



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 11:03 PM UTC

PDB ID : 5KV8 / pdb_00005kv8
Title : Crystal structure of a hPIV haemagglutinin-neuraminidase-inhibitor complex
Authors : Dirr, L.; El-Deeb, I.M.; Chavas, L.M.G.; Guillon, P.; von Itzstein, M.
Deposited on : 2016-07-13
Resolution : 1.95 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 : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

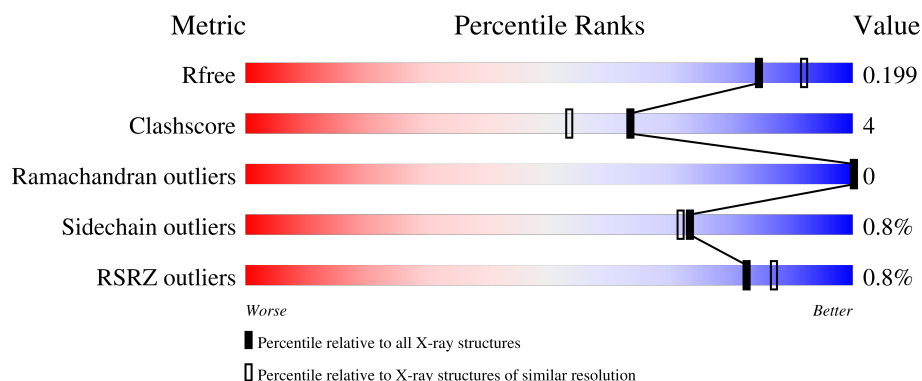
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.95 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}	180053	1452 (1.94-1.94)
Clashscore	190562	1494 (1.94-1.94)
Ramachandran outliers	187476	1479 (1.94-1.94)
Sidechain outliers	187428	1479 (1.94-1.94)
RSRZ outliers	180081	1453 (1.94-1.94)

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 $\leq 5\%$. 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	437	% 91% 7% .
1	B	437	% 89% 7% .

2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 7608 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.

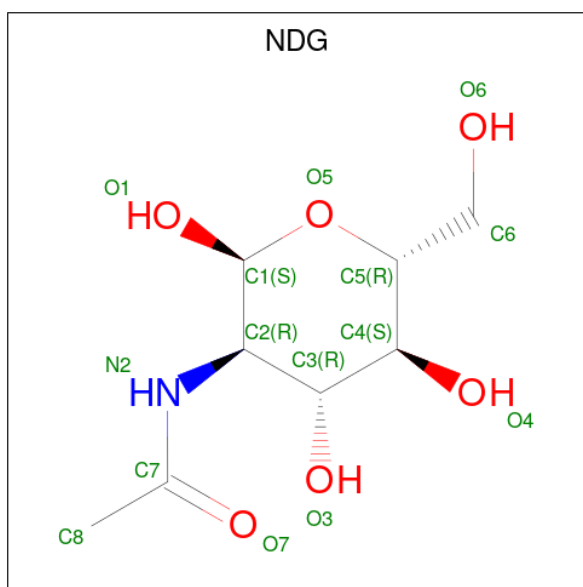
- Molecule 1 is a protein called Hemagglutinin-neuraminidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	430	Total	C	N	O	S	0	2	0
			3384	2139	582	643	20			
1	B	424	Total	C	N	O	S	0	0	0
			3326	2105	572	629	20			

There are 12 discrepancies between the modelled and reference sequences:

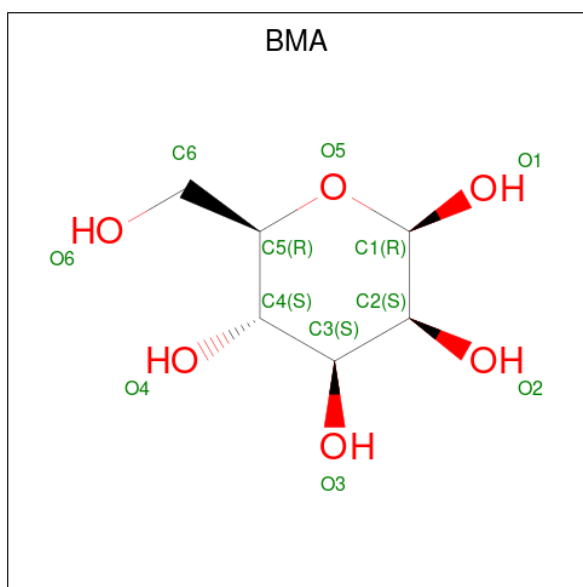
Chain	Residue	Modelled	Actual	Comment	Reference
A	573	HIS	-	expression tag	UNP G8G134
A	574	HIS	-	expression tag	UNP G8G134
A	575	HIS	-	expression tag	UNP G8G134
A	576	HIS	-	expression tag	UNP G8G134
A	577	HIS	-	expression tag	UNP G8G134
A	578	HIS	-	expression tag	UNP G8G134
B	573	HIS	-	expression tag	UNP G8G134
B	574	HIS	-	expression tag	UNP G8G134
B	575	HIS	-	expression tag	UNP G8G134
B	576	HIS	-	expression tag	UNP G8G134
B	577	HIS	-	expression tag	UNP G8G134
B	578	HIS	-	expression tag	UNP G8G134

- Molecule 2 is 2-acetamido-2-deoxy-alpha-D-glucopyranose (CCD ID: NDG) (formula: C₈H₁₅NO₆).



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	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		

- Molecule 3 is beta-D-mannopyranose (CCD ID: BMA) (formula: C₆H₁₂O₆).

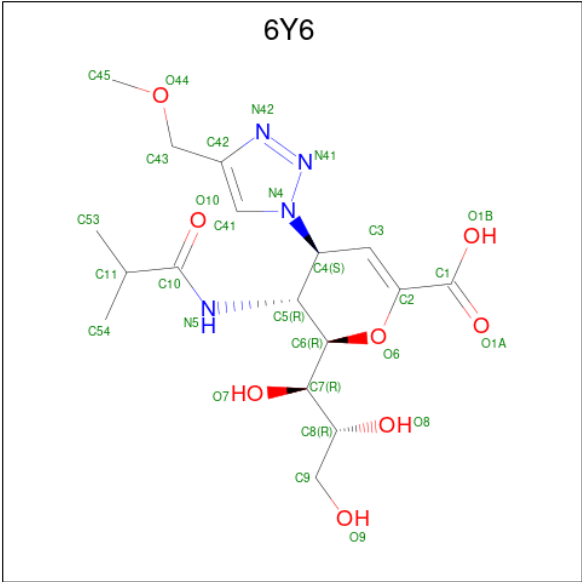


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			11	6	5		
3	B	1	Total	C	O	0	0
			11	6	5		

- Molecule 4 is CALCIUM ION (CCD ID: CA) (formula: Ca).

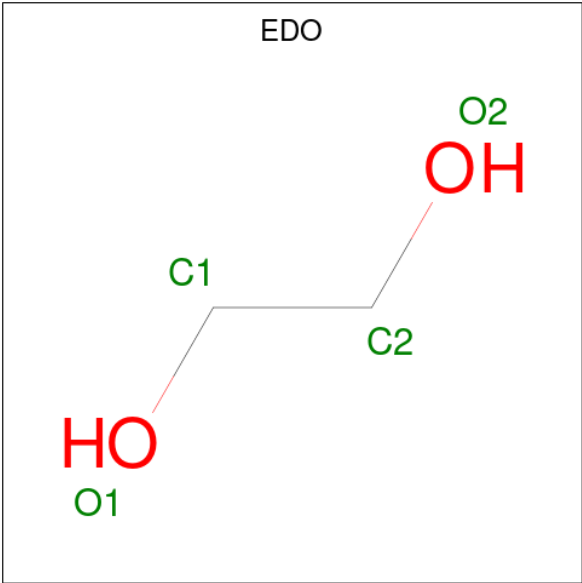
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Ca	0	0
			1	1		
4	B	1	Total	Ca	0	0
			1	1		

- Molecule 5 is 2,6-anhydro-3,4,5-trideoxy-4-[4-(methoxymethyl)-1H-1,2,3-triazol-1-yl]-5-[(2-methylpropanoyl)amino]-D-glycero-D-galacto -non-2-enonic acid (CCD ID: 6Y6) (formula: C₁₇H₂₆N₄O₈).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	N	O	0	0
			29	17	4	8		
5	B	1	Total	C	N	O	0	0
			29	17	4	8		

- Molecule 6 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



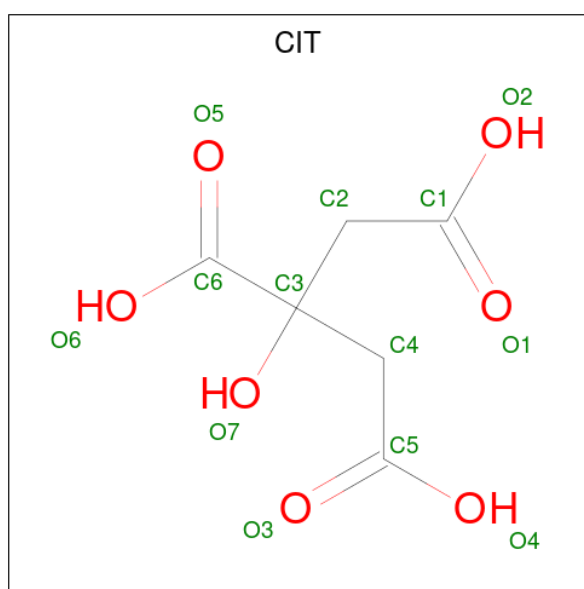
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			4	2	2		
6	A	1	Total	C	O	0	0
			4	2	2		

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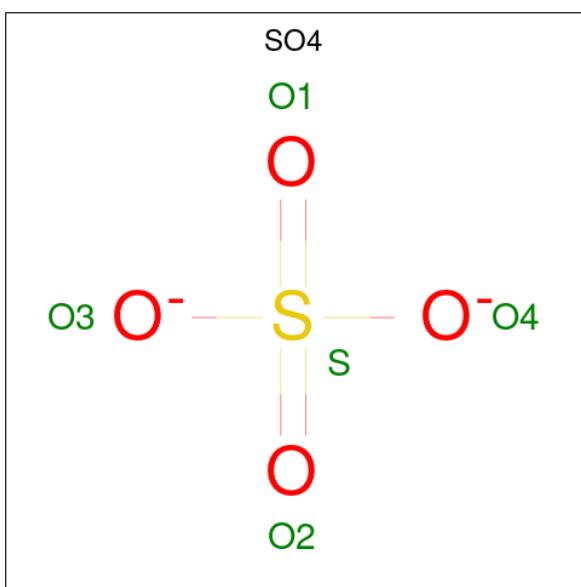
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			4	2	2		
6	B	1	Total	C	O	0	0
			4	2	2		
6	B	1	Total	C	O	0	0
			4	2	2		
6	B	1	Total	C	O	0	0
			4	2	2		

- Molecule 7 is CITRIC ACID (CCD ID: CIT) (formula: $C_6H_8O_7$).



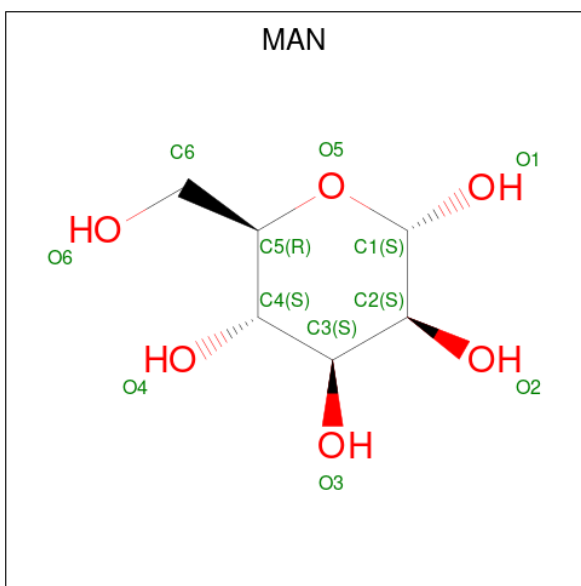
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	C	O	0	0
			13	6	7		

- Molecule 8 is SULFATE ION (CCD ID: SO4) (formula: O_4S).



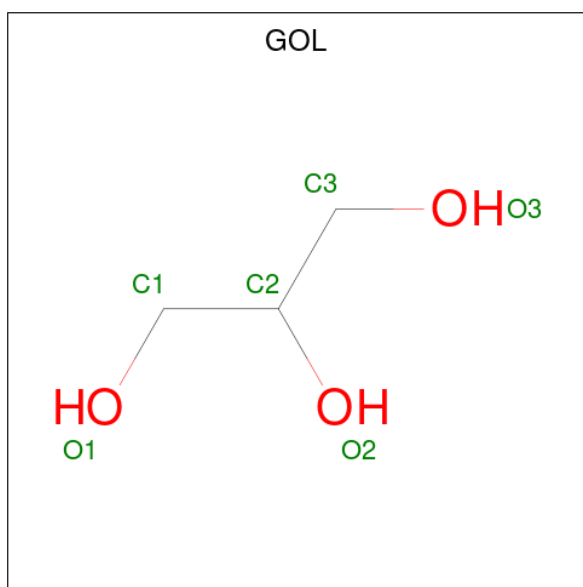
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	B	1	Total	O	S	0	0
			5	4	1		

- Molecule 9 is alpha-D-mannopyranose (CCD ID: MAN) (formula: $C_6H_{12}O_6$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	B	1	Total	C	O	0	0
			11	6	5		

- Molecule 10 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	B	1	Total	C	O	0	0
			6	3	3		

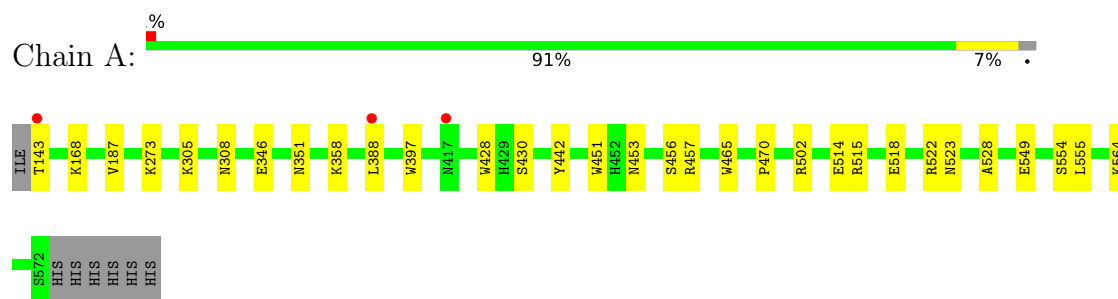
- Molecule 11 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	A	353	Total	O	0	0
			353	353		
11	B	292	Total	O	0	0
			292	292		

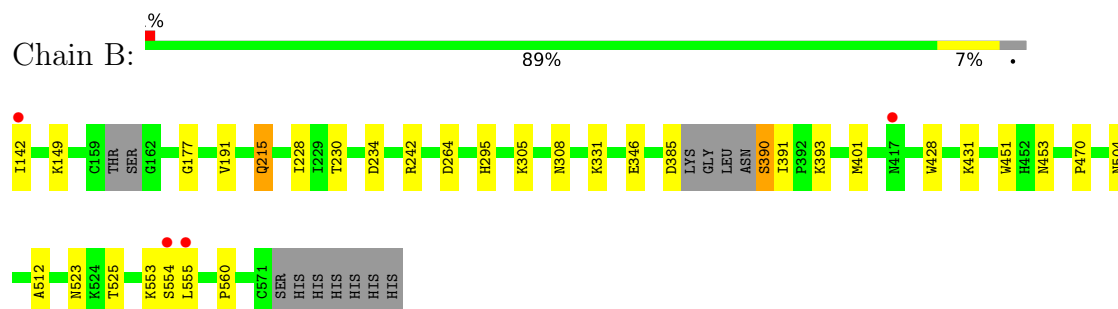
3 Residue-property plots [i](#)

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: Hemagglutinin-neuraminidase



• Molecule 1: Hemagglutinin-neuraminidase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	81.57Å 98.61Å 103.39Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	45.78 – 1.95 45.78 – 1.95	Depositor EDS
% Data completeness (in resolution range)	99.9 (45.78-1.95) 99.9 (45.78-1.95)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.97 (at 1.95Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.161 , 0.200 0.161 , 0.199	Depositor DCC
R_{free} test set	3137 reflections (5.10%)	wwPDB-VP
Wilson B-factor (Å ²)	23.9	Xtriage
Anisotropy	0.212	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 44.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.013 for -h,l,k	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	7608	wwPDB-VP
Average B, all atoms (Å ²)	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.62% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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: CIT, EDO, GOL, 6Y6, SO4, MAN, BMA, CA, NDG

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	0.51	0/3466	0.77	0/4724
1	B	0.51	0/3405	0.78	2/4639 (0.0%)
All	All	0.51	0/6871	0.77	2/9363 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	177	GLY	CA-C-N	-5.67	114.14	120.14
1	B	177	GLY	C-N-CA	-5.67	114.14	120.14

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3384	0	3337	25	1
1	B	3326	0	3285	21	1
2	A	56	0	48	8	0
2	B	56	0	48	7	1
3	A	11	0	10	1	0
3	B	11	0	10	1	0
4	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	1	0	0	0	0
5	A	29	0	0	0	0
5	B	29	0	0	0	0
6	A	12	0	18	0	0
6	B	12	0	18	0	0
7	A	13	0	5	1	0
8	B	5	0	0	1	0
9	B	11	0	10	2	0
10	B	6	0	8	0	0
11	A	353	0	0	7	1
11	B	292	0	0	5	0
All	All	7608	0	6797	55	3

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

All (55) 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:555:LEU:O	11:A:701:HOH:O	1.92	0.87
1:A:143:THR:N	11:A:703:HOH:O	2.09	0.85
1:B:215:GLN:NE2	11:B:703:HOH:O	2.15	0.79
2:B:601:NDG:H4	2:B:602:NDG:C1	2.13	0.78
1:A:554:SER:OG	8:B:610:SO4:O4	1.99	0.77
1:A:351:ASN:HD21	2:A:601:NDG:C1	2.00	0.74
1:B:393:LYS:NZ	11:B:704:HOH:O	2.20	0.73
1:A:523:ASN:HD21	2:A:603:NDG:C1	2.02	0.72
1:B:308:ASN:HD21	2:B:611:NDG:C1	2.01	0.72
2:B:601:NDG:O3	11:B:701:HOH:O	2.10	0.70
1:A:308:ASN:HD21	2:A:610:NDG:C1	2.05	0.68
2:B:603:NDG:O6	11:B:702:HOH:O	2.13	0.65
2:B:601:NDG:H8C1	2:B:601:NDG:H3	1.78	0.65
2:A:601:NDG:H4	2:A:602:NDG:C1	2.31	0.60
1:A:305:LYS:O	1:A:308:ASN:HB2	2.01	0.59
1:B:554:SER:OG	1:B:555:LEU:N	2.36	0.57
1:B:305:LYS:O	1:B:308:ASN:HB2	2.06	0.55
1:B:191:VAL:HB	1:B:560:PRO:HD3	1.88	0.54
1:B:428:TRP:CD2	1:B:470:PRO:HA	2.42	0.54
1:B:228:ILE:HD11	1:B:242:ARG:NH2	2.22	0.54
2:A:602:NDG:H4	3:A:604:BMA:C1	2.37	0.54
3:B:604:BMA:O3	9:B:612:MAN:H3	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:168:LYS:NZ	1:A:514:GLU:OE2	2.43	0.52
1:A:549:GLU:OE2	11:A:705:HOH:O	2.18	0.51
1:A:351:ASN:ND2	2:A:601:NDG:C1	2.73	0.50
2:A:601:NDG:C4	2:A:602:NDG:C1	2.90	0.50
1:B:264:ASP:OD1	1:B:295:HIS:HD2	1.95	0.49
1:A:515:ARG:HD2	1:A:518:GLU:OE1	2.12	0.48
1:B:428:TRP:CG	1:B:470:PRO:HA	2.49	0.47
1:A:428:TRP:CG	1:A:470:PRO:HA	2.50	0.47
1:B:504:ASN:OD1	1:B:523:ASN:HA	2.15	0.46
1:A:451:TRP:CH2	1:A:453:ASN:HB2	2.51	0.46
1:A:428:TRP:CD2	1:A:470:PRO:HA	2.50	0.46
1:A:456:SER:HB3	1:A:465:TRP:CD2	2.50	0.46
1:B:512:ALA:HB3	9:B:612:MAN:H62	1.97	0.45
2:B:601:NDG:H3	2:B:601:NDG:C8	2.45	0.44
1:B:431:LYS:NZ	1:B:453:ASN:OD1	2.49	0.44
1:B:149:LYS:HE3	11:B:916:HOH:O	2.18	0.44
1:A:351:ASN:HD21	2:A:601:NDG:C2	2.30	0.44
1:A:397:TRP:CD2	1:A:442:TYR:HB3	2.53	0.44
1:A:187:VAL:HG22	11:A:887:HOH:O	2.17	0.43
1:B:346:GLU:HG3	1:B:401:MET:HE3	2.00	0.43
1:B:390:SER:HB2	1:B:391:ILE:H	1.30	0.43
1:B:308:ASN:HD21	2:B:611:NDG:C2	2.30	0.43
1:A:522:ARG:HB3	1:A:523:ASN:H	1.65	0.42
1:A:273:LYS:HE3	11:A:937:HOH:O	2.19	0.42
1:A:346:GLU:HB3	11:A:774:HOH:O	2.20	0.41
1:A:502:ARG:HB3	1:A:528:ALA:O	2.21	0.41
1:A:430:SER:HB2	1:A:457:ARG:CZ	2.51	0.41
1:B:331:LYS:NZ	1:B:385:ASP:OD1	2.51	0.41
1:B:451:TRP:CH2	1:B:453:ASN:HB2	2.56	0.41
1:A:358:LYS:HD3	1:A:358:LYS:HA	1.81	0.41
7:A:611:CIT:H42	1:B:230:THR:HB	2.03	0.41
1:A:523:ASN:ND2	11:A:717:HOH:O	2.50	0.41
1:B:525:THR:O	1:B:553:LYS:NZ	2.54	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:273:LYS:NZ	2:B:602:NDG:O6[2_544]	2.18	0.02
11:A:972:HOH:O	11:A:994:HOH:O[2_554]	2.18	0.02
1:B:215:GLN:OE1	1:B:390:SER:OG[4_545]	2.18	0.02

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	430/437 (98%)	412 (96%)	18 (4%)	0	100	100
1	B	418/437 (96%)	396 (95%)	22 (5%)	0	100	100
All	All	848/874 (97%)	808 (95%)	40 (5%)	0	100	100

There are no Ramachandran outliers to report.

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	390/395 (99%)	388 (100%)	2 (0%)	81	82
1	B	383/395 (97%)	379 (99%)	4 (1%)	68	64
All	All	773/790 (98%)	767 (99%)	6 (1%)	73	71

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	388	LEU
1	A	564	LYS
1	B	142	ILE
1	B	215	GLN
1	B	234	ASP
1	B	390	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such

sidechains are listed below:

Mol	Chain	Res	Type
1	A	342	HIS
1	A	461	ASN
1	B	295	HIS
1	B	351	ASN
1	B	365	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 24 ligands modelled in this entry, 2 are monoatomic - leaving 22 for Mogul analysis.

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	$\# Z > 2$
8	SO4	B	610	-	4,4,4	0.24	0	6,6,6	0.10	0
2	NDG	B	603	-	14,14,15	0.96	1 (7%)	17,19,21	0.76	0
2	NDG	B	602	-	14,14,15	1.34	2 (14%)	17,19,21	1.61	3 (17%)
6	EDO	B	608	-	3,3,3	0.42	0	2,2,2	0.46	0
9	MAN	B	612	-	11,11,12	1.87	3 (27%)	15,15,17	1.56	4 (26%)
2	NDG	A	610	-	14,14,15	1.42	1 (7%)	17,19,21	0.81	1 (5%)
7	CIT	A	611	-	12,12,12	1.06	0	17,17,17	1.55	2 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	NDG	A	603	-	14,14,15	1.57	1 (7%)	17,19,21	1.15	2 (11%)
2	NDG	B	601	-	14,14,15	1.54	1 (7%)	17,19,21	2.15	3 (17%)
5	6Y6	A	606	-	30,30,30	1.92	6 (20%)	31,42,42	1.76	9 (29%)
2	NDG	A	601	-	14,14,15	2.39	2 (14%)	17,19,21	1.67	2 (11%)
6	EDO	B	609	-	3,3,3	0.45	0	2,2,2	0.31	0
6	EDO	A	609	-	3,3,3	0.44	0	2,2,2	0.25	0
10	GOL	B	613	-	5,5,5	0.30	0	5,5,5	0.60	0
6	EDO	A	607	-	3,3,3	0.47	0	2,2,2	0.46	0
2	NDG	B	611	-	14,14,15	1.40	1 (7%)	17,19,21	0.84	1 (5%)
3	BMA	B	604	-	11,11,12	2.19	4 (36%)	15,15,17	1.92	3 (20%)
3	BMA	A	604	-	11,11,12	2.48	5 (45%)	15,15,17	2.73	3 (20%)
2	NDG	A	602	-	14,14,15	1.93	2 (14%)	17,19,21	1.70	2 (11%)
5	6Y6	B	606	-	30,30,30	1.93	6 (20%)	31,42,42	1.81	8 (25%)
6	EDO	B	607	-	3,3,3	0.40	0	2,2,2	0.49	0
6	EDO	A	608	-	3,3,3	0.52	0	2,2,2	0.36	0

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	NDG	B	603	-	-	0/6/23/26	0/1/1/1
2	NDG	B	602	-	-	1/6/23/26	0/1/1/1
6	EDO	B	608	-	-	0/1/1/1	-
9	MAN	B	612	-	-	0/2/19/22	0/1/1/1
2	NDG	A	610	-	-	1/6/23/26	0/1/1/1
7	CIT	A	611	-	-	6/16/16/16	-
2	NDG	A	603	-	-	2/6/23/26	0/1/1/1
2	NDG	B	601	-	-	5/6/23/26	0/1/1/1
5	6Y6	A	606	-	-	2/29/45/45	0/2/2/2
2	NDG	A	601	-	-	2/6/23/26	0/1/1/1
6	EDO	B	609	-	-	1/1/1/1	-
6	EDO	A	609	-	-	1/1/1/1	-
10	GOL	B	613	-	-	0/4/4/4	-
6	EDO	A	607	-	-	1/1/1/1	-
2	NDG	B	611	-	-	0/6/23/26	0/1/1/1
3	BMA	B	604	-	-	1/2/19/22	0/1/1/1
3	BMA	A	604	-	-	1/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NDG	A	602	-	-	2/6/23/26	0/1/1/1
5	6Y6	B	606	-	-	2/29/45/45	0/2/2/2
6	EDO	B	607	-	-	1/1/1/1	-
6	EDO	A	608	-	-	1/1/1/1	-

All (35) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	601	NDG	O5-C1	-7.45	1.31	1.43
5	A	606	6Y6	C2-C1	-6.12	1.35	1.48
5	B	606	6Y6	C2-C1	-5.97	1.35	1.48
2	A	602	NDG	O5-C1	-5.54	1.34	1.43
2	A	603	NDG	O5-C1	-5.51	1.34	1.43
5	B	606	6Y6	N42-N41	5.19	1.40	1.32
2	B	601	NDG	O5-C1	-5.16	1.35	1.43
3	A	604	BMA	C4-C5	5.08	1.63	1.53
2	B	611	NDG	O5-C1	-4.97	1.35	1.43
5	A	606	6Y6	N42-N41	4.91	1.40	1.32
2	A	610	NDG	O5-C1	-4.90	1.35	1.43
3	B	604	BMA	C4-C5	4.59	1.62	1.53
2	A	601	NDG	C1-C2	-4.56	1.46	1.52
2	A	602	NDG	C1-C2	-4.16	1.46	1.52
3	A	604	BMA	C4-C3	4.05	1.62	1.52
9	B	612	MAN	O5-C5	3.83	1.50	1.43
5	B	606	6Y6	N4-N41	3.80	1.40	1.35
3	B	604	BMA	O5-C1	-3.79	1.37	1.43
5	A	606	6Y6	N4-N41	3.56	1.39	1.35
2	B	602	NDG	C1-C2	-3.54	1.47	1.52
2	B	603	NDG	O5-C1	-3.40	1.38	1.43
2	B	602	NDG	O5-C1	-3.24	1.38	1.43
9	B	612	MAN	C1-C2	3.20	1.59	1.52
3	A	604	BMA	C2-C3	-3.09	1.47	1.52
5	B	606	6Y6	C10-N5	-3.02	1.27	1.34
5	A	606	6Y6	C10-N5	-2.96	1.27	1.34
3	B	604	BMA	C2-C3	-2.79	1.48	1.52
3	B	604	BMA	C4-C3	2.45	1.58	1.52
5	A	606	6Y6	O6-C2	2.39	1.45	1.37
5	B	606	6Y6	O6-C2	2.39	1.45	1.37
5	A	606	6Y6	O1B-C1	-2.37	1.24	1.30
5	B	606	6Y6	O1B-C1	-2.31	1.24	1.30
3	A	604	BMA	C1-C2	-2.26	1.46	1.52
3	A	604	BMA	O5-C1	-2.24	1.39	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	B	612	MAN	C2-C3	2.11	1.55	1.52

All (43) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	604	BMA	C1-C2-C3	-9.08	96.42	109.64
2	B	601	NDG	C2-N2-C7	5.69	130.53	122.90
2	A	602	NDG	C3-C4-C5	5.16	119.59	110.23
2	B	601	NDG	C3-C4-C5	4.94	119.19	110.23
2	A	601	NDG	C3-C4-C5	4.85	119.03	110.23
3	B	604	BMA	C1-O5-C5	-4.30	106.42	112.19
2	A	601	NDG	C1-O5-C5	-4.24	106.50	112.19
5	B	606	6Y6	O6-C2-C3	-4.23	119.88	124.62
5	A	606	6Y6	C43-C42-C41	-3.94	123.42	130.22
7	A	611	CIT	O6-C6-C3	3.92	120.66	113.14
3	B	604	BMA	C3-C4-C5	3.82	117.15	110.23
9	B	612	MAN	C1-O5-C5	3.81	117.30	112.19
2	A	602	NDG	C1-O5-C5	-3.80	107.10	112.19
5	A	606	6Y6	C43-C42-N42	3.78	127.75	121.49
2	B	602	NDG	C3-C4-C5	3.77	117.06	110.23
5	B	606	6Y6	C43-C42-C41	-3.73	123.79	130.22
5	B	606	6Y6	N4-N41-N42	-3.64	104.02	107.09
3	A	604	BMA	C1-O5-C5	-3.63	107.33	112.19
5	A	606	6Y6	O6-C2-C3	-3.62	120.57	124.62
2	B	602	NDG	C1-O5-C5	-3.58	107.39	112.19
5	B	606	6Y6	C43-C42-N42	3.58	127.42	121.49
5	A	606	6Y6	N4-N41-N42	-3.50	104.14	107.09
5	B	606	6Y6	O6-C2-C1	3.12	118.24	112.02
5	A	606	6Y6	O1B-C1-C2	3.05	120.97	114.06
2	B	602	NDG	O4-C4-C3	-2.95	103.41	110.38
2	A	603	NDG	O3-C3-C2	-2.94	103.30	109.40
3	B	604	BMA	C1-C2-C3	-2.77	105.61	109.64
5	B	606	6Y6	C6-C5-N5	-2.61	106.75	110.91
5	B	606	6Y6	C8-C7-C6	-2.58	108.20	113.05
5	B	606	6Y6	O1B-C1-C2	2.55	119.84	114.06
5	A	606	6Y6	O6-C2-C1	2.50	117.00	112.02
3	A	604	BMA	O3-C3-C4	2.42	116.09	110.38
2	A	603	NDG	C3-C4-C5	2.39	114.56	110.23
2	B	601	NDG	C1-C2-N2	2.39	114.19	110.43
7	A	611	CIT	O2-C1-O1	-2.26	117.53	123.33
9	B	612	MAN	O5-C1-C2	2.24	116.14	110.79
5	A	606	6Y6	C6-C5-N5	-2.23	107.34	110.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	B	612	MAN	O3-C3-C2	2.23	114.60	110.05
2	B	611	NDG	C3-C4-C5	2.14	114.12	110.23
9	B	612	MAN	O2-C2-C1	2.14	114.11	109.22
2	A	610	NDG	C3-C4-C5	2.13	114.10	110.23
5	A	606	6Y6	O1B-C1-O1A	-2.12	118.85	123.90
5	A	606	6Y6	C8-C7-C6	-2.06	109.19	113.05

There are no chirality outliers.

All (30) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	603	NDG	O5-C5-C6-O6
2	A	601	NDG	C4-C5-C6-O6
2	A	603	NDG	C4-C5-C6-O6
2	A	601	NDG	O5-C5-C6-O6
2	B	601	NDG	C8-C7-N2-C2
2	B	601	NDG	O7-C7-N2-C2
2	A	602	NDG	C4-C5-C6-O6
3	B	604	BMA	O5-C5-C6-O6
2	A	602	NDG	O5-C5-C6-O6
3	A	604	BMA	O5-C5-C6-O6
2	B	601	NDG	C4-C5-C6-O6
5	A	606	6Y6	C41-C42-C43-O44
5	A	606	6Y6	N42-C42-C43-O44
5	B	606	6Y6	C41-C42-C43-O44
5	B	606	6Y6	N42-C42-C43-O44
6	B	609	EDO	O1-C1-C2-O2
2	B	601	NDG	O5-C5-C6-O6
7	A	611	CIT	O7-C3-C6-O5
6	A	608	EDO	O1-C1-C2-O2
7	A	611	CIT	C2-C3-C6-O6
7	A	611	CIT	C4-C3-C6-O5
7	A	611	CIT	C4-C3-C6-O6
2	A	610	NDG	C4-C5-C6-O6
2	B	601	NDG	C3-C2-N2-C7
7	A	611	CIT	O7-C3-C6-O6
6	A	609	EDO	O1-C1-C2-O2
2	B	602	NDG	C4-C5-C6-O6
6	B	607	EDO	O1-C1-C2-O2
7	A	611	CIT	C2-C3-C6-O5
6	A	607	EDO	O1-C1-C2-O2

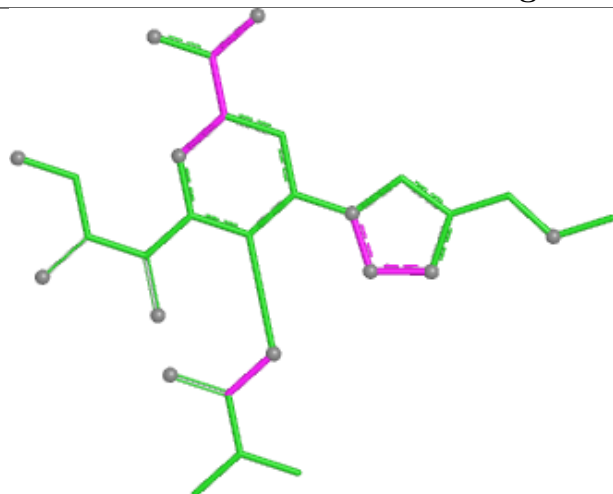
There are no ring outliers.

13 monomers are involved in 20 short contacts:

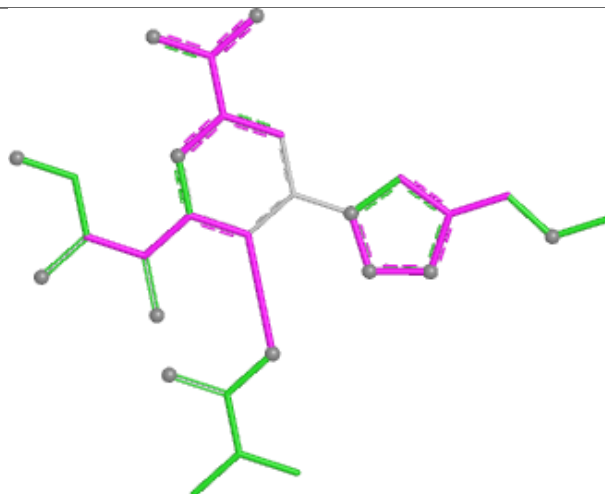
Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	B	610	SO4	1	0
2	B	603	NDG	1	0
2	B	602	NDG	1	1
9	B	612	MAN	2	0
2	A	610	NDG	1	0
7	A	611	CIT	1	0
2	A	603	NDG	1	0
2	B	601	NDG	4	0
2	A	601	NDG	5	0
2	B	611	NDG	2	0
3	B	604	BMA	1	0
3	A	604	BMA	1	0
2	A	602	NDG	3	0

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.

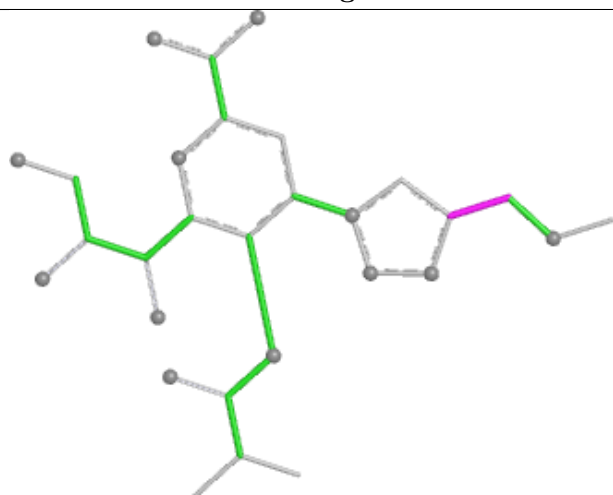
Ligand 6Y6 A 606



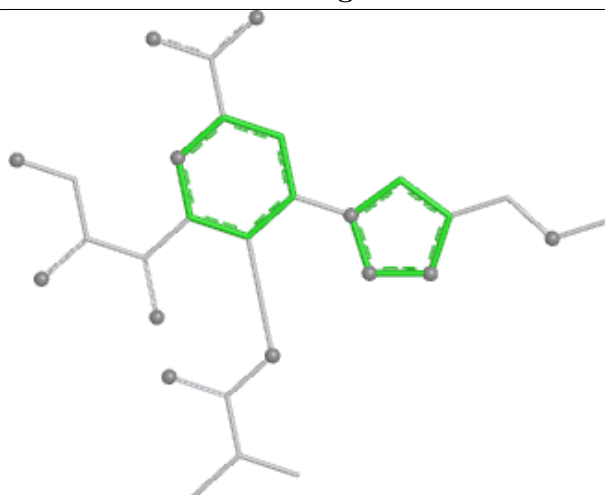
Bond lengths



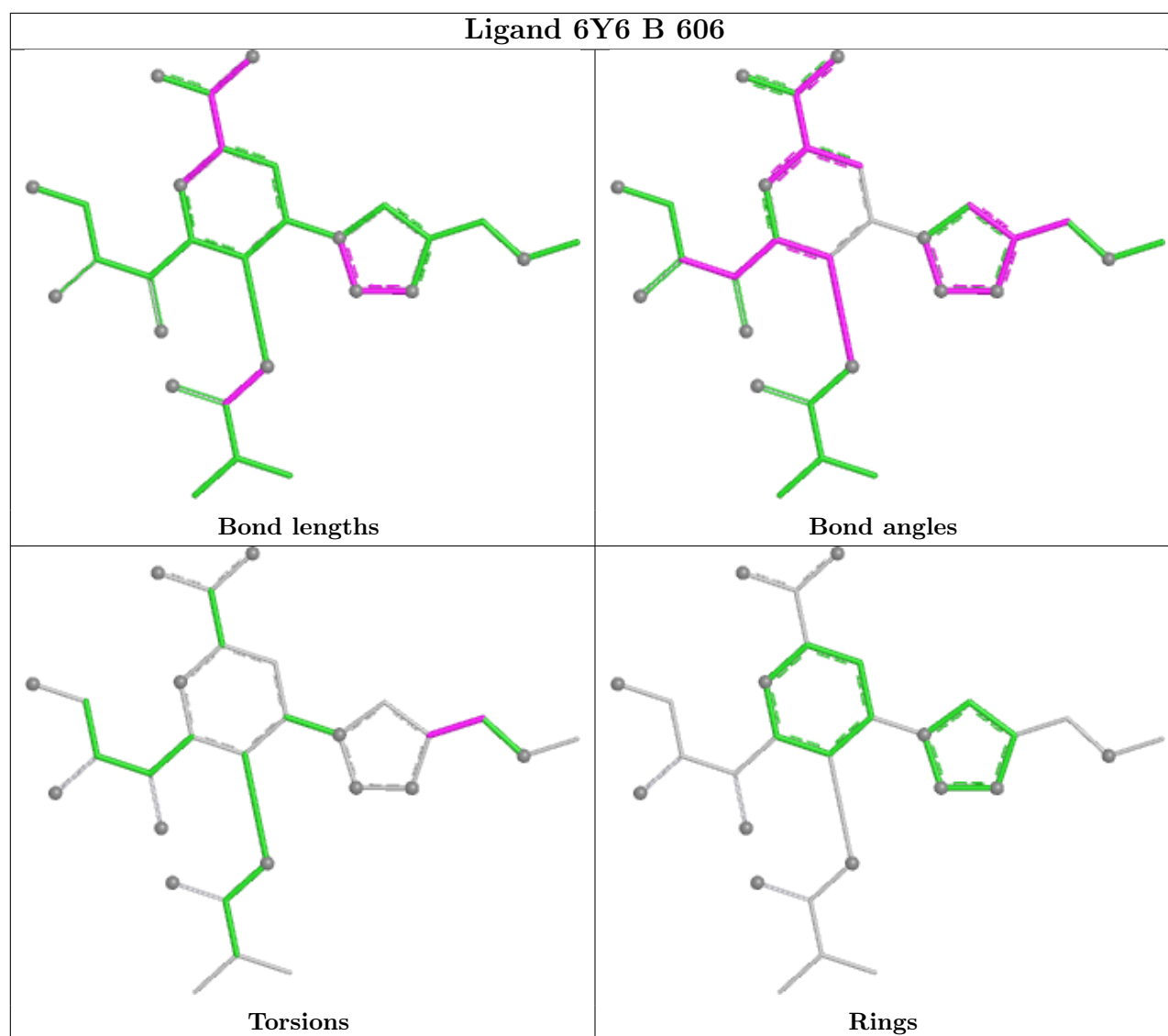
Bond angles



Torsions



Rings



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	430/437 (98%)	-0.37	3 (0%) 84 88	9, 23, 39, 58	2 (0%)
1	B	424/437 (97%)	-0.24	4 (0%) 81 85	16, 25, 44, 60	0
All	All	854/874 (97%)	-0.30	7 (0%) 82 87	9, 24, 42, 60	2 (0%)

All (7) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	417	ASN	3.5
1	A	388	LEU	3.2
1	B	142	ILE	3.2
1	A	417	ASN	3.0
1	A	143	THR	2.5
1	B	554	SER	2.4
1	B	555	LEU	2.1

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 oligosaccharides in this entry.

6.4 Ligands [i](#)

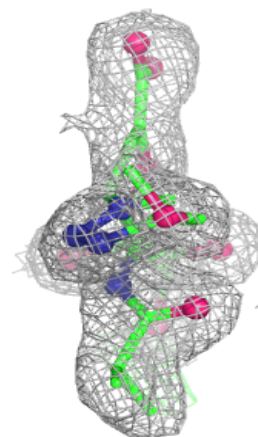
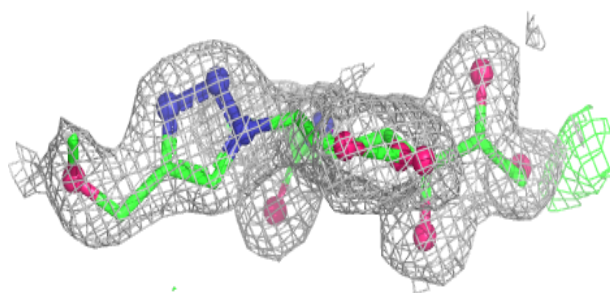
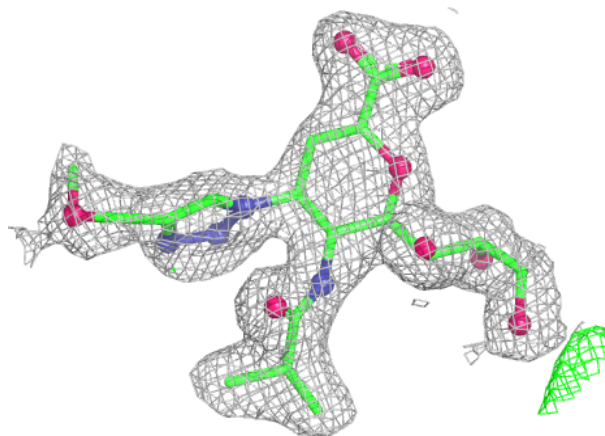
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q < 0.9’ lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	NDG	B	601	14/15	0.61	0.21	40,52,63,73	0
9	MAN	B	612	11/12	0.63	0.16	45,48,61,66	0
3	BMA	B	604	11/12	0.69	0.15	38,52,62,63	0
3	BMA	A	604	11/12	0.70	0.14	55,61,68,68	0
2	NDG	B	611	14/15	0.71	0.13	46,54,64,68	0
2	NDG	A	603	14/15	0.72	0.14	42,52,65,66	0
2	NDG	A	610	14/15	0.74	0.13	41,59,64,65	0
6	EDO	A	608	4/4	0.75	0.14	34,35,36,39	0
2	NDG	A	601	14/15	0.75	0.15	39,42,51,66	0
2	NDG	B	603	14/15	0.77	0.13	40,50,56,60	0
6	EDO	B	607	4/4	0.80	0.14	34,36,37,38	0
2	NDG	B	602	14/15	0.80	0.15	37,44,56,58	0
2	NDG	A	602	14/15	0.81	0.14	39,44,54,63	0
6	EDO	B	608	4/4	0.86	0.13	35,39,40,59	0
7	CIT	A	611	13/13	0.87	0.10	30,39,51,61	0
6	EDO	A	609	4/4	0.87	0.14	46,48,48,48	0
6	EDO	B	609	4/4	0.89	0.14	38,43,46,52	0
6	EDO	A	607	4/4	0.90	0.10	27,35,37,42	0
5	6Y6	B	606	29/29	0.91	0.09	24,31,43,48	0
5	6Y6	A	606	29/29	0.93	0.08	21,28,41,49	0
8	SO4	B	610	5/5	0.95	0.11	32,43,52,52	0
10	GOL	B	613	6/6	0.95	0.07	23,27,30,31	0
4	CA	A	605	1/1	0.99	0.02	23,23,23,23	0
4	CA	B	605	1/1	0.99	0.04	27,27,27,27	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.

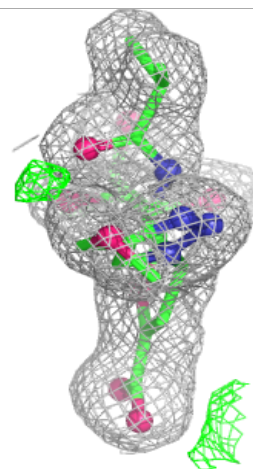
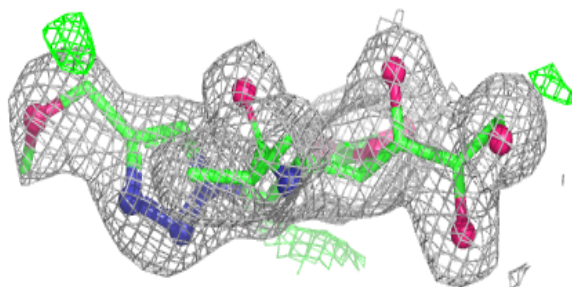
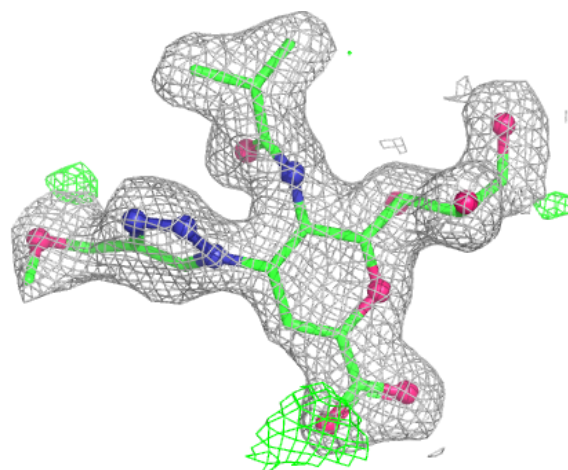
Electron density around 6Y6 B 606:

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



Electron density around 6Y6 A 606:

$2mF_o-DF_c$ (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.