	0.67
1:D:82:GLN:O	4:D:601:HOH:O	2.14	0.66
1:C:62:GLU:HG3	1:C:64:GLU:H	1.59	0.66
1:A:335:GLU:OE2	2:A:507:NAG:H61	1.97	0.65
1:D:298:ARG:NH2	1:D:439:ILE:O	2.28	0.65
1:A:52:LEU:HD22	1:A:219:ALA:HA	1.79	0.65
1:A:78:ASP:OD2	4:A:602:HOH:O	2.14	0.65
1:B:49:LYS:N	4:B:603:HOH:O	2.30	0.64
1:C:392:ASN:OD1	1:C:406:THR:OG1	2.16	0.64
1:A:353:PHE:C	1:A:357:LYS:CE	2.63	0.64
1:C:226:LEU:HD12	1:C:489:VAL:HG11	1.80	0.64
1:A:331:CYS:O	1:A:415:THR:HA	1.98	0.64
1:D:101:VAL:HG21	1:D:480:ARG:HG2	1.82	0.62
1:D:231:LYS:HD2	1:D:231:LYS:H	1.63	0.62
1:C:274:SER:OG	4:C:602:HOH:O	2.15	0.61
1:C:331:CYS:O	1:C:415:THR:HA	2.01	0.61
1:C:231:LYS:HE2	1:C:267:GLU:OE1	2.00	0.61
1:C:231:LYS:CE	1:C:267:GLU:OE1	2.49	0.61
1:C:59:LYS:C	1:C:61:TYR:N	2.53	0.60
1:C:298:ARG:HH21	1:C:326:ILE:HB	1.67	0.60
1:C:61:TYR:C	1:C:61:TYR:CD2	2.73	0.59
1:A:297:THR:HG23	1:A:444:THR:HG22	1.83	0.59
1:C:358:THR:HG23	1:C:396:ARG:HB2	1.84	0.58
1:D:408:ARG:NH2	1:D:410:SER:HB2	2.19	0.58
1:C:49:LYS:HE2	1:C:99:ASP:HB2	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:231:LYS:NZ	1:C:267:GLU:OE1	2.35	0.57
1:A:79:PRO:O	1:A:81:PRO:HD3	2.04	0.57
1:D:225:ILE:HB	1:D:245:VAL:HG23	1.85	0.57
1:D:353:PHE:HB3	1:D:357:LYS:HE3	1.86	0.57
2:D:503:NAG:H83	2:D:503:NAG:H3	1.86	0.57
1:B:59:LYS:O	4:B:601:HOH:O	2.18	0.56
1:D:207:LYS:HG2	1:D:439:ILE:CG2	2.36	0.56
1:A:60:ALA:HA	1:A:71:THR:HG21	1.88	0.56
2:A:503:NAG:H83	2:A:503:NAG:H3	1.86	0.56
1:C:69:TRP:CE3	1:C:111:LEU:HD12	2.41	0.55
1:C:84:MET:HB3	1:C:244:THR:HB	1.89	0.55
1:C:430:VAL:HA	3:C:506:7IW:N28	2.21	0.55
1:D:64:GLU:HA	1:D:209:SER:HB3	1.89	0.54
1:B:434:ILE:HD11	1:C:434:ILE:HD12	1.88	0.54
1:C:60:ALA:CA	1:C:71:THR:HG21	2.38	0.54
1:D:230:ASN:HB3	1:D:233:PHE:HB2	1.88	0.54
1:A:354:PRO:N	1:A:357:LYS:CE	2.71	0.54
1:C:60:ALA:HA	1:C:71:THR:HG21	1.90	0.52
1:D:207:LYS:HE2	1:D:436:ALA:HB3	1.91	0.52
1:D:83:GLU:HG3	1:D:243:SER:OG	2.10	0.52
1:B:62:GLU:HG3	1:B:64:GLU:H	1.74	0.52
1:C:79:PRO:C	1:C:81:PRO:HD3	2.30	0.51
1:D:350:ALA:O	1:D:354:PRO:HA	2.10	0.51
1:C:89:VAL:HG22	1:C:90:THR:H	1.76	0.51
1:C:399:THR:HA	1:C:403:TYR:N	2.25	0.51
1:A:226:LEU:HD22	1:A:242:VAL:HG12	1.93	0.51
1:A:298:ARG:HD2	1:A:326:ILE:O	2.10	0.51
1:B:359:ILE:HB	1:B:395:TYR:HB3	1.93	0.51
2:B:503:NAG:H83	2:B:503:NAG:H3	1.94	0.50
2:C:503:NAG:H3	2:C:503:NAG:H83	1.92	0.50
1:B:358:THR:HG23	1:B:465:THR:HG22	1.93	0.50
1:B:207:LYS:HE2	1:B:436:ALA:HB3	1.94	0.49
1:B:331:CYS:HB2	1:B:416:LEU:HD12	1.95	0.49
1:C:90:THR:HB	1:C:240:ARG:HA	1.95	0.49
1:C:276:ASN:O	4:C:602:HOH:O	2.20	0.49
1:A:343:GLN:HB3	1:A:403:TYR:HB3	1.94	0.49
1:B:104:MET:O	1:B:108:ILE:HG12	2.13	0.49
1:B:370:GLU:CD	1:B:425:ASN:HB2	2.33	0.48
1:D:231:LYS:H	1:D:231:LYS:CD	2.24	0.48
1:A:340:ASN:HA	1:A:343:GLN:HG2	1.96	0.48
1:B:61:TYR:HA	1:D:59:LYS:HE2	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:408:ARG:NH1	1:B:403:TYR:O	2.47	0.48
1:A:229:ASN:OD1	1:A:243:SER:OG	2.24	0.47
1:A:79:PRO:C	1:A:81:PRO:HD3	2.34	0.47
1:D:386:ASN:O	1:D:416:LEU:HB3	2.14	0.47
1:A:254:VAL:HG11	1:A:261:LEU:HB2	1.95	0.47
1:B:101:VAL:HG21	1:B:480:ARG:HG2	1.96	0.47
1:D:86:LEU:HD23	1:D:89:VAL:HG21	1.96	0.47
1:C:59:LYS:O	1:C:61:TYR:N	2.48	0.46
1:A:101:VAL:HG21	1:A:480:ARG:HG2	1.98	0.46
1:B:434:ILE:HG21	1:C:122:LEU:HD21	1.97	0.46
1:D:291:SER:OG	1:D:448:ASN:HB3	2.16	0.46
1:A:104:MET:O	1:A:108:ILE:HG12	2.16	0.46
1:D:298:ARG:NH1	1:D:441:GLY:O	2.48	0.46
1:A:354:PRO:N	1:A:357:LYS:HE3	2.31	0.46
1:A:465:THR:OG1	1:A:466:GLU:N	2.49	0.45
1:A:338:TRP:CZ2	1:A:390:LEU:HG	2.52	0.45
1:C:268:GLU:O	2:C:504:NAG:H83	2.16	0.45
1:B:430:VAL:HA	3:B:507:7IW:N28	2.31	0.45
1:D:90:THR:HB	1:D:240:ARG:HA	1.98	0.45
1:D:223:PHE:CE2	1:D:490:GLU:HG3	2.52	0.45
1:B:434:ILE:HD12	1:C:120:VAL:HG11	1.99	0.44
1:B:477:ASP:OD1	1:B:480:ARG:NH1	2.51	0.44
1:A:359:ILE:HB	1:A:395:TYR:HB3	1.98	0.44
1:A:327:ARG:O	1:A:419:LYS:HA	2.18	0.44
1:A:419:LYS:HB2	1:A:419:LYS:HE2	1.79	0.44
1:D:60:ALA:HA	1:D:71:THR:HG21	1.99	0.44
1:D:207:LYS:HG2	1:D:439:ILE:HG22	1.99	0.44
1:A:64:GLU:OE1	1:A:67:ASN:ND2	2.43	0.44
1:B:334:ASN:HB3	1:B:337:LYS:HD2	2.00	0.44
1:C:60:ALA:N	1:C:71:THR:HG21	2.32	0.44
1:B:219:ALA:H	1:B:225:ILE:HD11	1.82	0.44
1:B:366:GLY:CA	4:B:602:HOH:O	2.65	0.44
1:D:86:LEU:HB3	1:D:89:VAL:CB	2.46	0.43
1:C:83:GLU:HG3	1:C:243:SER:OG	2.17	0.43
1:A:386:ASN:O	1:A:416:LEU:HB3	2.18	0.43
1:B:227:LYS:HA	1:B:485:LYS:O	2.18	0.43
1:A:120:VAL:HB	1:A:434:ILE:HB	2.01	0.43
1:D:387:THR:HA	1:D:416:LEU:HD22	1.99	0.43
1:A:476:ARG:O	1:A:480:ARG:HG3	2.19	0.43
1:C:231:LYS:HE2	1:C:267:GLU:CD	2.38	0.43
1:B:363:PRO:HG3	1:B:388:SER:HA	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:384:TYR:CE1	1:C:421:LYS:HB2	2.54	0.43
1:A:439:ILE:HG22	1:A:440:GLU:N	2.34	0.43
1:A:63:LYS:HB3	1:A:63:LYS:HE3	1.73	0.42
1:A:80:ASN:O	1:A:80:ASN:ND2	2.52	0.42
1:B:52:LEU:HD23	1:B:103:GLN:NE2	2.34	0.42
1:D:399:THR:HA	1:D:403:TYR:N	2.34	0.42
1:A:117:LYS:HE2	1:A:204:ALA:O	2.19	0.42
1:B:59:LYS:H	1:B:67:ASN:HD22	1.68	0.42
1:B:90:THR:CG2	1:B:240:ARG:HG2	2.49	0.42
1:C:90:THR:HG21	1:C:240:ARG:CD	2.50	0.42
1:D:298:ARG:HG2	1:D:328:GLN:O	2.20	0.42
1:C:84:MET:O	1:C:243:SER:HA	2.19	0.42
1:A:90:THR:HB	1:A:240:ARG:HA	2.02	0.42
1:B:65:VAL:HB	1:B:115:SER:HB3	2.01	0.42
1:C:90:THR:CB	1:C:240:ARG:HA	2.50	0.41
1:C:396:ARG:O	1:C:399:THR:O	2.38	0.41
1:D:257:THR:O	1:D:259:LEU:N	2.46	0.41
1:A:55:ALA:HA	1:A:75:VAL:O	2.21	0.41
1:C:386:ASN:O	1:C:416:LEU:HB3	2.20	0.41
1:D:427:TRP:HB3	3:D:507:7IW:C17	2.51	0.41
1:D:476:ARG:O	1:D:480:ARG:HG3	2.20	0.41
1:A:332:ASN:OD1	1:A:415:THR:HG22	2.20	0.41
1:A:427:TRP:HB3	3:A:508:7IW:C17	2.51	0.41
1:B:408:ARG:HB2	2:B:506:NAG:O6	2.20	0.41
1:C:64:GLU:HA	1:C:209:SER:HB3	2.03	0.41
1:C:343:GLN:NE2	1:C:398:GLY:O	2.41	0.41
1:B:476:ARG:O	1:B:480:ARG:HG3	2.21	0.41
1:C:93:PHE:HB2	1:C:233:PHE:CZ	2.55	0.41
1:C:393:GLY:HA3	1:C:403:TYR:CE1	2.56	0.41
1:C:421:LYS:HB3	1:C:421:LYS:HE2	1.68	0.41
1:B:330:HIS:HA	1:B:416:LEU:O	2.22	0.41
1:D:353:PHE:HA	1:D:357:LYS:HZ2	1.86	0.40
1:D:285:ILE:HG12	1:D:453:LEU:HD23	2.03	0.40
1:D:342:LEU:HD23	1:D:342:LEU:HA	1.75	0.40
1:A:337:LYS:O	1:A:341:THR:OG1	2.27	0.40
1:C:90:THR:HG22	1:C:240:ARG:HA	2.04	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	327/362 (90%)	314 (96%)	11 (3%)	2 (1%)	25	50
1	B	325/362 (90%)	315 (97%)	10 (3%)	0	100	100
1	C	327/362 (90%)	306 (94%)	19 (6%)	2 (1%)	25	50
1	D	325/362 (90%)	317 (98%)	8 (2%)	0	100	100
All	All	1304/1448 (90%)	1252 (96%)	48 (4%)	4 (0%)	41	66

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	85	VAL
1	A	411	ASN
1	A	365	SER
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	297/316 (94%)	291 (98%)	6 (2%)	55	81
1	B	297/316 (94%)	293 (99%)	4 (1%)	69	87
1	C	297/316 (94%)	291 (98%)	6 (2%)	55	81
1	D	297/316 (94%)	289 (97%)	8 (3%)	44	74
All	All	1188/1264 (94%)	1164 (98%)	24 (2%)	55	81



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

Mol	Chain	Res	Type
1	A	82	GLN
1	A	84	MET
1	A	94	ASN
1	A	379	ARG
1	A	396	ARG
1	A	475	MET
1	B	231	LYS
1	B	337	LYS
1	B	410	SER
1	B	475	MET
1	C	78	ASP
1	C	81	PRO
1	C	113	ASP
1	C	240	ARG
1	C	298	ARG
1	C	327	ARG
1	D	231	LYS
1	D	240	ARG
1	D	243	SER
1	D	264	SER
1	D	291	SER
1	D	337	LYS
1	D	365	SER
1	D	419	LYS

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

Mol	Chain	Res	Type
1	A	293	ASN
1	C	404	ASN
1	D	340	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

28 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	504	1	14,14,15	0.27	0	17,19,21	0.53	0
2	NAG	A	506	1	14,14,15	0.49	0	17,19,21	0.54	0
2	NAG	B	503	1	14,14,15	0.32	0	17,19,21	1.39	2 (11%)
2	NAG	B	505	1	14,14,15	0.24	0	17,19,21	0.44	0
2	NAG	B	501	1	14,14,15	0.21	0	17,19,21	0.33	0
2	NAG	D	501	1	14,14,15	0.26	0	17,19,21	0.50	0
2	NAG	D	504	1	14,14,15	0.18	0	17,19,21	0.56	0
2	NAG	D	505	1	14,14,15	0.24	0	17,19,21	0.44	0
2	NAG	A	501	1	14,14,15	0.17	0	17,19,21	0.41	0
3	7IW	D	507	-	37,39,39	2.90	12 (32%)	45,54,54	1.65	11 (24%)
2	NAG	C	501	1	14,14,15	0.21	0	17,19,21	0.35	0
2	NAG	D	502	1	14,14,15	0.22	0	17,19,21	0.61	1 (5%)
3	7IW	C	506	-	37,39,39	2.90	12 (32%)	45,54,54	1.63	11 (24%)
2	NAG	B	502	1	14,14,15	0.19	0	17,19,21	0.58	0
2	NAG	D	503	1	14,14,15	0.35	0	17,19,21	1.32	2 (11%)
3	7IW	A	508	-	37,39,39	2.90	12 (32%)	45,54,54	1.64	11 (24%)
2	NAG	C	505	1	14,14,15	0.25	0	17,19,21	0.39	0
2	NAG	C	504	1	14,14,15	0.17	0	17,19,21	0.48	0
2	NAG	A	505	1	14,14,15	0.26	0	17,19,21	0.47	0
2	NAG	A	503	1	14,14,15	0.40	0	17,19,21	1.25	1 (5%)
2	NAG	B	504	1	14,14,15	0.35	0	17,19,21	0.59	0
2	NAG	D	506	1	14,14,15	0.53	0	17,19,21	0.84	1 (5%)
2	NAG	A	507	1	14,14,15	1.06	2 (14%)	17,19,21	1.04	1 (5%)
3	7IW	B	507	-	37,39,39	2.91	12 (32%)	45,54,54	1.63	11 (24%)
2	NAG	C	502	1	14,14,15	0.25	0	17,19,21	0.67	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	NAG	B	506	1	14,14,15	0.22	0	17,19,21	0.75	1 (5%)
2	NAG	C	503	1	14,14,15	0.30	0	17,19,21	1.45	2 (11%)
2	NAG	A	502	1	14,14,15	0.20	0	17,19,21	0.69	1 (5%)

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	504	1	-	2/6/23/26	0/1/1/1
2	NAG	A	506	1	-	4/6/23/26	0/1/1/1
2	NAG	B	503	1	-	5/6/23/26	0/1/1/1
2	NAG	B	505	1	-	2/6/23/26	0/1/1/1
2	NAG	B	501	1	-	2/6/23/26	0/1/1/1
2	NAG	D	501	1	-	0/6/23/26	0/1/1/1
2	NAG	D	504	1	-	3/6/23/26	0/1/1/1
2	NAG	D	505	1	-	2/6/23/26	0/1/1/1
2	NAG	A	501	1	-	0/6/23/26	0/1/1/1
3	7IW	D	507	-	-	5/26/43/43	0/3/3/3
2	NAG	C	501	1	-	0/6/23/26	0/1/1/1
2	NAG	D	502	1	-	2/6/23/26	0/1/1/1
3	7IW	C	506	-	-	5/26/43/43	0/3/3/3
2	NAG	B	502	1	-	1/6/23/26	0/1/1/1
2	NAG	D	503	1	-	5/6/23/26	0/1/1/1
3	7IW	A	508	-	-	5/26/43/43	0/3/3/3
2	NAG	C	505	1	-	2/6/23/26	0/1/1/1
2	NAG	C	504	1	-	4/6/23/26	0/1/1/1
2	NAG	A	505	1	-	2/6/23/26	0/1/1/1
2	NAG	A	503	1	-	5/6/23/26	0/1/1/1
2	NAG	B	504	1	-	2/6/23/26	0/1/1/1
2	NAG	D	506	1	-	4/6/23/26	0/1/1/1
2	NAG	A	507	1	-	0/6/23/26	0/1/1/1
3	7IW	B	507	-	-	5/26/43/43	0/3/3/3
2	NAG	C	502	1	-	2/6/23/26	0/1/1/1
2	NAG	B	506	1	-	4/6/23/26	0/1/1/1
2	NAG	C	503	1	-	3/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	A	502	1	-	0/6/23/26	0/1/1/1

All (50) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	507	7IW	C15-N14	8.07	1.50	1.34
3	B	507	7IW	C15-N14	8.04	1.50	1.34
3	A	508	7IW	C15-N14	8.01	1.50	1.34
3	C	506	7IW	C15-N14	8.00	1.50	1.34
3	A	508	7IW	C02-N03	7.29	1.47	1.33
3	D	507	7IW	C02-N03	7.23	1.47	1.33
3	B	507	7IW	C02-N03	7.22	1.47	1.33
3	C	506	7IW	C02-N03	7.16	1.47	1.33
3	B	507	7IW	C07-C06	5.84	1.59	1.51
3	D	507	7IW	C17-N19	5.78	1.48	1.35
3	A	508	7IW	C07-C06	5.77	1.59	1.51
3	A	508	7IW	C17-N19	5.77	1.48	1.35
3	C	506	7IW	C07-C06	5.76	1.59	1.51
3	C	506	7IW	C17-N19	5.74	1.48	1.35
3	B	507	7IW	C17-N19	5.73	1.48	1.35
3	D	507	7IW	C07-C06	5.72	1.59	1.51
3	C	506	7IW	C20-N19	5.64	1.53	1.41
3	B	507	7IW	C20-N19	5.57	1.52	1.41
3	A	508	7IW	C20-N19	5.54	1.52	1.41
3	D	507	7IW	C20-N19	5.53	1.52	1.41
3	C	506	7IW	C06-C05	-4.64	1.47	1.55
3	B	507	7IW	C06-C05	-4.62	1.47	1.55
3	D	507	7IW	C06-C05	-4.57	1.47	1.55
3	A	508	7IW	C06-C05	-4.50	1.48	1.55
3	D	507	7IW	C00-C09	4.09	1.60	1.51
3	C	506	7IW	C00-C09	4.08	1.60	1.51
3	B	507	7IW	C00-C09	4.08	1.60	1.51
3	A	508	7IW	C00-C09	4.08	1.60	1.51
3	A	508	7IW	C08-C07	3.55	1.45	1.39
3	D	507	7IW	C08-C07	3.54	1.45	1.39
3	B	507	7IW	C08-C07	3.47	1.45	1.39
3	C	506	7IW	C08-C07	3.42	1.45	1.39
3	C	506	7IW	C10-C09	3.10	1.45	1.38
3	A	508	7IW	C10-C09	3.04	1.45	1.38
3	B	507	7IW	C10-C09	3.03	1.45	1.38
3	D	507	7IW	C10-C09	3.02	1.45	1.38
2	A	507	NAG	O5-C1	3.02	1.48	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	508	7IW	C11-C12	2.42	1.42	1.39
3	B	507	7IW	C11-C12	2.41	1.42	1.39
2	A	507	NAG	C1-C2	2.39	1.55	1.52
3	C	506	7IW	C11-C12	2.36	1.42	1.39
3	D	507	7IW	C11-C12	2.35	1.42	1.39
3	D	507	7IW	O16-C15	-2.34	1.19	1.23
3	B	507	7IW	O16-C15	-2.33	1.19	1.23
3	C	506	7IW	O16-C15	-2.31	1.19	1.23
3	A	508	7IW	O16-C15	-2.28	1.19	1.23
3	C	506	7IW	O31-C33	-2.25	1.36	1.43
3	D	507	7IW	O31-C33	-2.22	1.36	1.43
3	B	507	7IW	O31-C33	-2.21	1.36	1.43
3	A	508	7IW	O31-C33	-2.20	1.36	1.43

All (57) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	506	7IW	C12-C13-N14	-5.51	105.76	114.61
3	D	507	7IW	C12-C13-N14	-5.50	105.78	114.61
3	A	508	7IW	C12-C13-N14	-5.49	105.81	114.61
3	B	507	7IW	C12-C13-N14	-5.49	105.81	114.61
2	C	503	NAG	C2-N2-C7	4.47	129.27	122.90
2	A	503	NAG	C2-N2-C7	4.43	129.21	122.90
2	D	503	NAG	C2-N2-C7	4.40	129.17	122.90
2	B	503	NAG	C2-N2-C7	4.36	129.11	122.90
2	A	507	NAG	C1-O5-C5	3.61	117.08	112.19
3	D	507	7IW	C17-C15-N14	3.02	120.97	113.73
3	C	506	7IW	C17-C15-N14	3.02	120.97	113.73
3	B	507	7IW	C17-C15-N14	3.02	120.97	113.73
3	A	508	7IW	C17-C15-N14	3.01	120.95	113.73
2	D	506	NAG	C1-O5-C5	2.94	116.18	112.19
3	D	507	7IW	C26-C24-C22	2.89	121.26	118.94
3	A	508	7IW	C20-C21-C22	-2.89	116.39	118.76
3	D	507	7IW	C20-C21-C22	-2.88	116.40	118.76
3	A	508	7IW	C26-C24-C22	2.82	121.20	118.94
3	B	507	7IW	C26-C24-C22	2.79	121.17	118.94
3	C	506	7IW	C20-C21-C22	-2.78	116.48	118.76
3	B	507	7IW	C20-C21-C22	-2.75	116.51	118.76
2	B	503	NAG	C1-C2-N2	2.67	115.05	110.49
3	D	507	7IW	O16-C15-N14	-2.64	118.45	123.08
3	A	508	7IW	O16-C15-N14	-2.63	118.47	123.08
3	B	507	7IW	O16-C15-N14	-2.62	118.49	123.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	508	7IW	C31-C06-C07	2.61	120.14	113.03
3	C	506	7IW	O16-C15-N14	-2.60	118.51	123.08
3	D	507	7IW	C31-C06-C07	2.59	120.09	113.03
3	C	506	7IW	C26-C24-C22	2.58	121.01	118.94
3	C	506	7IW	C31-C06-C07	2.57	120.04	113.03
3	B	507	7IW	C31-C06-C07	2.57	120.02	113.03
2	C	503	NAG	C1-C2-N2	2.56	114.87	110.49
3	A	508	7IW	C15-C17-N19	2.47	116.22	112.31
3	D	507	7IW	C15-C17-N19	2.46	116.20	112.31
2	B	506	NAG	C1-O5-C5	2.45	115.51	112.19
3	B	507	7IW	C15-C17-N19	2.45	116.18	112.31
3	C	506	7IW	C15-C17-N19	2.44	116.16	112.31
3	C	506	7IW	C20-N19-C17	-2.41	123.35	127.53
3	B	507	7IW	C20-N19-C17	-2.38	123.41	127.53
2	C	502	NAG	C1-O5-C5	2.36	115.38	112.19
3	D	507	7IW	C20-N19-C17	-2.34	123.46	127.53
2	A	502	NAG	C1-O5-C5	2.33	115.35	112.19
3	A	508	7IW	C20-N19-C17	-2.32	123.50	127.53
3	D	507	7IW	C08-C07-C12	-2.25	118.61	121.36
3	A	508	7IW	C08-C07-C12	-2.21	118.66	121.36
3	C	506	7IW	C08-C07-C12	-2.19	118.68	121.36
3	B	507	7IW	C08-C07-C12	-2.17	118.71	121.36
2	D	503	NAG	C1-C2-N2	2.13	114.13	110.49
3	A	508	7IW	C07-C08-C09	-2.12	120.00	121.98
3	B	507	7IW	C07-C08-C09	-2.12	120.00	121.98
3	D	507	7IW	C07-C08-C09	-2.11	120.01	121.98
2	D	502	NAG	C1-O5-C5	2.10	115.03	112.19
3	D	507	7IW	C12-C13-C05	2.08	106.42	104.41
3	A	508	7IW	C12-C13-C05	2.05	106.39	104.41
3	C	506	7IW	C12-C13-C05	2.05	106.39	104.41
3	C	506	7IW	C07-C08-C09	-2.05	120.06	121.98
3	B	507	7IW	C12-C13-C05	2.03	106.37	104.41

There are no chirality outliers.

All (76) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	508	7IW	N03-C04-C05-C13
3	B	507	7IW	N03-C04-C05-C13
3	C	506	7IW	N03-C04-C05-C13
3	D	507	7IW	N03-C04-C05-C13
2	D	505	NAG	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
2	A	503	NAG	O5-C5-C6-O6
2	C	505	NAG	O5-C5-C6-O6
2	A	505	NAG	O5-C5-C6-O6
2	B	503	NAG	O5-C5-C6-O6
2	B	505	NAG	O5-C5-C6-O6
2	C	505	NAG	C4-C5-C6-O6
2	B	503	NAG	C4-C5-C6-O6
2	D	505	NAG	C4-C5-C6-O6
2	B	505	NAG	C4-C5-C6-O6
2	A	503	NAG	C4-C5-C6-O6
2	A	503	NAG	C8-C7-N2-C2
2	A	503	NAG	O7-C7-N2-C2
2	A	504	NAG	C8-C7-N2-C2
2	A	504	NAG	O7-C7-N2-C2
2	A	506	NAG	C8-C7-N2-C2
2	A	506	NAG	O7-C7-N2-C2
2	B	503	NAG	C8-C7-N2-C2
2	B	503	NAG	O7-C7-N2-C2
2	B	504	NAG	C8-C7-N2-C2
2	B	504	NAG	O7-C7-N2-C2
2	B	506	NAG	C8-C7-N2-C2
2	B	506	NAG	O7-C7-N2-C2
2	C	503	NAG	C8-C7-N2-C2
2	C	503	NAG	O7-C7-N2-C2
2	C	504	NAG	C8-C7-N2-C2
2	C	504	NAG	O7-C7-N2-C2
2	D	503	NAG	C8-C7-N2-C2
2	D	503	NAG	O7-C7-N2-C2
2	D	504	NAG	C8-C7-N2-C2
2	D	504	NAG	O7-C7-N2-C2
2	D	506	NAG	C8-C7-N2-C2
2	D	506	NAG	O7-C7-N2-C2
2	D	506	NAG	O5-C5-C6-O6
2	A	505	NAG	C4-C5-C6-O6
2	A	506	NAG	O5-C5-C6-O6
2	A	506	NAG	C4-C5-C6-O6
2	C	504	NAG	O5-C5-C6-O6
3	A	508	7IW	C32-C33-C34-O32
3	B	507	7IW	C32-C33-C34-O32
3	C	506	7IW	C32-C33-C34-O32
3	D	507	7IW	C32-C33-C34-O32
2	D	502	NAG	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
2	D	502	NAG	C4-C5-C6-O6
3	A	508	7IW	O31-C33-C34-O32
3	C	506	7IW	O31-C33-C34-O32
3	D	507	7IW	O31-C33-C34-O32
2	D	503	NAG	C4-C5-C6-O6
2	D	503	NAG	O5-C5-C6-O6
2	D	506	NAG	C4-C5-C6-O6
3	B	507	7IW	O31-C33-C34-O32
2	B	506	NAG	C4-C5-C6-O6
3	A	508	7IW	C07-C06-C31-C32
3	B	507	7IW	C07-C06-C31-C32
3	C	506	7IW	C07-C06-C31-C32
3	D	507	7IW	C07-C06-C31-C32
2	C	502	NAG	C4-C5-C6-O6
2	B	501	NAG	C4-C5-C6-O6
2	C	502	NAG	O5-C5-C6-O6
3	A	508	7IW	N03-C04-C05-C06
3	B	507	7IW	N03-C04-C05-C06
3	C	506	7IW	N03-C04-C05-C06
3	D	507	7IW	N03-C04-C05-C06
2	C	504	NAG	C4-C5-C6-O6
2	D	504	NAG	C4-C5-C6-O6
2	B	506	NAG	O5-C5-C6-O6
2	B	501	NAG	O5-C5-C6-O6
2	B	502	NAG	C4-C5-C6-O6
2	A	503	NAG	C3-C2-N2-C7
2	B	503	NAG	C3-C2-N2-C7
2	C	503	NAG	C3-C2-N2-C7
2	D	503	NAG	C3-C2-N2-C7

There are no ring outliers.

11 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	503	NAG	1	0
3	D	507	7IW	1	0
3	C	506	7IW	1	0
2	D	503	NAG	1	0
3	A	508	7IW	1	0
2	C	504	NAG	1	0
2	A	503	NAG	1	0
2	A	507	NAG	1	0

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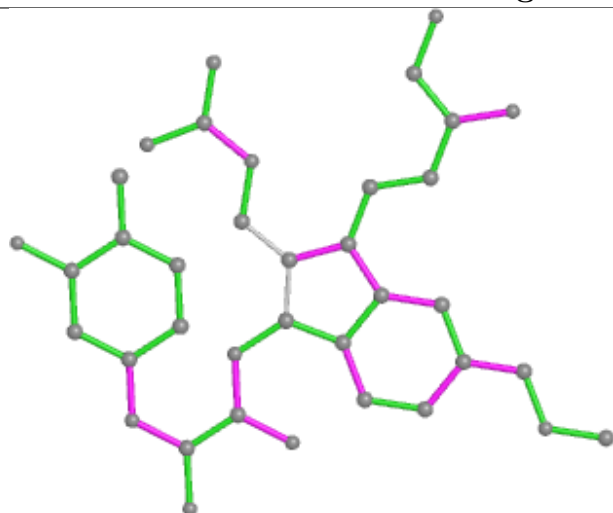


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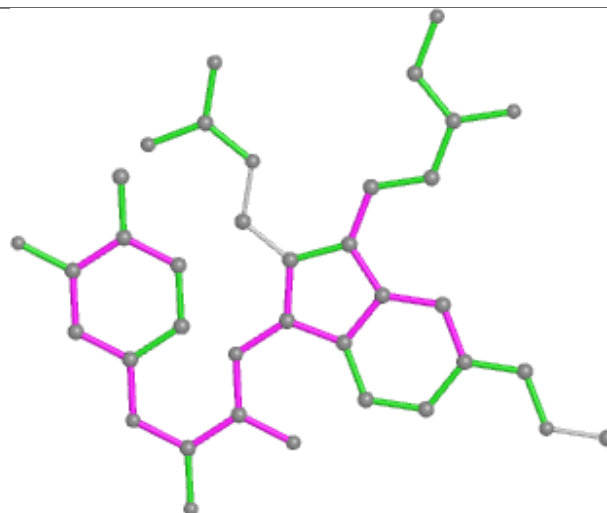
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	507	7IW	1	0
2	B	506	NAG	1	0
2	C	503	NAG	1	0

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

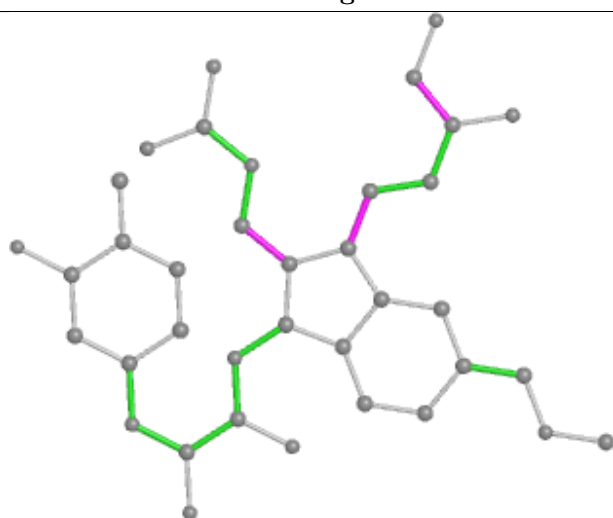
## Ligand 7IW D 507



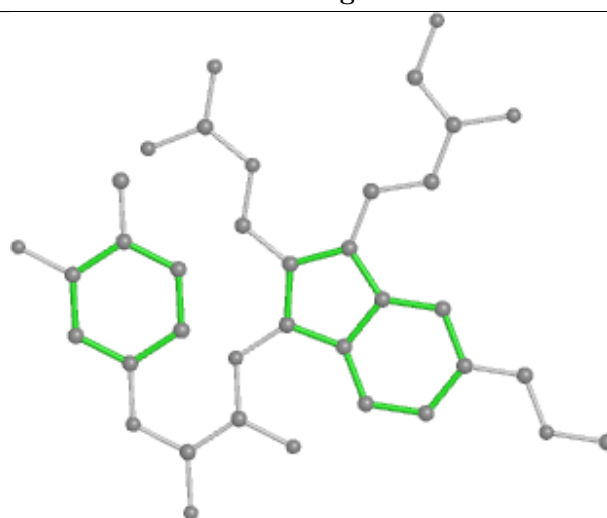
Bond lengths



Bond angles

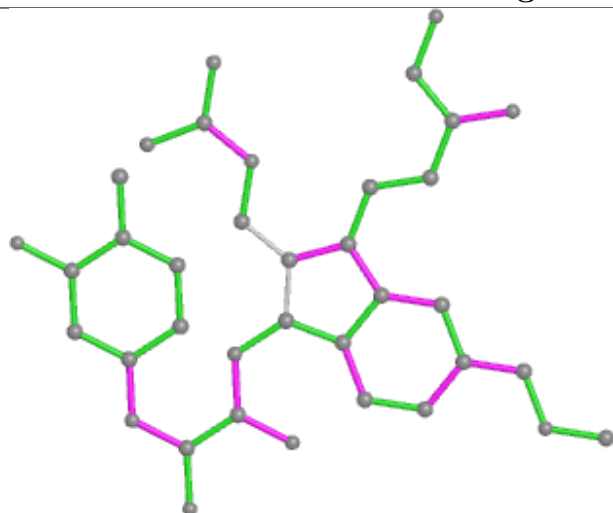


Torsions

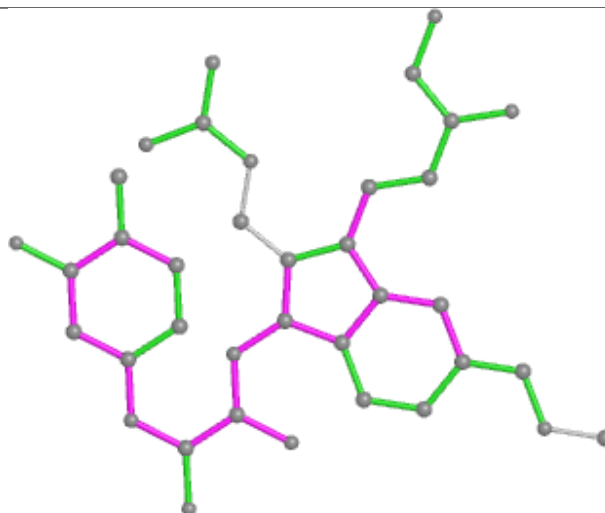


Rings

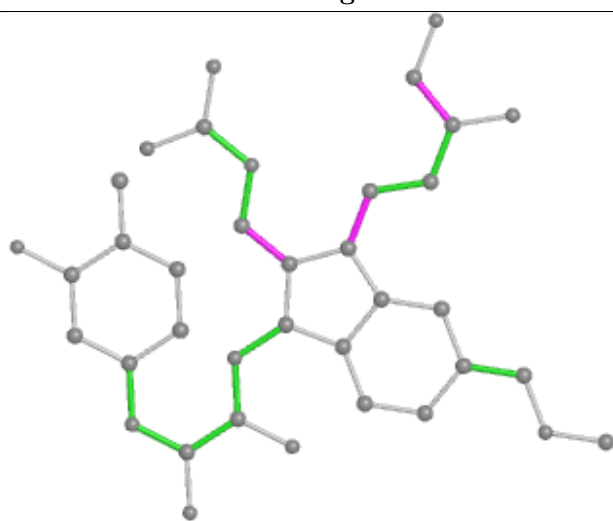
## Ligand 7IW C 506



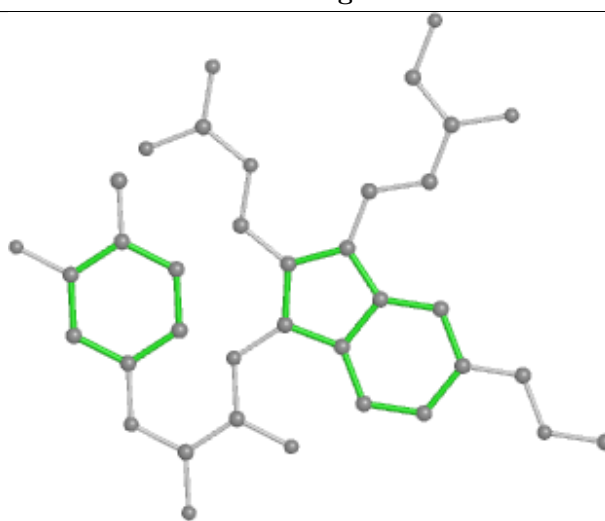
Bond lengths



Bond angles

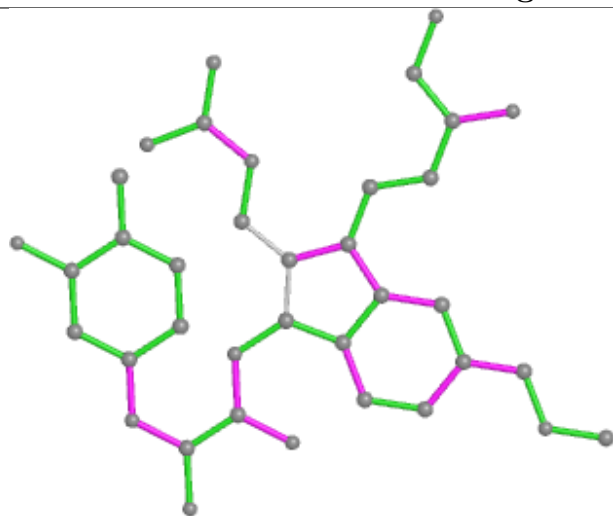


Torsions

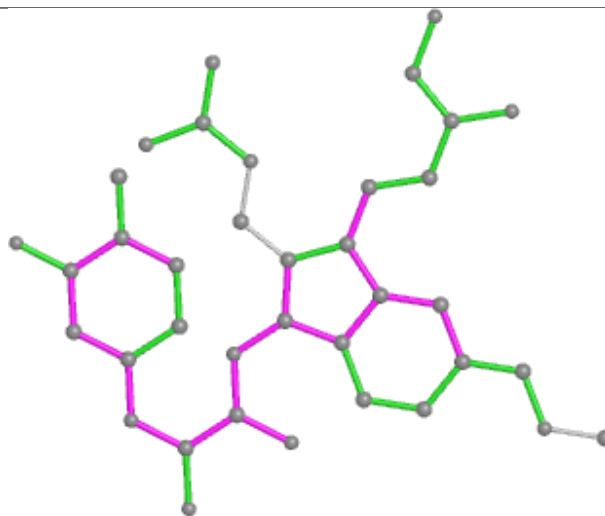


Rings

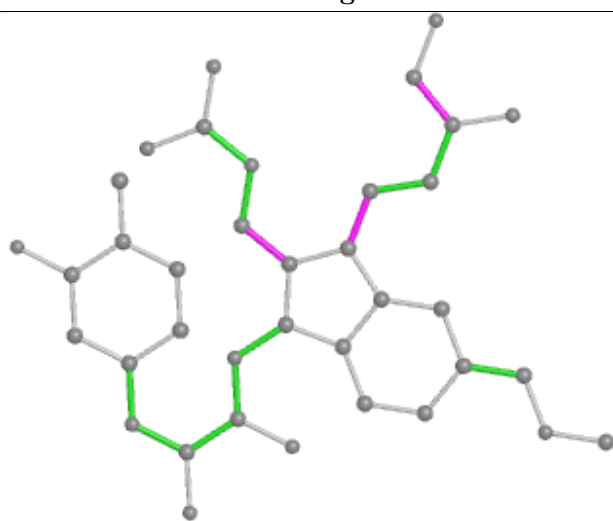
## Ligand 7IW A 508



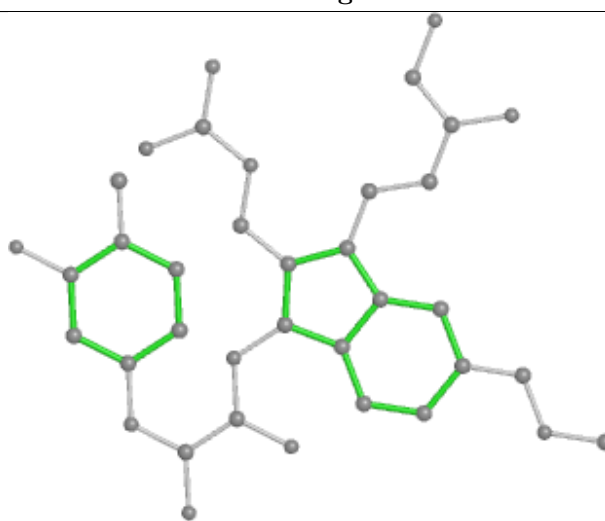
Bond lengths



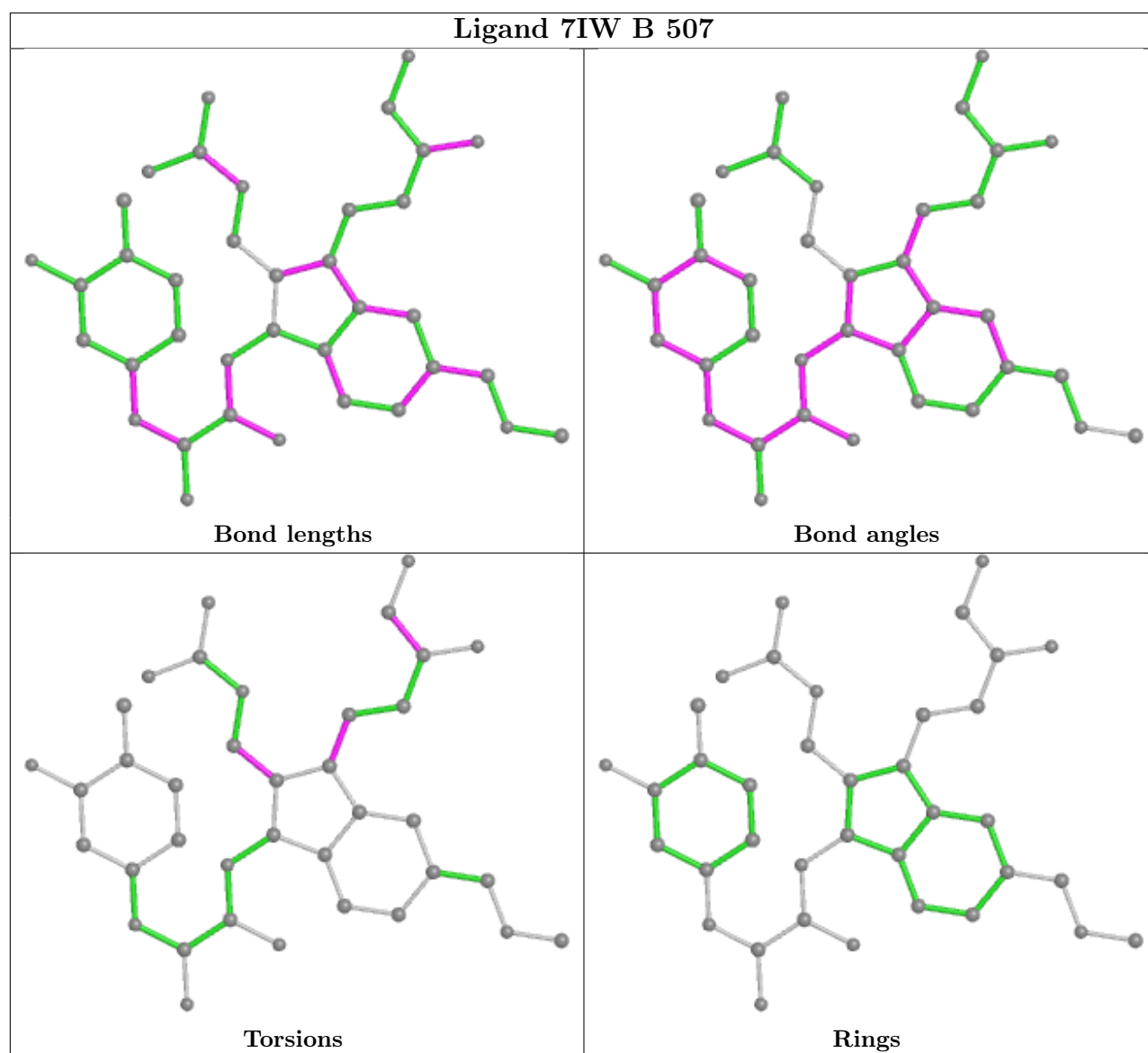
Bond angles



Torsions



Rings



## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	D	2
1	B	2
1	A	1
1	C	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	D	354:PRO	C	356:SER	N	4.57
1	A	354:PRO	C	356:SER	N	4.15
1	C	399:THR	C	403:TYR	N	3.57
1	B	354:PRO	C	356:SER	N	3.48
1	D	399:THR	C	403:TYR	N	3.19
1	B	399:THR	C	403:TYR	N	2.91

## 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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	335/362 (92%)	0.31	14 (4%) 36 35	43, 61, 89, 110	0
1	B	335/362 (92%)	0.27	11 (3%) 46 46	43, 59, 89, 104	0
1	C	335/362 (92%)	0.54	30 (8%) 9 7	46, 67, 92, 114	0
1	D	335/362 (92%)	0.49	23 (6%) 16 15	47, 69, 96, 116	0
All	All	1340/1448 (92%)	0.40	78 (5%) 23 22	43, 64, 92, 116	0

All (78) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	354	PRO	6.5
1	A	87	ALA	6.5
1	A	89	VAL	6.0
1	C	86	LEU	5.6
1	D	87	ALA	5.0
1	D	86	LEU	4.9
1	C	60	ALA	4.8
1	D	89	VAL	4.8
1	A	356	SER	4.6
1	C	240	ARG	4.5
1	C	50	THR	4.5
1	A	86	LEU	4.4
1	D	242	VAL	4.3
1	A	240	ARG	4.0
1	C	399	THR	3.9
1	D	88	ASN	3.8
1	A	226	LEU	3.7
1	C	61	TYR	3.7
1	A	88	ASN	3.6
1	D	85	VAL	3.6
1	C	88	ASN	3.5

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Mol	Chain	Res	Type	RSRZ
1	D	232	THR	3.5
1	D	326	ILE	3.5
1	C	354	PRO	3.5
1	B	89	VAL	3.5
1	D	399	THR	3.5
1	C	91	GLU	3.4
1	A	242	VAL	3.4
1	B	240	ARG	3.3
1	A	85	VAL	3.3
1	B	85	VAL	3.3
1	B	86	LEU	3.3
1	D	488	VAL	3.1
1	D	356	SER	3.0
1	C	89	VAL	2.9
1	C	72	HIS	2.9
1	C	85	VAL	2.9
1	C	237	GLY	2.8
1	D	240	ARG	2.8
1	C	51	THR	2.8
1	C	87	ALA	2.8
1	D	226	LEU	2.7
1	C	356	SER	2.7
1	B	225	ILE	2.6
1	D	354	PRO	2.5
1	C	265	LEU	2.5
1	D	82	GLN	2.5
1	C	359	ILE	2.5
1	D	246	GLN	2.4
1	B	61	TYR	2.4
1	C	489	VAL	2.4
1	B	87	ALA	2.3
1	C	226	LEU	2.3
1	B	88	ASN	2.3
1	A	78	ASP	2.3
1	B	84	MET	2.3
1	C	342	LEU	2.3
1	D	341	THR	2.3
1	B	490	GLU	2.3
1	D	239	CYS	2.3
1	D	291	SER	2.2
1	C	220	PRO	2.2
1	C	84	MET	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	90	THR	2.2
1	D	243	SER	2.2
1	A	222	GLY	2.2
1	C	408	ARG	2.2
1	A	79	PRO	2.2
1	A	51	THR	2.2
1	C	291	SER	2.1
1	C	223	PHE	2.1
1	D	50	THR	2.1
1	C	396	ARG	2.1
1	B	399	THR	2.1
1	D	223	PHE	2.1
1	D	84	MET	2.0
1	C	360	LYS	2.0
1	C	488	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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
2	NAG	A	503	14/15	0.66	0.38	87,105,108,110	0
2	NAG	B	503	14/15	0.79	0.28	81,90,98,99	0
3	7IW	B	507	37/37	0.80	0.30	50,70,84,94	0
3	7IW	D	507	37/37	0.81	0.30	56,77,85,93	0
3	7IW	C	506	37/37	0.82	0.33	55,74,83,99	0
3	7IW	A	508	37/37	0.84	0.31	57,74,86,98	0
2	NAG	D	506	14/15	0.85	0.19	66,77,81,85	0
2	NAG	D	505	14/15	0.86	0.18	61,70,81,91	0

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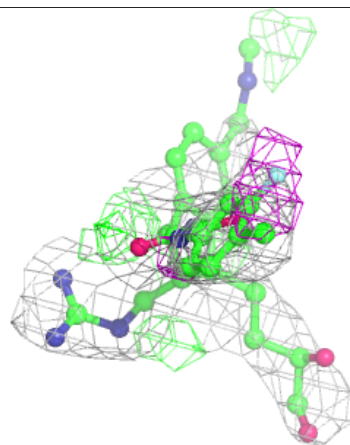
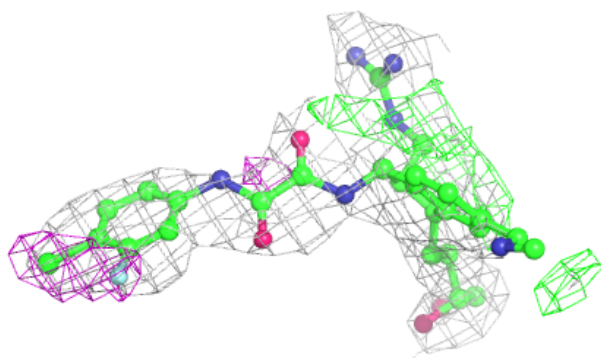
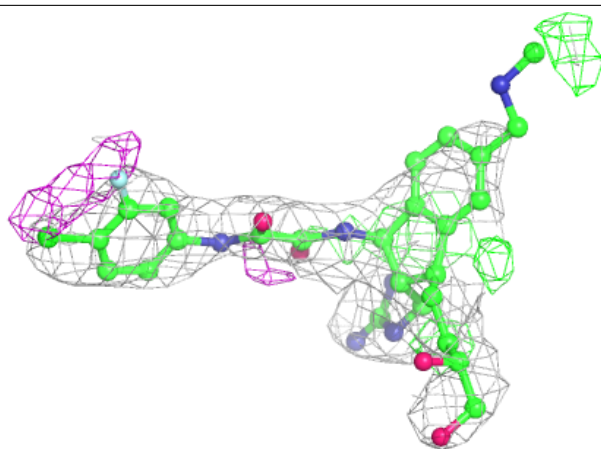
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	NAG	A	507	14/15	0.87	0.32	50,69,73,75	0
2	NAG	A	505	14/15	0.87	0.22	61,68,77,78	0
2	NAG	B	501	14/15	0.88	0.20	65,71,75,78	0
2	NAG	D	503	14/15	0.88	0.24	61,72,81,89	0
2	NAG	D	501	14/15	0.89	0.17	72,82,85,96	0
2	NAG	A	501	14/15	0.89	0.20	73,82,89,92	0
2	NAG	C	504	14/15	0.90	0.19	69,77,81,82	0
2	NAG	B	504	14/15	0.90	0.24	68,73,76,81	0
2	NAG	B	505	14/15	0.90	0.16	50,62,68,71	0
2	NAG	C	503	14/15	0.91	0.22	59,64,75,82	0
2	NAG	D	504	14/15	0.91	0.14	76,81,85,91	0
2	NAG	A	504	14/15	0.91	0.17	63,70,77,79	0
2	NAG	C	501	14/15	0.91	0.17	70,81,89,92	0
2	NAG	C	502	14/15	0.92	0.23	53,64,70,77	0
2	NAG	B	506	14/15	0.93	0.19	50,55,65,66	0
2	NAG	D	502	14/15	0.94	0.25	47,57,70,73	0
2	NAG	C	505	14/15	0.94	0.15	65,68,73,81	0
2	NAG	A	506	14/15	0.94	0.16	46,49,63,65	0
2	NAG	B	502	14/15	0.95	0.26	48,55,63,68	0
2	NAG	A	502	14/15	0.95	0.25	42,54,60,60	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.

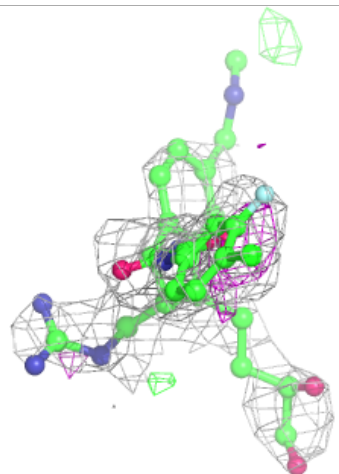
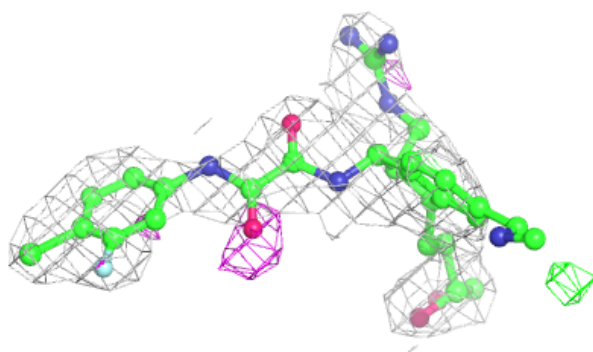
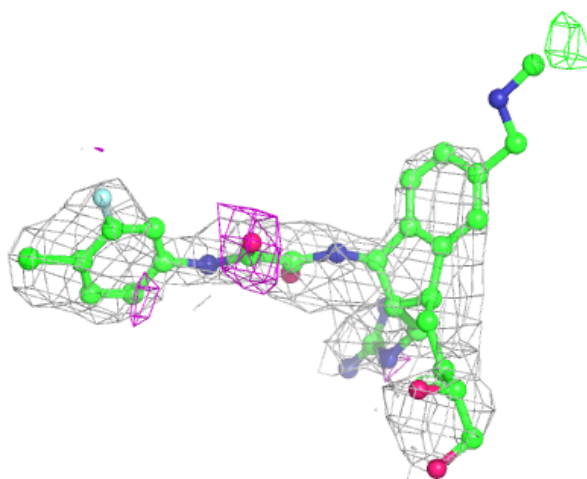
**Electron density around 7IW B 507:**

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



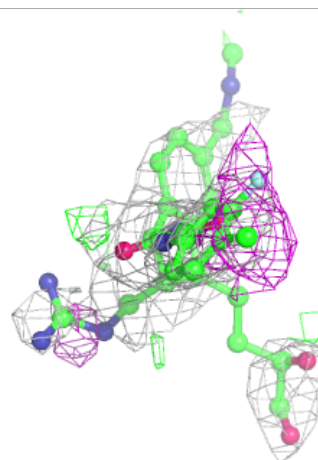
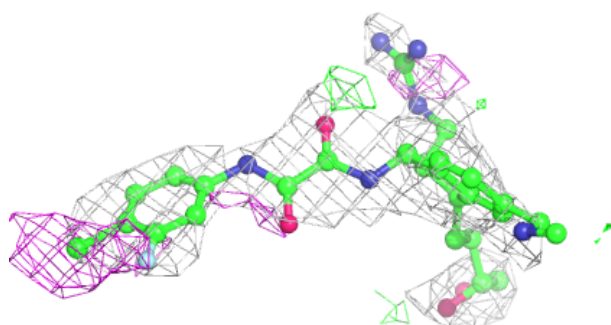
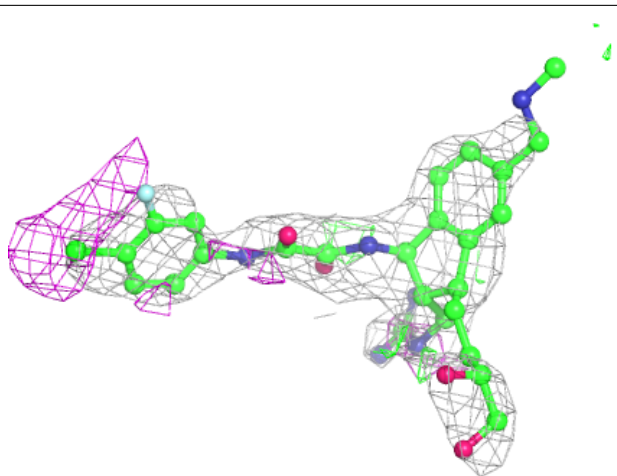
**Electron density around 7IW D 507:**

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



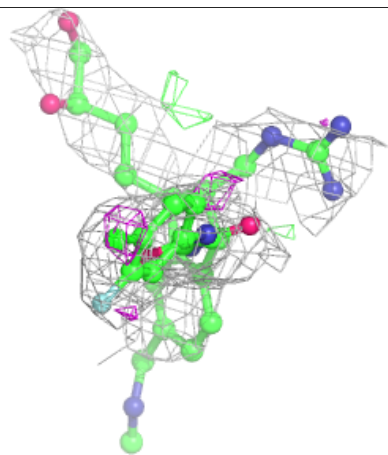
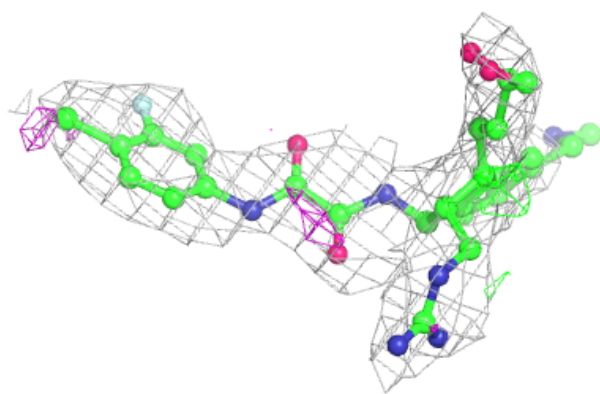
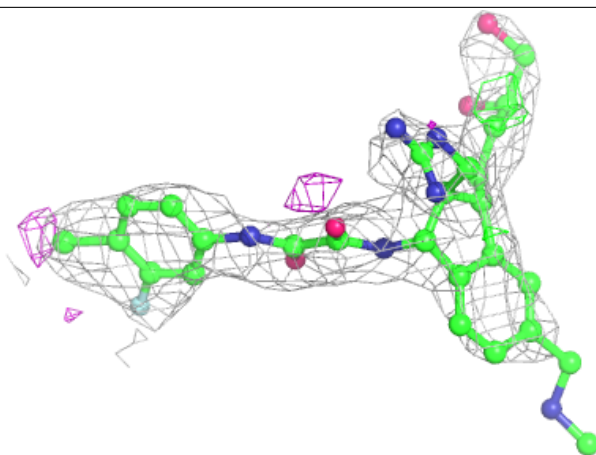
**Electron density around 7IW C 506:**

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



**Electron density around 7IW A 508:**

$2mF_o-DF_c$  (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.