



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 06:20 PM UTC

PDB ID : 6TBK / pdb_00006tbk
Title : Structure of a beta galactosidase with inhibitor
Authors : Offen, W.; Davies, G.
Deposited on : 2019-11-01
Resolution : 1.60 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

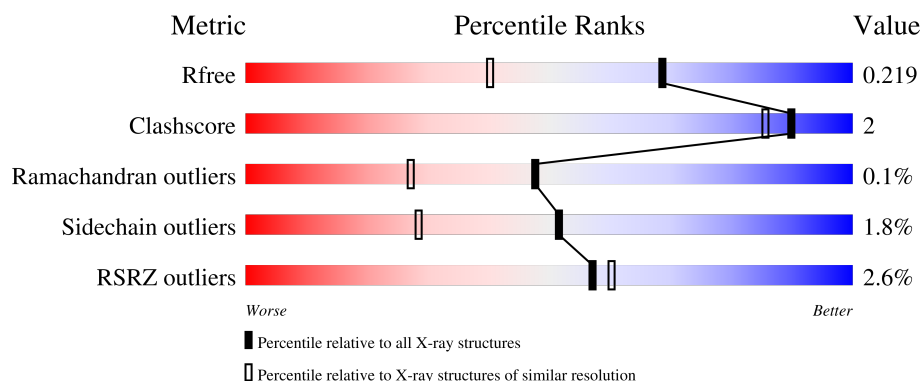
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

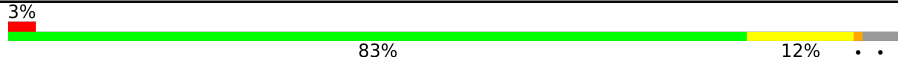
The reported resolution of this entry is 1.60 Å.

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	4673 (1.60-1.60)
Clashscore	190562	4931 (1.60-1.60)
Ramachandran outliers	187476	4831 (1.60-1.60)
Sidechain outliers	187428	4830 (1.60-1.60)
RSRZ outliers	180081	4672 (1.60-1.60)

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	550	
1	B	550	
1	C	550	
1	D	550	
1	E	550	

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Mol	Chain	Length	Quality of chain
1	F	550	3% 84% 12%
1	G	550	% 87% 9%
1	H	550	3% 83% 13%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 36143 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 Beta-galactosidase, putative, bgl35A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	527	Total	C	N	O	S	0	0	0
			4138	2655	699	769	15			
1	B	533	Total	C	N	O	S	0	1	0
			4182	2683	708	776	15			
1	C	533	Total	C	N	O	S	0	0	0
			4153	2664	702	772	15			
1	D	537	Total	C	N	O	S	0	3	0
			4227	2708	718	785	16			
1	E	537	Total	C	N	O	S	0	2	0
			4207	2698	710	784	15			
1	F	535	Total	C	N	O	S	0	5	0
			4245	2718	721	791	15			
1	G	526	Total	C	N	O	S	0	4	0
			4162	2673	706	767	16			
1	H	532	Total	C	N	O	S	0	2	0
			4170	2673	708	774	15			

There are 80 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	26	MET	-	initiating methionine	UNP B3PBE0
A	27	GLY	-	expression tag	UNP B3PBE0
A	28	SER	-	expression tag	UNP B3PBE0
A	29	SER	-	expression tag	UNP B3PBE0
A	30	HIS	-	expression tag	UNP B3PBE0
A	31	HIS	-	expression tag	UNP B3PBE0
A	32	HIS	-	expression tag	UNP B3PBE0
A	33	HIS	-	expression tag	UNP B3PBE0
A	34	HIS	-	expression tag	UNP B3PBE0
A	35	HIS	-	expression tag	UNP B3PBE0
B	26	MET	-	initiating methionine	UNP B3PBE0
B	27	GLY	-	expression tag	UNP B3PBE0
B	28	SER	-	expression tag	UNP B3PBE0

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Chain	Residue	Modelled	Actual	Comment	Reference
B	29	SER	-	expression tag	UNP B3PBE0
B	30	HIS	-	expression tag	UNP B3PBE0
B	31	HIS	-	expression tag	UNP B3PBE0
B	32	HIS	-	expression tag	UNP B3PBE0
B	33	HIS	-	expression tag	UNP B3PBE0
B	34	HIS	-	expression tag	UNP B3PBE0
B	35	HIS	-	expression tag	UNP B3PBE0
C	26	MET	-	initiating methionine	UNP B3PBE0
C	27	GLY	-	expression tag	UNP B3PBE0
C	28	SER	-	expression tag	UNP B3PBE0
C	29	SER	-	expression tag	UNP B3PBE0
C	30	HIS	-	expression tag	UNP B3PBE0
C	31	HIS	-	expression tag	UNP B3PBE0
C	32	HIS	-	expression tag	UNP B3PBE0
C	33	HIS	-	expression tag	UNP B3PBE0
C	34	HIS	-	expression tag	UNP B3PBE0
C	35	HIS	-	expression tag	UNP B3PBE0
D	26	MET	-	initiating methionine	UNP B3PBE0
D	27	GLY	-	expression tag	UNP B3PBE0
D	28	SER	-	expression tag	UNP B3PBE0
D	29	SER	-	expression tag	UNP B3PBE0
D	30	HIS	-	expression tag	UNP B3PBE0
D	31	HIS	-	expression tag	UNP B3PBE0
D	32	HIS	-	expression tag	UNP B3PBE0
D	33	HIS	-	expression tag	UNP B3PBE0
D	34	HIS	-	expression tag	UNP B3PBE0
D	35	HIS	-	expression tag	UNP B3PBE0
E	26	MET	-	initiating methionine	UNP B3PBE0
E	27	GLY	-	expression tag	UNP B3PBE0
E	28	SER	-	expression tag	UNP B3PBE0
E	29	SER	-	expression tag	UNP B3PBE0
E	30	HIS	-	expression tag	UNP B3PBE0
E	31	HIS	-	expression tag	UNP B3PBE0
E	32	HIS	-	expression tag	UNP B3PBE0
E	33	HIS	-	expression tag	UNP B3PBE0
E	34	HIS	-	expression tag	UNP B3PBE0
E	35	HIS	-	expression tag	UNP B3PBE0
F	26	MET	-	initiating methionine	UNP B3PBE0
F	27	GLY	-	expression tag	UNP B3PBE0
F	28	SER	-	expression tag	UNP B3PBE0
F	29	SER	-	expression tag	UNP B3PBE0
F	30	HIS	-	expression tag	UNP B3PBE0

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Chain	Residue	Modelled	Actual	Comment	Reference
F	31	HIS	-	expression tag	UNP B3PBE0
F	32	HIS	-	expression tag	UNP B3PBE0
F	33	HIS	-	expression tag	UNP B3PBE0
F	34	HIS	-	expression tag	UNP B3PBE0
F	35	HIS	-	expression tag	UNP B3PBE0
G	26	MET	-	initiating methionine	UNP B3PBE0
G	27	GLY	-	expression tag	UNP B3PBE0
G	28	SER	-	expression tag	UNP B3PBE0
G	29	SER	-	expression tag	UNP B3PBE0
G	30	HIS	-	expression tag	UNP B3PBE0
G	31	HIS	-	expression tag	UNP B3PBE0
G	32	HIS	-	expression tag	UNP B3PBE0
G	33	HIS	-	expression tag	UNP B3PBE0
G	34	HIS	-	expression tag	UNP B3PBE0
G	35	HIS	-	expression tag	UNP B3PBE0
H	26	MET	-	initiating methionine	UNP B3PBE0
H	27	GLY	-	expression tag	UNP B3PBE0
H	28	SER	-	expression tag	UNP B3PBE0
H	29	SER	-	expression tag	UNP B3PBE0
H	30	HIS	-	expression tag	UNP B3PBE0
H	31	HIS	-	expression tag	UNP B3PBE0
H	32	HIS	-	expression tag	UNP B3PBE0
H	33	HIS	-	expression tag	UNP B3PBE0
H	34	HIS	-	expression tag	UNP B3PBE0
H	35	HIS	-	expression tag	UNP B3PBE0

- Molecule 2 is SODIUM ION (CCD ID: NA) (formula: Na).

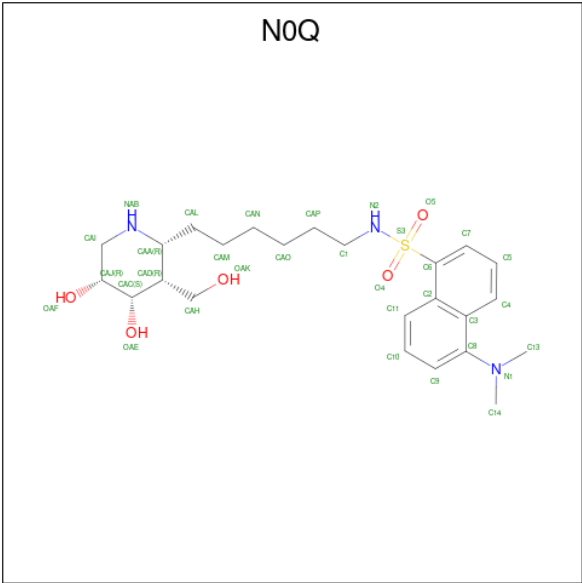
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	4	Total Na 4 4	0	0
2	B	3	Total Na 3 3	0	0
2	C	4	Total Na 4 4	0	0
2	D	5	Total Na 5 5	0	0
2	E	5	Total Na 5 5	0	0
2	F	4	Total Na 4 4	0	0
2	G	5	Total Na 5 5	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	H	2	Total	Na	0	0
			2	2		

- Molecule 3 is 5-(dimethylamino)- {N}-[6-[(2 {R},3 {R},4 {S},5 {R})-3-(hydroxymethyl)-4,5-bis(oxidanyl)piperidin-2-yl]hexyl]naphthalene-1-sulfonamide (CCD ID: N0Q) (formula: C₂₄H₃₇N₃O₅S) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	S	0	0
			21	13	2	5	1		
3	B	1	Total	C	N	O		0	0
			14	10	1	3			
3	C	1	Total	C	N	O		0	0
			13	9	1	3			
3	D	1	Total	C	N	O	S	0	0
			21	13	2	5	1		
3	E	1	Total	C	N	O		0	0
			13	9	1	3			
3	F	1	Total	C	N	O		0	0
			15	11	1	3			
3	G	1	Total	C	N	O		0	0
			15	11	1	3			
3	H	1	Total	C	N	O		0	0
			13	9	1	3			

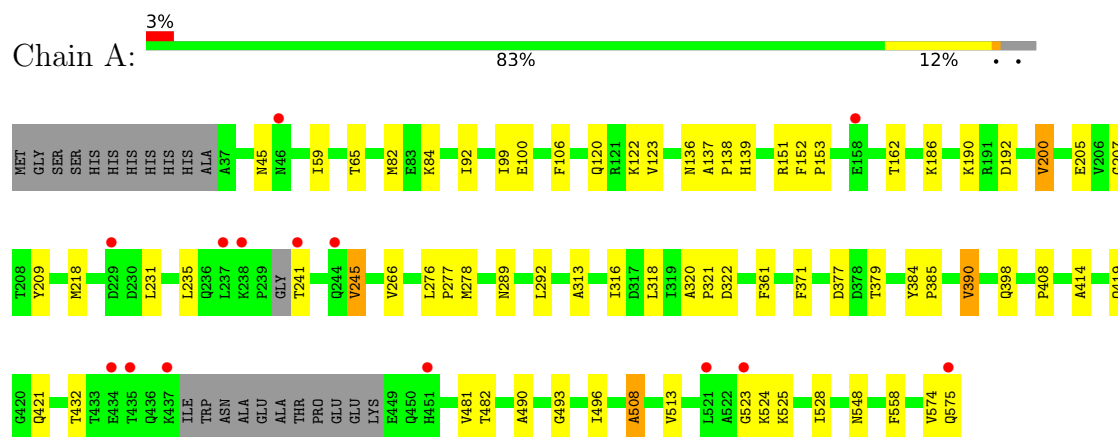
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	238	Total 238	O 238	0	0
4	B	300	Total 300	O 300	0	0
4	C	286	Total 286	O 286	0	0
4	D	344	Total 344	O 344	0	0
4	E	359	Total 359	O 359	0	0
4	F	308	Total 308	O 308	0	0
4	G	390	Total 390	O 390	0	0
4	H	277	Total 277	O 277	0	0

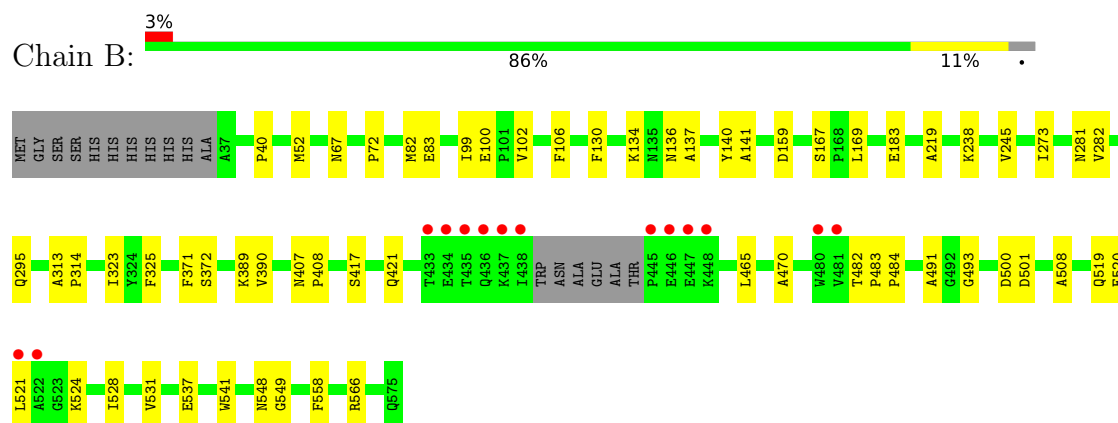
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

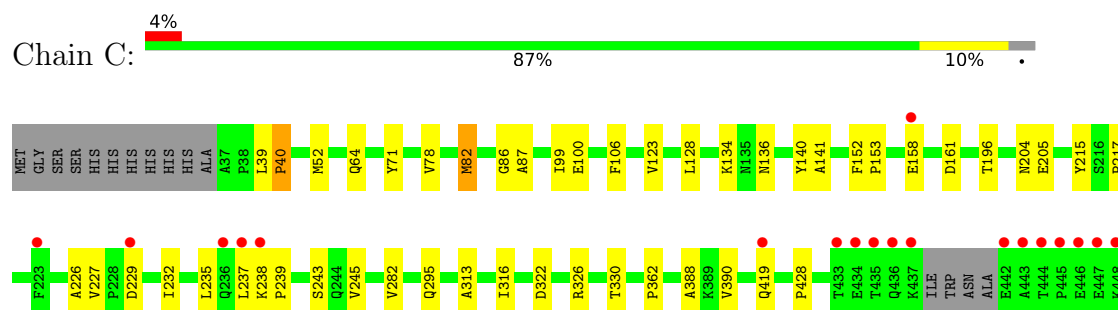
- Molecule 1: Beta-galactosidase, putative, bgl35A

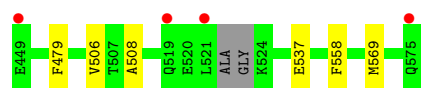


- Molecule 1: Beta-galactosidase, putative, bgl35A

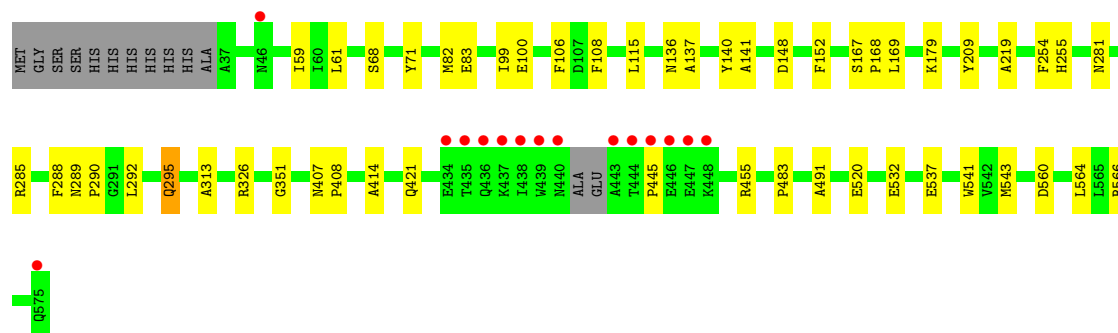
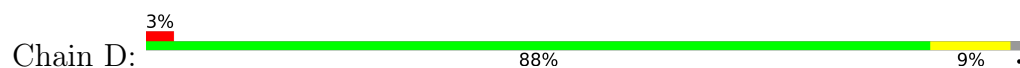


- Molecule 1: Beta-galactosidase, putative, bgl35A

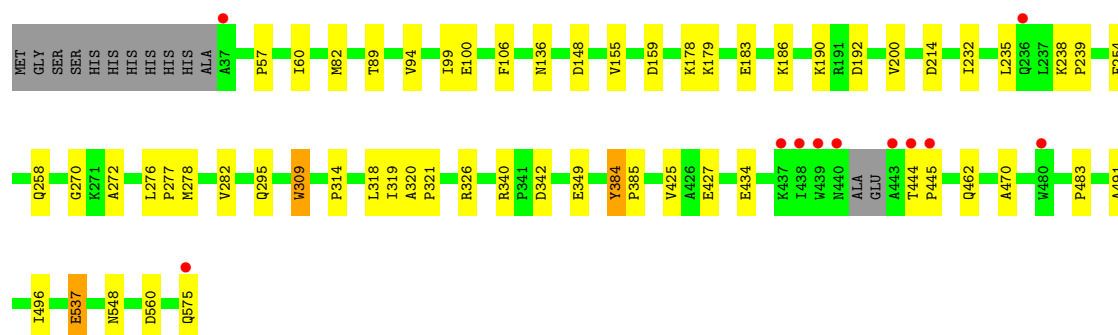
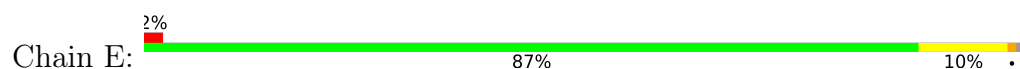




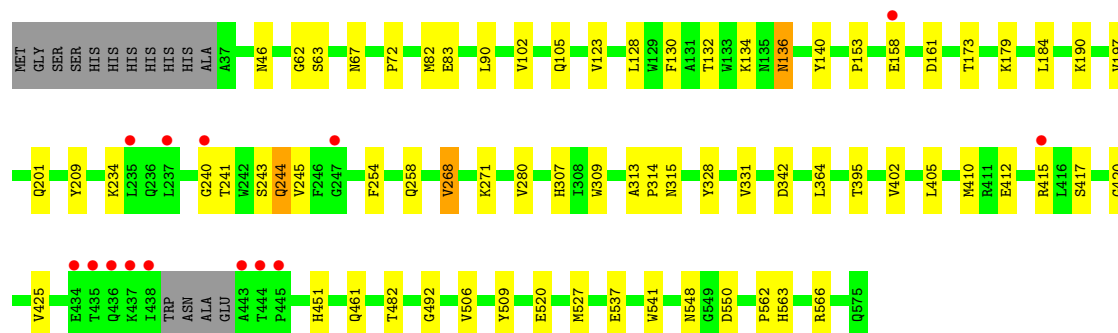
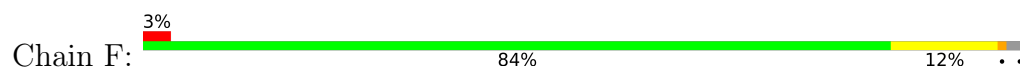
- Molecule 1: Beta-galactosidase, putative, bgl35A



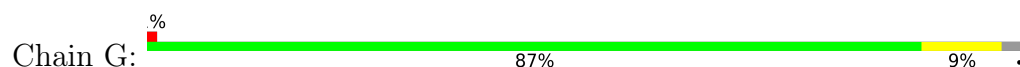
- Molecule 1: Beta-galactosidase, putative, bgl35A

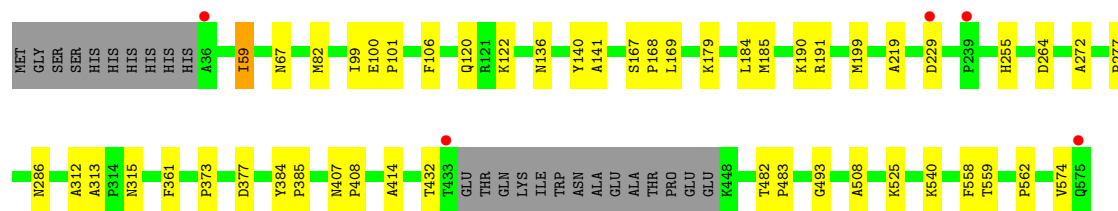


- Molecule 1: Beta-galactosidase, putative, bgl35A

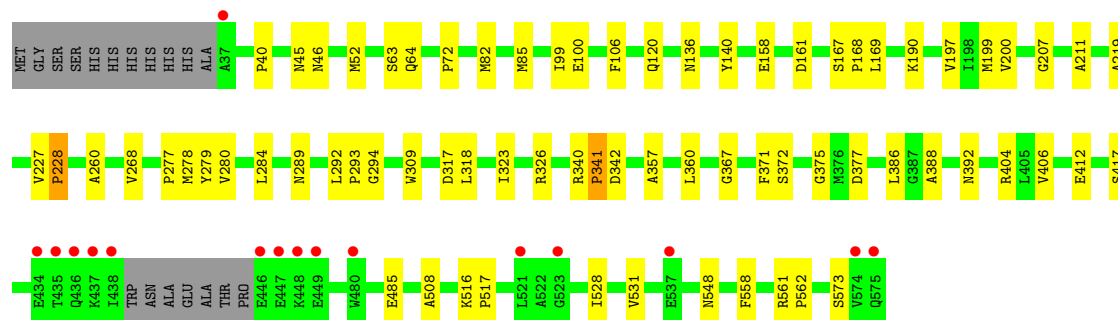
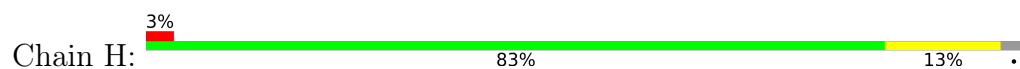


- Molecule 1: Beta-galactosidase, putative, bgl35A





● Molecule 1: Beta-galactosidase, putative, bgl35A



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	98.95Å 116.05Å 115.58Å 89.84° 90.07° 89.98°	Depositor
Resolution (Å)	63.20 – 1.60 63.20 – 1.60	Depositor EDS
% Data completeness (in resolution range)	95.8 (63.20-1.60) 95.8 (63.20-1.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.48 (at 1.60Å)	Xtriage
Refinement program	REFMAC 5.8.0253	Depositor
R, R_{free}	0.152 , 0.212 0.163 , 0.219	Depositor DCC
R_{free} test set	32511 reflections (4.57%)	wwPDB-VP
Wilson B-factor (Å ²)	23.6	Xtriage
Anisotropy	0.249	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 48.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	0.076 for h,l,-k 0.076 for h,-l,k 0.048 for h,-k,-l 0.032 for -h,-k,l 0.034 for -h,k,-l 0.036 for -h,-l,-k 0.033 for -h,l,k	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	36143	wwPDB-VP
Average B, all atoms (Å ²)	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.05% 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 ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: NA, N0Q

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	1.34	21/4249 (0.5%)	1.42	25/5792 (0.4%)
1	B	1.31	11/4297 (0.3%)	1.44	31/5857 (0.5%)
1	C	1.33	20/4264 (0.5%)	1.43	18/5816 (0.3%)
1	D	1.30	12/4339 (0.3%)	1.42	25/5914 (0.4%)
1	E	1.32	18/4322 (0.4%)	1.47	30/5893 (0.5%)
1	F	1.37	23/4360 (0.5%)	1.41	19/5940 (0.3%)
1	G	1.31	11/4280 (0.3%)	1.41	21/5832 (0.4%)
1	H	1.36	25/4285 (0.6%)	1.46	31/5843 (0.5%)
All	All	1.33	141/34396 (0.4%)	1.43	200/46887 (0.4%)

All (141) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	482	THR	C-N	8.15	1.40	1.33
1	C	390	VAL	C-O	7.90	1.31	1.24
1	H	72	PRO	C-O	-7.63	1.14	1.24
1	C	569	MET	C-O	7.33	1.32	1.23
1	A	390	VAL	C-O	7.21	1.31	1.24
1	D	520	GLU	C-O	7.10	1.32	1.23
1	H	268	VAL	C-O	7.10	1.32	1.24
1	A	508	ALA	C-O	7.08	1.32	1.23
1	B	323	ILE	C-O	7.05	1.31	1.24
1	H	161	ASP	C-O	7.03	1.32	1.23
1	A	523	GLY	C-O	7.00	1.33	1.24
1	D	254	PHE	C-O	6.84	1.31	1.24
1	C	64	GLN	C-O	6.78	1.32	1.24
1	C	326	ARG	C-O	6.78	1.32	1.24
1	F	364	LEU	C-O	6.78	1.32	1.24
1	B	273	ILE	C-O	-6.74	1.17	1.24
1	D	285	ARG	C-O	6.68	1.32	1.23
1	B	484	PRO	N-CA	6.66	1.55	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	362	PRO	C-O	-6.65	1.16	1.24
1	C	153	PRO	N-CA	6.64	1.55	1.47
1	D	564	LEU	C-O	6.59	1.31	1.24
1	C	123	VAL	C-O	6.57	1.31	1.23
1	C	388	ALA	C-O	6.56	1.31	1.23
1	C	239	PRO	C-O	-6.55	1.15	1.23
1	E	94	VAL	C-O	6.50	1.31	1.24
1	A	575	GLN	C-O	6.46	1.36	1.23
1	H	392	ASN	C-O	6.46	1.31	1.23
1	D	255	HIS	CE1-NE2	6.44	1.39	1.32
1	A	277	PRO	N-CA	6.41	1.54	1.47
1	D	281	ASN	C-O	6.37	1.31	1.24
1	F	102	VAL	C-O	6.36	1.30	1.24
1	G	255	HIS	CE1-NE2	6.35	1.38	1.32
1	C	78	VAL	C-O	6.35	1.30	1.23
1	H	561	ARG	C-N	6.35	1.40	1.33
1	H	372	SER	CA-CB	-6.25	1.45	1.53
1	A	200	VAL	C-O	-6.23	1.17	1.24
1	F	563	HIS	CE1-NE2	6.23	1.38	1.32
1	H	260	ALA	C-O	6.22	1.31	1.24
1	F	197	VAL	C-O	6.20	1.30	1.24
1	A	123	VAL	C-O	6.17	1.31	1.23
1	C	128	LEU	C-O	-6.15	1.16	1.24
1	A	398	GLN	N-CA	6.11	1.53	1.46
1	F	417	SER	C-O	6.01	1.31	1.24
1	H	517	PRO	N-CA	5.98	1.54	1.47
1	A	218	MET	C-O	5.98	1.30	1.24
1	D	560	ASP	CG-OD2	-5.96	1.14	1.25
1	B	417	SER	C-O	5.95	1.31	1.24
1	B	281	ASN	C-O	5.90	1.31	1.24
1	A	84	LYS	C-O	-5.89	1.16	1.24
1	F	240	GLY	C-O	5.88	1.31	1.23
1	F	425	VAL	N-CA	5.84	1.52	1.46
1	C	428	PRO	C-O	-5.83	1.17	1.24
1	E	57	PRO	C-O	-5.83	1.16	1.23
1	E	282	VAL	C-O	-5.82	1.17	1.24
1	C	238	LYS	C-N	5.82	1.41	1.33
1	G	286	ASN	C-N	5.82	1.40	1.33
1	F	105	GLN	C-O	5.81	1.30	1.23
1	G	373	PRO	C-O	-5.81	1.17	1.23
1	A	513	VAL	C-O	-5.80	1.17	1.24
1	H	168	PRO	N-CA	5.77	1.55	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	408	PRO	C-O	-5.76	1.16	1.24
1	G	141	ALA	C-N	5.75	1.40	1.33
1	C	86	GLY	C-O	-5.75	1.16	1.23
1	H	284	LEU	C-O	5.75	1.30	1.23
1	H	293	PRO	N-CA	5.74	1.53	1.47
1	H	190	LYS	C-O	-5.73	1.16	1.24
1	F	123	VAL	C-O	5.73	1.30	1.23
1	E	321	PRO	N-CA	5.72	1.54	1.47
1	F	309	TRP	C-O	5.72	1.30	1.24
1	C	40	PRO	N-CA	5.70	1.53	1.47
1	H	485	GLU	C-O	5.68	1.31	1.24
1	F	527	MET	C-O	5.68	1.30	1.23
1	D	148	ASP	C-O	5.66	1.31	1.23
1	H	326	ARG	C-O	5.66	1.31	1.24
1	F	509	TYR	C-O	-5.65	1.17	1.23
1	G	101	PRO	C-O	-5.65	1.17	1.24
1	F	72	PRO	C-O	-5.61	1.16	1.24
1	A	379	THR	C-O	5.60	1.31	1.24
1	H	323	ILE	C-O	-5.59	1.18	1.24
1	A	321	PRO	N-CA	5.58	1.54	1.47
1	F	506	VAL	C-O	5.56	1.29	1.24
1	F	328	TYR	C-O	-5.56	1.17	1.24
1	H	562	PRO	N-CA	5.56	1.54	1.47
1	H	228	PRO	N-CA	5.54	1.54	1.47
1	E	277	PRO	N-CA	5.54	1.53	1.47
1	F	62	GLY	C-O	-5.53	1.16	1.23
1	H	360	LEU	C-O	5.52	1.30	1.24
1	F	90	LEU	N-CA	5.50	1.52	1.46
1	F	280	VAL	C-O	5.50	1.29	1.24
1	A	138	PRO	C-O	-5.50	1.16	1.24
1	B	314	PRO	N-CA	5.50	1.54	1.47
1	H	377	ASP	C-O	5.49	1.30	1.23
1	E	560	ASP	CG-OD1	-5.49	1.15	1.25
1	C	282	VAL	C-O	5.46	1.30	1.24
1	H	292	LEU	C-N	5.45	1.40	1.33
1	B	183	GLU	C-O	-5.44	1.17	1.24
1	H	197	VAL	C-O	5.44	1.29	1.23
1	G	168	PRO	N-CA	5.43	1.54	1.47
1	G	255	HIS	ND1-CE1	-5.43	1.27	1.32
1	D	168	PRO	N-CA	5.43	1.54	1.47
1	A	490	ALA	C-O	5.42	1.30	1.23
1	E	239	PRO	N-CA	5.42	1.54	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	282	VAL	C-O	5.41	1.30	1.24
1	A	320	ALA	C-N	5.40	1.40	1.33
1	F	410	MET	C-O	-5.39	1.18	1.24
1	G	312	ALA	C-O	-5.38	1.17	1.24
1	G	562	PRO	C-O	-5.38	1.18	1.23
1	E	314	PRO	C-O	-5.38	1.16	1.24
1	E	470	ALA	C-O	5.33	1.30	1.23
1	C	479	PHE	C-O	-5.30	1.17	1.23
1	E	309	TRP	C-O	-5.29	1.18	1.24
1	A	209	TYR	C-O	5.29	1.30	1.23
1	E	183	GLU	N-CA	5.28	1.52	1.46
1	F	451	HIS	C-O	5.28	1.30	1.24
1	H	357	ALA	C-O	5.25	1.30	1.24
1	A	496	ILE	C-O	5.22	1.29	1.24
1	C	506	VAL	C-O	5.21	1.29	1.24
1	D	68	SER	CA-CB	-5.21	1.46	1.53
1	C	204	ASN	C-O	-5.21	1.17	1.24
1	A	528	ILE	C-O	5.20	1.29	1.24
1	F	492	GLY	N-CA	5.20	1.51	1.45
1	H	280	VAL	C-O	5.20	1.29	1.24
1	E	496	ILE	C-O	5.18	1.29	1.24
1	B	102	VAL	C-O	5.16	1.29	1.24
1	E	575	GLN	C-O	5.16	1.33	1.23
1	H	375	GLY	C-O	5.16	1.30	1.23
1	G	59	ILE	C-O	-5.16	1.18	1.24
1	E	178	LYS	C-O	-5.15	1.18	1.24
1	B	372	SER	C-O	-5.14	1.19	1.24
1	F	307	HIS	CE1-NE2	5.14	1.37	1.32
1	E	326	ARG	C-O	5.12	1.30	1.24
1	C	226	ALA	C-O	5.12	1.29	1.23
1	E	270	GLY	C-O	5.12	1.29	1.23
1	E	272	ALA	C-O	-5.12	1.17	1.24
1	D	288	PHE	C-O	-5.12	1.17	1.24
1	E	340	ARG	N-CA	5.09	1.50	1.45
1	F	461	GLN	C-O	-5.09	1.17	1.24
1	H	388	ALA	C-O	-5.08	1.17	1.23
1	D	290	PRO	C-O	-5.07	1.18	1.24
1	G	167	SER	C-N	5.06	1.39	1.34
1	B	72	PRO	C-O	5.03	1.31	1.24

All (200) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	483	PRO	O-C-N	-11.93	115.82	121.31
1	E	276	LEU	CA-C-N	11.25	131.37	119.90
1	E	276	LEU	C-N-CA	11.25	131.37	119.90
1	H	167	SER	CA-C-N	11.12	130.91	119.56
1	H	167	SER	C-N-CA	11.12	130.91	119.56
1	A	320	ALA	CA-C-N	10.68	131.11	119.90
1	A	320	ALA	C-N-CA	10.68	131.11	119.90
1	C	152	PHE	CA-C-N	10.63	130.40	119.76
1	C	152	PHE	C-N-CA	10.63	130.40	119.76
1	D	167	SER	CA-C-N	10.61	130.21	119.82
1	D	167	SER	C-N-CA	10.61	130.21	119.82
1	E	320	ALA	CA-C-N	10.59	131.02	119.90
1	E	320	ALA	C-N-CA	10.59	131.02	119.90
1	A	276	LEU	CA-C-N	10.57	130.68	119.90
1	A	276	LEU	C-N-CA	10.57	130.68	119.90
1	G	313	ALA	CA-C-N	10.50	130.27	119.56
1	G	313	ALA	C-N-CA	10.50	130.27	119.56
1	G	483	PRO	O-C-N	-9.99	116.72	121.31
1	D	313	ALA	CA-C-N	9.76	129.51	119.56
1	D	313	ALA	C-N-CA	9.76	129.51	119.56
1	C	39	LEU	CA-C-N	9.74	129.83	119.90
1	C	39	LEU	C-N-CA	9.74	129.83	119.90
1	G	167	SER	CA-C-N	9.70	129.96	119.87
1	G	167	SER	C-N-CA	9.70	129.96	119.87
1	B	167	SER	CA-C-N	9.67	129.30	119.82
1	B	167	SER	C-N-CA	9.67	129.30	119.82
1	D	152	PHE	O-C-N	-9.35	112.96	121.37
1	B	483	PRO	O-C-N	-9.23	117.06	121.31
1	B	313	ALA	CA-C-N	9.10	129.28	119.28
1	B	313	ALA	C-N-CA	9.10	129.28	119.28
1	H	227	VAL	CA-C-N	9.00	131.09	119.84
1	H	227	VAL	C-N-CA	9.00	131.09	119.84
1	A	137	ALA	CA-C-N	8.97	131.06	119.84
1	A	137	ALA	C-N-CA	8.97	131.06	119.84
1	H	516	LYS	CA-C-N	8.80	128.83	119.76
1	H	516	LYS	C-N-CA	8.80	128.83	119.76
1	H	340	ARG	CA-C-N	8.58	129.10	119.32
1	H	340	ARG	C-N-CA	8.58	129.10	119.32
1	A	419	GLN	CA-C-N	-8.45	115.66	122.16
1	A	419	GLN	C-N-CA	-8.45	115.66	122.16
1	H	292	LEU	CA-C-N	8.25	128.76	119.93
1	H	292	LEU	C-N-CA	8.25	128.76	119.93
1	C	71	TYR	O-C-N	-7.83	115.07	121.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	341	PRO	N-CA-C	-7.60	102.43	113.75
1	A	482	THR	CA-C-N	7.58	125.19	119.66
1	A	482	THR	C-N-CA	7.58	125.19	119.66
1	H	517	PRO	N-CA-C	-7.49	99.46	111.14
1	H	561	ARG	CA-C-N	7.48	129.43	120.23
1	H	561	ARG	C-N-CA	7.48	129.43	120.23
1	C	100	GLU	O-C-N	-7.39	114.99	121.20
1	D	141	ALA	O-C-N	-7.32	113.48	121.53
1	D	295	GLN	N-CA-C	-7.22	103.34	111.14
1	B	483	PRO	CA-C-N	7.08	127.48	119.83
1	B	483	PRO	C-N-CA	7.08	127.48	119.83
1	F	153	PRO	N-CA-C	6.93	122.06	111.19
1	E	238	LYS	CA-C-N	6.92	128.49	119.84
1	E	238	LYS	C-N-CA	6.92	128.49	119.84
1	B	295	GLN	N-CA-C	-6.91	103.67	111.14
1	G	482	THR	CA-CB-OG1	-6.90	99.25	109.60
1	A	100	GLU	CA-C-N	6.81	126.41	119.19
1	A	100	GLU	C-N-CA	6.81	126.41	119.19
1	A	266	VAL	N-CA-C	-6.64	104.02	110.72
1	H	46	ASN	CA-C-O	-6.59	113.89	121.54
1	D	71	TYR	O-C-N	-6.58	117.21	121.88
1	C	295	GLN	N-CA-C	-6.51	103.46	111.40
1	C	141	ALA	O-C-N	-6.50	114.71	121.60
1	E	100	GLU	O-C-N	-6.50	115.13	121.17
1	B	501	ASP	CA-CB-CG	-6.49	106.11	112.60
1	B	159	ASP	CA-CB-CG	6.41	119.01	112.60
1	C	227	VAL	N-CA-C	-6.39	102.69	108.95
1	H	573	SER	CA-C-N	6.37	130.18	122.16
1	H	573	SER	C-N-CA	6.37	130.18	122.16
1	F	402	VAL	CA-C-O	-6.36	113.90	120.71
1	G	286	ASN	CA-C-N	6.32	126.00	119.56
1	G	286	ASN	C-N-CA	6.32	126.00	119.56
1	F	130	PHE	CA-CB-CG	6.29	120.09	113.80
1	E	277	PRO	N-CA-C	-6.24	101.28	111.15
1	B	141	ALA	O-C-N	-6.17	114.74	121.53
1	G	100	GLU	CA-C-N	6.16	125.78	119.56
1	G	100	GLU	C-N-CA	6.16	125.78	119.56
1	C	238	LYS	CA-C-N	6.15	126.50	119.92
1	C	238	LYS	C-N-CA	6.15	126.50	119.92
1	F	173	THR	CA-CB-OG1	-6.14	100.38	109.60
1	E	483	PRO	N-CA-C	6.12	116.35	110.47
1	A	377	ASP	CA-CB-CG	6.12	118.72	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	483	PRO	CA-C-N	6.11	126.06	119.76
1	D	483	PRO	C-N-CA	6.11	126.06	119.76
1	A	277	PRO	N-CA-C	-6.09	101.53	111.15
1	G	377	ASP	CA-CB-CG	6.00	118.61	112.60
1	E	537	GLU	CB-CA-C	5.97	120.07	110.16
1	A	100	GLU	O-C-N	-5.95	116.20	121.20
1	C	100	GLU	CA-C-N	5.93	125.47	119.19
1	C	100	GLU	C-N-CA	5.93	125.47	119.19
1	E	295	GLN	N-CA-C	-5.92	104.17	111.40
1	A	162	THR	CB-CA-C	5.88	119.37	109.48
1	B	482	THR	CA-CB-OG1	-5.87	100.80	109.60
1	D	209	TYR	CA-C-O	-5.84	114.20	120.92
1	B	493	GLY	CA-C-O	-5.83	115.94	121.60
1	C	196	THR	N-CA-C	-5.83	104.93	111.28
1	D	115	LEU	N-CA-C	-5.81	104.95	111.28
1	C	71	TYR	CA-C-N	5.81	125.94	119.32
1	C	71	TYR	C-N-CA	5.81	125.94	119.32
1	G	141	ALA	O-C-N	-5.81	115.14	121.53
1	A	153	PRO	N-CA-C	5.79	120.59	111.38
1	G	483	PRO	CB-CA-C	-5.78	105.96	111.39
1	D	168	PRO	N-CA-C	-5.76	106.55	113.98
1	E	444	THR	CA-C-N	5.75	127.03	119.84
1	E	444	THR	C-N-CA	5.75	127.03	119.84
1	F	313	ALA	CA-C-N	5.75	125.85	119.87
1	F	313	ALA	C-N-CA	5.75	125.85	119.87
1	H	309	TRP	CA-C-O	-5.72	114.48	120.55
1	E	192	ASP	CA-C-N	5.71	128.50	120.28
1	E	192	ASP	C-N-CA	5.71	128.50	120.28
1	E	321	PRO	CB-CA-C	5.69	118.34	111.46
1	D	61	LEU	CA-C-N	-5.68	116.45	122.30
1	D	61	LEU	C-N-CA	-5.68	116.45	122.30
1	E	148	ASP	CA-CB-CG	5.67	118.27	112.60
1	E	425	VAL	CA-C-O	-5.67	115.72	121.67
1	F	482	THR	CA-CB-OG1	-5.67	101.10	109.60
1	A	482	THR	O-C-N	-5.66	116.26	121.30
1	A	192	ASP	CA-C-N	5.63	128.39	120.28
1	A	192	ASP	C-N-CA	5.63	128.39	120.28
1	B	100	GLU	CA-C-N	5.63	125.16	119.19
1	B	100	GLU	C-N-CA	5.63	125.16	119.19
1	G	272	ALA	N-CA-C	-5.63	105.68	112.54
1	D	141	ALA	CA-C-N	5.61	125.92	119.92
1	D	141	ALA	C-N-CA	5.61	125.92	119.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	141	ALA	CA-C-N	5.60	125.91	119.92
1	B	141	ALA	C-N-CA	5.60	125.91	119.92
1	B	137	ALA	CA-C-N	5.59	126.82	119.84
1	B	137	ALA	C-N-CA	5.59	126.82	119.84
1	B	134	LYS	CB-CA-C	5.57	119.04	110.62
1	B	549	GLY	CA-C-N	5.55	127.98	120.38
1	B	549	GLY	C-N-CA	5.55	127.98	120.38
1	B	130	PHE	CA-CB-CG	5.51	119.31	113.80
1	G	286	ASN	O-C-N	-5.51	116.52	121.31
1	F	132	THR	CA-CB-OG1	-5.49	101.37	109.60
1	H	289	ASN	CA-CB-CG	5.49	118.09	112.60
1	F	190	LYS	CA-C-O	-5.48	114.15	120.24
1	B	67	ASN	CA-CB-CG	5.47	118.07	112.60
1	F	331	VAL	CA-C-O	-5.47	115.37	121.17
1	G	122	LYS	CB-CA-C	5.46	119.18	111.86
1	G	559	THR	O-C-N	5.44	126.17	121.65
1	F	395	THR	CB-CA-C	-5.43	101.78	110.79
1	F	268	VAL	N-CA-CB	5.43	118.72	110.58
1	E	342	ASP	CA-C-O	-5.42	112.87	119.43
1	G	141	ALA	CA-C-N	5.42	125.71	119.92
1	G	141	ALA	C-N-CA	5.42	125.71	119.92
1	H	100	GLU	O-C-N	-5.41	116.66	121.20
1	B	325	PHE	CA-C-O	-5.41	114.59	120.81
1	C	330	THR	N-CA-C	-5.40	105.48	111.36
1	B	520	GLU	CB-CA-C	5.38	118.36	109.70
1	A	289	ASN	CA-CB-CG	5.37	117.97	112.60
1	E	232	ILE	CA-C-O	-5.33	115.73	121.27
1	A	432	THR	CB-CA-C	5.32	117.82	110.16
1	E	100	GLU	CA-C-N	5.32	124.83	119.19
1	E	100	GLU	C-N-CA	5.32	124.83	119.19
1	F	161	ASP	CA-CB-CG	5.32	117.92	112.60
1	H	279	TYR	CA-C-O	-5.31	115.77	121.45
1	A	207	GLY	CA-C-O	-5.29	116.87	122.01
1	F	314	PRO	CB-CA-C	5.29	119.43	111.44
1	E	427	GLU	CA-C-O	5.29	124.19	119.59
1	B	371	PHE	CA-CB-CG	5.29	119.09	113.80
1	E	235	LEU	CA-C-N	-5.28	114.53	122.24
1	E	235	LEU	C-N-CA	-5.28	114.53	122.24
1	H	317	ASP	CA-C-O	-5.28	115.26	120.70
1	E	560	ASP	CA-CB-CG	5.28	117.88	112.60
1	B	389	LYS	N-CA-C	-5.27	105.62	111.36
1	D	137	ALA	CA-C-N	5.27	126.42	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	137	ALA	C-N-CA	5.27	126.42	119.84
1	H	371	PHE	CA-CB-CG	5.26	119.06	113.80
1	F	209	TYR	CA-C-O	-5.25	114.88	120.92
1	H	211	ALA	CA-C-O	-5.25	115.61	121.23
1	D	289	ASN	CA-CB-CG	5.25	117.85	112.60
1	H	412	GLU	CB-CG-CD	5.24	121.51	112.60
1	F	184	LEU	CA-C-O	-5.23	115.33	120.82
1	H	64	GLN	CB-CG-CD	5.23	121.49	112.60
1	D	108	PHE	CA-C-O	-5.22	113.57	119.78
1	E	159	ASP	CA-CB-CG	5.20	117.80	112.60
1	E	434	GLU	CA-C-N	5.20	127.77	120.28
1	E	434	GLU	C-N-CA	5.20	127.77	120.28
1	F	550	ASP	CA-CB-CG	5.18	117.78	112.60
1	G	67	ASN	CA-CB-CG	5.17	117.77	112.60
1	B	500	ASP	CA-CB-CG	5.16	117.76	112.60
1	F	412	GLU	CB-CG-CD	5.16	121.38	112.60
1	H	168	PRO	CB-CA-C	5.15	119.16	111.85
1	D	100	GLU	CA-C-N	5.13	124.92	119.28
1	D	100	GLU	C-N-CA	5.13	124.92	119.28
1	H	207	GLY	O-C-N	5.12	128.07	123.00
1	G	100	GLU	O-C-N	-5.11	116.91	121.20
1	H	100	GLU	CA-C-N	5.11	124.90	119.28
1	H	100	GLU	C-N-CA	5.11	124.90	119.28
1	B	100	GLU	O-C-N	-5.11	116.91	121.20
1	D	351	GLY	CA-C-O	-5.08	115.92	121.71
1	C	40	PRO	N-CA-C	-5.07	103.14	111.15
1	F	173	THR	N-CA-C	-5.06	105.67	111.14
1	A	371	PHE	CA-CB-CG	5.05	118.85	113.80
1	E	384	TYR	O-C-N	-5.04	117.25	121.38
1	B	238	LYS	CB-CA-C	5.04	115.97	108.87
1	H	406	VAL	CA-C-O	-5.02	115.92	120.73

There are no chirality outliers.

There are no planarity outliers.

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	4138	0	3969	19	0
1	B	4182	0	4008	11	0
1	C	4153	0	3950	15	0
1	D	4227	0	4051	13	0
1	E	4207	0	4028	11	0
1	F	4245	0	4068	20	0
1	G	4162	0	4026	15	0
1	H	4170	0	3990	16	0
2	A	4	0	0	0	0
2	B	3	0	0	0	0
2	C	4	0	0	0	0
2	D	5	0	0	0	0
2	E	5	0	0	0	0
2	F	4	0	0	0	0
2	G	5	0	0	0	0
2	H	2	0	0	0	0
3	A	21	0	0	0	0
3	B	14	0	0	0	0
3	C	13	0	0	0	0
3	D	21	0	0	0	0
3	E	13	0	0	1	0
3	F	15	0	0	0	0
3	G	15	0	0	0	0
3	H	13	0	0	0	0
4	A	238	0	0	2	0
4	B	300	0	0	0	0
4	C	286	0	0	0	0
4	D	344	0	0	3	0
4	E	359	0	0	0	0
4	F	308	0	0	5	0
4	G	390	0	0	1	0
4	H	277	0	0	2	0
All	All	36143	0	32090	115	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 2.

All (115) 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:F:241:THR:OG1	1:F:244:GLN:HG3	1.79	0.81
1:F:179:LYS:HE2	4:F:742:HOH:O	1.81	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:169:LEU:HD12	1:H:219:ALA:HA	1.66	0.77
1:F:415[C]:ARG:HH21	1:F:415[C]:ARG:HG3	1.55	0.72
1:A:139:HIS:HB2	4:A:899:HOH:O	1.89	0.71
1:D:421:GLN:NE2	4:D:701:HOH:O	2.23	0.71
1:H:169:LEU:CD1	1:H:219:ALA:HA	2.22	0.70
1:G:432:THR:HG23	4:G:714:HOH:O	1.97	0.63
1:C:158:GLU:HG3	1:C:215:TYR:CD1	2.34	0.62
1:C:232:ILE:HG23	1:C:237:LEU:O	2.00	0.62
1:F:46:ASN:HB3	4:F:703:HOH:O	1.98	0.62
1:C:235:LEU:HB3	1:C:237:LEU:HD13	1.83	0.61
1:F:46:ASN:CG	4:F:703:HOH:O	2.44	0.60
1:F:415[C]:ARG:HG3	1:F:415[C]:ARG:NH2	2.14	0.60
1:G:169:LEU:HD13	1:G:219:ALA:HA	1.84	0.59
1:A:481:VAL:HG22	1:A:481:VAL:O	2.04	0.57
1:D:532:GLU:OE1	1:D:543[B]:MET:HG3	2.05	0.57
1:C:99:ILE:O	1:C:106:PHE:HA	2.06	0.56
1:C:140:TYR:CZ	1:H:548:ASN:HB3	2.41	0.56
1:C:237:LEU:HD23	1:C:245:VAL:HG13	1.87	0.56
1:D:541:TRP:CE2	1:D:566:ARG:HD3	2.41	0.55
1:F:420:GLY:N	4:F:704:HOH:O	2.40	0.55
1:B:407:ASN:N	1:B:408:PRO:HD2	2.21	0.55
1:H:294:GLY:HA3	4:H:929:HOH:O	2.07	0.54
1:H:99:ILE:O	1:H:106:PHE:HA	2.08	0.54
1:A:525:LYS:HD3	1:A:574:VAL:HG11	1.90	0.53
1:E:155:VAL:HG13	1:E:214:ASP:HA	1.91	0.52
1:C:237:LEU:HD23	1:C:245:VAL:CG1	2.39	0.52
1:F:46:ASN:CB	4:F:703:HOH:O	2.57	0.51
1:A:186:LYS:O	1:A:190:LYS:HG3	2.11	0.51
1:A:361:PHE:CD2	1:A:493:GLY:HA3	2.46	0.50
1:C:313:ALA:HB1	1:C:316:ILE:HD12	1.94	0.50
1:D:140:TYR:CZ	1:E:548:ASN:HB3	2.47	0.49
1:H:508:ALA:HB3	1:H:558:PHE:CD1	2.47	0.49
1:A:99:ILE:O	1:A:106:PHE:HA	2.12	0.49
1:G:508:ALA:HB3	1:G:558:PHE:CD1	2.48	0.49
1:B:528:ILE:HG21	1:B:531:VAL:HG23	1.95	0.48
1:D:532:GLU:CD	1:D:543[B]:MET:HG3	2.38	0.48
1:D:179:LYS:HE2	4:D:730:HOH:O	2.12	0.48
1:G:184:LEU:HG	1:G:185[A]:MET:HE2	1.96	0.48
1:A:65:THR:HG21	1:A:92:ILE:HD12	1.95	0.47
1:F:548:ASN:HB3	1:G:140:TYR:CZ	2.49	0.47
1:A:508:ALA:HB3	1:A:558:PHE:CD1	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:405:LEU:HD12	1:F:562:PRO:HB3	1.96	0.47
1:B:548:ASN:HB3	1:H:140:TYR:CZ	2.49	0.47
1:B:99:ILE:O	1:B:106:PHE:HA	2.14	0.47
1:B:169:LEU:HD13	1:B:219:ALA:HA	1.96	0.47
1:E:186:LYS:O	1:E:190:LYS:HG2	2.15	0.47
1:A:548:ASN:HB3	1:B:140:TYR:CZ	2.49	0.47
1:A:313:ALA:HB1	1:A:316:ILE:HD12	1.95	0.47
1:A:59:ILE:HG12	1:A:414:ALA:HB2	1.97	0.47
1:G:169:LEU:CD1	1:G:219:ALA:HA	2.44	0.47
1:G:190:LYS:HG3	1:G:191:ARG:HG2	1.96	0.46
1:D:407:ASN:N	1:D:408:PRO:HD2	2.30	0.46
1:E:99:ILE:O	1:E:106:PHE:HA	2.15	0.46
1:A:205:GLU:OE2	1:A:322:ASP:OD2	2.34	0.46
1:G:407:ASN:N	1:G:408:PRO:HD2	2.31	0.46
1:D:292:LEU:O	1:D:295:GLN:HB2	2.16	0.46
1:C:508:ALA:HB3	1:C:558:PHE:CD1	2.51	0.45
1:D:99:ILE:O	1:D:106:PHE:HA	2.16	0.45
1:H:528:ILE:HG21	1:H:531:VAL:HG23	1.99	0.45
1:A:151:ARG:HD3	1:A:152:PHE:CE2	2.52	0.45
1:G:264:ASP:OD1	1:G:315:ASN:HB2	2.17	0.45
1:B:40:PRO:HA	1:B:52:MET:O	2.16	0.45
1:E:60:ILE:HG23	1:E:89:THR:HB	1.99	0.44
1:E:384:TYR:CD1	1:E:385:PRO:HA	2.52	0.44
1:B:521:LEU:HB3	1:B:524:LYS:HB2	1.98	0.44
1:F:134:LYS:HD3	1:F:134:LYS:C	2.43	0.44
1:G:384:TYR:CD1	1:G:385:PRO:HA	2.53	0.44
1:D:169:LEU:CD1	1:D:219:ALA:HA	2.48	0.44
1:C:134:LYS:HD3	1:C:134:LYS:C	2.43	0.43
1:C:313:ALA:CB	1:C:316:ILE:HD12	2.49	0.43
1:H:404:ARG:HD2	4:H:703:HOH:O	2.17	0.43
1:F:342:ASP:OD1	1:F:342:ASP:C	2.61	0.43
1:B:465:LEU:HD11	1:B:470:ALA:HB2	1.99	0.43
1:F:271:LYS:HE3	1:F:315:ASN:O	2.19	0.43
1:H:200:VAL:O	1:H:278:MET:HA	2.18	0.43
1:C:205:GLU:OE2	1:C:322:ASP:OD2	2.37	0.43
1:D:59:ILE:HG12	1:D:414:ALA:HB2	2.00	0.42
1:E:254:PHE:O	1:E:258:GLN:HG2	2.19	0.42
1:A:384:TYR:CD1	1:A:385:PRO:HA	2.54	0.42
1:E:200:VAL:O	1:E:278:MET:HA	2.20	0.42
1:G:99:ILE:O	1:G:106:PHE:HA	2.19	0.42
1:H:342:ASP:OD1	1:H:342:ASP:C	2.61	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:541:TRP:CG	1:F:566:ARG:HH11	2.38	0.42
1:G:361:PHE:CD2	1:G:493:GLY:HA3	2.54	0.42
1:A:200:VAL:O	1:A:278:MET:HA	2.19	0.42
1:H:367:GLY:HA2	1:H:417:SER:OG	2.19	0.42
1:A:524:LYS:NZ	4:A:708:HOH:O	2.49	0.42
1:H:318:LEU:HD12	1:H:318:LEU:C	2.45	0.42
1:E:349:GLU:OE1	3:E:606:N0Q:NAB	2.53	0.42
1:H:40:PRO:HA	1:H:52:MET:O	2.20	0.42
1:B:541:TRP:CG	1:B:566:ARG:HH11	2.38	0.41
1:F:136:ASN:ND2	1:F:136:ASN:C	2.78	0.41
1:E:318:LEU:C	1:E:318:LEU:HD12	2.44	0.41
1:B:508:ALA:HB3	1:B:558:PHE:CD1	2.55	0.41
1:A:231:LEU:HD11	1:A:235:LEU:HD11	2.01	0.41
1:F:128:LEU:HA	1:F:201:GLN:HB3	2.02	0.41
1:H:199:MET:HG2	1:H:277:PRO:HB2	2.02	0.41
1:C:40:PRO:HA	1:C:52:MET:O	2.20	0.41
1:F:415[C]:ARG:HH21	1:F:415[C]:ARG:CG	2.25	0.41
1:C:158:GLU:HG3	1:C:215:TYR:CG	2.56	0.41
1:D:455:ARG:NH1	4:D:719:HOH:O	2.54	0.41
1:G:59:ILE:HG12	1:G:414:ALA:HB2	2.03	0.41
1:F:67:ASN:HB3	1:F:140:TYR:OH	2.21	0.41
1:F:254:PHE:O	1:F:258:GLN:HG2	2.20	0.40
1:D:169:LEU:HD12	1:D:219:ALA:HA	2.03	0.40
1:G:199:MET:HG2	1:G:277:PRO:HB2	2.02	0.40
1:G:525:LYS:HD3	1:G:574:VAL:HG11	2.03	0.40
1:H:63:SER:HB3	1:H:85:MET:SD	2.62	0.40
1:A:241:THR:O	1:A:245:VAL:HG13	2.21	0.40
1:C:82:MET:HG2	1:C:87:ALA:HB3	2.03	0.40
1:E:309:TRP:HB3	1:E:319:ILE:HD11	2.03	0.40
1:F:241:THR:O	1:F:245:VAL:HG23	2.21	0.40
1:A:318:LEU:HD12	1:A:318:LEU:C	2.47	0.40

There are no symmetry-related clashes.

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	521/550 (95%)	503 (96%)	18 (4%)	0	100	100
1	B	530/550 (96%)	515 (97%)	14 (3%)	1 (0%)	43	24
1	C	527/550 (96%)	507 (96%)	20 (4%)	0	100	100
1	D	536/550 (98%)	516 (96%)	18 (3%)	2 (0%)	30	14
1	E	535/550 (97%)	517 (97%)	16 (3%)	2 (0%)	30	14
1	F	537/550 (98%)	519 (97%)	18 (3%)	0	100	100
1	G	526/550 (96%)	510 (97%)	16 (3%)	0	100	100
1	H	530/550 (96%)	511 (96%)	19 (4%)	0	100	100
All	All	4242/4400 (96%)	4098 (97%)	139 (3%)	5 (0%)	48	27

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	445	PRO
1	B	491	ALA
1	D	491	ALA
1	E	491	ALA
1	D	445	PRO

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	425/461 (92%)	416 (98%)	9 (2%)	47	23
1	B	427/461 (93%)	419 (98%)	8 (2%)	50	27
1	C	421/461 (91%)	413 (98%)	8 (2%)	50	27
1	D	433/461 (94%)	428 (99%)	5 (1%)	63	43
1	E	430/461 (93%)	424 (99%)	6 (1%)	59	38
1	F	435/461 (94%)	424 (98%)	11 (2%)	42	18

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	G	429/461 (93%)	423 (99%)	6 (1%)	59	38
1	H	426/461 (92%)	418 (98%)	8 (2%)	50	27
All	All	3426/3688 (93%)	3365 (98%)	61 (2%)	51	28

All (61) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	45	ASN
1	A	82	MET
1	A	120	GLN
1	A	122	LYS
1	A	136	ASN
1	A	245	VAL
1	A	292	LEU
1	A	390	VAL
1	A	421	GLN
1	B	82	MET
1	B	83	GLU
1	B	136	ASN
1	B	245	VAL
1	B	390	VAL
1	B	421	GLN
1	B	519	GLN
1	B	537	GLU
1	C	82	MET
1	C	136	ASN
1	C	161	ASP
1	C	217	PRO
1	C	229	ASP
1	C	243	SER
1	C	419	GLN
1	C	537	GLU
1	D	82	MET
1	D	83	GLU
1	D	136	ASN
1	D	326	ARG
1	D	537	GLU
1	E	82	MET
1	E	136	ASN
1	E	179	LYS
1	E	462[A]	GLN

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Mol	Chain	Res	Type
1	E	462[B]	GLN
1	E	537	GLU
1	F	63	SER
1	F	82	MET
1	F	83	GLU
1	F	136	ASN
1	F	158	GLU
1	F	234	LYS
1	F	243	SER
1	F	244	GLN
1	F	268	VAL
1	F	520	GLU
1	F	537	GLU
1	G	82	MET
1	G	120	GLN
1	G	136	ASN
1	G	179	LYS
1	G	229	ASP
1	G	540	LYS
1	H	45	ASN
1	H	82	MET
1	H	120	GLN
1	H	136	ASN
1	H	158	GLU
1	H	228	PRO
1	H	341	PRO
1	H	386	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (30) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	172	ASN
1	A	275	ASN
1	A	289	ASN
1	A	315	ASN
1	A	419	GLN
1	A	421	GLN
1	B	120	GLN
1	B	275	ASN
1	B	354	GLN
1	B	487	ASN
1	C	64	GLN

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Mol	Chain	Res	Type
1	C	120	GLN
1	C	315	ASN
1	C	451	HIS
1	C	487	ASN
1	D	233	GLN
1	D	275	ASN
1	E	64	GLN
1	E	275	ASN
1	F	64	GLN
1	F	105	GLN
1	F	224	ASN
1	F	258	GLN
1	F	275	ASN
1	G	64	GLN
1	G	105	GLN
1	G	171	GLN
1	H	275	ASN
1	H	421	GLN
1	H	451	HIS

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 40 ligands modelled in this entry, 32 are monoatomic - leaving 8 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	$\# Z > 2$
3	N0Q	A	605	-	21,21,35	1.91	5 (23%)	21,28,49	2.43	8 (38%)
3	N0Q	C	605	-	13,13,35	0.93	1 (7%)	10,17,49	1.81	2 (20%)
3	N0Q	G	606	-	15,15,35	2.13	4 (26%)	13,19,49	1.52	3 (23%)
3	N0Q	F	605	-	15,15,35	3.01	5 (33%)	13,19,49	1.23	1 (7%)
3	N0Q	E	606	-	13,13,35	1.53	3 (23%)	10,17,49	1.57	3 (30%)
3	N0Q	D	606	-	21,21,35	2.37	7 (33%)	21,28,49	1.98	6 (28%)
3	N0Q	B	604	-	14,14,35	1.69	4 (28%)	12,18,49	1.81	3 (25%)
3	N0Q	H	603	-	13,13,35	1.73	2 (15%)	10,17,49	1.47	2 (20%)

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	N0Q	A	605	-	-	8/13/30/40	0/1/1/3
3	N0Q	C	605	-	-	2/5/22/40	0/1/1/3
3	N0Q	G	606	-	-	3/7/24/40	0/1/1/3
3	N0Q	F	605	-	-	4/7/24/40	0/1/1/3
3	N0Q	E	606	-	-	3/5/22/40	0/1/1/3
3	N0Q	D	606	-	-	7/13/30/40	0/1/1/3
3	N0Q	B	604	-	-	3/6/23/40	0/1/1/3
3	N0Q	H	603	-	-	2/5/22/40	0/1/1/3

All (31) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	605	N0Q	CAI-NAB	-6.62	1.38	1.47
3	D	606	N0Q	C6-S3	-6.37	1.61	1.75
3	F	605	N0Q	CAD-CAC	-6.36	1.46	1.53
3	A	605	N0Q	C6-S3	-5.65	1.62	1.75
3	F	605	N0Q	CAJ-CAC	-5.32	1.44	1.52
3	G	606	N0Q	CAD-CAC	5.32	1.58	1.53
3	H	603	N0Q	CAI-NAB	-4.15	1.41	1.47
3	A	605	N0Q	O4-S3	3.97	1.50	1.43
3	D	606	N0Q	O4-S3	3.91	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	G	606	N0Q	CAA-NAB	3.76	1.53	1.47
3	D	606	N0Q	CAL-CAA	3.56	1.60	1.52
3	G	606	N0Q	OAF-CAJ	3.50	1.50	1.43
3	H	603	N0Q	CAA-NAB	3.41	1.52	1.47
3	A	605	N0Q	CAD-CAC	-3.40	1.49	1.53
3	B	604	N0Q	CAI-NAB	-3.37	1.42	1.47
3	F	605	N0Q	CAH-CAD	3.32	1.57	1.52
3	G	606	N0Q	CAJ-CAC	-3.28	1.47	1.52
3	D	606	N0Q	CAD-CAC	-3.24	1.49	1.53
3	D	606	N0Q	OAE-CAC	3.11	1.50	1.43
3	D	606	N0Q	CAI-CAJ	3.00	1.55	1.52
3	E	606	N0Q	CAH-CAD	-2.88	1.47	1.52
3	B	604	N0Q	CAD-CAC	-2.74	1.50	1.53
3	B	604	N0Q	OAE-CAC	2.70	1.49	1.43
3	E	606	N0Q	CAD-CAC	-2.68	1.50	1.53
3	B	604	N0Q	CAI-CAJ	2.58	1.54	1.52
3	E	606	N0Q	CAJ-CAC	-2.51	1.48	1.52
3	F	605	N0Q	CAI-CAJ	-2.42	1.50	1.52
3	D	606	N0Q	CAJ-CAC	-2.41	1.48	1.52
3	A	605	N0Q	CAA-NAB	-2.41	1.44	1.47
3	C	605	N0Q	CAH-CAD	2.30	1.56	1.52
3	A	605	N0Q	CAJ-CAC	-2.09	1.49	1.52

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	605	N0Q	O5-S3-O4	-6.88	109.65	118.87
3	D	606	N0Q	O5-S3-O4	-4.87	112.34	118.87
3	C	605	N0Q	CAI-CAJ-CAC	4.36	115.58	110.25
3	B	604	N0Q	CAM-CAL-CAA	-4.15	106.03	113.94
3	A	605	N0Q	O4-S3-N2	3.77	112.58	107.33
3	D	606	N0Q	CAM-CAL-CAA	-3.58	107.12	113.94
3	A	605	N0Q	CAI-CAJ-CAC	-3.37	106.13	110.25
3	G	606	N0Q	CAC-CAD-CAA	3.16	116.19	109.26
3	D	606	N0Q	O5-S3-N2	3.13	111.69	107.33
3	H	603	N0Q	CAI-CAJ-CAC	-3.09	106.48	110.25
3	B	604	N0Q	CAC-CAD-CAA	3.07	115.99	109.26
3	A	605	N0Q	C6-S3-N2	-3.03	105.84	107.82
3	A	605	N0Q	CAP-C1-N2	-3.01	104.72	111.03
3	C	605	N0Q	CAC-CAD-CAA	3.01	115.87	109.26
3	A	605	N0Q	CAI-NAB-CAA	2.94	116.17	109.71
3	G	606	N0Q	OAF-CAJ-CAC	-2.91	104.12	110.15

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	606	N0Q	CAN-CAM-CAL	-2.89	102.71	113.62
3	F	605	N0Q	OAE-CAC-CAD	2.71	115.47	109.94
3	B	604	N0Q	CAI-NAB-CAA	2.69	115.61	109.71
3	A	605	N0Q	CAM-CAL-CAA	-2.68	108.84	113.94
3	D	606	N0Q	CAP-C1-N2	-2.61	105.56	111.03
3	A	605	N0Q	O5-S3-C6	2.47	112.16	108.26
3	E	606	N0Q	CAI-CAJ-CAC	-2.42	107.29	110.25
3	G	606	N0Q	OAE-CAC-CAD	-2.24	105.38	109.94
3	E	606	N0Q	OAF-CAJ-CAI	-2.20	105.40	109.65
3	H	603	N0Q	CAC-CAD-CAA	2.07	113.80	109.26
3	E	606	N0Q	CAI-NAB-CAA	2.03	114.18	109.71
3	D	606	N0Q	CAC-CAD-CAA	2.01	113.66	109.26

There are no chirality outliers.

All (32) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	605	N0Q	C1-N2-S3-C6
3	A	605	N0Q	C1-N2-S3-O4
3	A	605	N0Q	C1-N2-S3-O5
3	A	605	N0Q	N2-C1-CAP-CAO
3	A	605	N0Q	NAB-CAA-CAL-CAM
3	A	605	N0Q	CAD-CAA-CAL-CAM
3	B	604	N0Q	NAB-CAA-CAL-CAM
3	B	604	N0Q	CAD-CAA-CAL-CAM
3	C	605	N0Q	NAB-CAA-CAL-CAM
3	C	605	N0Q	CAD-CAA-CAL-CAM
3	D	606	N0Q	C1-N2-S3-C6
3	D	606	N0Q	N2-C1-CAP-CAO
3	E	606	N0Q	NAB-CAA-CAL-CAM
3	E	606	N0Q	CAD-CAA-CAL-CAM
3	F	605	N0Q	NAB-CAA-CAL-CAM
3	F	605	N0Q	CAD-CAA-CAL-CAM
3	G	606	N0Q	NAB-CAA-CAL-CAM
3	G	606	N0Q	CAD-CAA-CAL-CAM
3	H	603	N0Q	NAB-CAA-CAL-CAM
3	H	603	N0Q	CAD-CAA-CAL-CAM
3	D	606	N0Q	CAL-CAM-CAN-CAO
3	G	606	N0Q	CAL-CAM-CAN-CAO
3	A	605	N0Q	CAN-CAO-CAP-C1
3	F	605	N0Q	CAM-CAN-CAO-CAP
3	D	606	N0Q	CAA-CAL-CAM-CAN

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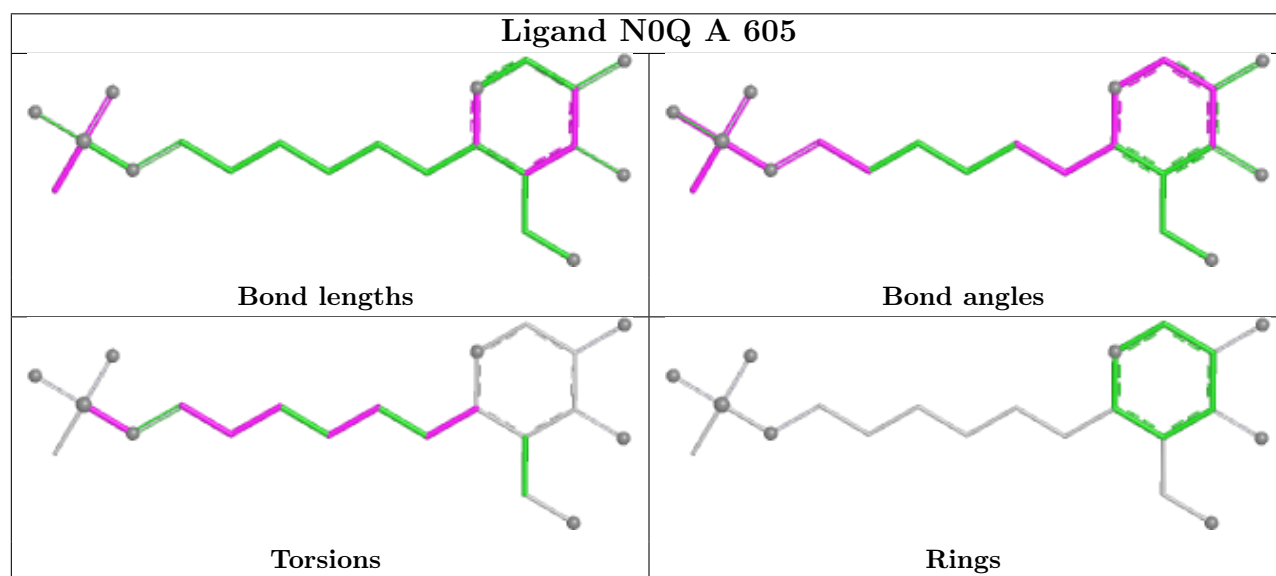
Mol	Chain	Res	Type	Atoms
3	F	605	N0Q	CAL-CAM-CAN-CAO
3	A	605	N0Q	CAL-CAM-CAN-CAO
3	B	604	N0Q	CAL-CAM-CAN-CAO
3	D	606	N0Q	CAM-CAN-CAO-CAP
3	D	606	N0Q	CAN-CAO-CAP-C1
3	D	606	N0Q	C1-N2-S3-O4
3	E	606	N0Q	CAA-CAD-CAH-OAK

There are no ring outliers.

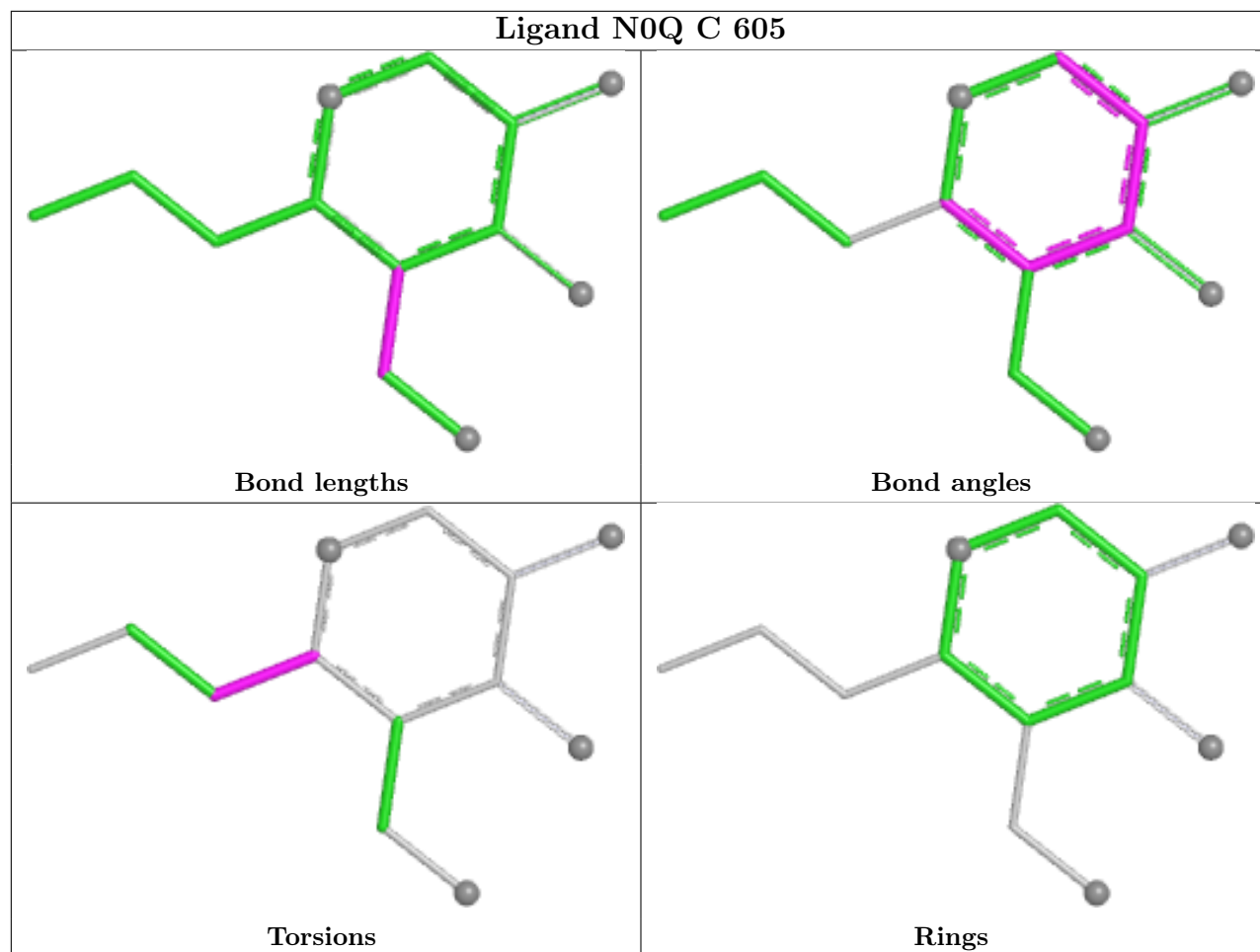
1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	E	606	N0Q	1	0

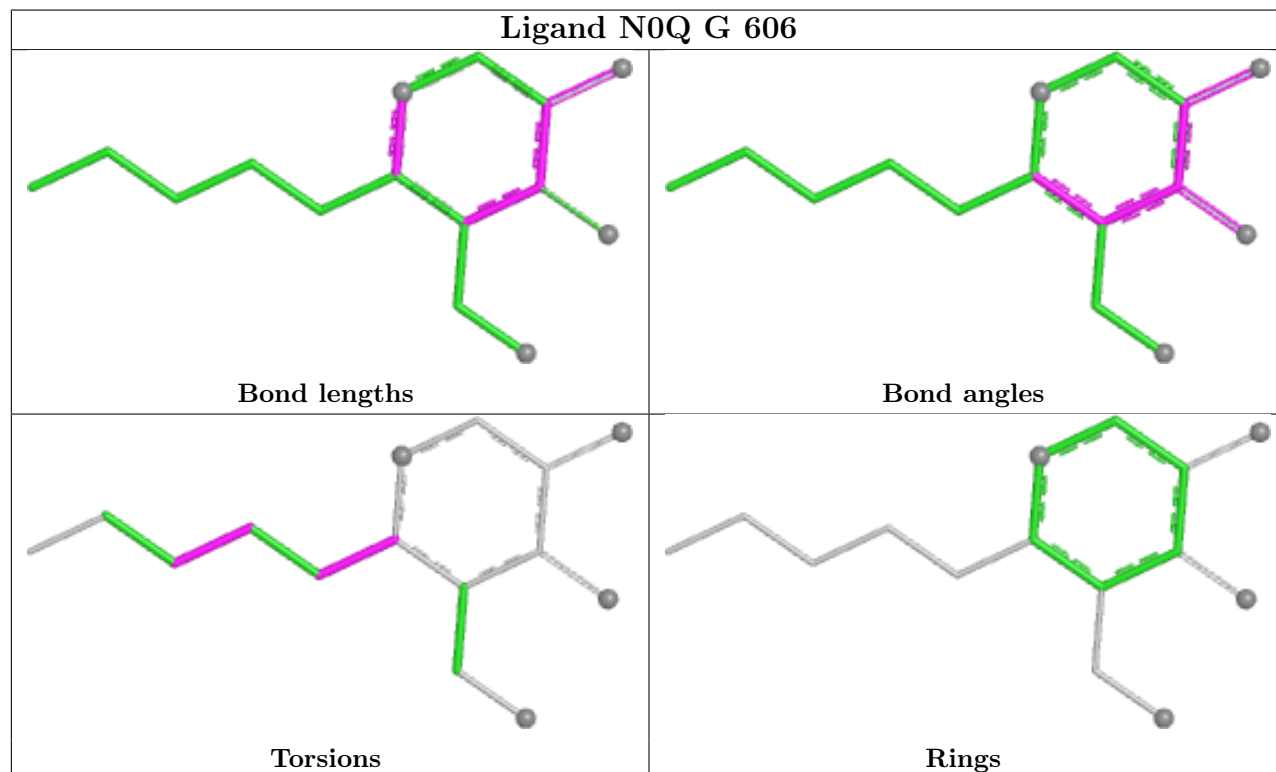
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

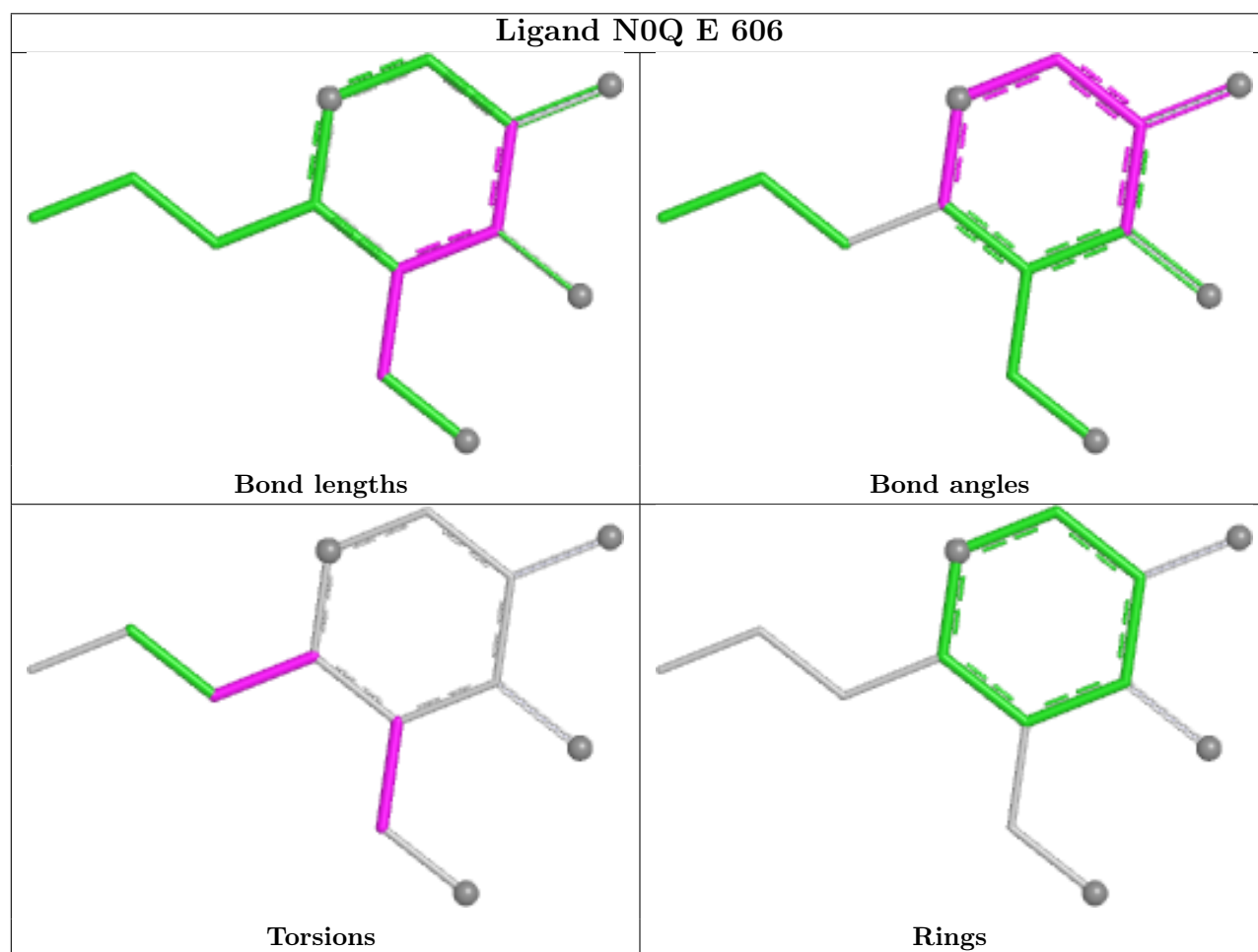
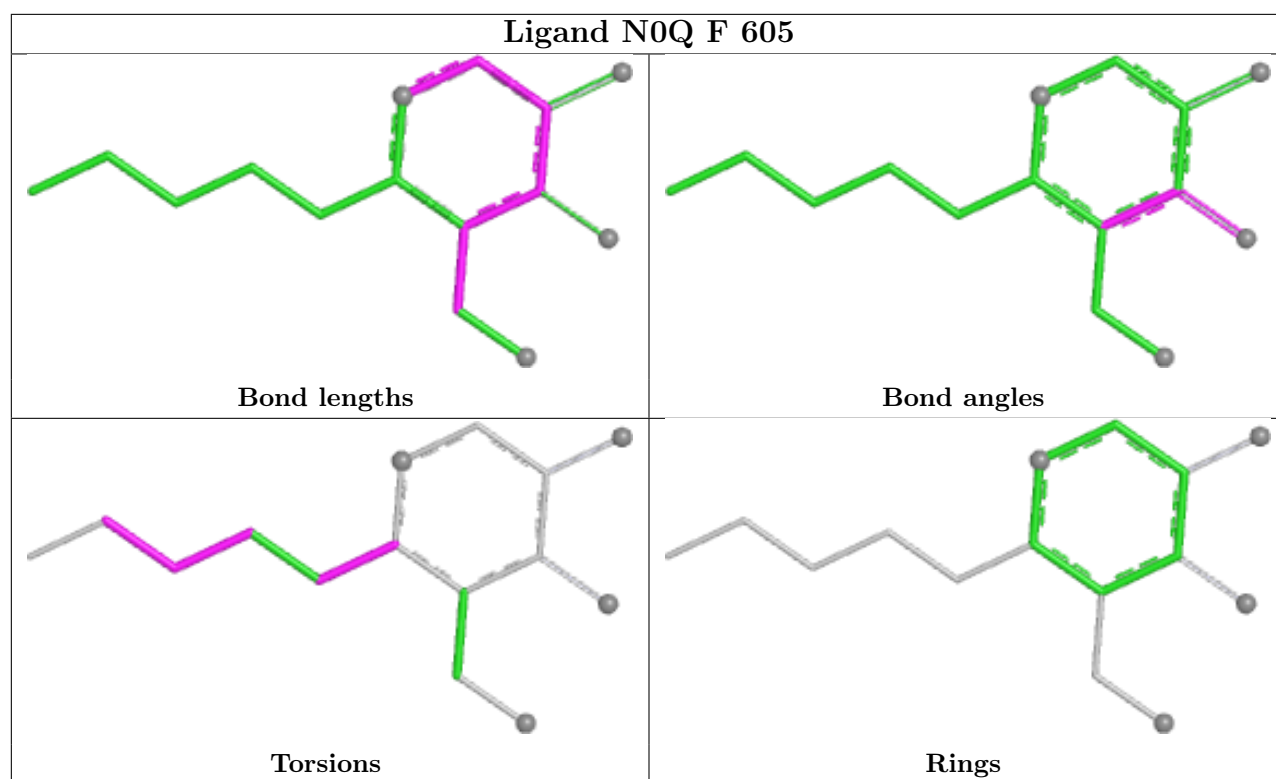


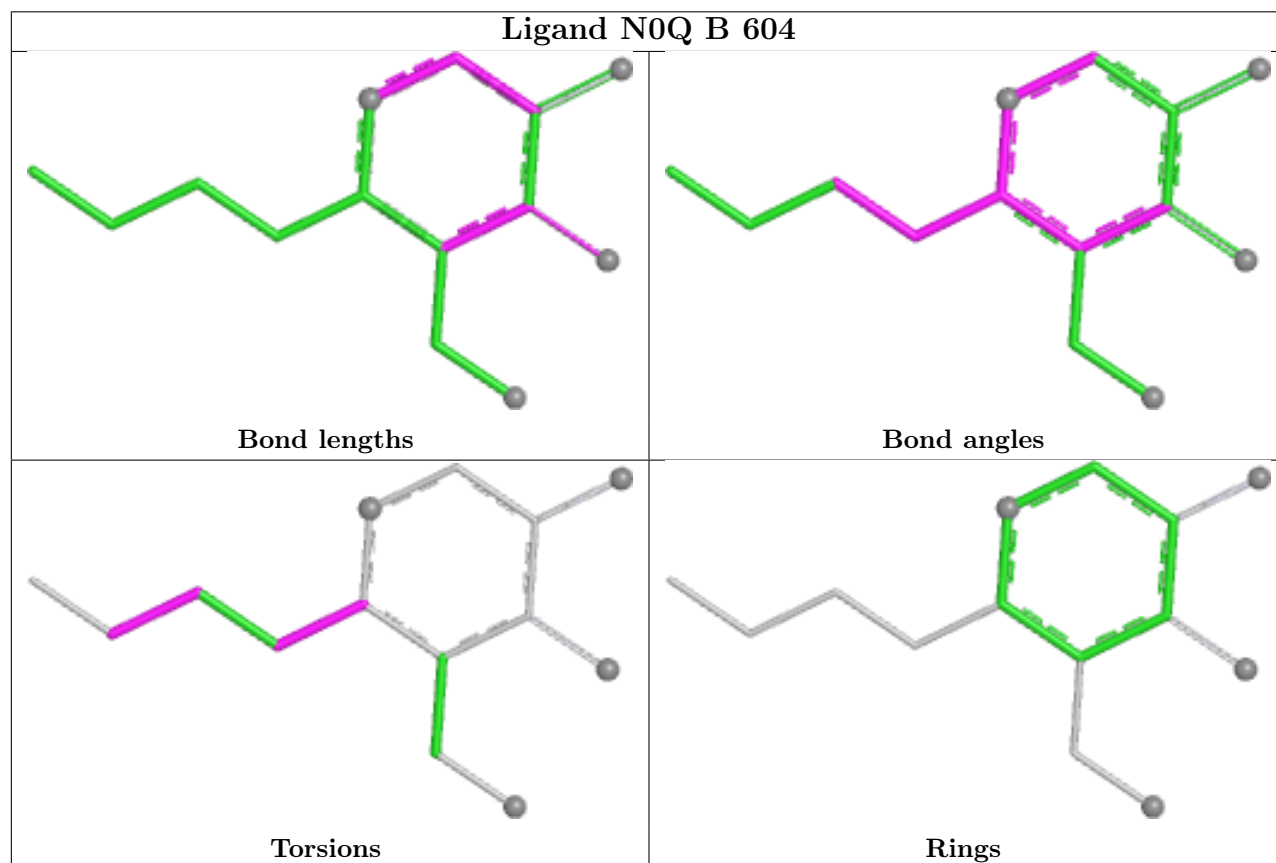
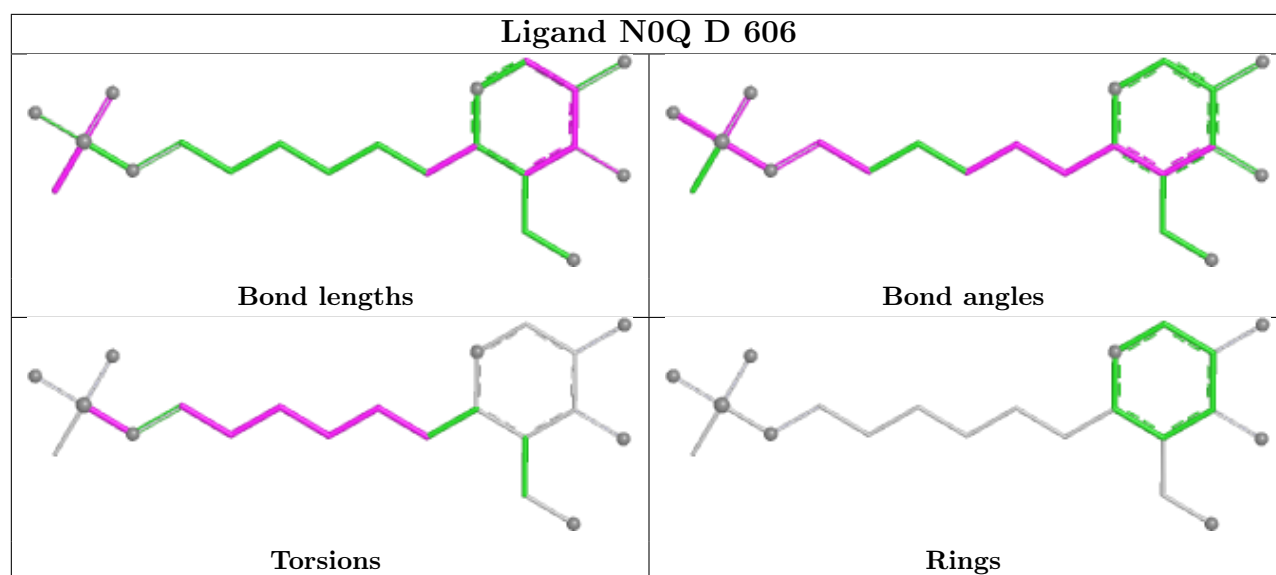
Ligand N0Q C 605

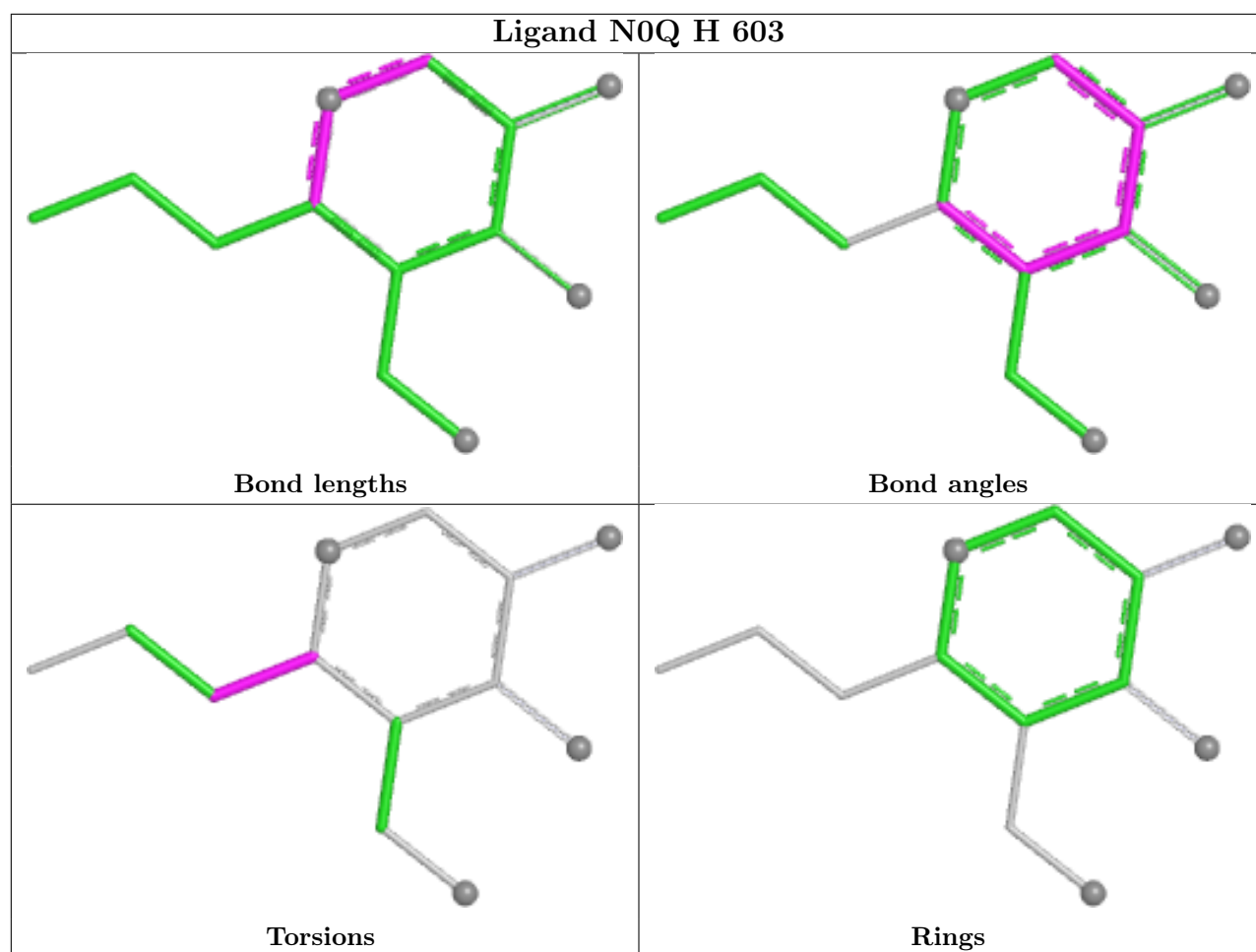


Ligand N0Q G 606









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	527/550 (95%)	-0.06	14 (2%)	56	59	20, 30, 49, 83	25 (4%)
1	B	533/550 (96%)	-0.13	14 (2%)	57	60	17, 26, 43, 62	21 (3%)
1	C	533/550 (96%)	0.03	23 (4%)	40	41	19, 28, 47, 56	32 (6%)
1	D	537/550 (97%)	-0.21	15 (2%)	55	58	15, 24, 41, 59	26 (4%)
1	E	537/550 (97%)	-0.28	11 (2%)	65	69	12, 24, 43, 61	19 (3%)
1	F	535/550 (97%)	-0.18	14 (2%)	57	60	13, 27, 48, 64	35 (6%)
1	G	526/550 (95%)	-0.31	5 (0%)	79	83	12, 25, 44, 65	16 (3%)
1	H	532/550 (96%)	-0.10	16 (3%)	52	55	15, 27, 43, 70	26 (4%)
All	All	4260/4400 (96%)	-0.15	112 (2%)	57	60	12, 26, 45, 83	200 (4%)

All (112) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	522	ALA	12.8
1	C	444	THR	9.2
1	D	445	PRO	9.2
1	B	438	ILE	8.9
1	C	521	LEU	8.8
1	C	238	LYS	8.6
1	F	438	ILE	8.2
1	C	435	THR	8.2
1	E	440	ASN	8.0
1	G	36	ALA	7.9
1	E	444	THR	7.8
1	H	435	THR	7.7
1	C	433	THR	7.7
1	E	438	ILE	7.6
1	C	575	GLN	7.5
1	D	438	ILE	7.2

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Mol	Chain	Res	Type	RSRZ
1	C	442	GLU	7.1
1	F	240	GLY	7.0
1	C	445	PRO	7.0
1	H	575	GLN	6.8
1	E	439	TRP	6.6
1	B	445	PRO	6.3
1	B	447	GLU	6.3
1	H	574	VAL	6.2
1	H	438	ILE	6.2
1	D	443	ALA	6.2
1	A	435	THR	6.2
1	C	443	ALA	6.1
1	H	448	LYS	6.1
1	D	435	THR	6.1
1	F	444	THR	6.1
1	H	446	GLU	6.1
1	H	436	GLN	6.0
1	D	439	TRP	5.9
1	A	575	GLN	5.7
1	E	575	GLN	5.7
1	B	437	LYS	5.6
1	B	446	GLU	5.5
1	C	434	GLU	5.5
1	F	443	ALA	5.4
1	G	575	GLN	5.4
1	B	433	THR	5.4
1	E	443	ALA	5.4
1	H	523	GLY	5.4
1	D	446	GLU	5.3
1	H	447	GLU	5.2
1	A	434	GLU	5.2
1	F	445	PRO	5.2
1	C	437	LYS	5.1
1	G	433	THR	5.1
1	A	241	THR	5.1
1	H	437	LYS	4.9
1	E	445	PRO	4.8
1	C	236	GLN	4.7
1	E	236	GLN	4.6
1	C	436	GLN	4.6
1	D	575	GLN	4.5
1	D	437	LYS	4.5

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Mol	Chain	Res	Type	RSRZ
1	B	521	LEU	4.4
1	E	437	LYS	4.4
1	B	435	THR	4.3
1	A	521	LEU	4.2
1	B	434	GLU	4.2
1	H	537	GLU	4.2
1	B	448	LYS	4.2
1	H	434	GLU	4.1
1	A	437	LYS	4.1
1	C	223	PHE	4.0
1	H	449	GLU	3.8
1	D	444	THR	3.8
1	D	448	LYS	3.7
1	A	523	GLY	3.7
1	C	237	LEU	3.6
1	C	446	GLU	3.4
1	H	521	LEU	3.3
1	D	436	GLN	3.3
1	D	440	ASN	3.3
1	D	434	GLU	3.2
1	F	247	GLY	3.2
1	C	447	GLU	3.1
1	D	447	GLU	3.1
1	C	519	GLN	2.9
1	B	480	TRP	2.9
1	A	229	ASP	2.8
1	E	480	TRP	2.8
1	C	419	GLN	2.7
1	F	415[A]	ARG	2.7
1	C	448	LYS	2.7
1	F	434	GLU	2.7
1	A	158	GLU	2.6
1	C	449	GLU	2.6
1	A	238	LYS	2.6
1	F	437	LYS	2.6
1	F	158	GLU	2.5
1	A	46	ASN	2.5
1	C	158	GLU	2.5
1	D	46	ASN	2.5
1	B	436	GLN	2.4
1	A	244	GLN	2.4
1	E	37	ALA	2.4

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Mol	Chain	Res	Type	RSRZ
1	H	480	TRP	2.2
1	A	451	HIS	2.2
1	H	37	ALA	2.2
1	F	235	LEU	2.2
1	F	237	LEU	2.2
1	F	436	GLN	2.2
1	F	435	THR	2.2
1	C	229	ASP	2.2
1	G	239	PRO	2.2
1	A	237	LEU	2.2
1	G	229	ASP	2.1
1	B	481	VAL	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(Å ²)	Q<0.9
2	NA	A	602	1/1	0.96	0.09	40,40,40,40	0
2	NA	H	601	1/1	0.96	0.08	42,42,42,42	0
2	NA	C	602	1/1	0.97	0.08	39,39,39,39	0
2	NA	B	603	1/1	0.97	0.17	36,36,36,36	0
3	N0Q	A	605	21/33	0.97	0.10	22,25,50,64	9
3	N0Q	D	606	21/33	0.97	0.09	18,22,52,61	8
3	N0Q	E	606	13/33	0.97	0.06	18,19,28,32	1
3	N0Q	F	605	15/33	0.97	0.08	20,22,38,41	3
2	NA	D	603	1/1	0.98	0.10	31,31,31,31	0
2	NA	D	604	1/1	0.98	0.14	33,33,33,33	0
2	NA	E	602	1/1	0.98	0.08	27,27,27,27	0

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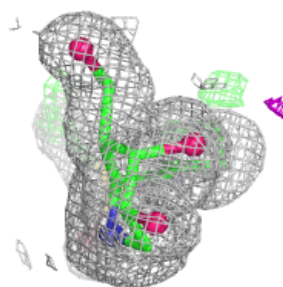
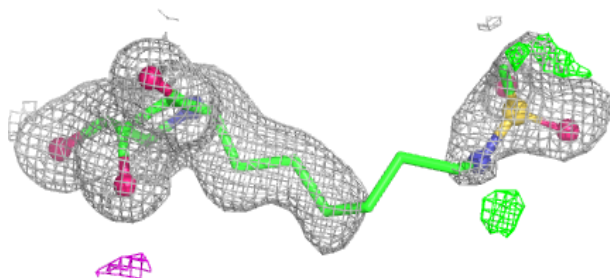
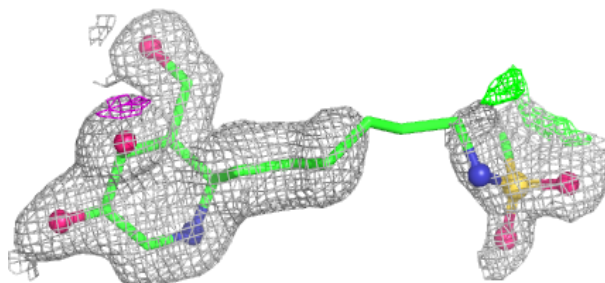
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	NA	E	604	1/1	0.98	0.07	35,35,35,35	0
2	NA	F	602	1/1	0.98	0.06	29,29,29,29	0
2	NA	G	604	1/1	0.98	0.07	34,34,34,34	0
2	NA	B	602	1/1	0.98	0.12	34,34,34,34	0
2	NA	A	604	1/1	0.98	0.06	39,39,39,39	0
3	N0Q	B	604	14/33	0.98	0.05	19,22,32,35	1
3	N0Q	C	605	13/33	0.98	0.06	19,24,31,40	0
2	NA	B	601	1/1	0.98	0.06	38,38,38,38	0
2	NA	C	603	1/1	0.98	0.04	47,47,47,47	0
2	NA	C	604	1/1	0.98	0.07	50,50,50,50	0
3	N0Q	G	606	15/33	0.98	0.06	17,22,33,37	2
3	N0Q	H	603	13/33	0.98	0.06	20,22,28,32	0
2	NA	F	603	1/1	0.99	0.04	35,35,35,35	0
2	NA	F	604	1/1	0.99	0.06	32,32,32,32	0
2	NA	G	601	1/1	0.99	0.02	26,26,26,26	0
2	NA	G	602	1/1	0.99	0.08	35,35,35,35	0
2	NA	G	603	1/1	0.99	0.04	29,29,29,29	0
2	NA	A	601	1/1	0.99	0.08	37,37,37,37	0
2	NA	G	605	1/1	0.99	0.11	33,33,33,33	0
2	NA	A	603	1/1	0.99	0.12	33,33,33,33	0
2	NA	H	602	1/1	0.99	0.07	30,30,30,30	0
2	NA	D	605	1/1	0.99	0.05	29,29,29,29	0
2	NA	E	601	1/1	0.99	0.03	30,30,30,30	0
2	NA	C	601	1/1	0.99	0.04	33,33,33,33	0
2	NA	E	603	1/1	0.99	0.05	28,28,28,28	0
2	NA	D	601	1/1	0.99	0.06	33,33,33,33	0
2	NA	E	605	1/1	0.99	0.09	29,29,29,29	0
2	NA	F	601	1/1	0.99	0.03	29,29,29,29	0
2	NA	D	602	1/1	0.99	0.05	31,31,31,31	0

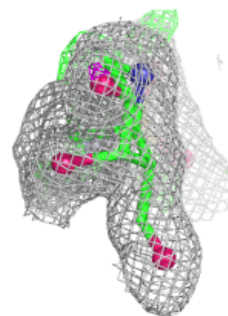
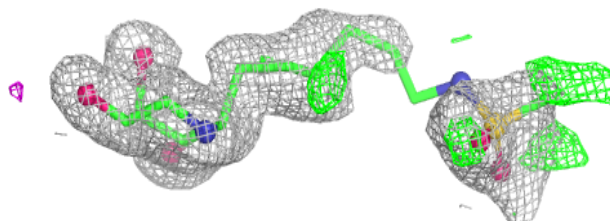
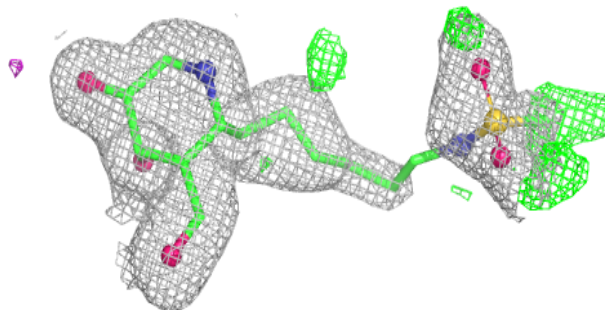
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around N0Q A 605:

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

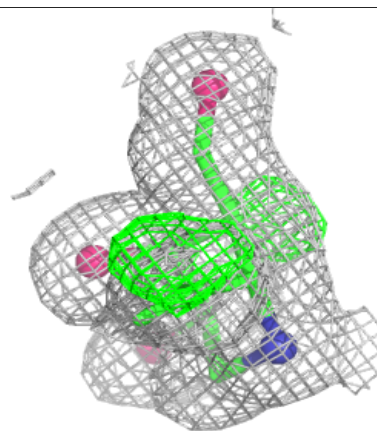
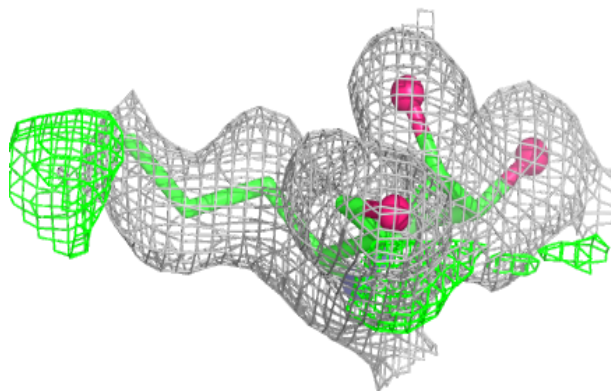
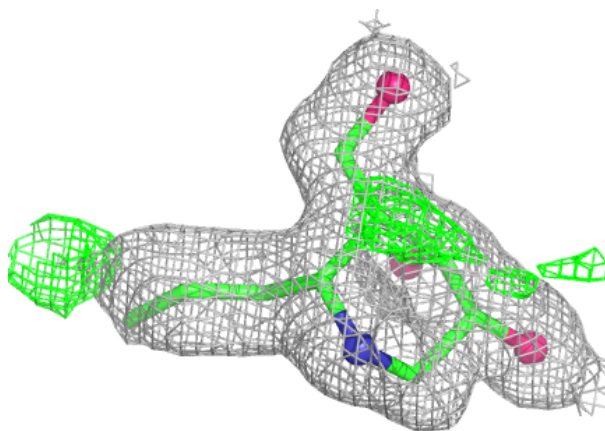
**Electron density around N0Q D 606:**

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



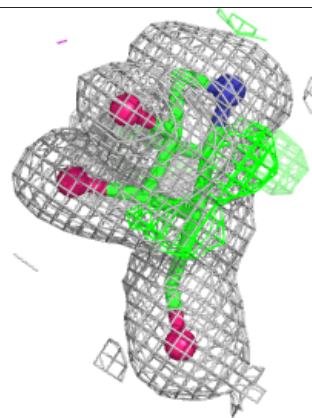
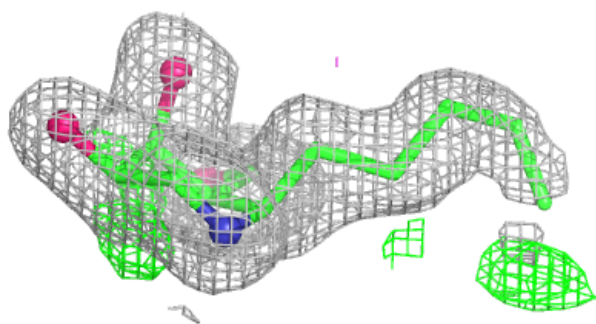
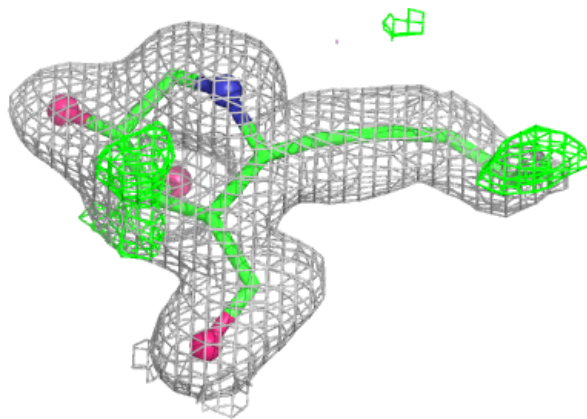
Electron density around N0Q E 606:

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



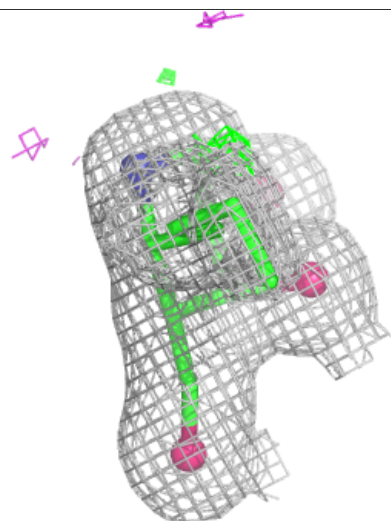
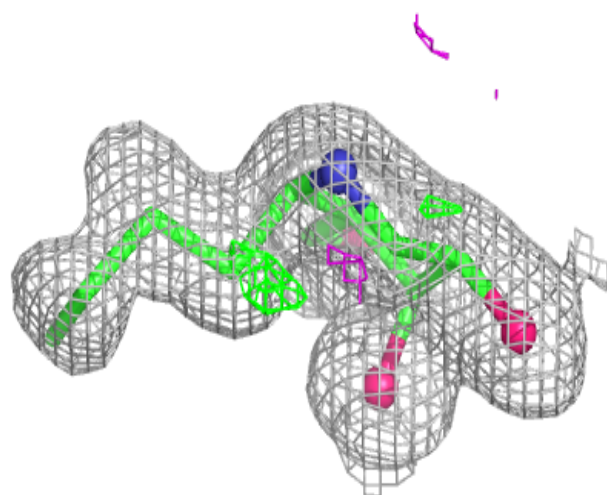
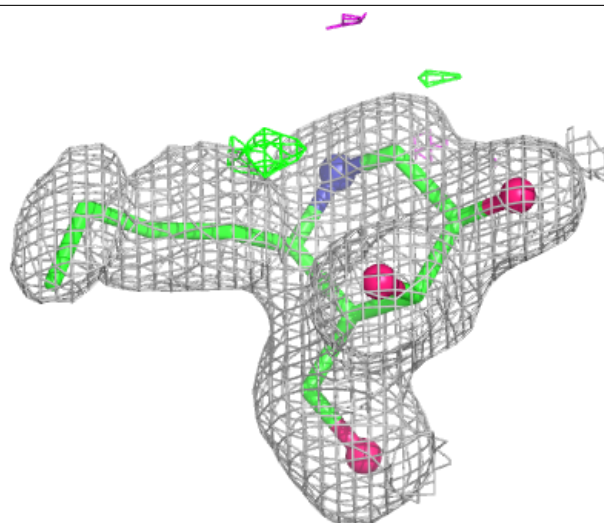
Electron density around N0Q F 605:

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



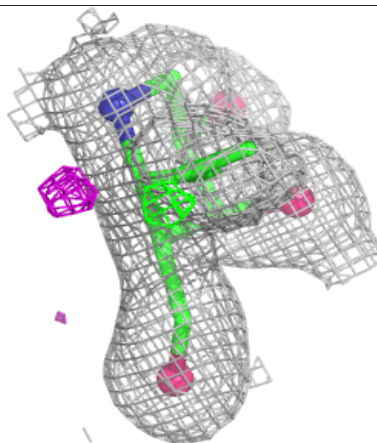
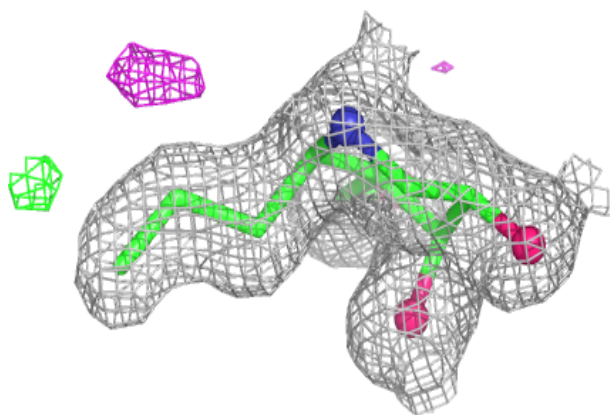
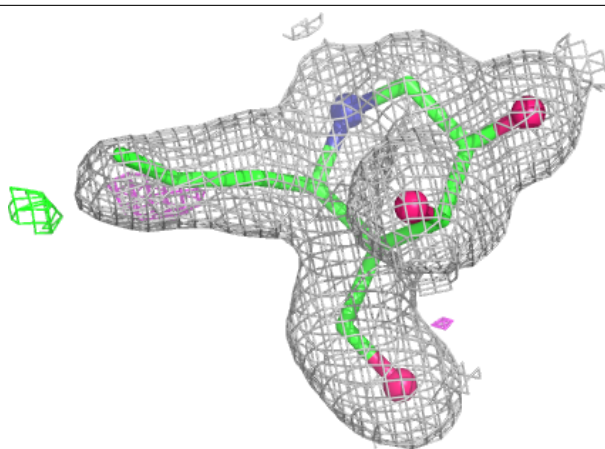
Electron density around N0Q B 604:

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

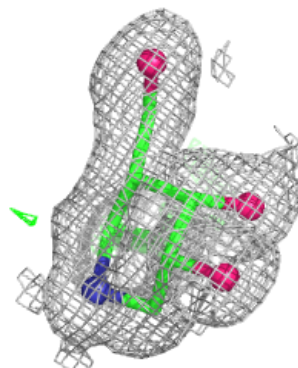
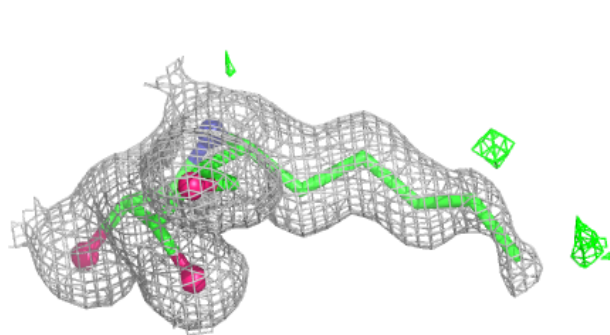
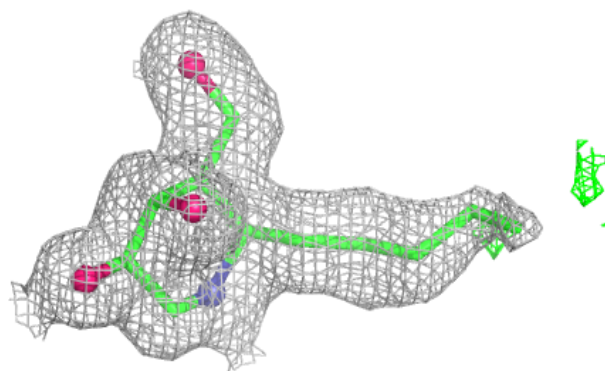


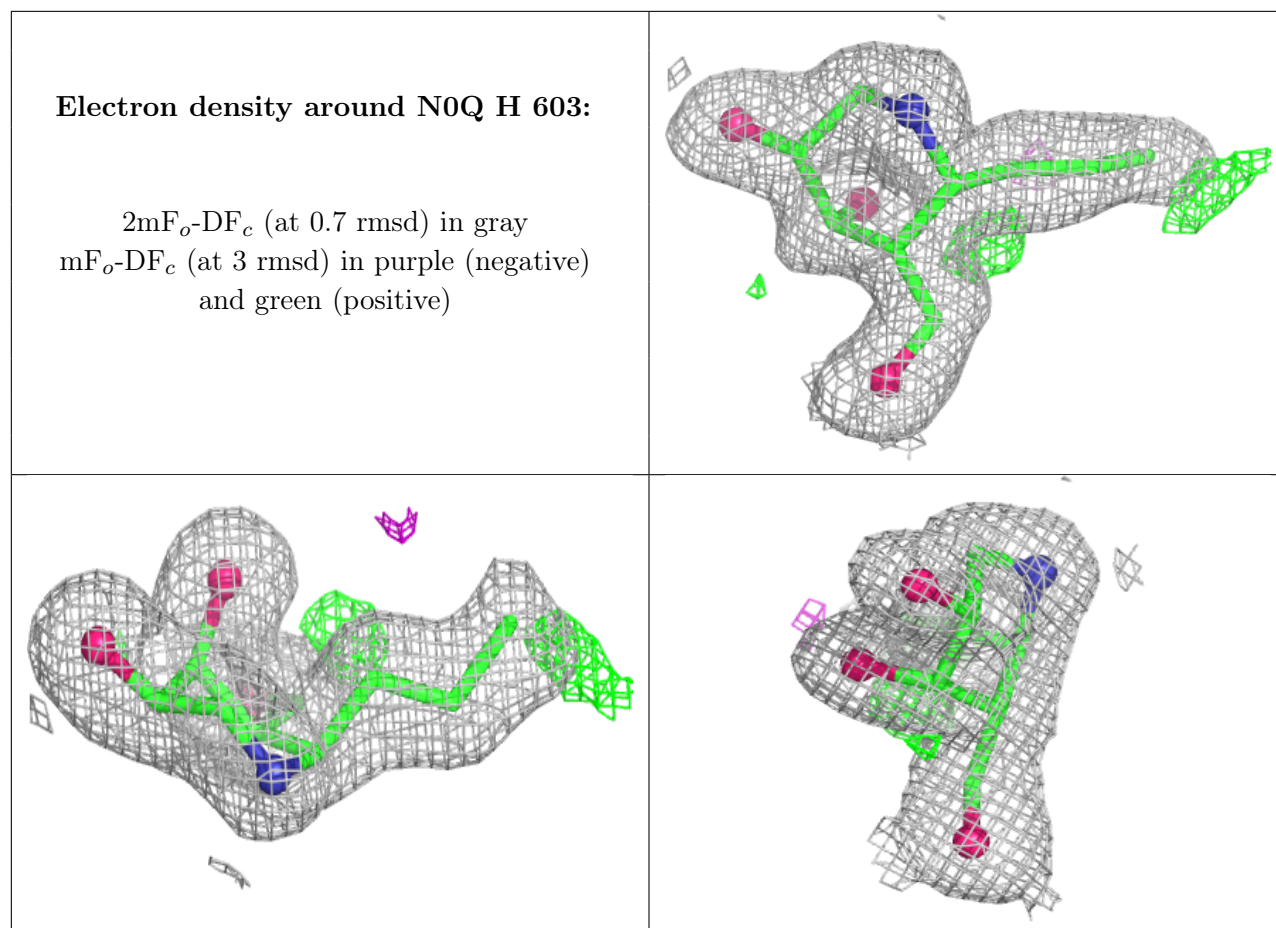
Electron density around N0Q C 605:

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

**Electron density around N0Q G 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 ⓘ

There are no such residues in this entry.