



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 11:12 AM UTC

PDB ID : 4CH8 / pdb_00004ch8
Title : High-salt crystal structure of a thrombin-GpIbalpha peptide complex
Authors : Lechtenberg, B.C.; Freund, S.M.V.; Huntington, J.A.
Deposited on : 2013-11-29
Resolution : 1.75 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:

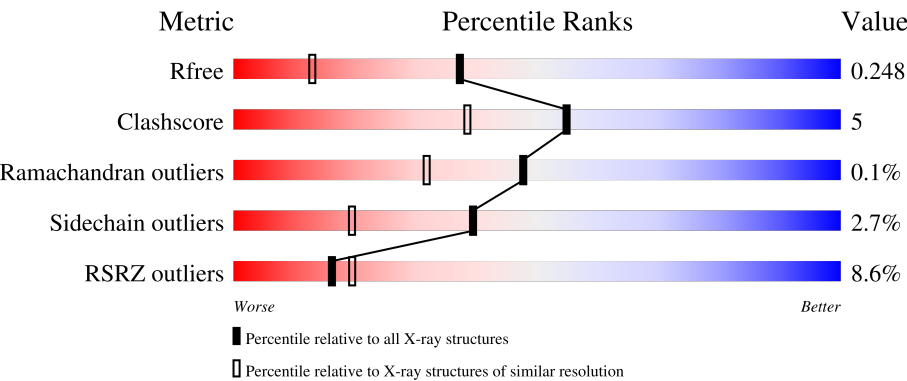
MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal 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 i

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

The reported resolution of this entry is 1.75 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	3183 (1.76-1.76)
Clashscore	190562	3299 (1.76-1.76)
Ramachandran outliers	187476	3274 (1.76-1.76)
Sidechain outliers	187428	3274 (1.76-1.76)
RSRZ outliers	180081	3183 (1.76-1.76)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	36	47% 67%6%28%
1	C	36	28% 78%8%11%
1	E	36	8% 72%28%
1	G	36	8% 67%6%25%
2	B	259	9% 80%14%

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Mol	Chain	Length	Quality of chain
2	D	259	3% 84% 13%
2	F	259	5% 89% 8%
2	H	259	7% 91% 8%
3	P	14	7% 14% 7% 79%
3	Q	14	21% 7% 71%
3	R	14	7% 14% 7% 79%
3	S	14	7% 7% 14% 79%

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 9557 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 THROMBIN, LIGHT CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	26	Total	C	N	O	S	0	0	0
			184	115	29	39	1			
1	C	32	Total	C	N	O	S	0	0	0
			243	151	40	51	1			
1	E	26	Total	C	N	O	S	0	0	0
			202	128	31	42	1			
1	G	27	Total	C	N	O	S	0	1	0
			222	140	34	47	1			

- Molecule 2 is a protein called THROMBIN, HEAVY CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	249	Total	C	N	O	S	1	4	0
			1995	1274	350	356	15			
2	D	252	Total	C	N	O	S	0	2	0
			2014	1289	348	363	14			
2	F	253	Total	C	N	O	S	3	2	0
			1985	1278	339	354	14			
2	H	259	Total	C	N	O	S	0	0	0
			2016	1289	356	357	14			

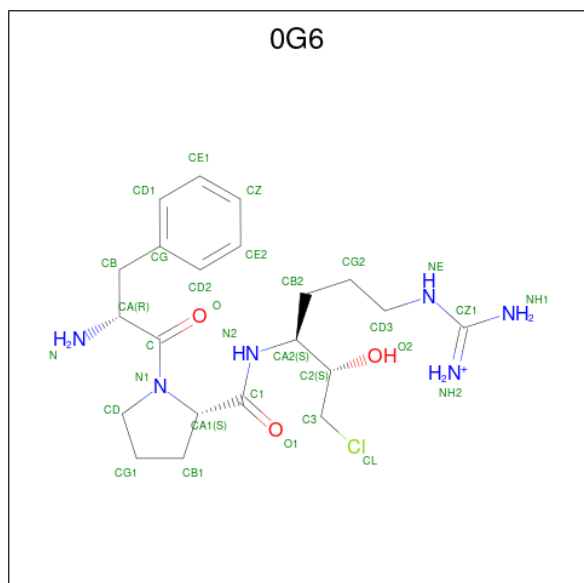
- Molecule 3 is a protein called PLATELET GLYCOPROTEIN IB ALPHA CHAIN, RESIDUES 287-300.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	P	3	Total	C	N	O	P	0	0	0
			32	19	3	9	1			
3	Q	4	Total	C	N	O	P	0	0	0
			40	23	4	12	1			
3	R	3	Total	C	N	O	P	0	0	0
			32	19	3	9	1			
3	S	3	Total	C	N	O	P	0	0	0
			32	19	3	9	1			

- Molecule 4 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total	Na	0	0
			1	1		
4	D	1	Total	Na	0	0
			1	1		
4	F	1	Total	Na	0	0
			1	1		
4	H	1	Total	Na	0	0
			1	1		

- Molecule 5 is D-phenylalanyl-N-[(2S,3S)-6-{[amino(iminio)methyl]amino}-1-chloro-2-hydroxyhexan-3-yl]-L-prolinamide (CCD ID: 0G6) (formula: C₂₁H₃₄ClN₆O₃).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	B	1	Total	C	N	O	0	0
			30	21	6	3		
5	D	1	Total	C	N	O	0	0
			30	21	6	3		
5	F	1	Total	C	N	O	0	0
			30	21	6	3		
5	H	1	Total	C	N	O	0	0
			30	21	6	3		

- Molecule 6 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



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

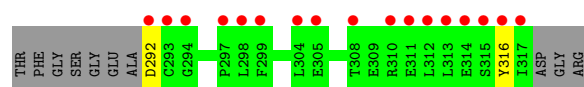
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	6	Total	O	0	0
			6	6		
7	B	94	Total	O	0	0
			94	94		
7	C	14	Total	O	0	0
			14	14		
7	D	108	Total	O	0	0
			108	108		
7	E	7	Total	O	0	0
			7	7		
7	F	94	Total	O	0	0
			94	94		
7	G	11	Total	O	0	0
			11	11		
7	H	90	Total	O	0	0
			90	90		

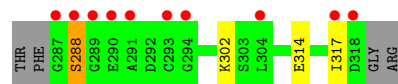
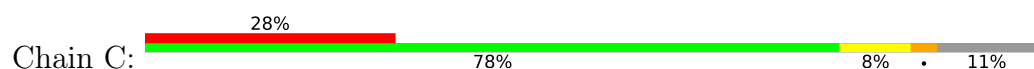
3 Residue-property plots [i](#)

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.

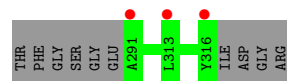
- Molecule 1: THROMBIN, LIGHT CHAIN



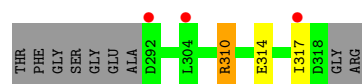
- Molecule 1: THROMBIN, LIGHT CHAIN



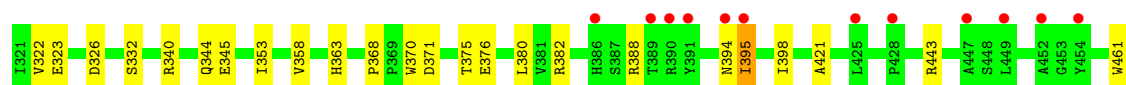
- Molecule 1: THROMBIN, LIGHT CHAIN



- Molecule 1: THROMBIN, LIGHT CHAIN

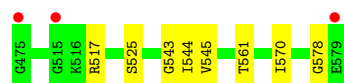
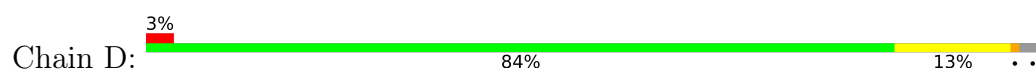


- Molecule 2: THROMBIN, HEAVY CHAIN

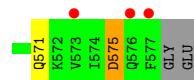
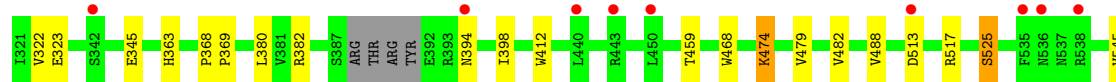
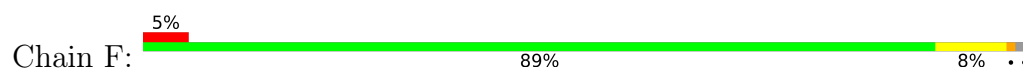




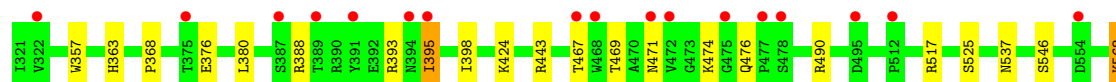
• Molecule 2: THROMBIN, HEAVY CHAIN



• Molecule 2: THROMBIN, HEAVY CHAIN



• Molecule 2: THROMBIN, HEAVY CHAIN



• Molecule 3: PLATELET GLYCOPROTEIN IB ALPHA CHAIN, RESIDUES 287-300



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- Molecule 3: PLATELET GLYCOPROTEIN IB ALPHA CHAIN, RESIDUES 287-300



- Molecule 3: PLATELET GLYCOPROTEIN IB ALPHA CHAIN, RESIDUES 287-300



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	74.22Å 51.33Å 150.08Å 90.00° 96.13° 90.00°	Depositor
Resolution (Å)	42.14 – 1.75 42.14 – 1.75	Depositor EDS
% Data completeness (in resolution range)	92.9 (42.14-1.75) 82.6 (42.14-1.75)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.81 (at 1.75Å)	Xtrriage
Refinement program	REFMAC 5.7.0029	Depositor
R, R_{free}	0.210 , 0.242 0.215 , 0.248	Depositor DCC
R_{free} test set	5305 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	23.3	Xtrriage
Anisotropy	0.499	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 50.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	9557	wwPDB-VP
Average B, all atoms (Å ²)	35.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 25.79 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 2.9676e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PTR, NA, GOL, OG6

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	0.88	0/186	0.81	0/253
1	C	0.93	0/245	1.06	1/327 (0.3%)
1	E	0.82	0/204	0.79	0/273
1	G	0.80	0/227	0.94	0/304
2	B	1.30	11/2046 (0.5%)	1.13	5/2772 (0.2%)
2	D	1.35	6/2069 (0.3%)	1.14	6/2802 (0.2%)
2	F	1.06	2/2043 (0.1%)	0.98	1/2774 (0.0%)
2	H	1.06	3/2068 (0.1%)	0.95	1/2803 (0.0%)
3	P	1.26	0/14	0.90	0/16
3	Q	0.94	0/22	0.89	0/27
3	R	0.94	0/14	0.73	0/16
3	S	1.48	0/14	1.56	0/16
All	All	1.17	22/9152 (0.2%)	1.04	14/12383 (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	C	0	1
2	D	0	1
2	H	0	1
All	All	0	3

All (22) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	525	SER	CB-OG	14.35	1.70	1.42
2	B	525	SER	CB-OG	11.36	1.64	1.42
2	H	525	SER	CB-OG	6.93	1.56	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	360	THR	CA-CB	6.73	1.64	1.53
2	D	525	SER	CB-OG	6.64	1.55	1.42
2	B	353	ILE	CA-CB	-6.49	1.47	1.54
2	F	545	VAL	N-CA	6.04	1.53	1.46
2	D	545	VAL	C-O	-5.87	1.18	1.24
2	B	561	THR	C-O	5.79	1.31	1.23
2	D	570	ILE	C-O	5.67	1.30	1.24
2	B	568	LYS	N-CA	5.59	1.53	1.46
2	H	490	ARG	C-O	-5.59	1.19	1.24
2	B	421	ALA	C-O	-5.49	1.17	1.23
2	B	527	GLY	C-O	5.44	1.31	1.24
2	B	368	PRO	C-O	-5.29	1.18	1.24
2	H	546	SER	CA-C	5.22	1.57	1.52
2	D	404	ILE	N-CA	5.20	1.52	1.46
2	B	528	PRO	C-O	-5.19	1.18	1.23
2	D	545	VAL	C-N	5.16	1.40	1.33
2	B	358	VAL	N-CA	5.14	1.52	1.46
2	B	510	TYR	N-CA	5.12	1.52	1.45
2	B	528	PRO	CA-C	5.05	1.57	1.52

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	571	GLN	CG-CD-OE1	-8.75	103.30	120.80
2	B	571	GLN	CG-CD-NE2	8.14	128.60	116.40
2	D	544	ILE	N-CA-C	-6.98	98.06	108.46
2	B	368	PRO	N-CA-C	6.75	118.93	110.70
2	D	368	PRO	N-CA-C	6.65	118.81	110.70
1	C	288	SER	N-CA-C	6.49	118.63	108.96
2	H	368	PRO	N-CA-C	5.92	117.92	110.70
2	D	353	ILE	N-CA-C	5.83	118.49	112.90
2	F	368	PRO	N-CA-C	5.61	117.54	110.70
2	D	379	LEU	N-CA-C	5.27	117.69	109.52
2	D	356	ARG	NE-CZ-NH2	-5.18	114.54	119.20
2	B	443	ARG	N-CA-C	5.16	116.59	111.07
2	B	571	GLN	OE1-CD-NE2	5.06	127.66	122.60
2	D	356	ARG	CB-CA-C	-5.02	100.94	109.38

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	288	SER	Peptide
2	D	578	GLY	Peptide
2	H	578	GLY	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	184	0	144	2	0
1	C	243	0	228	1	0
1	E	202	0	189	0	0
1	G	222	0	207	2	0
2	B	1995	0	1920	34	0
2	D	2014	0	1944	19	0
2	F	1985	0	1916	17	0
2	H	2016	0	1939	12	0
3	P	32	0	21	0	0
3	Q	40	0	25	0	0
3	R	32	0	22	1	0
3	S	32	0	21	3	0
4	B	1	0	0	0	0
4	D	1	0	0	0	0
4	F	1	0	0	0	0
4	H	1	0	0	0	0
5	B	30	0	31	4	0
5	D	30	0	31	2	0
5	F	30	0	31	4	0
5	H	30	0	31	3	0
6	B	6	0	8	2	0
6	F	6	0	8	2	0
7	A	6	0	0	0	0
7	B	94	0	0	2	0
7	C	14	0	0	0	0
7	D	108	0	0	3	0
7	E	7	0	0	0	0
7	F	94	0	0	1	0
7	G	11	0	0	1	0
7	H	90	0	0	1	0
All	All	9557	0	8716	85	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 5.

All (85) 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)
2:B:525:SER:OG	2:B:525:SER:CB	1.64	1.43
2:F:363:HIS:NE2	5:F:1579:OG6:C3	1.86	1.38
2:F:525:SER:OG	2:F:525:SER:CB	1.70	1.36
2:H:363:HIS:NE2	5:H:1581:OG6:C3	1.98	1.25
2:B:363:HIS:NE2	5:B:1579:OG6:C3	2.00	1.25
2:B:487:ILE:HD11	2:B:531[A]:MET:CE	1.67	1.22
2:D:363:HIS:NE2	5:D:1581:OG6:C3	2.02	1.22
2:B:487:ILE:CD1	2:B:531[A]:MET:HE1	1.83	1.08
2:B:487:ILE:HD11	2:B:531[A]:MET:HE1	1.03	1.00
2:F:525:SER:CB	5:F:1579:OG6:C2	2.59	0.80
2:F:459:THR:HG22	2:F:482[B]:VAL:HG22	1.64	0.80
2:D:340[B]:ARG:NH1	2:D:345:GLU:OE1	2.15	0.79
2:B:529:PHE:HE1	2:B:531[A]:MET:HE3	1.48	0.78
2:B:345:GLU:OE1	7:B:2010:HOH:O	2.05	0.75
2:B:487:ILE:CD1	2:B:531[A]:MET:CE	2.55	0.74
1:G:310:ARG:NH1	7:G:2006:HOH:O	2.20	0.74
2:B:326:ASP:CG	2:B:479:VAL:HG21	2.13	0.74
2:B:525:SER:CB	5:B:1579:OG6:C2	2.66	0.71
2:F:363:HIS:CD2	5:F:1579:OG6:C3	2.73	0.71
2:D:414:GLU:OE2	7:D:2045:HOH:O	2.09	0.70
2:B:340[A]:ARG:NH2	7:B:2009:HOH:O	2.25	0.70
2:F:382:ARG:HH12	2:F:398:ILE:HD11	1.58	0.68
2:F:345:GLU:OE1	7:F:2017:HOH:O	2.12	0.67
1:A:316:TYR:OH	2:B:532:LYS:O	2.08	0.65
2:B:382:ARG:HH12	2:B:398:ILE:HD11	1.62	0.64
2:D:382:ARG:HH12	2:D:398:ILE:HD11	1.62	0.63
2:B:511:LYS:HD2	2:B:511:LYS:H	1.64	0.62
2:B:529:PHE:CE1	2:B:531[A]:MET:HE3	2.34	0.61
2:D:375:THR:OG1	2:D:376:GLU:OE1	2.17	0.61
2:B:371:ASP:O	2:D:340[B]:ARG:NH2	2.34	0.60
2:D:427:LYS:O	7:D:2034:HOH:O	2.16	0.60
2:B:363:HIS:CD2	5:B:1579:OG6:C3	2.84	0.59
2:H:363:HIS:CD2	5:H:1581:OG6:C3	2.82	0.59
2:B:525:SER:OG	2:B:525:SER:CA	2.50	0.56
2:H:388:ARG:NH1	2:H:476:GLN:OE1	2.37	0.56
1:G:314[A]:GLU:OE2	1:G:317:ILE:HD11	2.06	0.55
2:D:376:GLU:H	2:D:376:GLU:CD	2.15	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:488:VAL:O	6:F:1580:GOL:C3	2.56	0.54
2:H:568:LYS:HE3	3:S:276:PTR:CE1	2.37	0.53
2:H:380:LEU:HD12	2:H:380:LEU:C	2.34	0.53
2:H:443:ARG:NH1	3:S:276:PTR:O2P	2.42	0.52
2:D:386:HIS:HB3	2:D:392:GLU:OE2	2.11	0.51
2:B:388:ARG:HG3	2:B:461[B]:TRP:CZ3	2.46	0.51
2:B:332:SER:C	6:B:1580:GOL:H11	2.36	0.51
2:H:393:ARG:O	2:H:395:ILE:HD13	2.11	0.51
2:B:326:ASP:OD2	2:B:479:VAL:HG21	2.13	0.49
2:F:382:ARG:NH1	2:F:398:ILE:HD11	2.27	0.48
2:F:525:SER:OG	2:F:525:SER:CA	2.51	0.48
2:F:488:VAL:O	6:F:1580:GOL:H32	2.13	0.48
2:B:363:HIS:NE2	5:B:1579:OG6:C2	2.73	0.47
2:D:363:HIS:CD2	5:D:1581:OG6:C3	2.92	0.47
2:D:394:ASN:O	7:D:2031:HOH:O	2.20	0.47
2:H:357:TRP:CZ2	2:H:424:LYS:HD2	2.50	0.46
2:H:537:ASN:HB3	7:H:2079:HOH:O	2.15	0.46
2:F:363:HIS:NE2	5:F:1579:OG6:C2	2.75	0.46
2:H:471:ASN:ND2	2:H:474:LYS:O	2.49	0.45
3:R:276:PTR:O	3:R:277:ASP:C	2.57	0.45
2:D:375:THR:N	2:D:378:ASP:OD2	2.39	0.44
2:F:571:GLN:O	2:F:575:ASP:HB2	2.18	0.44
2:B:382:ARG:NH1	2:B:398:ILE:HD11	2.30	0.44
2:D:357:TRP:CZ2	2:D:424:LYS:HD2	2.53	0.44
2:B:370:TRP:HB3	2:D:370:TRP:HB3	2.00	0.44
2:B:394:ASN:C	2:B:395:ILE:HD13	2.42	0.43
1:C:314:GLU:O	1:C:317:ILE:HG13	2.17	0.43
2:F:380:LEU:C	2:F:380:LEU:HD12	2.43	0.43
2:D:543:GLY:HA2	2:D:561:THR:O	2.17	0.43
2:H:363:HIS:NE2	5:H:1581:OG6:C2	2.76	0.43
2:D:380:LEU:HD12	2:D:380:LEU:C	2.43	0.43
2:B:376:GLU:H	2:B:376:GLU:CD	2.27	0.43
2:F:468:TRP:HA	2:F:474:LYS:HB2	2.00	0.43
2:B:322:VAL:HG12	2:B:323:GLU:HG2	1.99	0.43
2:H:376:GLU:H	2:H:376:GLU:CD	2.27	0.43
2:B:543:GLY:HA2	2:B:561:THR:O	2.19	0.43
1:A:316:TYR:CE2	2:B:534:PRO:HD3	2.55	0.42
2:B:332:SER:H	6:B:1580:GOL:C1	2.33	0.42
2:D:322:VAL:HG12	2:D:323:GLU:HG2	2.02	0.41
2:D:382:ARG:NH1	2:D:398:ILE:HD11	2.31	0.41
2:B:380:LEU:C	2:B:380:LEU:HD12	2.45	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:S:275:LEU:HD12	3:S:275:LEU:HA	1.92	0.41
2:B:326:ASP:CG	2:B:479:VAL:CG2	2.91	0.41
2:B:568:LYS:HA	2:B:571:GLN:HE21	1.86	0.41
2:F:369:PRO:HD3	2:F:412:TRP:CE3	2.56	0.41
2:D:337:MET:SD	2:D:385:LYS:HD3	2.61	0.41
2:B:511:LYS:H	2:B:511:LYS:CD	2.34	0.41
2:F:322:VAL:HG12	2:F:323:GLU:HG2	2.02	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	24/36 (67%)	23 (96%)	1 (4%)	0	100	100
1	C	30/36 (83%)	29 (97%)	1 (3%)	0	100	100
1	E	24/36 (67%)	23 (96%)	1 (4%)	0	100	100
1	G	26/36 (72%)	25 (96%)	1 (4%)	0	100	100
2	B	249/259 (96%)	245 (98%)	4 (2%)	0	100	100
2	D	250/259 (96%)	245 (98%)	5 (2%)	0	100	100
2	F	251/259 (97%)	244 (97%)	6 (2%)	1 (0%)	30	15
2	H	257/259 (99%)	252 (98%)	5 (2%)	0	100	100
3	Q	1/14 (7%)	1 (100%)	0	0	100	100
All	All	1112/1194 (93%)	1087 (98%)	24 (2%)	1 (0%)	48	32

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	F	474	LYS

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	16/31 (52%)	15 (94%)	1 (6%)	16	3
1	C	25/31 (81%)	24 (96%)	1 (4%)	28	9
1	E	21/31 (68%)	21 (100%)	0	100	100
1	G	24/31 (77%)	23 (96%)	1 (4%)	26	8
2	B	207/225 (92%)	201 (97%)	6 (3%)	37	17
2	D	211/225 (94%)	208 (99%)	3 (1%)	59	44
2	F	205/225 (91%)	200 (98%)	5 (2%)	43	23
2	H	205/225 (91%)	199 (97%)	6 (3%)	37	17
3	P	2/10 (20%)	2 (100%)	0	100	100
3	Q	3/10 (30%)	3 (100%)	0	100	100
3	R	2/10 (20%)	1 (50%)	1 (50%)	0	0
3	S	2/10 (20%)	1 (50%)	1 (50%)	0	0
All	All	923/1064 (87%)	898 (97%)	25 (3%)	39	19

All (25) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	292	ASP
2	B	344	GLN
2	B	375	THR
2	B	395	ILE
2	B	507	CYS
2	B	511	LYS
2	B	517	ARG
1	C	302	LYS
2	D	375	THR
2	D	378	ASP
2	D	517	ARG
2	F	394	ASN
2	F	479	VAL
2	F	513	ASP

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Mol	Chain	Res	Type
2	F	517	ARG
2	F	575	ASP
1	G	310	ARG
2	H	395	ILE
2	H	398	ILE
2	H	467	THR
2	H	469	THR
2	H	517	ARG
2	H	568	LYS
3	R	275	LEU
3	S	275	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	537	ASN
2	B	571	GLN
2	D	571	GLN
2	F	394	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

4 non-standard protein/DNA/RNA residues 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$
3	PTR	Q	276	3	15,16,17	1.24	1 (6%)	17,22,24	1.43	3 (17%)
3	PTR	P	276	3	15,16,17	0.99	0	17,22,24	1.23	2 (11%)
3	PTR	R	276	3	15,16,17	0.92	0	17,22,24	1.16	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	PTR	S	276	3	15,16,17	1.18	1 (6%)	17,22,24	1.35	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
3	PTR	Q	276	3	-	0/10/11/13	0/1/1/1
3	PTR	P	276	3	-	1/10/11/13	0/1/1/1
3	PTR	R	276	3	-	2/10/11/13	0/1/1/1
3	PTR	S	276	3	-	0/10/11/13	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	S	276	PTR	CD2-CG	2.23	1.43	1.38
3	Q	276	PTR	P-OH	2.02	1.63	1.59

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	Q	276	PTR	O3P-P-O2P	3.41	120.59	107.80
3	R	276	PTR	O3P-P-O2P	2.98	118.98	107.80
3	S	276	PTR	O3P-P-OH	-2.72	97.28	105.32
3	S	276	PTR	O3P-P-O2P	2.63	117.66	107.80
3	P	276	PTR	O2P-P-OH	2.54	112.83	105.32
3	Q	276	PTR	OH-CZ-CE1	2.11	125.53	119.22
3	Q	276	PTR	OH-P-O1P	-2.10	102.47	109.48
3	P	276	PTR	OH-P-O1P	-2.02	102.75	109.48

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	P	276	PTR	O-C-CA-CB
3	R	276	PTR	N-CA-CB-CG
3	R	276	PTR	CZ-OH-P-O2P

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	R	276	PTR	1	0
3	S	276	PTR	2	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 10 ligands modelled in this entry, 4 are monoatomic - leaving 6 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	$\# Z > 2$
5	OG6	H	1581	2	30,31,32	2.94	2 (6%)	37,41,42	1.88	5 (13%)
6	GOL	B	1580	-	5,5,5	0.76	0	5,5,5	1.07	0
5	OG6	F	1579	2	30,31,32	1.47	3 (10%)	37,41,42	1.53	7 (18%)
5	OG6	B	1579	2	30,31,32	1.49	5 (16%)	37,41,42	2.14	12 (32%)
5	OG6	D	1581	2	30,31,32	1.99	2 (6%)	37,41,42	1.60	8 (21%)
6	GOL	F	1580	-	5,5,5	0.50	0	5,5,5	0.92	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
5	OG6	H	1581	2	-	2/31/41/43	0/2/2/2
6	GOL	B	1580	-	-	4/4/4/4	-
5	OG6	F	1579	2	-	1/31/41/43	0/2/2/2
5	OG6	B	1579	2	-	0/31/41/43	0/2/2/2
5	OG6	D	1581	2	-	0/31/41/43	0/2/2/2
6	GOL	F	1580	-	-	2/4/4/4	-

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	H	1581	0G6	C1-N2	15.13	1.66	1.34
5	D	1581	0G6	C1-N2	9.38	1.54	1.34
5	F	1579	0G6	C1-N2	6.00	1.46	1.34
5	B	1579	0G6	CD3-NE	4.73	1.56	1.46
5	D	1581	0G6	CA2-N2	3.74	1.52	1.46
5	H	1581	0G6	O-C	2.61	1.27	1.22
5	B	1579	0G6	CB2-CA2	-2.44	1.47	1.52
5	F	1579	0G6	CD2-CG	2.27	1.43	1.38
5	B	1579	0G6	CE2-CD2	2.19	1.42	1.38
5	F	1579	0G6	CE1-CD1	2.09	1.42	1.38
5	B	1579	0G6	CG1-CB1	-2.04	1.43	1.51
5	B	1579	0G6	CZ1-NH2	-2.01	1.25	1.32

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	H	1581	0G6	CA2-N2-C1	-6.91	111.23	123.25
5	B	1579	0G6	NE-CZ1-NH2	6.59	131.99	120.67
5	H	1581	0G6	CB2-CA2-N2	-5.44	103.25	110.30
5	B	1579	0G6	NH1-CZ1-NE	-4.85	108.24	119.27
5	B	1579	0G6	CB2-CA2-N2	-4.66	104.26	110.30
5	F	1579	0G6	CB2-CA2-N2	-4.16	104.91	110.30
5	F	1579	0G6	CG2-CB2-CA2	-3.97	106.38	113.94
5	D	1581	0G6	C2-CA2-N2	3.82	117.84	110.90
5	H	1581	0G6	O2-C2-C3	-3.61	98.88	109.68
5	D	1581	0G6	O2-C2-C3	-3.28	99.89	109.68
5	B	1579	0G6	CG2-CD3-NE	-3.27	103.03	112.20
5	B	1579	0G6	CB2-CG2-CD3	-3.17	102.94	112.07
5	D	1581	0G6	CA2-N2-C1	-2.87	118.26	123.25
5	B	1579	0G6	O2-C2-C3	-2.86	101.14	109.68
5	F	1579	0G6	CD2-CG-CD1	2.81	122.42	118.23
5	D	1581	0G6	O1-C1-N2	2.78	127.94	122.96
5	B	1579	0G6	C2-CA2-N2	2.77	115.94	110.90
5	B	1579	0G6	CA1-C1-N2	2.61	122.25	116.52
5	H	1581	0G6	CD2-CG-CD1	2.49	121.94	118.23
5	F	1579	0G6	CB2-CG2-CD3	-2.48	104.91	112.07
5	B	1579	0G6	O1-C1-N2	-2.46	118.56	122.96
5	F	1579	0G6	CE1-CD1-CG	-2.42	117.20	120.61
5	B	1579	0G6	CB1-CA1-C1	-2.40	106.11	111.21
5	F	1579	0G6	O2-C2-C3	-2.35	102.66	109.68
5	H	1581	0G6	CA1-C1-N2	-2.29	111.49	116.52
5	D	1581	0G6	CG2-CB2-CA2	-2.22	109.71	113.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	1579	0G6	CD-N1-C	2.20	133.65	125.85
5	D	1581	0G6	NE-CZ1-NH2	2.15	124.36	120.67
5	D	1581	0G6	NH1-CZ1-NE	-2.13	114.43	119.27
5	D	1581	0G6	CD-N1-C	2.12	133.37	125.85
5	B	1579	0G6	CA1-N1-C	-2.04	114.27	121.45
5	F	1579	0G6	CE2-CZ-CE1	2.02	122.63	119.87

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	F	1580	GOL	C1-C2-C3-O3
6	B	1580	GOL	O1-C1-C2-C3
6	B	1580	GOL	C1-C2-C3-O3
6	B	1580	GOL	O2-C2-C3-O3
6	F	1580	GOL	O2-C2-C3-O3
5	F	1579	0G6	O2-C2-CA2-CB2
5	H	1581	0G6	NH1-CZ1-NE-CD3
6	B	1580	GOL	O1-C1-C2-O2
5	H	1581	0G6	O2-C2-CA2-CB2

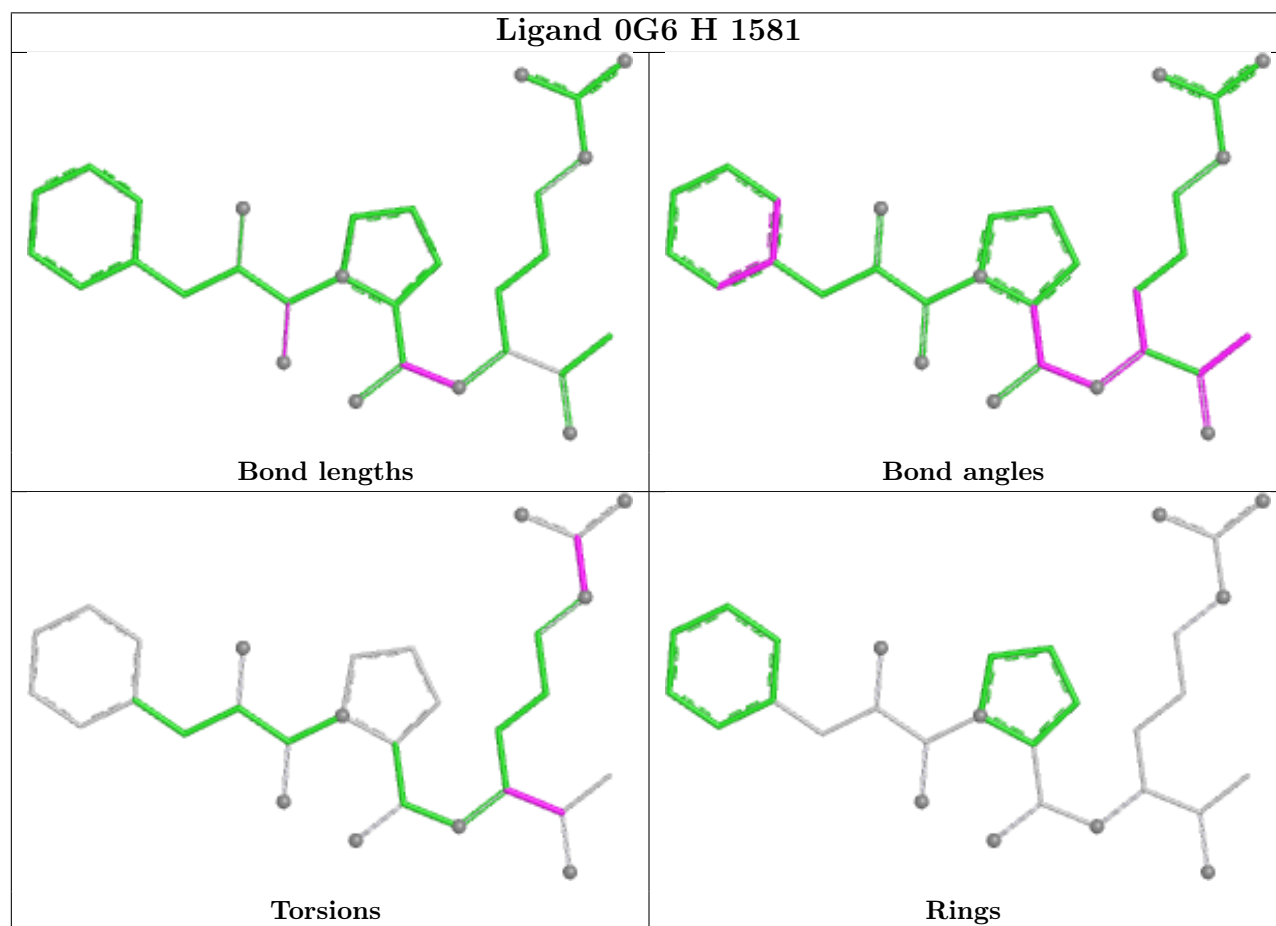
There are no ring outliers.

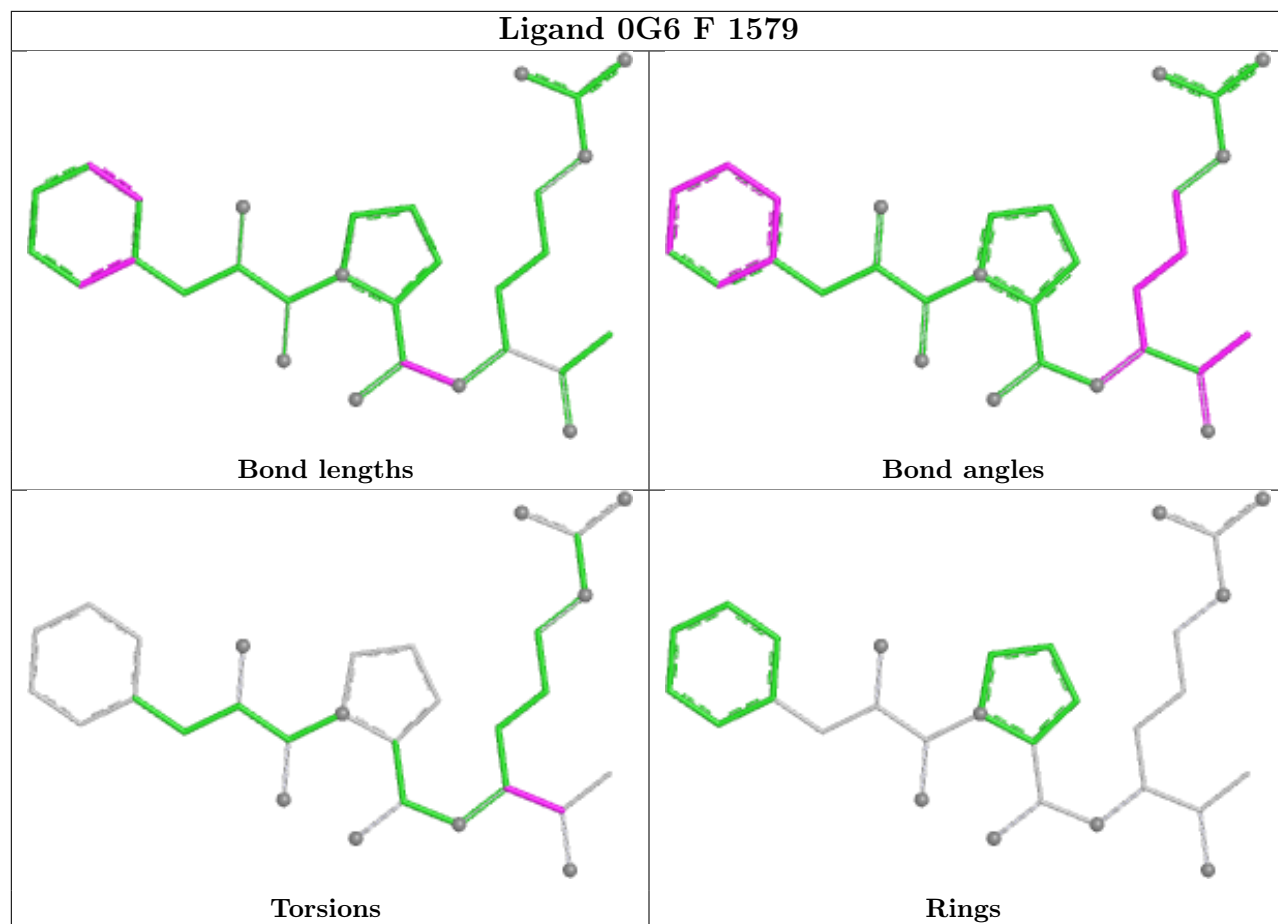
6 monomers are involved in 17 short contacts:

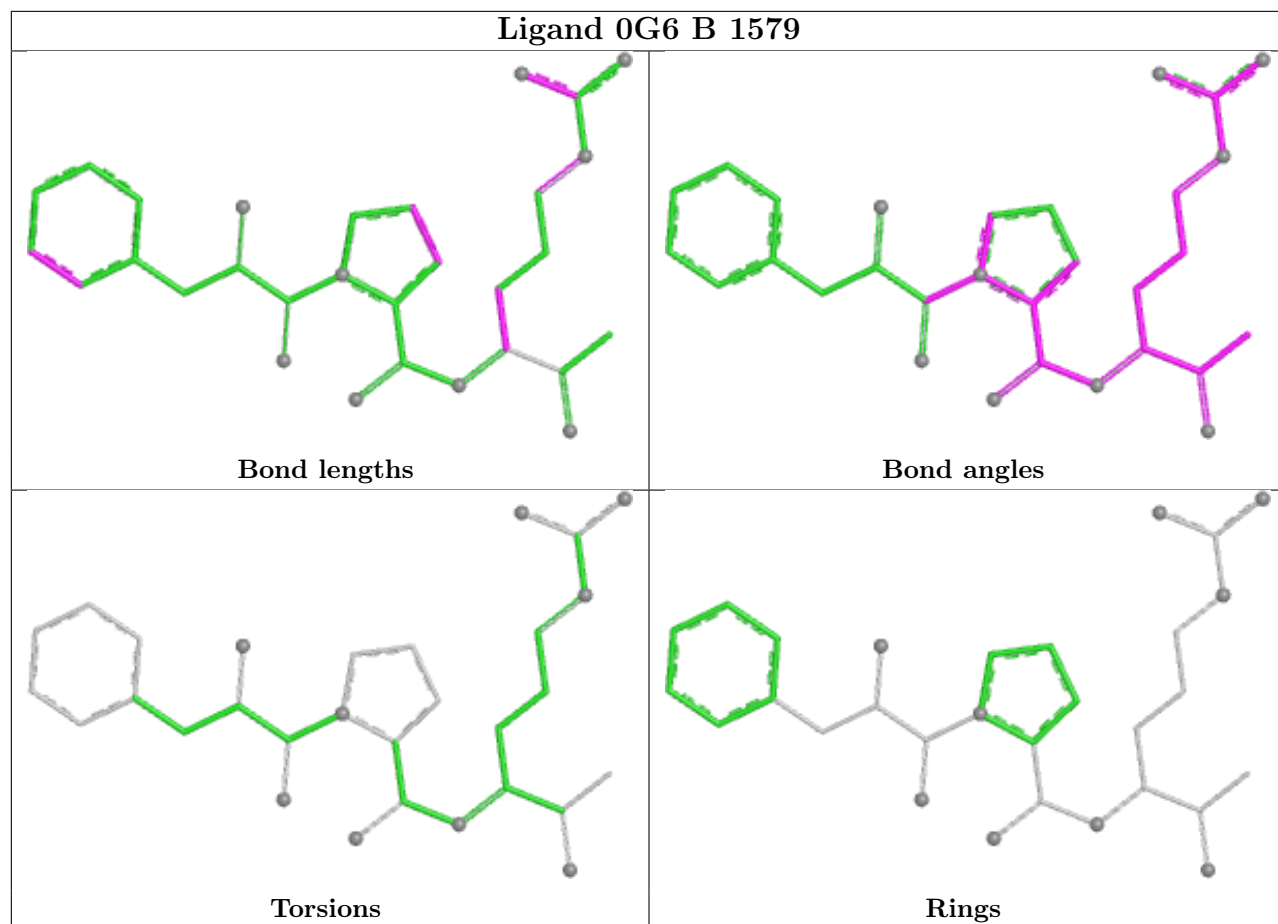
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	H	1581	0G6	3	0
6	B	1580	GOL	2	0
5	F	1579	0G6	4	0
5	B	1579	0G6	4	0
5	D	1581	0G6	2	0
6	F	1580	GOL	2	0

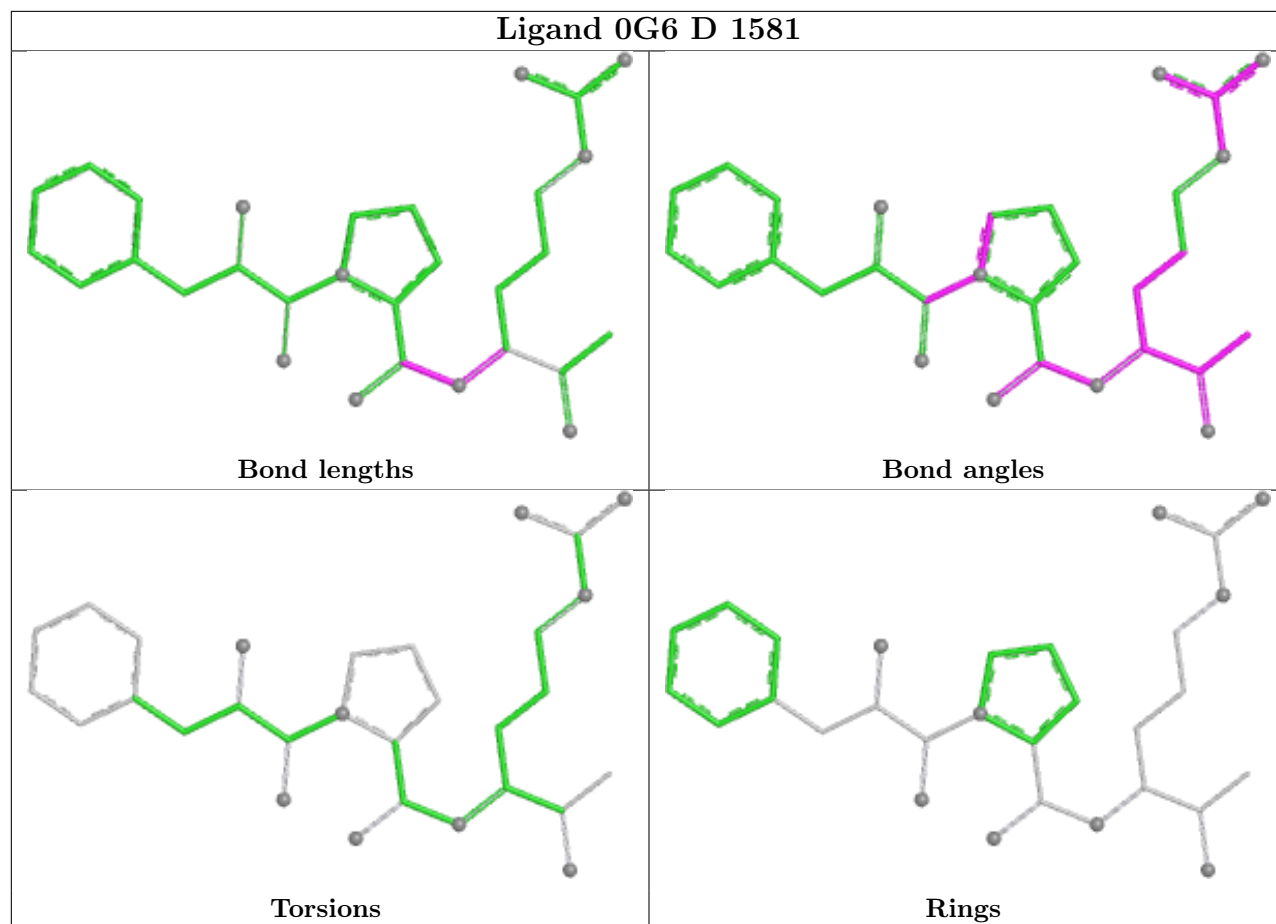
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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









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 ⓘ

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(Å ²)	Q<0.9
1	A	26/36 (72%)	2.44	17 (65%) 0 0	41, 60, 79, 102	0
1	C	32/36 (88%)	1.30	10 (31%) 1 1	23, 42, 71, 72	0
1	E	26/36 (72%)	1.21	3 (11%) 9 11	36, 46, 57, 66	0
1	G	27/36 (75%)	0.98	3 (11%) 10 11	22, 39, 54, 60	1 (3%)
2	B	249/259 (96%)	0.65	24 (9%) 13 16	11, 33, 54, 65	5 (2%)
2	D	252/259 (97%)	0.34	7 (2%) 55 61	14, 29, 51, 59	2 (0%)
2	F	253/259 (97%)	0.54	12 (4%) 36 42	14, 34, 53, 66	4 (1%)
2	H	259/259 (100%)	0.60	18 (6%) 23 26	17, 35, 63, 70	0
3	P	2/14 (14%)	1.95	1 (50%) 0 0	36, 36, 36, 54	0
3	Q	3/14 (21%)	0.53	0 100 100	32, 32, 39, 42	0
3	R	2/14 (14%)	2.65	1 (50%) 0 0	54, 54, 54, 68	0
3	S	2/14 (14%)	2.34	1 (50%) 0 0	35, 35, 35, 52	0
All	All	1133/1236 (91%)	0.63	97 (8%) 16 19	11, 34, 59, 102	12 (1%)

All (97) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	291	ALA	5.6
2	B	577	PHE	5.0
2	B	389	THR	4.9
1	A	313	LEU	4.9
1	A	317	ILE	4.9
1	A	304	LEU	4.6
3	S	275	LEU	4.4
2	H	472	VAL	4.2
3	R	275	LEU	4.2
2	F	535	PHE	4.0
1	C	294	GLY	4.0

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Mol	Chain	Res	Type	RSRZ
2	D	467	THR	3.8
2	H	389	THR	3.7
2	B	534	PRO	3.6
2	B	535	PHE	3.6
1	A	312	LEU	3.4
2	H	468	TRP	3.4
1	A	310	ARG	3.4
1	A	299	PHE	3.4
2	H	395	ILE	3.4
2	B	515	GLY	3.3
1	E	316	TYR	3.2
1	C	290	GLU	3.2
1	A	315	SER	3.1
2	F	576	GLN	3.1
1	A	294	GLY	3.1
2	D	342	SER	3.1
2	B	395	ILE	3.0
2	D	343	PRO	3.0
1	C	304	LEU	3.0
1	G	304	LEU	3.0
1	C	289	GLY	3.0
1	C	291	ALA	3.0
2	F	450	LEU	3.0
3	P	275	LEU	3.0
1	C	287	GLY	3.0
1	C	293	CYS	2.9
1	E	313	LEU	2.9
2	B	447	ALA	2.9
2	H	475	GLY	2.9
1	A	293	CYS	2.9
2	H	478	SER	2.9
1	A	316	TYR	2.8
2	H	579	GLU	2.8
2	F	573	VAL	2.8
2	H	391	TYR	2.8
1	G	292	ASP	2.8
2	H	554	ASP	2.8
2	F	394	ASN	2.7
1	C	318	ASP	2.7
1	A	297	PRO	2.7
1	C	317	ILE	2.7
2	H	512	PRO	2.6

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Mol	Chain	Res	Type	RSRZ
2	D	579	GLU	2.6
2	F	342	SER	2.6
2	H	471	ASN	2.6
2	B	454	TYR	2.6
2	H	322	VAL	2.6
2	H	375	THR	2.5
2	B	492	VAL	2.5
2	H	495	ASP	2.5
1	A	308	THR	2.5
1	A	298	LEU	2.5
2	B	425	LEU	2.4
2	F	443	ARG	2.4
2	B	452	ALA	2.4
2	D	375	THR	2.4
2	B	391	TYR	2.4
1	A	292	ASP	2.4
1	A	311	GLU	2.4
2	B	533	SER	2.4
2	B	513	ASP	2.3
2	B	576	GLN	2.3
2	D	475	GLY	2.3
2	B	394	ASN	2.3
1	C	288	SER	2.3
2	F	577	PHE	2.2
2	F	513	ASP	2.2
1	A	305	GLU	2.2
2	B	386	HIS	2.2
2	B	557	TYR	2.2
2	H	477	PRO	2.2
2	H	387	SER	2.2
2	F	538	ARG	2.2
2	B	537	ASN	2.2
1	G	317	ILE	2.2
2	B	574	ILE	2.2
2	B	390	ARG	2.1
2	B	511	LYS	2.1
1	A	314	GLU	2.1
2	H	394	ASN	2.1
2	H	467	THR	2.1
2	D	515	GLY	2.1
2	B	428	PRO	2.1
2	B	449	LEU	2.0

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Mol	Chain	Res	Type	RSRZ
2	F	440	LEU	2.0
2	F	536	ASN	2.0

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	PTR	R	276	16/17	0.89	0.14	45,66,73,76	0
3	PTR	S	276	16/17	0.90	0.11	33,40,48,56	0
3	PTR	P	276	16/17	0.92	0.10	35,40,50,52	0
3	PTR	Q	276	16/17	0.94	0.07	26,30,41,47	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

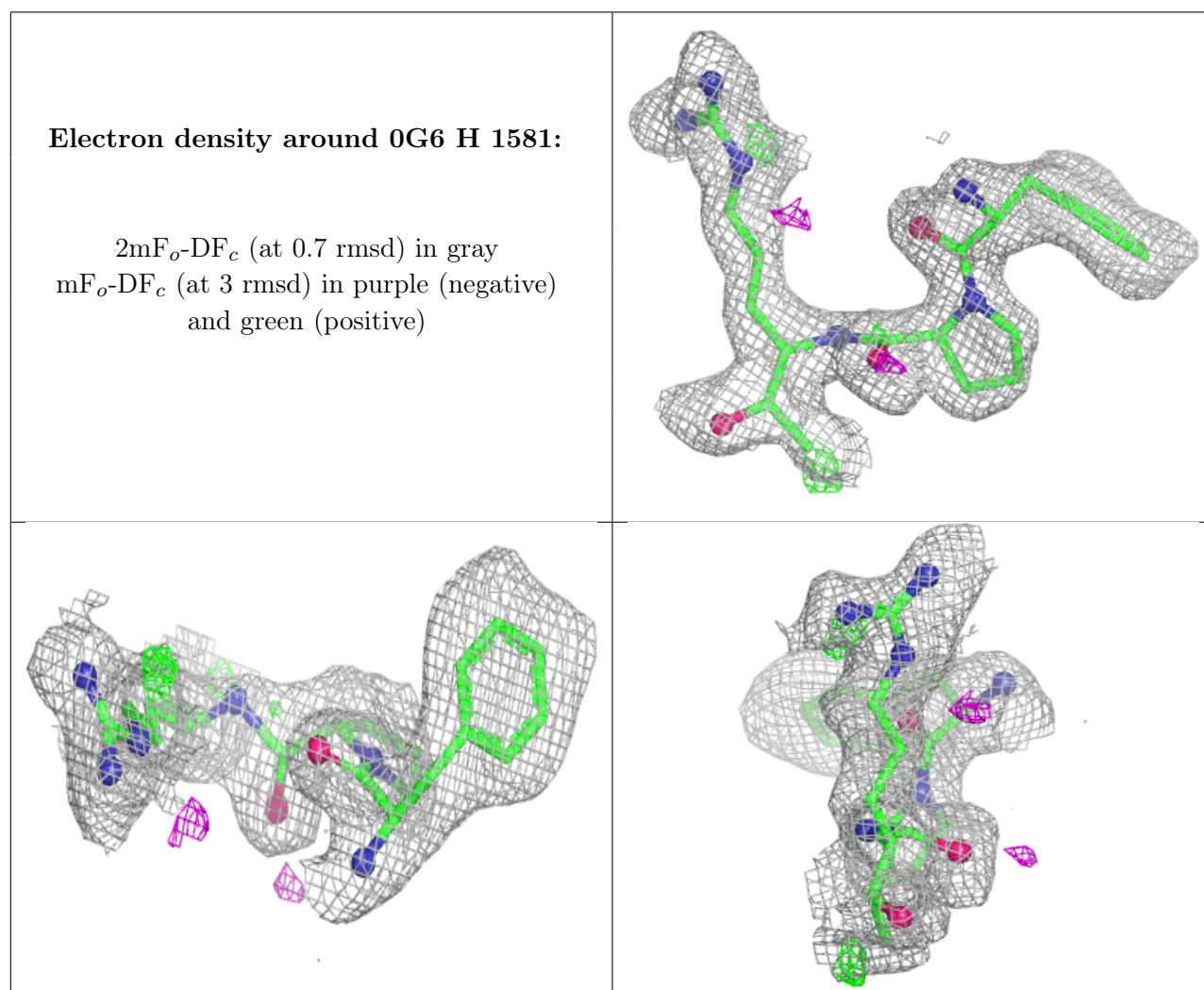
6.4 Ligands [i](#)

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(Å ²)	Q<0.9
4	NA	F	1578	1/1	0.85	0.21	38,38,38,38	0
6	GOL	F	1580	6/6	0.88	0.13	33,46,51,56	0
4	NA	B	1578	1/1	0.90	0.16	35,35,35,35	0
6	GOL	B	1580	6/6	0.91	0.10	33,40,44,47	0
4	NA	D	1580	1/1	0.92	0.09	45,45,45,45	0
4	NA	H	1580	1/1	0.93	0.08	45,45,45,45	0
5	0G6	H	1581	30/31	0.93	0.08	24,29,33,34	0
5	0G6	F	1579	30/31	0.94	0.07	20,23,26,26	0
5	0G6	B	1579	30/31	0.94	0.08	16,21,28,28	0
5	0G6	D	1581	30/31	0.95	0.07	18,22,25,29	0

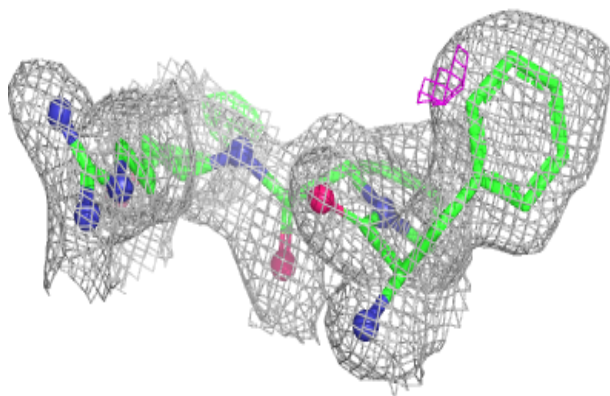
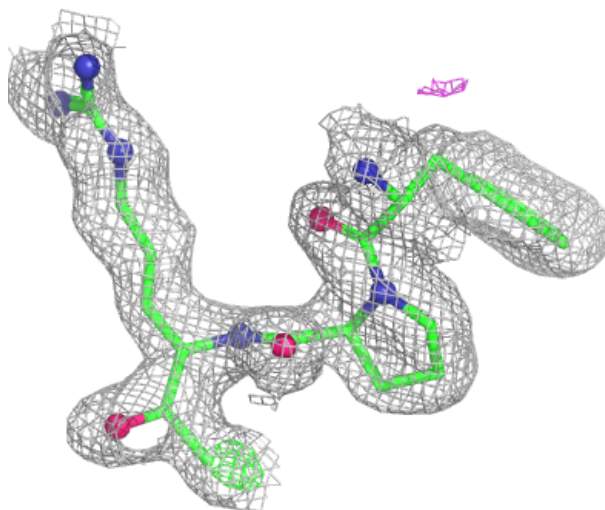
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers

as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.



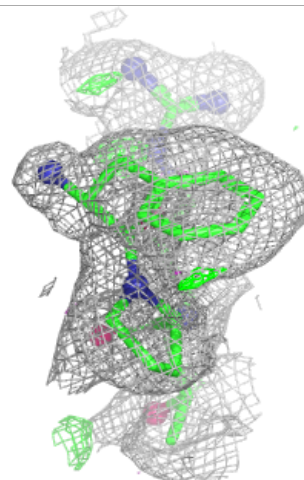
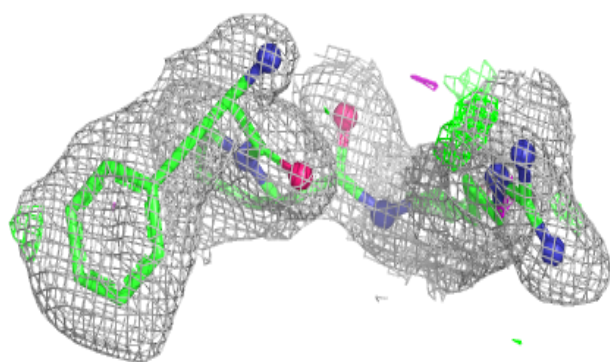
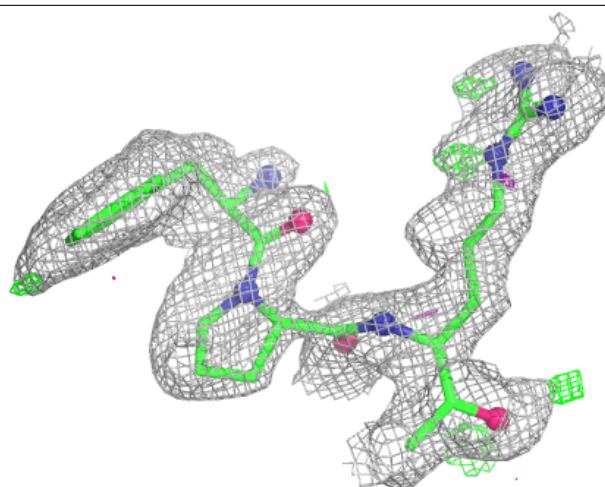
Electron density around 0G6 F 1579:

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



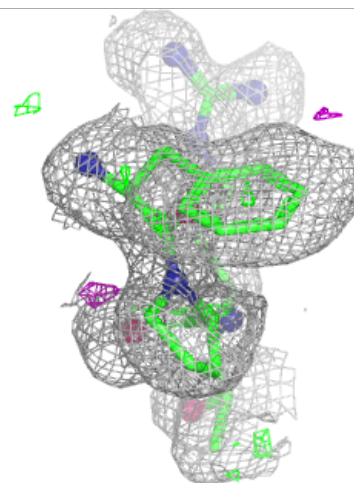
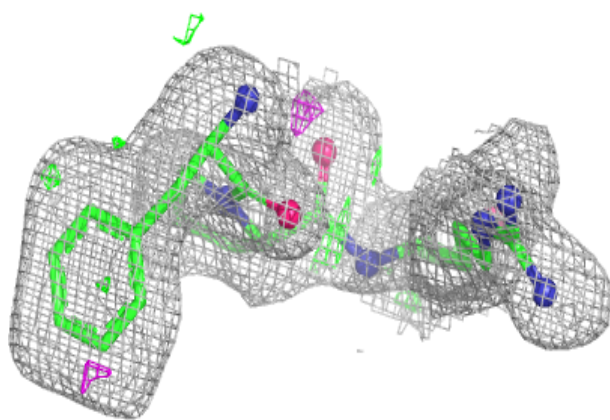
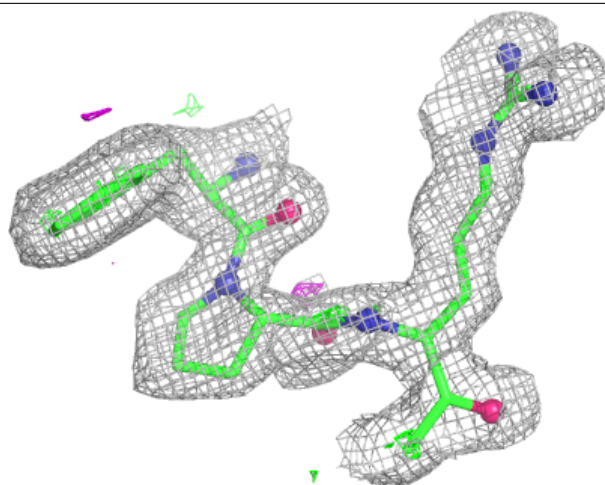
Electron density around 0G6 B 1579:

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



Electron density around 0G6 D 1581:

$2mF_o-DF_c$ (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.