WORLDWIDE PDB

PROTEIN DATA BANK

Full wwPDB X-ray Structure Validation Report ⓘ

Mar 27, 2023 – 03:03 PM EDT

PDB ID	:	8FM3
Title	:	HIV-1 gp120 complex with CJF-III-288
Authors	:	Gong, Z.; Hendrickson, W.A.
Deposited on	:	2022-12-22
Resolution	:	2.11 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:

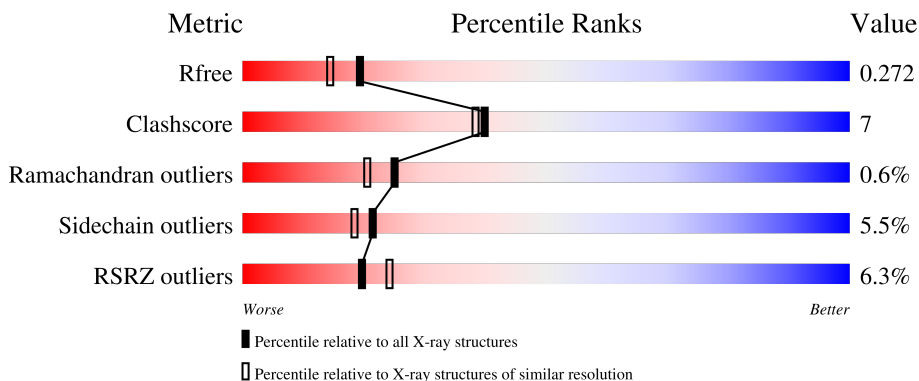|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.32.2
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.32.2

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 2.11 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	Percentile Ranks	Value
Rfree		0.272
Clashscore		7
Ramachandran outliers		0.6%
Sidechain outliers		5.5%
RSRZ outliers		6.3%

Worse   *Better*

■ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	6241 (2.14-2.10)
Clashscore	141614	6778 (2.14-2.10)
Ramachandran outliers	138981	6705 (2.14-2.10)
Sidechain outliers	138945	6706 (2.14-2.10)
RSRZ outliers	127900	6112 (2.14-2.10)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

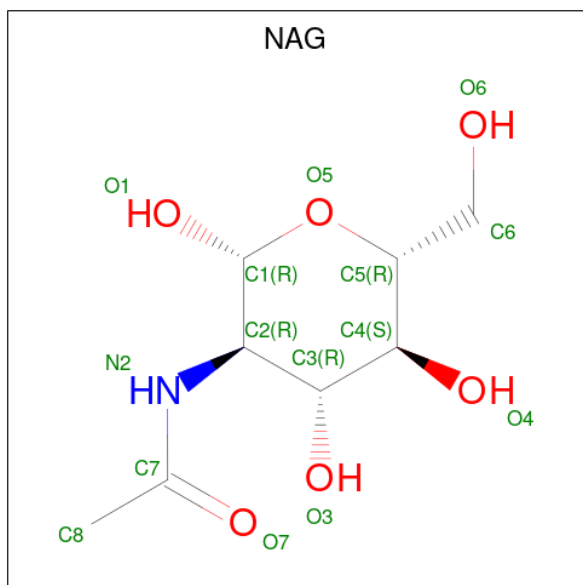| Mol	Chain	Length	Quality of chain
1	A	358	3% / 77% 14% · 6%
1	B	358	8% / 76% 14% · 6%
1	C	358	7% / 76% 16% · 6%
1	D	358	6% / 76% 15% ·· 6%

2 Entry composition ⓘ

There are 4 unique types of molecules in this entry. The entry contains 11216 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 Envelope glycoprotein gp120.

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

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

- Molecule 3 is propyl (2R,3S)-2-(carbamimidamidomethyl)-3-[2-(4-chloro-3-fluoroanilino)(oxo)acetamido]-6-[(methylamino)methyl]-2,3-dihydro-1H-indole-1-carboxylate (three-letter code: Y26) (formula: $C_{24}H_{29}ClFN_7O_4$) (labeled as "Ligand of Interest" by depositor).
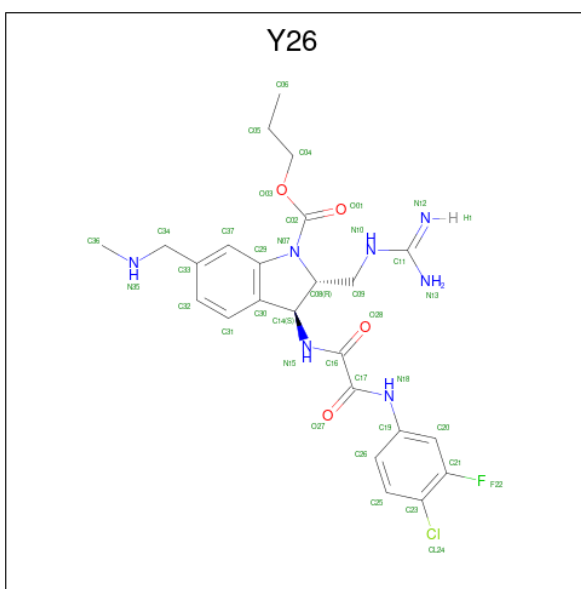
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	A	1	Total 37	C 24	Cl 1	F 1	N 7	O 4	0	0
3	C	1	Total 37	C 24	Cl 1	F 1	N 7	O 4	0	0
3	D	1	Total 37	C 24	Cl 1	F 1	N 7	O 4	0	0
3	B	1	Total 37	C 24	Cl 1	F 1	N 7	O 4	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	41	Total 41	O 41	0	0

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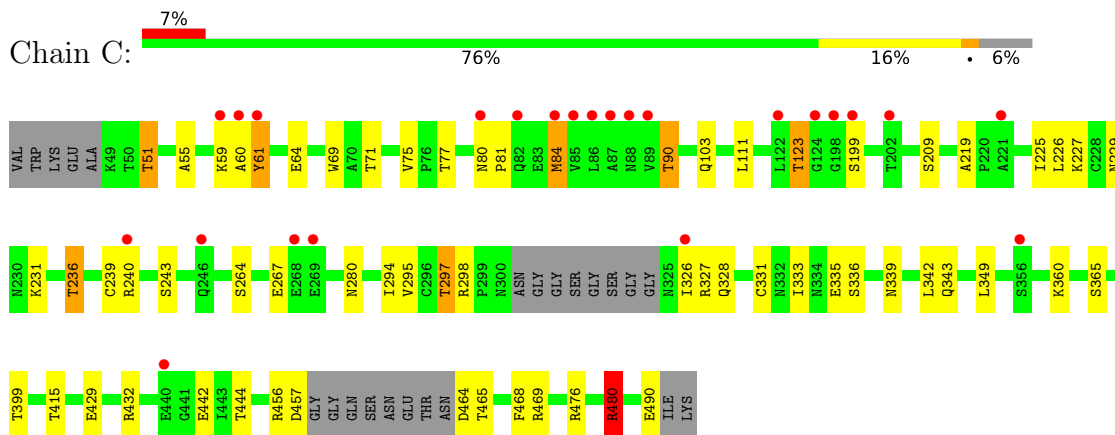| Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	C	54	Total 54	O 54	0	0
4	D	58	Total 58	O 58	0	0
4	B	43	Total 43	O 43	0	0

3 Residue-property plots ⓘ

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.
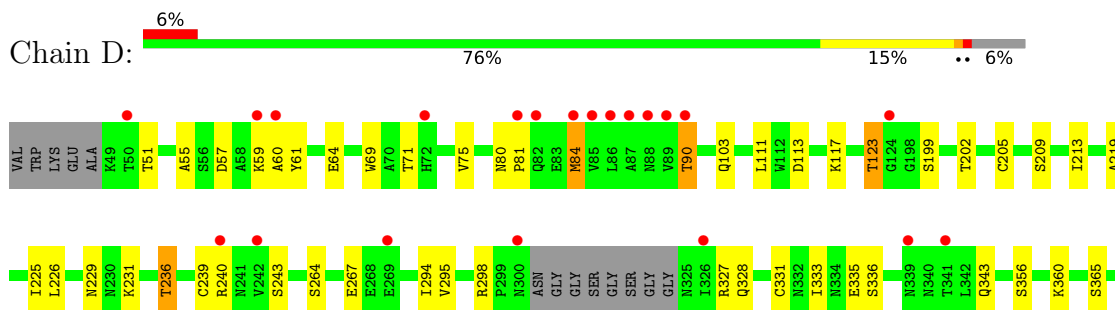
- Molecule 1: Envelope glycoprotein gp120

Chain A:

- Molecule 1: Envelope glycoprotein gp120

Chain C:

- Molecule 1: Envelope glycoprotein gp120

Chain D:

R396 T399 R408 T415 E429 R432 E442 N448 D457 GLY GLY GLN SER ASN GLU THR ASN D464 T465 R469 R475 R480 K485 E490 ILE LYS

• Molecule 1: Envelope glycoprotein gp120

Chain B:

8%

76% 14% 6%

VAL TRP LYS GLU ALA K49 T50 T51 A55 S56 D57 A58 K59 A60 Y61 E62 K63 E64 W69 A70 T71 H72 V75 P79 N80 P81 M84 V85 L86 A87 N88 V89 T90 E91 Q103 L111 G124 G198 S199 T202 S209 A219 P220 A221 I225 L226 K227 C228

N229 N230 K231 T236 C239 R240 S243 T244 S264 L265 A266 E267 N280 I294 V295 C296 T297 R298 P299 N300 ASN GLY GLY SER GLY GLY N325 I326 R327 Q328 C331 N332 I333 N334 E335 S336 L342 Q343 S356 K360 S365 R396 T399 R408

N411 T415 K421 Q422 R432 E442 I443 T444 R456 D457 GLY GLY GLN SER ASN GLU THR ASN D464 T465 R469 R476 R480 E490 ILE LYS

4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	71.46Å 121.72Å 195.18Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.80 – 2.11 48.80 – 2.11	Depositor EDS
% Data completeness (in resolution range)	56.3 (48.80-2.11) 56.3 (48.80-2.11)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.43 (at 2.12Å)	Xtriage
Refinement program	PHENIX 1.20rc3_4406	Depositor
R, R_{free}	0.247 , 0.273 0.245 , 0.272	Depositor DCC
R_{free} test set	2000 reflections (3.61%)	wwPDB-VP
Wilson B-factor (Å^2)	38.2	Xtriage
Anisotropy	0.088	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 39.5	EDS
L-test for twinning[2]	$< \lvert L \rvert > = 0.50, < L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	11216	wwPDB-VP
Average B, all atoms (Å^2)	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 16.15% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.
[2]Theoretical values of $< \lvert L \rvert >$, $< L^2 >$ 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: Y26, 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	0.46	0/2682	0.79	5/3640 (0.1%)
1	B	0.46	0/2682	0.79	5/3640 (0.1%)
1	C	0.46	0/2682	0.79	5/3640 (0.1%)
1	D	0.46	0/2682	0.79	5/3640 (0.1%)
All	All	0.46	0/10728	0.79	20/14560 (0.1%)

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

There are no bond length outliers.

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	84	MET	CA-CB-CG	6.12	123.70	113.30
1	B	84	MET	CA-CB-CG	6.11	123.68	113.30
1	A	84	MET	CA-CB-CG	6.10	123.67	113.30
1	C	84	MET	CA-CB-CG	6.10	123.67	113.30
1	B	327	ARG	CG-CD-NE	-6.09	99.01	111.80
1	A	327	ARG	CG-CD-NE	-6.08	99.02	111.80
1	D	327	ARG	CG-CD-NE	-6.07	99.05	111.80
1	C	327	ARG	CG-CD-NE	-6.07	99.06	111.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	327	ARG	CA-CB-CG	5.75	126.06	113.40
1	A	327	ARG	CA-CB-CG	5.75	126.04	113.40
1	D	327	ARG	CA-CB-CG	5.74	126.03	113.40
1	C	327	ARG	CA-CB-CG	5.72	125.99	113.40
1	C	480	ARG	CG-CD-NE	-5.64	99.96	111.80
1	B	480	ARG	CG-CD-NE	-5.63	99.97	111.80
1	A	480	ARG	CG-CD-NE	-5.62	99.99	111.80
1	D	480	ARG	CG-CD-NE	-5.61	100.02	111.80
1	C	327	ARG	CB-CG-CD	5.06	124.75	111.60
1	D	327	ARG	CB-CG-CD	5.05	124.72	111.60
1	A	327	ARG	CB-CG-CD	5.04	124.71	111.60
1	B	327	ARG	CB-CG-CD	5.02	124.66	111.60

There are no chirality outliers.

All (12) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	432	ARG	Sidechain
1	A	476	ARG	Sidechain
1	A	480	ARG	Sidechain
1	B	432	ARG	Sidechain
1	B	476	ARG	Sidechain
1	B	480	ARG	Sidechain
1	C	432	ARG	Sidechain
1	C	476	ARG	Sidechain
1	C	480	ARG	Sidechain
1	D	432	ARG	Sidechain
1	D	476	ARG	Sidechain
1	D	480	ARG	Sidechain

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	31	0
1	B	2627	0	2542	29	2
1	C	2627	0	2541	61	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	2627	0	2542	64	2
2	A	98	0	91	2	0
2	B	84	0	78	1	0
2	C	98	0	91	3	0
2	D	84	0	78	1	0
3	A	37	0	0	0	0
3	B	37	0	0	0	0
3	C	37	0	0	0	0
3	D	37	0	0	0	0
4	A	41	0	0	1	0
4	B	43	0	0	0	0
4	C	54	0	0	2	0
4	D	58	0	0	9	0
All	All	11216	0	10503	157	2

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:60:ALA:C	1:D:59:LYS:HE2	1.78	1.04
1:C:80:ASN:HB2	1:D:442:GLU:HB3	1.46	0.98
1:D:448:ASN:ND2	4:D:601:HOH:O	2.10	0.81
1:C:61:TYR:N	1:D:59:LYS:HE2	1.98	0.78
1:A:60:ALA:HB2	1:A:71:THR:HG21	1.67	0.76
1:C:60:ALA:HB2	1:C:71:THR:HG21	1.67	0.75
1:D:60:ALA:HB2	1:D:71:THR:HG21	1.67	0.75
1:B:60:ALA:HB2	1:B:71:THR:HG21	1.67	0.75
1:C:339:ASN:HD21	2:C:508:NAG:H83	1.52	0.75
1:C:61:TYR:HE1	4:C:648:HOH:O	1.70	0.74
1:C:80:ASN:CB	1:D:442:GLU:HB3	2.17	0.74
1:C:61:TYR:HD1	1:D:59:LYS:HE3	1.51	0.74
1:C:80:ASN:ND2	1:D:442:GLU:OE1	2.21	0.72
1:D:490:GLU:O	4:D:602:HOH:O	2.11	0.69
1:B:297:THR:OG1	1:B:444:THR:OG1	2.12	0.68
1:A:297:THR:OG1	1:A:444:THR:OG1	2.12	0.68
1:C:297:THR:OG1	1:C:444:THR:OG1	2.12	0.67
1:C:60:ALA:HB3	1:D:59:LYS:HZ3	1.59	0.66
1:C:59:LYS:HB3	1:C:61:TYR:CE1	2.31	0.66
1:A:480:ARG:NH1	4:A:601:HOH:O	2.28	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:59:LYS:HB3	1:A:61:TYR:CE1	2.31	0.65
1:B:59:LYS:HB3	1:B:61:TYR:CE1	2.31	0.65
1:D:480:ARG:NH1	4:D:605:HOH:O	2.30	0.63
1:D:117:LYS:HG3	4:D:608:HOH:O	1.99	0.62
1:A:343:GLN:HE22	1:A:399:THR:HA	1.65	0.62
1:C:60:ALA:H	1:D:59:LYS:HZ3	1.47	0.62
1:D:343:GLN:HE22	1:D:399:THR:HA	1.65	0.61
1:B:343:GLN:HE22	1:B:399:THR:HA	1.65	0.61
1:C:343:GLN:HE22	1:C:399:THR:HA	1.65	0.61
1:C:61:TYR:CD1	1:D:59:LYS:HE3	2.36	0.60
1:C:80:ASN:HB2	1:D:442:GLU:H	1.68	0.59
1:C:61:TYR:CE2	1:D:213:ILE:HG22	2.37	0.59
1:B:457:ASP:OD1	1:B:469:ARG:NH1	2.36	0.59
1:C:457:ASP:OD1	1:C:469:ARG:NH1	2.36	0.59
1:D:113:ASP:OD1	4:D:603:HOH:O	2.16	0.58
1:D:457:ASP:OD1	1:D:469:ARG:NH1	2.36	0.58
1:A:457:ASP:OD1	1:A:469:ARG:NH1	2.36	0.57
1:C:60:ALA:HB3	1:D:59:LYS:NZ	2.21	0.56
1:C:326:ILE:HD11	4:C:601:HOH:O	2.06	0.55
1:C:339:ASN:ND2	2:C:508:NAG:H83	2.21	0.55
1:D:59:LYS:HD3	1:D:61:TYR:CE2	2.41	0.55
1:D:485:LYS:NZ	4:D:607:HOH:O	2.40	0.55
1:C:61:TYR:N	1:D:59:LYS:CE	2.69	0.55
1:C:80:ASN:HD22	1:D:442:GLU:CB	2.19	0.55
1:A:294:ILE:HD12	1:A:333:ILE:HD11	1.90	0.54
1:B:90:THR:OG1	1:B:240:ARG:HG3	2.08	0.53
1:A:90:THR:OG1	1:A:240:ARG:HG3	2.08	0.53
1:D:90:THR:HA	1:D:239:CYS:O	2.09	0.53
1:A:90:THR:HA	1:A:239:CYS:O	2.09	0.53
1:C:90:THR:HA	1:C:239:CYS:O	2.09	0.53
1:C:90:THR:OG1	1:C:240:ARG:HG3	2.08	0.53
1:C:294:ILE:HD12	1:C:333:ILE:HD11	1.90	0.53
1:C:60:ALA:CA	1:D:59:LYS:HE2	2.37	0.53
1:B:90:THR:HA	1:B:239:CYS:O	2.09	0.53
1:D:294:ILE:HD12	1:D:333:ILE:HD11	1.90	0.53
1:B:294:ILE:HD12	1:B:333:ILE:HD11	1.90	0.53
1:C:60:ALA:H	1:D:59:LYS:NZ	2.06	0.52
1:C:60:ALA:CB	1:D:59:LYS:HZ3	2.23	0.52
1:D:90:THR:OG1	1:D:240:ARG:HG3	2.08	0.52
1:C:80:ASN:ND2	1:D:442:GLU:CB	2.73	0.51
1:C:69:TRP:CD2	1:C:111:LEU:HD12	2.47	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:69:TRP:CD2	1:A:111:LEU:HD12	2.47	0.50
1:C:80:ASN:ND2	1:D:442:GLU:HB3	2.28	0.49
1:D:69:TRP:CD2	1:D:111:LEU:HD12	2.47	0.49
1:B:69:TRP:CD2	1:B:111:LEU:HD12	2.47	0.49
1:A:231:LYS:HD2	1:A:267:GLU:HB2	1.95	0.48
1:C:231:LYS:HD2	1:C:267:GLU:HB2	1.95	0.48
1:D:231:LYS:HD2	1:D:267:GLU:HB2	1.95	0.48
1:B:69:TRP:CE3	1:B:111:LEU:HD12	2.49	0.48
1:C:69:TRP:CE3	1:C:111:LEU:HD12	2.49	0.48
1:D:267:GLU:O	4:D:604:HOH:O	2.20	0.48
1:D:69:TRP:CE3	1:D:111:LEU:HD12	2.49	0.48
1:B:231:LYS:HD2	1:B:267:GLU:HB2	1.95	0.48
1:A:335:GLU:O	1:A:335:GLU:HG2	2.14	0.48
1:A:69:TRP:CE3	1:A:111:LEU:HD12	2.49	0.48
1:A:339:ASN:ND2	2:A:508:NAG:H83	2.29	0.47
1:D:123:THR:HG21	1:D:429:GLU:OE2	2.14	0.47
1:C:123:THR:HG21	1:C:429:GLU:OE2	2.14	0.47
1:D:480:ARG:NH2	4:D:610:HOH:O	2.45	0.47
1:C:60:ALA:HB3	1:D:59:LYS:CE	2.45	0.47
1:D:205:CYS:HB2	4:D:628:HOH:O	2.14	0.47
1:B:295:VAL:O	1:B:331:CYS:HA	2.15	0.47
1:D:295:VAL:O	1:D:331:CYS:HA	2.15	0.47
1:A:295:VAL:O	1:A:331:CYS:HA	2.15	0.47
1:D:335:GLU:O	1:D:335:GLU:HG2	2.14	0.47
1:C:64:GLU:HA	1:C:209:SER:OG	2.15	0.46
1:C:335:GLU:HG2	1:C:335:GLU:O	2.14	0.46
1:B:335:GLU:HG2	1:B:335:GLU:O	2.14	0.46
1:A:55:ALA:HA	1:A:75:VAL:O	2.16	0.46
1:C:55:ALA:HA	1:C:75:VAL:O	2.16	0.46
1:C:80:ASN:HD22	1:D:442:GLU:HB3	1.80	0.46
1:A:64:GLU:HA	1:A:209:SER:OG	2.15	0.46
1:D:64:GLU:HA	1:D:209:SER:OG	2.15	0.46
1:B:55:ALA:HA	1:B:75:VAL:O	2.16	0.46
1:B:64:GLU:HA	1:B:209:SER:OG	2.15	0.46
1:C:61:TYR:CZ	1:D:213:ILE:HG22	2.51	0.46
1:B:236:THR:HG22	2:B:501:NAG:H5	1.98	0.46
1:B:62:GLU:HA	1:B:62:GLU:OE1	2.15	0.46
1:D:236:THR:HG22	2:D:501:NAG:H5	1.98	0.45
1:A:62:GLU:HA	1:A:62:GLU:OE1	2.15	0.45
1:C:236:THR:HG22	2:C:501:NAG:H5	1.98	0.45
1:A:236:THR:HG22	2:A:501:NAG:H5	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:295:VAL:O	1:C:331:CYS:HA	2.15	0.45
1:D:55:ALA:HA	1:D:75:VAL:O	2.16	0.45
1:C:60:ALA:N	1:D:59:LYS:HZ3	2.11	0.45
1:D:59:LYS:HD3	1:D:61:TYR:CZ	2.52	0.45
1:A:298:ARG:HG2	1:A:328:GLN:O	2.17	0.45
1:C:61:TYR:CB	1:D:57:ASP:O	2.65	0.45
1:C:61:TYR:N	1:C:61:TYR:CD1	2.85	0.44
1:C:298:ARG:HG2	1:C:328:GLN:O	2.17	0.44
1:D:298:ARG:HG2	1:D:328:GLN:O	2.17	0.44
1:A:421:LYS:HB3	1:A:421:LYS:HE3	1.65	0.44
1:C:80:ASN:HA	1:C:81:PRO:HD3	1.82	0.44
1:A:331:CYS:O	1:A:415:THR:HA	2.18	0.44
1:D:360:LYS:HD2	1:D:465:THR:HG21	2.00	0.44
1:A:476:ARG:HE	1:A:476:ARG:HB2	1.64	0.44
1:B:360:LYS:HD2	1:B:465:THR:HG21	2.00	0.43
1:A:61:TYR:CD1	1:A:61:TYR:N	2.85	0.43
1:C:226:LEU:HA	1:C:243:SER:O	2.18	0.43
1:B:298:ARG:HG2	1:B:328:GLN:O	2.17	0.43
1:A:226:LEU:HA	1:A:243:SER:O	2.18	0.43
1:C:360:LYS:HD2	1:C:465:THR:HG21	2.00	0.43
1:B:60:ALA:HB2	1:B:71:THR:CG2	2.44	0.43
1:C:331:CYS:O	1:C:415:THR:HA	2.18	0.43
1:C:342:LEU:HD23	1:C:342:LEU:HA	1.83	0.43
1:C:61:TYR:HD1	1:D:59:LYS:CE	2.26	0.43
1:D:331:CYS:O	1:D:415:THR:HA	2.18	0.43
1:B:331:CYS:O	1:B:415:THR:HA	2.18	0.43
1:D:226:LEU:HA	1:D:243:SER:O	2.18	0.42
1:C:80:ASN:HD22	1:D:442:GLU:CD	2.18	0.42
1:A:360:LYS:HD2	1:A:465:THR:HG21	2.00	0.42
1:B:226:LEU:HA	1:B:243:SER:O	2.18	0.42
1:C:61:TYR:HB3	1:D:57:ASP:O	2.20	0.42
1:D:219:ALA:HB2	1:D:225:ILE:HG13	2.01	0.42
1:B:219:ALA:HB2	1:B:225:ILE:HG13	2.01	0.42
1:A:342:LEU:HD23	1:A:342:LEU:HA	1.83	0.42
1:D:476:ARG:HE	1:D:476:ARG:HB2	1.54	0.41
1:A:60:ALA:HB2	1:A:71:THR:CG2	2.44	0.41
1:A:219:ALA:HB2	1:A:225:ILE:HG13	2.01	0.41
1:C:51:THR:HA	1:C:103:GLN:HE22	1.85	0.41
1:A:51:THR:HA	1:A:103:GLN:HE22	1.85	0.41
1:D:51:THR:HA	1:D:103:GLN:HE22	1.86	0.41
1:B:421:LYS:HE3	1:B:421:LYS:HB3	1.65	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:60:ALA:HB2	1:C:71:THR:CG2	2.44	0.41
1:D:59:LYS:HB3	1:D:61:TYR:CE1	2.55	0.41
1:B:51:THR:HA	1:B:103:GLN:HE22	1.86	0.41
1:B:61:TYR:CD1	1:B:61:TYR:N	2.85	0.41
1:C:80:ASN:CG	1:D:442:GLU:HB3	2.41	0.41
1:D:80:ASN:HA	1:D:81:PRO:HD3	1.82	0.41
1:A:340:ASN:O	1:A:343:GLN:HB3	2.22	0.40
1:B:80:ASN:HA	1:B:81:PRO:HD3	1.82	0.40
1:B:342:LEU:HA	1:B:342:LEU:HD23	1.83	0.40
1:C:219:ALA:HB2	1:C:225:ILE:HG13	2.01	0.40
1:C:280:ASN:HB2	1:C:456:ARG:O	2.22	0.40
1:C:349:LEU:HD13	1:C:468:PHE:CE1	2.57	0.40
1:D:60:ALA:HB2	1:D:71:THR:CG2	2.44	0.40
1:B:280:ASN:HB2	1:B:456:ARG:O	2.22	0.40

All (2) 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:D:356:SER:OG	1:B:356:SER:OG[3_454]	1.99	0.21
1:D:202:THR:OG1	1:B:202:THR:O[4_555]	2.00	0.20

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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%)	314 (95%)	13 (4%)	2 (1%)	25	20
1	B	329/358 (92%)	314 (95%)	13 (4%)	2 (1%)	25	20
1	C	329/358 (92%)	314 (95%)	13 (4%)	2 (1%)	25	20
1	D	329/358 (92%)	314 (95%)	13 (4%)	2 (1%)	25	20

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	1316/1432 (92%)	1256 (95%)	52 (4%)	8 (1%)	25 20

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	365	SER
1	C	365	SER
1	D	365	SER
1	B	365	SER
1	A	90	THR
1	C	90	THR
1	D	90	THR
1	B	90	THR

5.3.2   Protein sidechains ⓘ

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%)	278 (94%)	19 (6%)	17 14
1	B	297/312 (95%)	278 (94%)	19 (6%)	17 14
1	C	297/312 (95%)	281 (95%)	16 (5%)	22 19
1	D	297/312 (95%)	286 (96%)	11 (4%)	34 34
All	All	1188/1248 (95%)	1123 (94%)	65 (6%)	21 18

All (65) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	51	THR
1	A	61	TYR
1	A	62	GLU
1	A	77	THR
1	A	84	MET
1	A	199	SER
1	A	202	THR

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Mol	Chain	Res	Type
1	A	229	ASN
1	A	236	THR
1	A	264	SER
1	A	297	THR
1	A	327	ARG
1	A	336	SER
1	A	408	ARG
1	A	442	GLU
1	A	464	ASP
1	A	480	ARG
1	A	488	VAL
1	A	490	GLU
1	C	51	THR
1	C	61	TYR
1	C	77	THR
1	C	84	MET
1	C	123	THR
1	C	199	SER
1	C	227	LYS
1	C	229	ASN
1	C	236	THR
1	C	264	SER
1	C	297	THR
1	C	336	SER
1	C	442	GLU
1	C	464	ASP
1	C	480	ARG
1	C	490	GLU
1	D	84	MET
1	D	123	THR
1	D	199	SER
1	D	229	ASN
1	D	236	THR
1	D	264	SER
1	D	336	SER
1	D	464	ASP
1	D	476	ARG
1	D	480	ARG
1	D	490	GLU
1	B	51	THR
1	B	61	TYR
1	B	62	GLU

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Mol	Chain	Res	Type
1	B	84	MET
1	B	199	SER
1	B	202	THR
1	B	227	LYS
1	B	229	ASN
1	B	236	THR
1	B	264	SER
1	B	297	THR
1	B	327	ARG
1	B	336	SER
1	B	399	THR
1	B	422	GLN
1	B	442	GLU
1	B	464	ASP
1	B	480	ARG
1	B	490	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	246	GLN
1	A	325	ASN
1	A	343	GLN
1	A	422	GLN
1	C	80	ASN
1	C	246	GLN
1	C	325	ASN
1	C	343	GLN
1	D	246	GLN
1	D	325	ASN
1	D	343	GLN
1	B	246	GLN
1	B	325	ASN
1	B	343	GLN
1	B	417	GLN
1	B	422	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

30 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	0.58	0	17,19,21	0.46	0
2	NAG	D	505	1	14,14,15	0.31	0	17,19,21	0.50	0
2	NAG	D	503	1	14,14,15	0.92	2 (14%)	17,19,21	0.69	0
2	NAG	C	503	1	14,14,15	0.92	2 (14%)	17,19,21	0.69	0
2	NAG	B	506	1	14,14,15	0.74	1 (7%)	17,19,21	2.01	2 (11%)
2	NAG	A	502	1	14,14,15	0.35	0	17,19,21	0.82	1 (5%)
3	Y26	A	507	-	38,39,39	3.28	16 (42%)	48,54,54	2.34	13 (27%)
3	Y26	B	507	-	38,39,39	3.28	16 (42%)	48,54,54	2.33	13 (27%)
2	NAG	A	505	1	14,14,15	0.31	0	17,19,21	0.50	0
2	NAG	C	508	1	14,14,15	0.79	1 (7%)	17,19,21	0.62	0
2	NAG	D	504	1	14,14,15	0.58	0	17,19,21	0.46	0
2	NAG	C	501	1	14,14,15	0.33	0	17,19,21	0.45	0
3	Y26	D	507	-	38,39,39	3.28	16 (42%)	48,54,54	2.34	13 (27%)
3	Y26	C	507	-	38,39,39	3.28	16 (42%)	48,54,54	2.34	13 (27%)
2	NAG	C	502	1	14,14,15	0.35	0	17,19,21	0.82	1 (5%)
2	NAG	B	501	1	14,14,15	0.33	0	17,19,21	0.45	0
2	NAG	B	505	1	14,14,15	0.31	0	17,19,21	0.50	0
2	NAG	A	503	1	14,14,15	0.92	2 (14%)	17,19,21	0.69	0
2	NAG	C	505	1	14,14,15	0.31	0	17,19,21	0.50	0
2	NAG	D	501	1	14,14,15	0.33	0	17,19,21	0.45	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	NAG	C	506	1	14,14,15	0.74	1 (7%)	17,19,21	2.01	2 (11%)
2	NAG	D	506	1	14,14,15	0.74	1 (7%)	17,19,21	2.01	2 (11%)
2	NAG	C	504	1	14,14,15	0.58	0	17,19,21	0.46	0
2	NAG	A	508	1	14,14,15	0.51	0	17,19,21	0.95	2 (11%)
2	NAG	B	504	1	14,14,15	0.58	0	17,19,21	0.45	0
2	NAG	D	502	1	14,14,15	0.35	0	17,19,21	0.82	1 (5%)
2	NAG	A	501	1	14,14,15	0.33	0	17,19,21	0.45	0
2	NAG	B	503	1	14,14,15	0.92	2 (14%)	17,19,21	0.69	0
2	NAG	B	502	1	14,14,15	0.35	0	17,19,21	0.82	1 (5%)
2	NAG	A	506	1	14,14,15	0.74	1 (7%)	17,19,21	2.01	2 (11%)

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	D	505	1	-	2/6/23/26	0/1/1/1
2	NAG	D	503	1	-	2/6/23/26	0/1/1/1
2	NAG	C	503	1	-	2/6/23/26	0/1/1/1
2	NAG	B	506	1	-	2/6/23/26	0/1/1/1
2	NAG	A	502	1	-	0/6/23/26	0/1/1/1
3	Y26	A	507	-	-	1/27/44/44	0/3/3/3
3	Y26	B	507	-	-	1/27/44/44	0/3/3/3
2	NAG	A	505	1	-	2/6/23/26	0/1/1/1
2	NAG	C	508	1	-	4/6/23/26	0/1/1/1
2	NAG	D	504	1	-	2/6/23/26	0/1/1/1
2	NAG	C	501	1	-	0/6/23/26	0/1/1/1
3	Y26	D	507	-	-	1/27/44/44	0/3/3/3
3	Y26	C	507	-	-	1/27/44/44	0/3/3/3
2	NAG	C	502	1	-	0/6/23/26	0/1/1/1
2	NAG	B	501	1	-	0/6/23/26	0/1/1/1
2	NAG	B	505	1	-	2/6/23/26	0/1/1/1
2	NAG	A	503	1	-	2/6/23/26	0/1/1/1
2	NAG	C	505	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	506	1	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	D	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	A	508	1	-	3/6/23/26	0/1/1/1
2	NAG	B	504	1	-	2/6/23/26	0/1/1/1
2	NAG	D	502	1	-	0/6/23/26	0/1/1/1
2	NAG	A	501	1	-	0/6/23/26	0/1/1/1
2	NAG	B	503	1	-	2/6/23/26	0/1/1/1
2	NAG	B	502	1	-	0/6/23/26	0/1/1/1
2	NAG	A	506	1	-	2/6/23/26	0/1/1/1

All (77) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	507	Y26	C02-N07	8.41	1.49	1.37
3	A	507	Y26	C02-N07	8.40	1.49	1.37
3	B	507	Y26	C02-N07	8.40	1.49	1.37
3	C	507	Y26	C02-N07	8.40	1.49	1.37
3	B	507	Y26	C30-C14	6.84	1.58	1.51
3	A	507	Y26	C30-C14	6.84	1.58	1.51
3	C	507	Y26	C30-C14	6.84	1.58	1.51
3	D	507	Y26	C30-C14	6.83	1.58	1.51
3	A	507	Y26	C11-N10	6.42	1.45	1.33
3	B	507	Y26	C11-N10	6.41	1.45	1.33
3	C	507	Y26	C11-N10	6.41	1.45	1.33
3	D	507	Y26	C11-N10	6.41	1.45	1.33
3	B	507	Y26	C16-N15	6.40	1.46	1.34
3	C	507	Y26	C16-N15	6.39	1.46	1.34
3	D	507	Y26	C16-N15	6.39	1.46	1.34
3	A	507	Y26	C16-N15	6.39	1.46	1.34
3	B	507	Y26	C17-N18	6.10	1.48	1.35
3	A	507	Y26	C17-N18	6.10	1.48	1.35
3	D	507	Y26	C17-N18	6.10	1.48	1.35
3	C	507	Y26	C17-N18	6.09	1.48	1.35
3	A	507	Y26	C08-N07	-6.00	1.40	1.48
3	D	507	Y26	C08-N07	-6.00	1.40	1.48
3	B	507	Y26	C08-N07	-6.00	1.40	1.48
3	C	507	Y26	C08-N07	-6.00	1.40	1.48
3	B	507	Y26	C14-N15	-5.29	1.36	1.46
3	C	507	Y26	C14-N15	-5.28	1.36	1.46
3	D	507	Y26	C14-N15	-5.28	1.36	1.46
3	A	507	Y26	C14-N15	-5.28	1.36	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	507	Y26	C11-N12	4.33	1.49	1.32
3	D	507	Y26	C11-N12	4.33	1.49	1.32
3	C	507	Y26	C11-N12	4.33	1.49	1.32
3	A	507	Y26	C11-N12	4.33	1.49	1.32
3	C	507	Y26	C19-N18	3.86	1.49	1.41
3	D	507	Y26	C19-N18	3.86	1.49	1.41
3	A	507	Y26	C19-N18	3.86	1.49	1.41
3	B	507	Y26	C19-N18	3.85	1.49	1.41
3	D	507	Y26	C14-C08	-3.57	1.51	1.55
3	A	507	Y26	C14-C08	-3.56	1.51	1.55
3	B	507	Y26	C14-C08	-3.55	1.51	1.55
3	C	507	Y26	C14-C08	-3.55	1.51	1.55
3	C	507	Y26	O01-C02	-3.21	1.16	1.21
3	D	507	Y26	O01-C02	-3.21	1.16	1.21
3	A	507	Y26	O01-C02	-3.20	1.16	1.21
3	B	507	Y26	O01-C02	-3.20	1.16	1.21
3	C	507	Y26	O03-C02	2.67	1.39	1.34
3	D	507	Y26	O03-C02	2.67	1.39	1.34
3	A	507	Y26	O03-C02	2.67	1.39	1.34
3	B	507	Y26	O03-C02	2.67	1.39	1.34
2	D	506	NAG	O5-C1	2.47	1.47	1.43
2	B	506	NAG	O5-C1	2.47	1.47	1.43
2	A	506	NAG	O5-C1	2.47	1.47	1.43
2	C	506	NAG	O5-C1	2.47	1.47	1.43
2	C	503	NAG	O5-C1	2.33	1.47	1.43
2	B	503	NAG	O5-C1	2.33	1.47	1.43
2	A	503	NAG	O5-C1	2.33	1.47	1.43
2	D	503	NAG	O5-C1	2.33	1.47	1.43
2	A	503	NAG	C1-C2	2.32	1.55	1.52
2	D	503	NAG	C1-C2	2.32	1.55	1.52
3	A	507	Y26	O27-C17	-2.32	1.19	1.23
2	C	503	NAG	C1-C2	2.32	1.55	1.52
3	D	507	Y26	O27-C17	-2.32	1.19	1.23
2	B	503	NAG	C1-C2	2.32	1.55	1.52
3	C	507	Y26	O27-C17	-2.31	1.19	1.23
3	B	507	Y26	O27-C17	-2.31	1.19	1.23
3	D	507	Y26	C32-C31	2.19	1.42	1.38
3	B	507	Y26	C32-C31	2.19	1.42	1.38
3	A	507	Y26	C32-C31	2.19	1.42	1.38
3	C	507	Y26	C32-C31	2.19	1.42	1.38
3	B	507	Y26	O28-C16	-2.16	1.19	1.23
3	D	507	Y26	O28-C16	-2.16	1.19	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	507	Y26	O28-C16	-2.15	1.19	1.23
3	C	507	Y26	O28-C16	-2.15	1.19	1.23
3	A	507	Y26	C29-C30	2.09	1.42	1.39
3	C	507	Y26	C29-C30	2.09	1.42	1.39
3	D	507	Y26	C29-C30	2.08	1.42	1.39
3	B	507	Y26	C29-C30	2.08	1.42	1.39
2	C	508	NAG	C1-C2	2.04	1.55	1.52

All (66) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	507	Y26	C08-C14-N15	-8.00	106.27	115.01
3	A	507	Y26	C08-C14-N15	-8.00	106.27	115.01
3	D	507	Y26	C08-C14-N15	-8.00	106.27	115.01
3	B	507	Y26	C08-C14-N15	-8.00	106.27	115.01
2	B	506	NAG	C1-O5-C5	7.73	122.67	112.19
2	C	506	NAG	C1-O5-C5	7.73	122.67	112.19
2	D	506	NAG	C1-O5-C5	7.73	122.66	112.19
2	A	506	NAG	C1-O5-C5	7.73	122.66	112.19
3	A	507	Y26	C30-C14-N15	-6.70	103.86	114.61
3	D	507	Y26	C30-C14-N15	-6.70	103.86	114.61
3	C	507	Y26	C30-C14-N15	-6.70	103.86	114.61
3	B	507	Y26	C30-C14-N15	-6.70	103.86	114.61
3	D	507	Y26	O03-C02-N07	5.87	119.89	111.07
3	B	507	Y26	O03-C02-N07	5.87	119.88	111.07
3	C	507	Y26	O03-C02-N07	5.87	119.88	111.07
3	A	507	Y26	O03-C02-N07	5.87	119.88	111.07
3	D	507	Y26	C30-C29-N07	-3.50	106.39	109.41
3	A	507	Y26	C30-C29-N07	-3.50	106.39	109.41
3	B	507	Y26	C30-C29-N07	-3.49	106.39	109.41
3	C	507	Y26	C30-C29-N07	-3.49	106.39	109.41
3	A	507	Y26	C19-N18-C17	-3.39	121.65	127.53
3	D	507	Y26	C19-N18-C17	-3.39	121.65	127.53
3	C	507	Y26	C19-N18-C17	-3.38	121.66	127.53
3	B	507	Y26	C19-N18-C17	-3.38	121.66	127.53
3	D	507	Y26	C37-C29-N07	3.32	134.19	128.50
3	A	507	Y26	C37-C29-N07	3.32	134.19	128.50
3	B	507	Y26	C37-C29-N07	3.32	134.19	128.50
3	C	507	Y26	C37-C29-N07	3.32	134.19	128.50
3	C	507	Y26	O03-C02-O01	-3.02	119.64	124.78
3	D	507	Y26	O03-C02-O01	-3.02	119.64	124.78
3	A	507	Y26	O03-C02-O01	-3.02	119.64	124.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	507	Y26	O03-C02-O01	-3.01	119.64	124.78
3	B	507	Y26	C14-N15-C16	-2.99	117.49	122.32
3	A	507	Y26	C14-N15-C16	-2.99	117.50	122.32
3	C	507	Y26	C14-N15-C16	-2.99	117.50	122.32
3	D	507	Y26	C14-N15-C16	-2.99	117.50	122.32
3	C	507	Y26	C16-C17-N18	2.91	116.92	112.31
3	B	507	Y26	C16-C17-N18	2.91	116.92	112.31
3	A	507	Y26	C16-C17-N18	2.91	116.92	112.31
3	D	507	Y26	C16-C17-N18	2.91	116.92	112.31
3	A	507	Y26	C30-C14-C08	2.83	106.09	102.76
3	C	507	Y26	C30-C14-C08	2.83	106.09	102.76
3	D	507	Y26	C30-C14-C08	2.83	106.09	102.76
3	B	507	Y26	C30-C14-C08	2.83	106.09	102.76
2	A	508	NAG	C1-O5-C5	2.80	115.99	112.19
2	A	502	NAG	C1-O5-C5	2.70	115.85	112.19
2	D	502	NAG	C1-O5-C5	2.70	115.85	112.19
2	B	502	NAG	C1-O5-C5	2.70	115.84	112.19
2	C	502	NAG	C1-O5-C5	2.69	115.84	112.19
3	A	507	Y26	C31-C30-C14	2.59	132.44	128.99
3	D	507	Y26	C31-C30-C14	2.59	132.43	128.99
3	C	507	Y26	C31-C30-C14	2.58	132.43	128.99
3	B	507	Y26	C31-C30-C14	2.58	132.43	128.99
3	C	507	Y26	C17-C16-N15	2.36	119.38	113.73
3	D	507	Y26	C17-C16-N15	2.36	119.38	113.73
3	A	507	Y26	C17-C16-N15	2.36	119.38	113.73
3	B	507	Y26	C17-C16-N15	2.35	119.38	113.73
2	C	506	NAG	C3-C4-C5	2.16	114.09	110.24
2	D	506	NAG	C3-C4-C5	2.16	114.09	110.24
3	B	507	Y26	O01-C02-N07	-2.16	120.47	124.09
2	A	506	NAG	C3-C4-C5	2.16	114.09	110.24
3	D	507	Y26	O01-C02-N07	-2.16	120.47	124.09
2	B	506	NAG	C3-C4-C5	2.16	114.09	110.24
3	A	507	Y26	O01-C02-N07	-2.16	120.48	124.09
3	C	507	Y26	O01-C02-N07	-2.15	120.48	124.09
2	A	508	NAG	C4-C3-C2	-2.09	107.95	111.02

There are no chirality outliers.

All (43) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	505	NAG	O5-C5-C6-O6
2	C	505	NAG	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
2	D	505	NAG	O5-C5-C6-O6
2	B	505	NAG	O5-C5-C6-O6
2	A	504	NAG	O5-C5-C6-O6
2	C	504	NAG	O5-C5-C6-O6
2	D	504	NAG	O5-C5-C6-O6
2	B	504	NAG	O5-C5-C6-O6
2	A	503	NAG	O5-C5-C6-O6
2	C	503	NAG	O5-C5-C6-O6
2	D	503	NAG	O5-C5-C6-O6
2	B	503	NAG	O5-C5-C6-O6
2	A	506	NAG	C4-C5-C6-O6
2	C	506	NAG	C4-C5-C6-O6
2	D	506	NAG	C4-C5-C6-O6
2	B	506	NAG	C4-C5-C6-O6
2	A	505	NAG	C4-C5-C6-O6
2	C	505	NAG	C4-C5-C6-O6
2	D	505	NAG	C4-C5-C6-O6
2	B	505	NAG	C4-C5-C6-O6
2	C	508	NAG	C4-C5-C6-O6
2	A	503	NAG	C4-C5-C6-O6
2	C	503	NAG	C4-C5-C6-O6
2	D	503	NAG	C4-C5-C6-O6
2	B	503	NAG	C4-C5-C6-O6
2	A	508	NAG	C8-C7-N2-C2
2	A	508	NAG	O7-C7-N2-C2
2	C	508	NAG	C8-C7-N2-C2
2	C	508	NAG	O7-C7-N2-C2
2	A	504	NAG	C4-C5-C6-O6
2	C	504	NAG	C4-C5-C6-O6
2	D	504	NAG	C4-C5-C6-O6
2	B	504	NAG	C4-C5-C6-O6
2	A	506	NAG	O5-C5-C6-O6
2	C	506	NAG	O5-C5-C6-O6
2	D	506	NAG	O5-C5-C6-O6
2	B	506	NAG	O5-C5-C6-O6
2	C	508	NAG	O5-C5-C6-O6
3	A	507	Y26	C08-C09-N10-C11
3	C	507	Y26	C08-C09-N10-C11
3	D	507	Y26	C08-C09-N10-C11
3	B	507	Y26	C08-C09-N10-C11
2	A	508	NAG	C4-C5-C6-O6

There are no ring outliers.

6 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	508	NAG	2	0
2	C	501	NAG	1	0
2	B	501	NAG	1	0
2	D	501	NAG	1	0
2	A	508	NAG	1	0
2	A	501	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 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 Y26 A 507

Bond lengths

Bond angles

Torsions

Rings

Ligand Y26 B 507

Bond lengths

Bond angles

Torsions

Rings

Ligand Y26 D 507

Bond lengths

Bond angles

Torsions

Rings

Ligand Y26 C 507

Bond lengths | Bond angles
Torsions | Rings
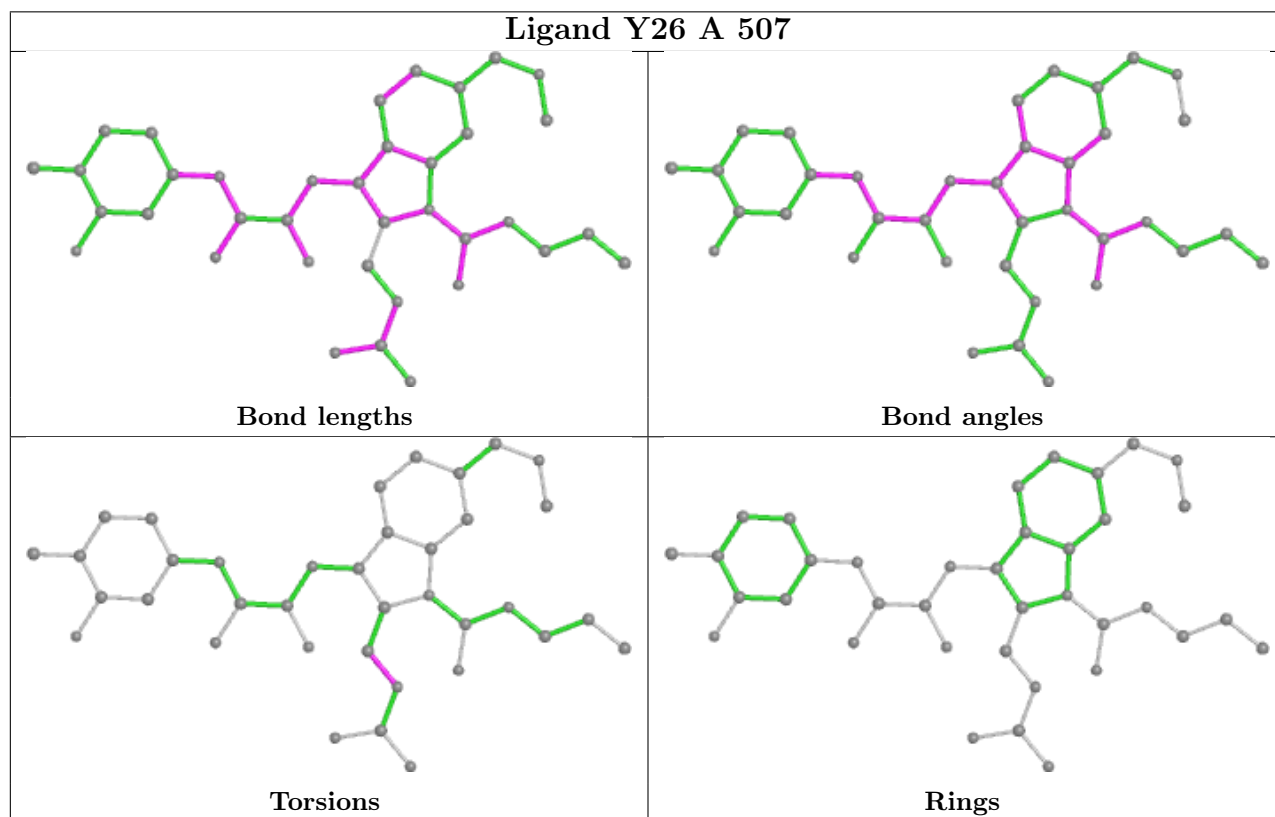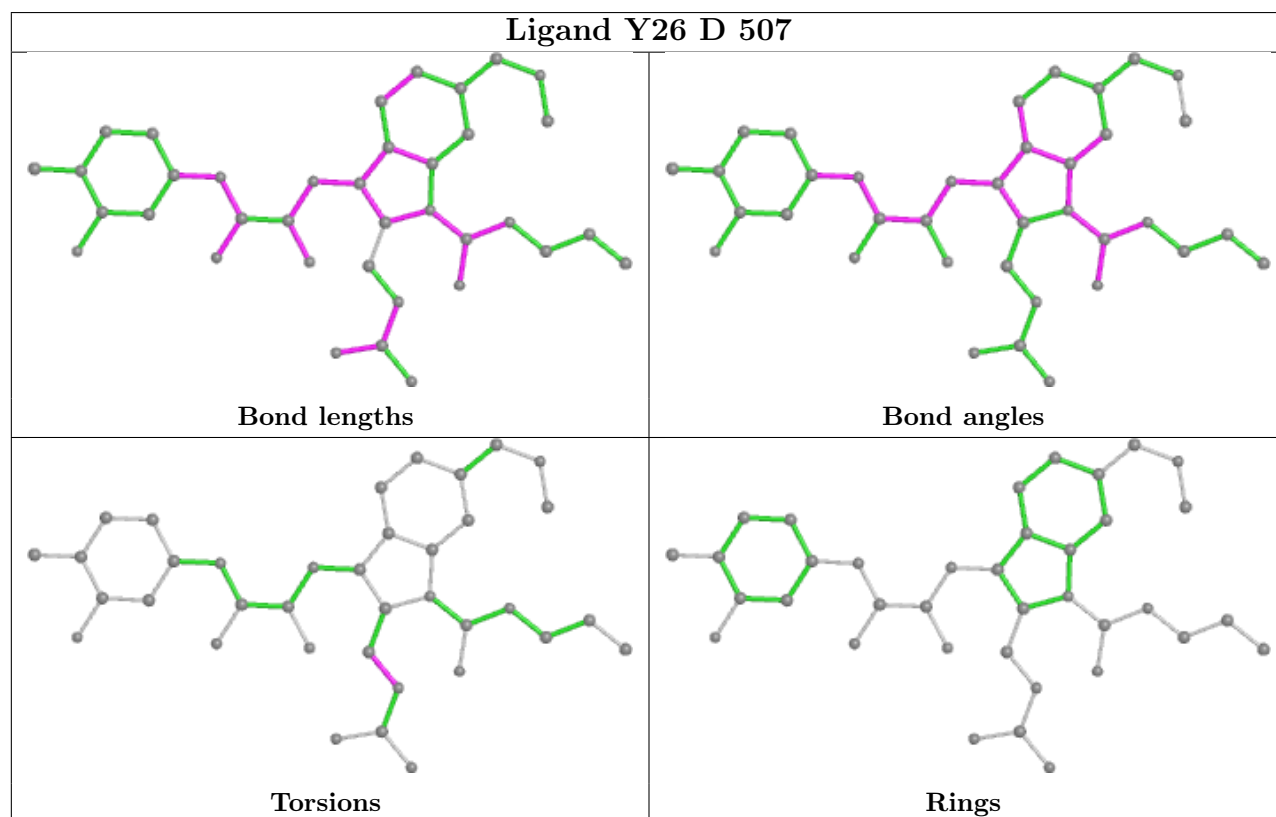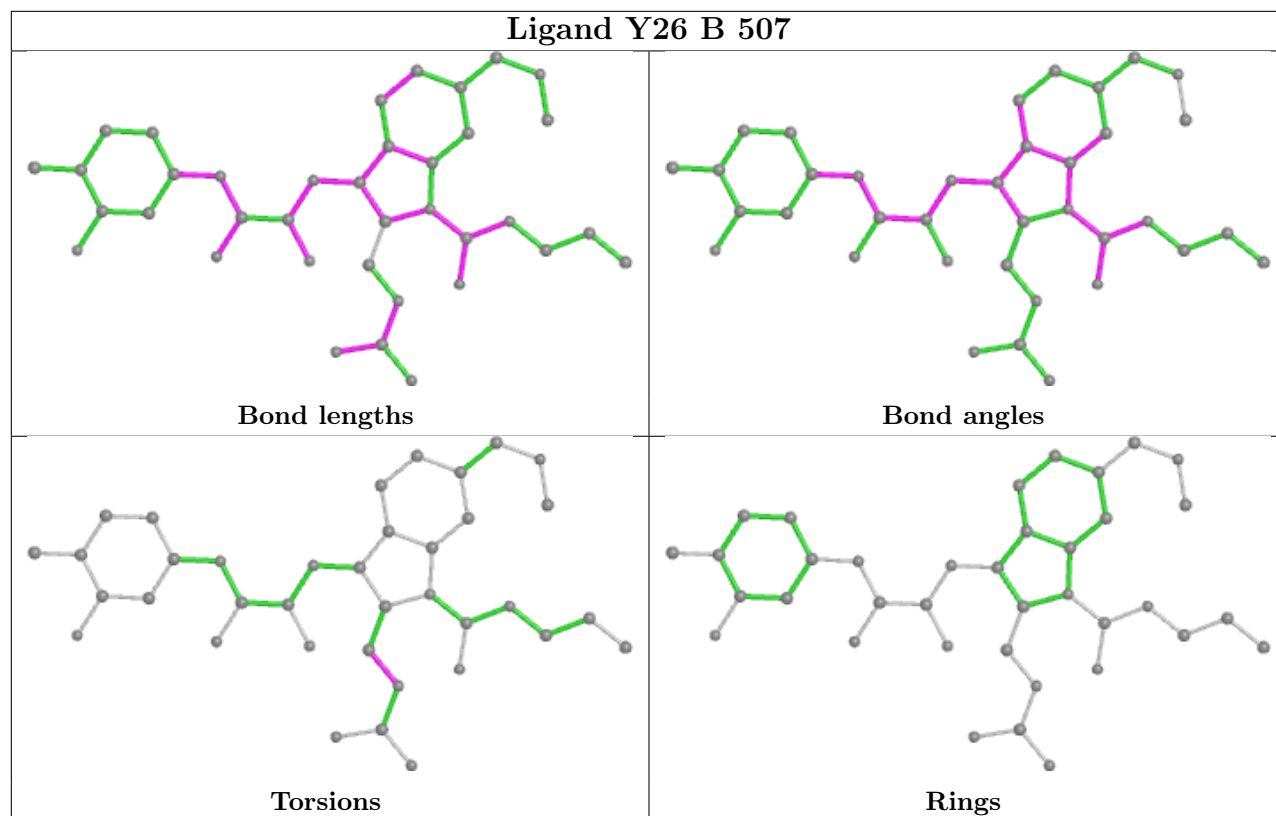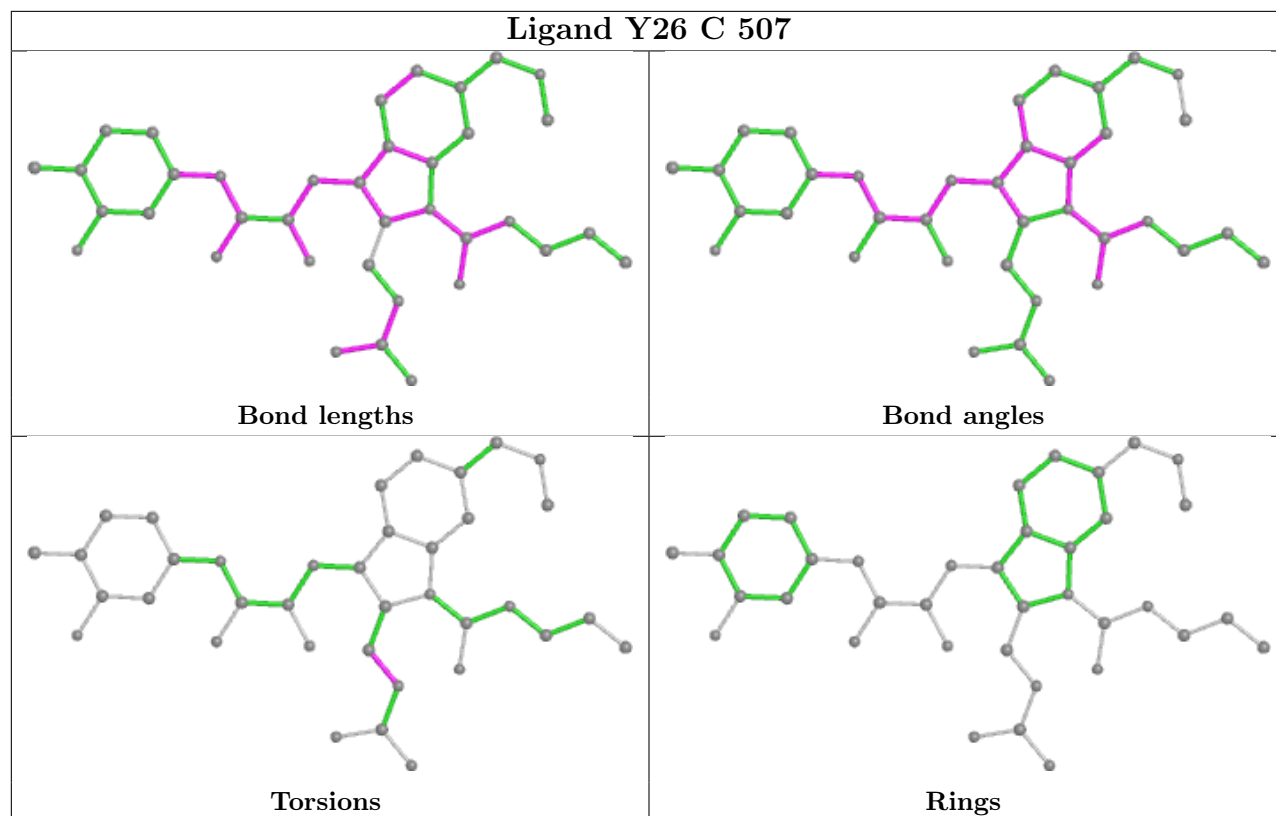
5.7 Other polymers ⓘ

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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å²)	Q<0.9
1	A	335/358 (93%)	0.18	11 (3%)	46	53	23, 37, 57, 91	0
1	B	335/358 (93%)	0.43	27 (8%)	12	15	25, 40, 77, 111	0
1	C	335/358 (93%)	0.41	24 (7%)	15	19	23, 36, 62, 122	0
1	D	335/358 (93%)	0.46	23 (6%)	16	20	25, 40, 66, 100	0
All	All	1340/1432 (93%)	0.37	85 (6%)	20	24	23, 38, 66, 122	0

All (85) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	60	ALA	10.6
1	C	61	TYR	8.7
1	D	89	VAL	7.6
1	C	89	VAL	6.8
1	B	89	VAL	6.4
1	B	240	ARG	6.1
1	D	87	ALA	6.1
1	C	88	ASN	6.0
1	B	88	ASN	5.9
1	D	240	ARG	5.8
1	C	124	GLY	5.4
1	B	60	ALA	5.4
1	B	72	HIS	5.2
1	A	198	GLY	5.1
1	C	198	GLY	4.7
1	D	88	ASN	4.6
1	C	86	LEU	4.6
1	B	50	THR	4.4
1	A	87	ALA	4.4
1	D	86	LEU	4.3
1	C	240	ARG	4.2

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Mol	Chain	Res	Type	RSRZ
1	C	80	ASN	4.1
1	B	408	ARG	4.1
1	B	61	TYR	4.1
1	C	84	MET	4.1
1	D	85	VAL	4.1
1	D	300	ASN	3.8
1	A	88	ASN	3.8
1	C	326	ILE	3.7
1	A	356	SER	3.7
1	C	199	SER	3.7
1	D	408	ARG	3.5
1	C	59	LYS	3.4
1	B	226	LEU	3.4
1	D	326	ILE	3.4
1	B	396	ARG	3.3
1	B	84	MET	3.2
1	D	60	ALA	3.1
1	B	411	ASN	3.1
1	A	89	VAL	3.1
1	D	82	GLN	3.1
1	B	59	LYS	3.0
1	C	122	LEU	3.0
1	B	86	LEU	3.0
1	B	91	GLU	3.0
1	D	396	ARG	2.9
1	B	90	THR	2.9
1	B	244	THR	2.9
1	B	231	LYS	2.9
1	D	124	GLY	2.8
1	A	84	MET	2.8
1	C	85	VAL	2.8
1	D	72	HIS	2.8
1	A	226	LEU	2.7
1	D	242	VAL	2.7
1	D	339	ASN	2.7
1	C	87	ALA	2.4
1	B	356	SER	2.4
1	C	246	GLN	2.4
1	B	57	ASP	2.4
1	D	90	THR	2.4
1	B	63	LYS	2.4
1	B	80	ASN	2.3

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Mol	Chain	Res	Type	RSRZ
1	D	341	THR	2.3
1	D	81	PRO	2.3
1	B	79	PRO	2.3
1	C	440	GLU	2.3
1	B	221	ALA	2.2
1	A	85	VAL	2.2
1	A	86	LEU	2.2
1	D	59	LYS	2.2
1	C	269	GLU	2.2
1	A	82	GLN	2.2
1	B	87	ALA	2.2
1	C	202	THR	2.2
1	C	268	GLU	2.1
1	C	82	GLN	2.1
1	A	354	PRO	2.1
1	C	221	ALA	2.1
1	C	356	SER	2.1
1	D	269	GLU	2.1
1	B	124	GLY	2.1
1	B	265	LEU	2.1
1	D	50	THR	2.0
1	D	84	MET	2.0

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

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

6.3　Carbohydrates ⓘ

There are no monosaccharides in this entry.

6.4　Ligands ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($Å^2$)	Q<0.9
2	NAG	D	506	14/15	0.53	0.35	52,61,69,70	0

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| Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å²)	Q<0.9
2	NAG	A	506	14/15	0.76	0.23	64,79,87,95	0
2	NAG	B	506	14/15	0.77	0.23	45,53,62,65	0
2	NAG	C	506	14/15	0.78	0.17	48,54,62,67	0
2	NAG	B	504	14/15	0.82	0.16	37,44,47,48	0
2	NAG	D	503	14/15	0.82	0.17	49,54,60,70	0
2	NAG	D	505	14/15	0.84	0.19	50,55,57,63	0
2	NAG	D	501	14/15	0.84	0.14	34,48,56,57	0
2	NAG	B	503	14/15	0.85	0.16	49,53,62,69	0
2	NAG	D	504	14/15	0.85	0.17	43,51,56,58	0
2	NAG	B	501	14/15	0.85	0.16	36,50,58,58	0
3	Y26	A	507	37/37	0.85	0.15	20,26,40,101	0
2	NAG	A	508	14/15	0.86	0.14	45,51,54,64	0
2	NAG	A	501	14/15	0.87	0.14	39,48,52,61	0
2	NAG	C	508	14/15	0.88	0.12	48,52,57,59	0
3	Y26	B	507	37/37	0.88	0.15	22,27,34,84	0
2	NAG	A	503	14/15	0.89	0.13	36,41,49,50	0
3	Y26	D	507	37/37	0.90	0.16	21,30,45,69	0
2	NAG	B	505	14/15	0.90	0.15	45,48,53,56	0
2	NAG	B	502	14/15	0.91	0.14	27,39,43,46	0
2	NAG	C	505	14/15	0.91	0.13	32,37,43,44	0
2	NAG	C	501	14/15	0.91	0.10	33,40,48,50	0
2	NAG	C	504	14/15	0.91	0.14	32,37,48,49	0
2	NAG	A	504	14/15	0.92	0.13	44,47,55,58	0
2	NAG	C	503	14/15	0.92	0.13	40,43,51,53	0
2	NAG	A	505	14/15	0.93	0.12	31,35,44,46	0
3	Y26	C	507	37/37	0.93	0.15	18,25,42,46	0
2	NAG	D	502	14/15	0.94	0.14	28,37,40,47	0
2	NAG	C	502	14/15	0.96	0.14	28,32,36,39	0
2	NAG	A	502	14/15	0.97	0.14	26,32,39,40	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 Y26 A 507:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
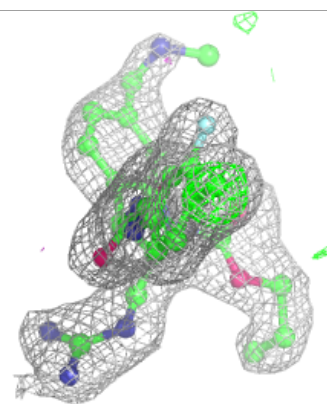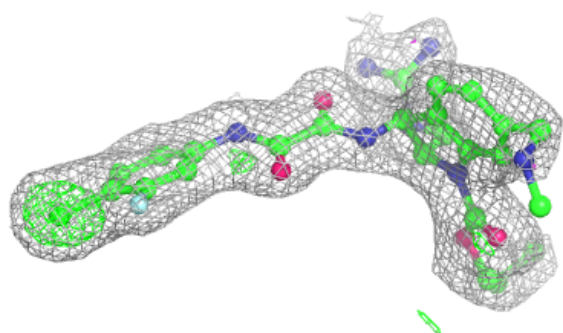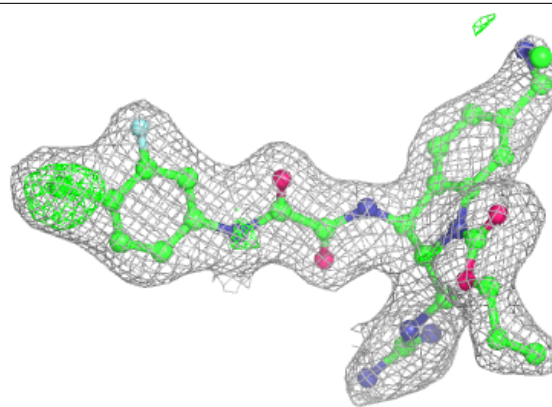$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)
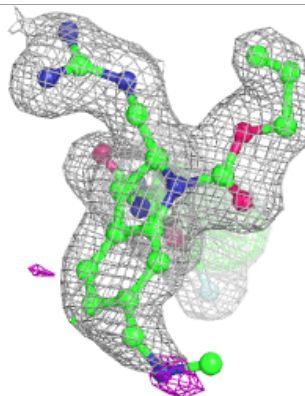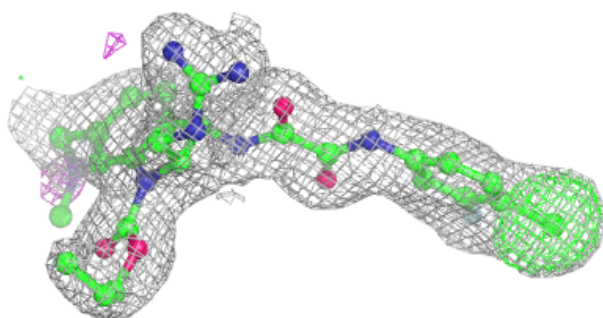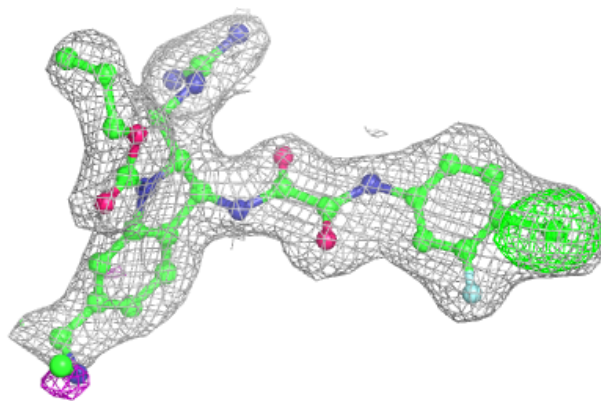
Electron density around Y26 B 507:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
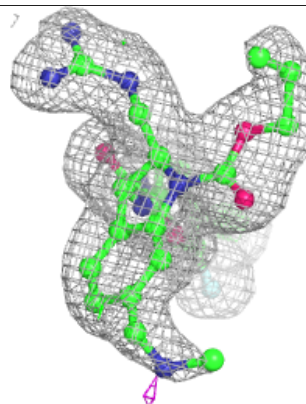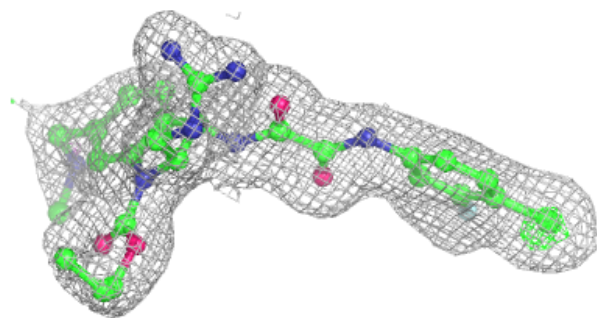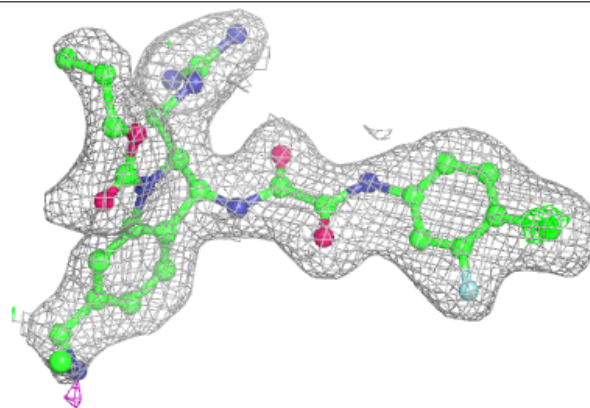and green (positive)
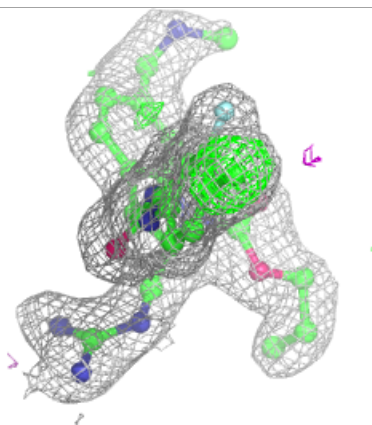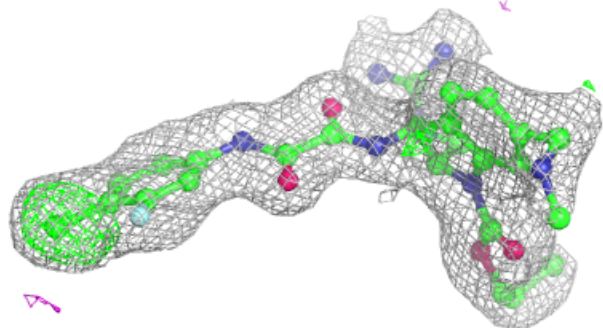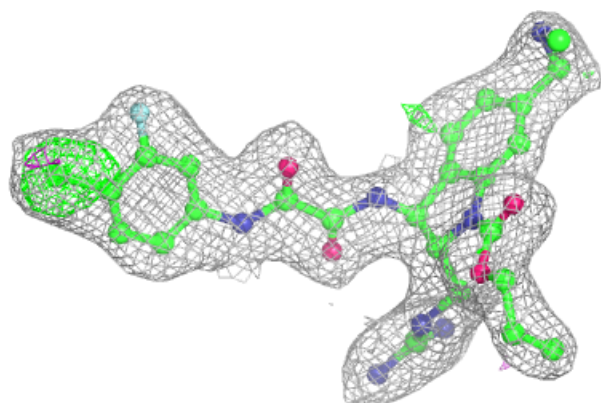
Electron density around Y26 D 507:

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 Y26 C 507:

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.