



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 03:57 AM UTC

PDB ID : 5OHS / pdb_00005ohs
Title : A GH31 family sulfoquinovosidase mutant D455N in complex with pNPSQ
Authors : Jin, Y.; Williams, S.J.; Goddard-Borger, E.; Davies, G.J.
Deposited on : 2017-07-18
Resolution : 1.97 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:

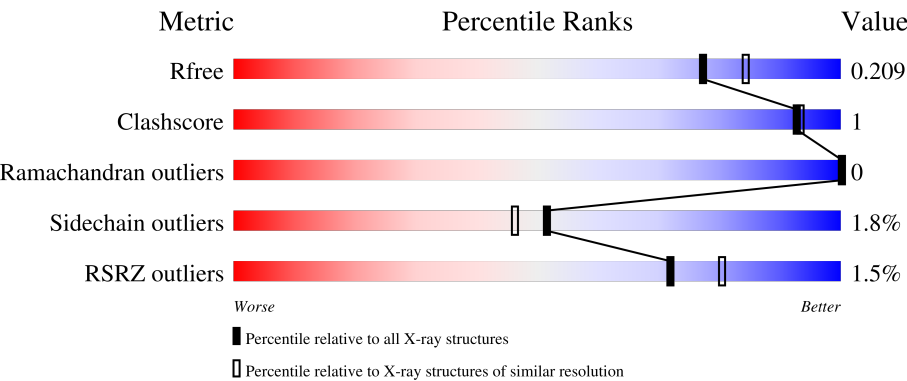
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal 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 1.97 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.



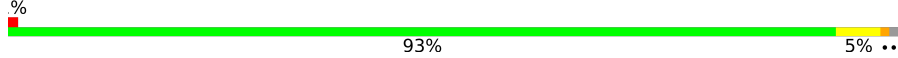
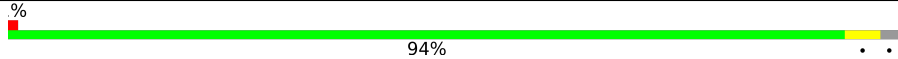
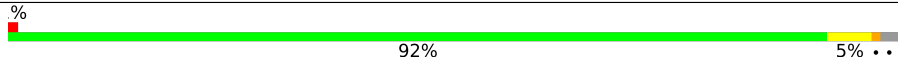
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R _{free}	180053	1506 (1.98-1.98)
Clashscore	190562	1534 (1.98-1.98)
Ramachandran outliers	187476	1518 (1.98-1.98)
Sidechain outliers	187428	1518 (1.98-1.98)
RSRZ outliers	180081	1506 (1.98-1.98)

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	672	% 92%6% .
1	B	672	% 93%5% ..
1	C	672	6% 92%6% ..
1	D	672	% 92%5% ..
1	E	672	94%. . .

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Mol	Chain	Length	Quality of chain
1	F	672	
1	G	672	
1	H	672	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	EDO	D	707	-	-	X	-

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 44146 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 Alpha-glucosidase yihQ.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	661	Total	C	N	O	S	0	1	0
			5207	3324	897	964	22			
1	B	663	Total	C	N	O	S	0	1	0
			5215	3330	897	966	22			
1	C	661	Total	C	N	O	S	0	1	0
			5183	3309	890	962	22			
1	D	662	Total	C	N	O	S	0	0	0
			5187	3314	890	962	21			
1	E	661	Total	C	N	O	S	0	1	0
			5206	3325	897	963	21			
1	F	664	Total	C	N	O	S	0	0	0
			5219	3331	899	968	21			
1	G	661	Total	C	N	O	S	0	0	0
			5186	3310	894	961	21			
1	H	661	Total	C	N	O	S	0	0	0
			5197	3318	894	964	21			

There are 88 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	370	ALA	GLU	engineered mutation	UNP A0A083ZKV2
A	371	ALA	GLU	engineered mutation	UNP A0A083ZKV2
A	455	ASN	ASP	engineered mutation	UNP A0A083ZKV2
A	665	LEU	-	expression tag	UNP A0A083ZKV2
A	666	GLU	-	expression tag	UNP A0A083ZKV2
A	667	HIS	-	expression tag	UNP A0A083ZKV2
A	668	HIS	-	expression tag	UNP A0A083ZKV2
A	669	HIS	-	expression tag	UNP A0A083ZKV2
A	670	HIS	-	expression tag	UNP A0A083ZKV2
A	671	HIS	-	expression tag	UNP A0A083ZKV2
A	672	HIS	-	expression tag	UNP A0A083ZKV2
B	370	ALA	GLU	engineered mutation	UNP A0A083ZKV2
B	371	ALA	GLU	engineered mutation	UNP A0A083ZKV2

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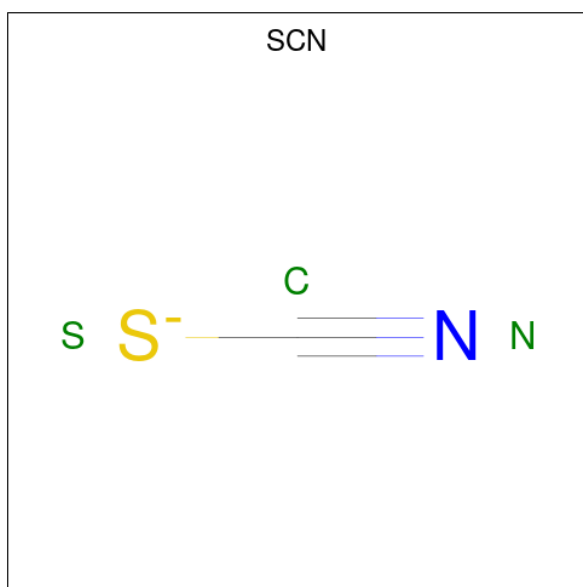
Chain	Residue	Modelled	Actual	Comment	Reference
B	455	ASN	ASP	engineered mutation	UNP A0A083ZKV2
B	665	LEU	-	expression tag	UNP A0A083ZKV2
B	666	GLU	-	expression tag	UNP A0A083ZKV2
B	667	HIS	-	expression tag	UNP A0A083ZKV2
B	668	HIS	-	expression tag	UNP A0A083ZKV2
B	669	HIS	-	expression tag	UNP A0A083ZKV2
B	670	HIS	-	expression tag	UNP A0A083ZKV2
B	671	HIS	-	expression tag	UNP A0A083ZKV2
B	672	HIS	-	expression tag	UNP A0A083ZKV2
C	370	ALA	GLU	engineered mutation	UNP A0A083ZKV2
C	371	ALA	GLU	engineered mutation	UNP A0A083ZKV2
C	455	ASN	ASP	engineered mutation	UNP A0A083ZKV2
C	665	LEU	-	expression tag	UNP A0A083ZKV2
C	666	GLU	-	expression tag	UNP A0A083ZKV2
C	667	HIS	-	expression tag	UNP A0A083ZKV2
C	668	HIS	-	expression tag	UNP A0A083ZKV2
C	669	HIS	-	expression tag	UNP A0A083ZKV2
C	670	HIS	-	expression tag	UNP A0A083ZKV2
C	671	HIS	-	expression tag	UNP A0A083ZKV2
C	672	HIS	-	expression tag	UNP A0A083ZKV2
D	370	ALA	GLU	engineered mutation	UNP A0A083ZKV2
D	371	ALA	GLU	engineered mutation	UNP A0A083ZKV2
D	455	ASN	ASP	engineered mutation	UNP A0A083ZKV2
D	665	LEU	-	expression tag	UNP A0A083ZKV2
D	666	GLU	-	expression tag	UNP A0A083ZKV2
D	667	HIS	-	expression tag	UNP A0A083ZKV2
D	668	HIS	-	expression tag	UNP A0A083ZKV2
D	669	HIS	-	expression tag	UNP A0A083ZKV2
D	670	HIS	-	expression tag	UNP A0A083ZKV2
D	671	HIS	-	expression tag	UNP A0A083ZKV2
D	672	HIS	-	expression tag	UNP A0A083ZKV2
E	370	ALA	GLU	engineered mutation	UNP A0A083ZKV2
E	371	ALA	GLU	engineered mutation	UNP A0A083ZKV2
E	455	ASN	ASP	engineered mutation	UNP A0A083ZKV2
E	665	LEU	-	expression tag	UNP A0A083ZKV2
E	666	GLU	-	expression tag	UNP A0A083ZKV2
E	667	HIS	-	expression tag	UNP A0A083ZKV2
E	668	HIS	-	expression tag	UNP A0A083ZKV2
E	669	HIS	-	expression tag	UNP A0A083ZKV2
E	670	HIS	-	expression tag	UNP A0A083ZKV2
E	671	HIS	-	expression tag	UNP A0A083ZKV2
E	672	HIS	-	expression tag	UNP A0A083ZKV2

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Chain	Residue	Modelled	Actual	Comment	Reference
F	370	ALA	GLU	engineered mutation	UNP A0A083ZKV2
F	371	ALA	GLU	engineered mutation	UNP A0A083ZKV2
F	455	ASN	ASP	engineered mutation	UNP A0A083ZKV2
F	665	LEU	-	expression tag	UNP A0A083ZKV2
F	666	GLU	-	expression tag	UNP A0A083ZKV2
F	667	HIS	-	expression tag	UNP A0A083ZKV2
F	668	HIS	-	expression tag	UNP A0A083ZKV2
F	669	HIS	-	expression tag	UNP A0A083ZKV2
F	670	HIS	-	expression tag	UNP A0A083ZKV2
F	671	HIS	-	expression tag	UNP A0A083ZKV2
F	672	HIS	-	expression tag	UNP A0A083ZKV2
G	370	ALA	GLU	engineered mutation	UNP A0A083ZKV2
G	371	ALA	GLU	engineered mutation	UNP A0A083ZKV2
G	455	ASN	ASP	engineered mutation	UNP A0A083ZKV2
G	665	LEU	-	expression tag	UNP A0A083ZKV2
G	666	GLU	-	expression tag	UNP A0A083ZKV2
G	667	HIS	-	expression tag	UNP A0A083ZKV2
G	668	HIS	-	expression tag	UNP A0A083ZKV2
G	669	HIS	-	expression tag	UNP A0A083ZKV2
G	670	HIS	-	expression tag	UNP A0A083ZKV2
G	671	HIS	-	expression tag	UNP A0A083ZKV2
G	672	HIS	-	expression tag	UNP A0A083ZKV2
H	370	ALA	GLU	engineered mutation	UNP A0A083ZKV2
H	371	ALA	GLU	engineered mutation	UNP A0A083ZKV2
H	455	ASN	ASP	engineered mutation	UNP A0A083ZKV2
H	665	LEU	-	expression tag	UNP A0A083ZKV2
H	666	GLU	-	expression tag	UNP A0A083ZKV2
H	667	HIS	-	expression tag	UNP A0A083ZKV2
H	668	HIS	-	expression tag	UNP A0A083ZKV2
H	669	HIS	-	expression tag	UNP A0A083ZKV2
H	670	HIS	-	expression tag	UNP A0A083ZKV2
H	671	HIS	-	expression tag	UNP A0A083ZKV2
H	672	HIS	-	expression tag	UNP A0A083ZKV2

- Molecule 2 is THIOCYANATE ION (CCD ID: SCN) (formula: CNS).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	S	0	0
			3	1	1	1		
2	A	1	Total	C	N	S	0	0
			3	1	1	1		
2	D	1	Total	C	N	S	0	0
			3	1	1	1		
2	E	1	Total	C	N	S	0	0
			3	1	1	1		
2	F	1	Total	C	N	S	0	0
			3	1	1	1		
2	F	1	Total	C	N	S	0	0
			3	1	1	1		
2	G	1	Total	C	N	S	0	0
			3	1	1	1		
2	H	1	Total	C	N	S	0	0
			3	1	1	1		

- Molecule 3 is (4S)-2-METHYL-2,4-PENTANEDIOL (CCD ID: MPD) (formula: C₆H₁₄O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			8	6	2		
3	A	1	Total	C	O	0	0
			8	6	2		
3	A	1	Total	C	O	0	0
			8	6	2		
3	B	1	Total	C	O	0	0
			8	6	2		
3	D	1	Total	C	O	0	0
			8	6	2		
3	D	1	Total	C	O	0	0
			8	6	2		
3	E	1	Total	C	O	0	0
			8	6	2		
3	F	1	Total	C	O	0	0
			8	6	2		
3	F	1	Total	C	O	0	0
			8	6	2		

- Molecule 4 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

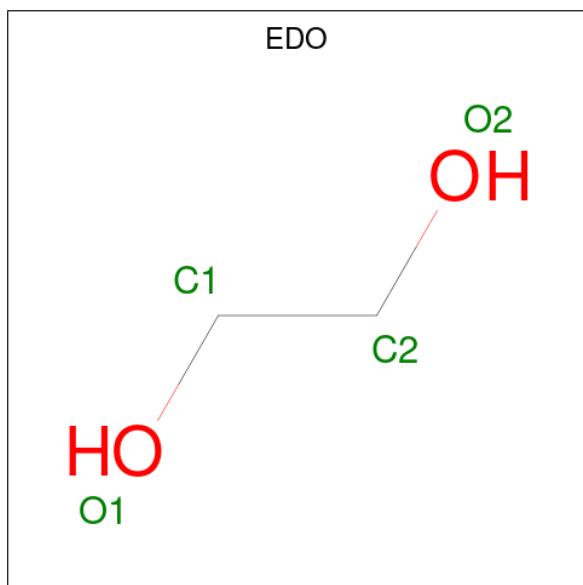
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Cl	0	0
			1	1		
4	B	1	Total	Cl	0	0
			1	1		
4	E	1	Total	Cl	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	F	1	Total	Cl	0	0
			1	1		
4	G	1	Total	Cl	0	0
			1	1		
4	H	1	Total	Cl	0	0
			1	1		

- Molecule 5 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: $C_2H_6O_2$).



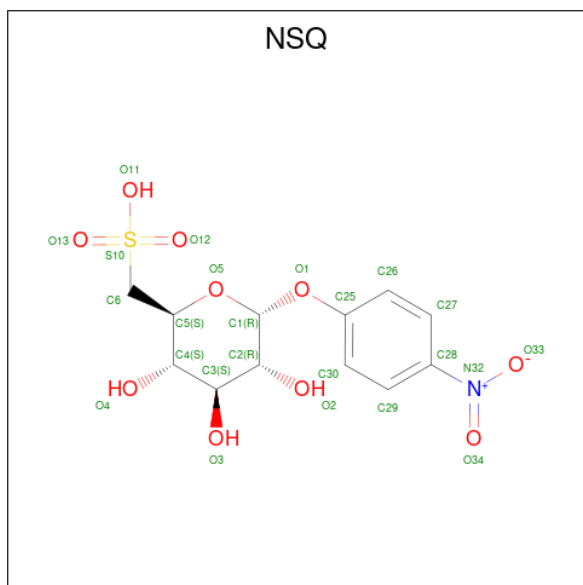
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			4	2	2		
5	A	1	Total	C	O	0	0
			4	2	2		
5	B	1	Total	C	O	0	0
			4	2	2		
5	B	1	Total	C	O	0	0
			4	2	2		
5	C	1	Total	C	O	0	0
			4	2	2		
5	D	1	Total	C	O	0	0
			4	2	2		
5	D	1	Total	C	O	0	0
			4	2	2		
5	D	1	Total	C	O	0	0
			4	2	2		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	E	1	Total	C	O	0	0
			4	2	2		
5	F	1	Total	C	O	0	0
			4	2	2		
5	F	1	Total	C	O	0	0
			4	2	2		
5	F	1	Total	C	O	0	0
			4	2	2		
5	F	1	Total	C	O	0	0
			4	2	2		
5	G	1	Total	C	O	0	0
			4	2	2		
5	G	1	Total	C	O	0	0
			4	2	2		
5	G	1	Total	C	O	0	0
			4	2	2		
5	H	1	Total	C	O	0	0
			4	2	2		

- Molecule 6 is 4-nitrophenyl alpha-D-6-sulfoquinovoside (CCD ID: NSQ) (formula: $C_{12}H_{15}NO_{10}S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	A	1	Total	C	N	O	S	0	0
			24	12	1	10	1		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	B	1	Total	C	N	O	S	0	0
			24	12	1	10	1		
6	C	1	Total	C	N	O	S	0	0
			24	12	1	10	1		
6	D	1	Total	C	N	O	S	0	0
			24	12	1	10	1		
6	E	1	Total	C	N	O	S	0	0
			24	12	1	10	1		
6	F	1	Total	C	N	O	S	0	0
			24	12	1	10	1		
6	G	1	Total	C	N	O	S	0	0
			24	12	1	10	1		
6	H	1	Total	C	N	O	S	0	0
			24	12	1	10	1		

- Molecule 7 is POTASSIUM ION (CCD ID: K) (formula: K).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	C	1	Total	K	0	0
			1	1		
7	D	1	Total	K	0	0
			1	1		

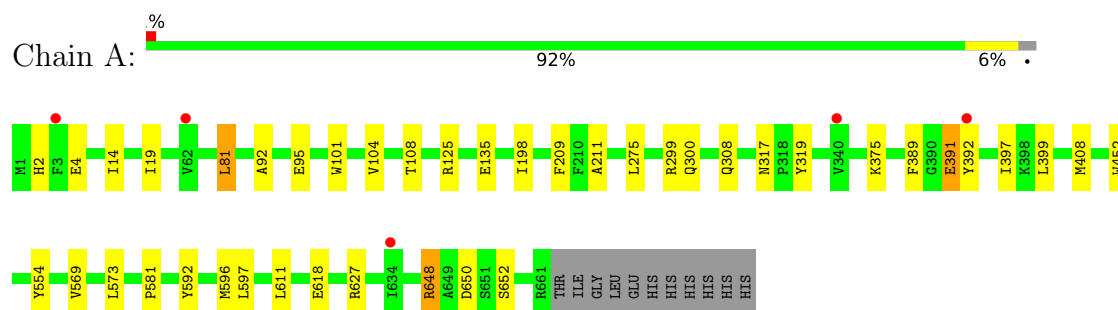
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	296	Total	O	0	2
			298	298		
8	B	265	Total	O	0	0
			265	265		
8	C	237	Total	O	0	1
			238	238		
8	D	305	Total	O	0	2
			307	307		
8	E	270	Total	O	0	2
			272	272		
8	F	292	Total	O	0	2
			294	294		
8	G	231	Total	O	0	0
			231	231		
8	H	272	Total	O	0	1
			273	273		

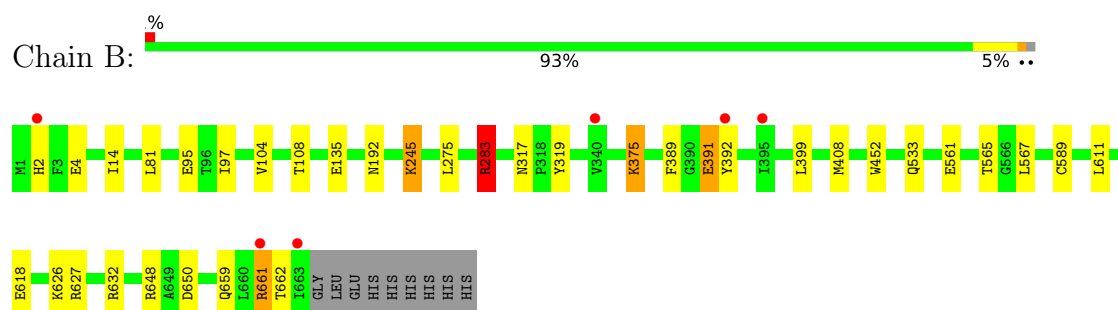
3 Residue-property plots

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

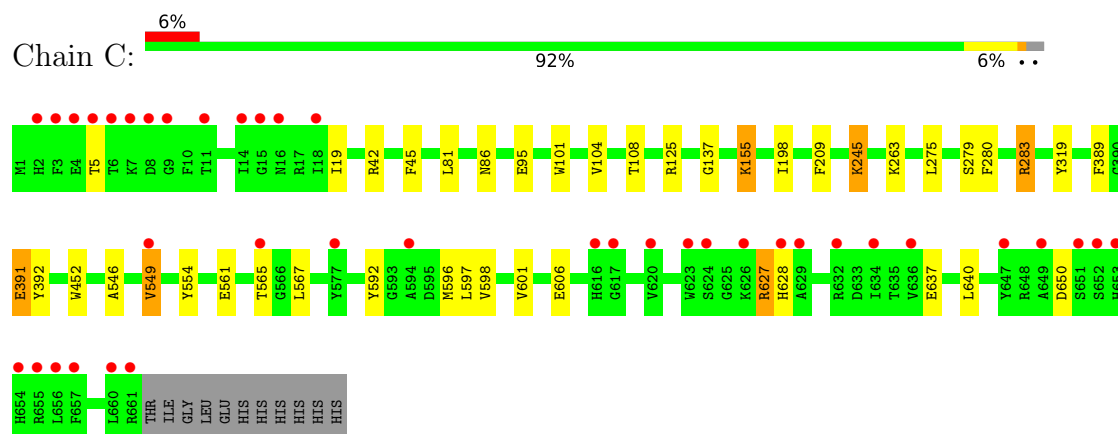
- Molecule 1: Alpha-glucosidase yihQ



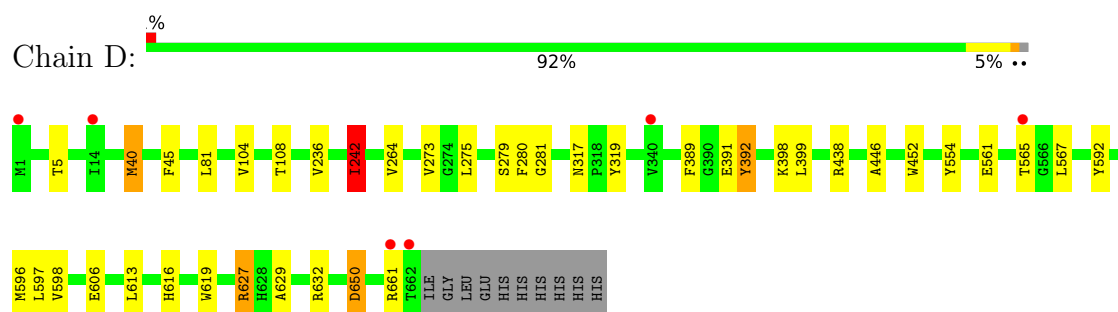
- Molecule 1: Alpha-glucosidase yihQ



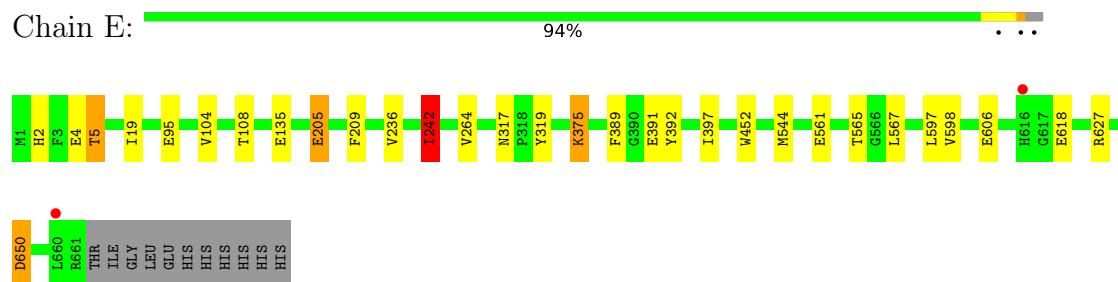
- Molecule 1: Alpha-glucosidase yihQ



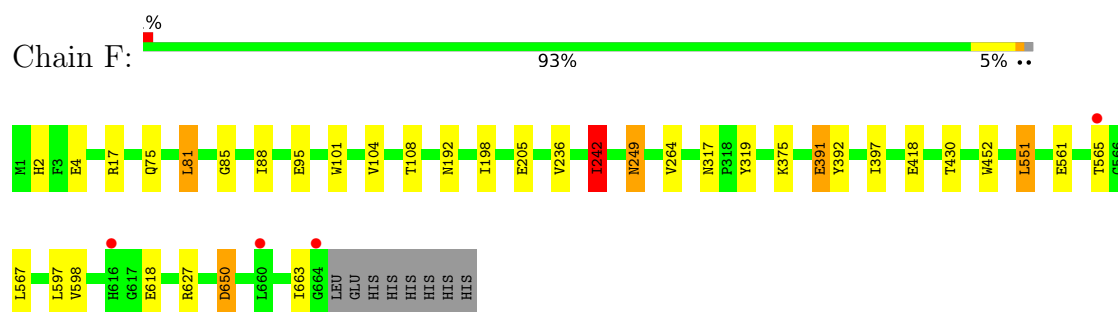
- Molecule 1: Alpha-glucosidase yihQ



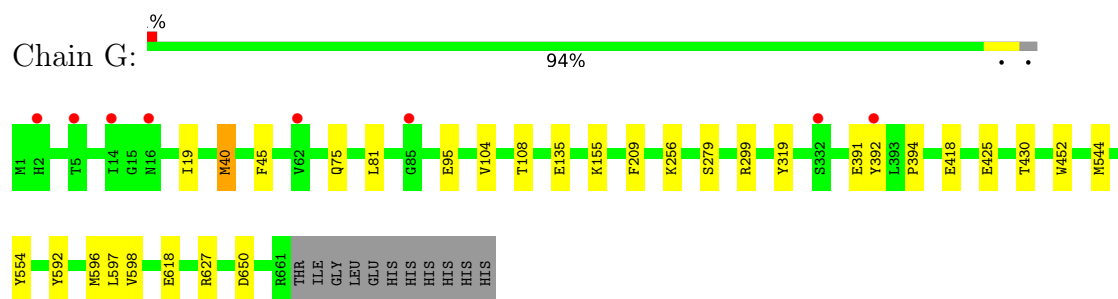
- Molecule 1: Alpha-glucosidase yihQ



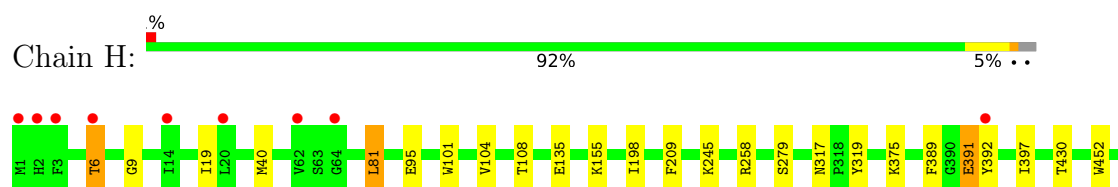
- Molecule 1: Alpha-glucosidase yihQ



- Molecule 1: Alpha-glucosidase yihQ



- Molecule 1: Alpha-glucosidase yihQ





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	104.20Å 169.19Å 169.69Å 90.00° 92.80° 90.00°	Depositor
Resolution (Å)	75.77 – 1.97 75.77 – 1.97	Depositor EDS
% Data completeness (in resolution range)	99.8 (75.77-1.97) 99.8 (75.77-1.97)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.34 (at 1.97Å)	Xtriage
Refinement program	REFMAC 5.8.0158	Depositor
R, R_{free}	0.181 , 0.203 0.188 , 0.209	Depositor DCC
R_{free} test set	20006 reflections (4.86%)	wwPDB-VP
Wilson B-factor (Å ²)	25.8	Xtriage
Anisotropy	0.395	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 44.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.000 for -h,l,k 0.000 for -h,-l,-k 0.020 for h,-k,-l	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	44146	wwPDB-VP
Average B, all atoms (Å ²)	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 40.30 % 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 2.7939e-04. 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: CL, NSQ, SCN, MPD, EDO, K

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	1.16	11/5359 (0.2%)	1.02	5/7286 (0.1%)
1	B	1.14	10/5367 (0.2%)	1.06	14/7299 (0.2%)
1	C	1.14	7/5332 (0.1%)	1.05	13/7251 (0.2%)
1	D	1.17	11/5334 (0.2%)	1.05	13/7254 (0.2%)
1	E	1.11	4/5358 (0.1%)	1.02	10/7284 (0.1%)
1	F	1.16	8/5368 (0.1%)	1.03	9/7300 (0.1%)
1	G	1.08	9/5335 (0.2%)	0.98	7/7257 (0.1%)
1	H	1.12	9/5345 (0.2%)	1.01	11/7268 (0.2%)
All	All	1.14	69/42798 (0.2%)	1.03	82/58199 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	F	0	1
All	All	0	2

All (69) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	245	LYS	CB-CG	-9.70	1.23	1.52
1	G	319	TYR	CZ-OH	7.98	1.54	1.38
1	B	245	LYS	CB-CG	-7.91	1.28	1.52
1	H	319	TYR	CZ-OH	7.86	1.54	1.38
1	B	319	TYR	CZ-OH	7.75	1.54	1.38
1	C	245	LYS	CA-CB	7.62	1.64	1.53
1	D	438	ARG	CZ-NH2	7.37	1.43	1.33
1	H	650	ASP	CB-CG	-7.26	1.33	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	391	GLU	CD-OE1	-6.98	1.12	1.25
1	D	650	ASP	CB-CG	-6.95	1.34	1.52
1	A	648	ARG	CD-NE	-6.93	1.36	1.46
1	G	430	THR	C-O	-6.88	1.15	1.23
1	F	650	ASP	CB-CG	-6.84	1.34	1.52
1	B	245	LYS	CA-CB	6.83	1.63	1.53
1	E	650	ASP	CB-CG	-6.67	1.35	1.52
1	H	430	THR	C-O	-6.66	1.16	1.23
1	A	135	GLU	CD-OE1	6.59	1.37	1.25
1	A	211	ALA	C-O	-6.59	1.15	1.23
1	A	319	TYR	CZ-OH	6.54	1.51	1.38
1	A	569	VAL	CA-C	6.42	1.61	1.52
1	H	245	LYS	CD-CE	-6.34	1.33	1.52
1	D	280	PHE	CA-CB	6.26	1.64	1.53
1	G	391	GLU	CD-OE1	-6.17	1.13	1.25
1	A	92	ALA	C-O	-6.16	1.16	1.24
1	B	275	LEU	C-O	-6.14	1.16	1.23
1	C	42	ARG	CZ-NH1	6.08	1.41	1.32
1	H	391	GLU	CD-OE1	-6.08	1.13	1.25
1	F	85	GLY	C-O	-6.06	1.15	1.24
1	F	249	ASN	CG-OD1	6.02	1.34	1.23
1	D	281	GLY	N-CA	6.00	1.52	1.45
1	B	283	ARG	CD-NE	-5.97	1.37	1.46
1	G	45	PHE	C-O	-5.96	1.16	1.24
1	E	319	TYR	CZ-OH	5.89	1.50	1.38
1	B	97	ILE	C-O	-5.89	1.18	1.24
1	F	249	ASN	CB-CG	-5.86	1.37	1.52
1	D	273	VAL	C-O	-5.85	1.17	1.24
1	C	391	GLU	C-O	-5.83	1.16	1.24
1	C	279	SER	C-O	-5.82	1.16	1.24
1	F	249	ASN	CG-ND2	5.78	1.45	1.33
1	D	279	SER	C-O	-5.78	1.16	1.24
1	F	319	TYR	CZ-OH	5.74	1.50	1.38
1	H	135	GLU	CD-OE1	5.73	1.36	1.25
1	C	280	PHE	CA-CB	5.57	1.62	1.53
1	A	81	LEU	CB-CG	-5.54	1.42	1.53
1	D	399	LEU	N-CA	-5.54	1.39	1.45
1	D	616	HIS	C-O	-5.54	1.16	1.24
1	E	135	GLU	CD-OE1	5.54	1.35	1.25
1	F	418	GLU	CA-C	5.46	1.59	1.52
1	A	275	LEU	C-O	-5.43	1.17	1.23
1	D	629	ALA	C-O	5.38	1.30	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	H	649	ALA	C-O	-5.35	1.17	1.24
1	E	205	GLU	CD-OE2	5.33	1.35	1.25
1	B	135	GLU	CD-OE1	5.30	1.35	1.25
1	G	279	SER	CB-OG	-5.26	1.31	1.42
1	G	418	GLU	CA-C	5.22	1.59	1.52
1	G	544	MET	SD-CE	-5.21	1.66	1.79
1	G	425	GLU	CG-CD	5.19	1.65	1.52
1	H	81	LEU	CB-CG	-5.18	1.43	1.53
1	H	279	SER	CB-OG	-5.18	1.31	1.42
1	A	300	GLN	CD-OE1	5.15	1.33	1.23
1	F	430	THR	C-O	-5.12	1.17	1.24
1	B	533	GLN	C-O	-5.12	1.17	1.24
1	C	137	GLY	C-O	-5.11	1.18	1.24
1	D	81	LEU	CB-CG	-5.10	1.43	1.53
1	G	40	MET	C-O	-5.06	1.17	1.24
1	A	391	GLU	CD-OE1	-5.06	1.15	1.25
1	D	40	MET	C-O	-5.04	1.18	1.24
1	B	192	ASN	CG-ND2	5.02	1.43	1.33
1	A	299	ARG	NE-CZ	5.01	1.38	1.33

All (82) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	283	ARG	NE-CZ-NH2	14.21	131.99	119.20
1	C	245	LYS	N-CA-CB	-14.12	91.88	111.65
1	B	245	LYS	N-CA-CB	-13.78	92.36	111.65
1	B	283	ARG	NE-CZ-NH1	-12.30	109.20	121.50
1	D	650	ASP	N-CA-C	8.83	123.82	112.34
1	E	650	ASP	N-CA-C	8.77	123.74	112.34
1	F	650	ASP	N-CA-C	8.74	123.70	112.34
1	C	86	ASN	CA-CB-CG	-8.30	104.30	112.60
1	D	392	TYR	CA-CB-CG	8.10	128.49	113.90
1	C	392	TYR	CA-CB-CG	8.09	128.46	113.90
1	H	650	ASP	N-CA-C	8.03	122.78	112.34
1	G	425	GLU	CA-CB-CG	7.66	129.41	114.10
1	C	650	ASP	N-CA-C	7.49	122.00	113.01
1	H	632	ARG	CA-CB-CG	7.43	128.97	114.10
1	H	650	ASP	CB-CA-C	-7.29	93.85	110.18
1	A	650	ASP	N-CA-C	6.94	121.45	113.19
1	F	650	ASP	CB-CA-C	-6.84	94.85	110.18
1	E	650	ASP	CB-CA-C	-6.84	94.85	110.18
1	G	650	ASP	N-CA-C	6.83	121.32	113.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	650	ASP	CB-CA-C	-6.76	95.03	110.18
1	E	242	ILE	CB-CG1-CD1	-6.76	99.60	113.80
1	F	242	ILE	CB-CG1-CD1	-6.76	99.60	113.80
1	E	375	LYS	CA-CB-CG	6.68	127.46	114.10
1	E	4	GLU	CB-CG-CD	6.61	123.84	112.60
1	C	549	VAL	CA-CB-CG1	6.56	121.55	110.40
1	B	650	ASP	N-CA-C	6.55	120.99	113.19
1	C	125	ARG	NE-CZ-NH2	6.55	125.09	119.20
1	H	632	ARG	CB-CA-C	-6.38	95.40	109.56
1	D	242	ILE	CB-CG1-CD1	-6.23	100.71	113.80
1	F	17	ARG	NE-CZ-NH1	6.17	127.67	121.50
1	B	661	ARG	CD-NE-CZ	5.98	132.78	124.40
1	E	2	HIS	N-CA-CB	5.93	120.65	110.68
1	B	392	TYR	CB-CA-C	-5.93	101.47	111.02
1	G	544	MET	CG-SD-CE	-5.93	87.85	100.90
1	D	627	ARG	CG-CD-NE	-5.91	98.99	112.00
1	C	391	GLU	N-CA-C	5.89	120.47	113.28
1	C	627	ARG	CG-CD-NE	-5.89	99.04	112.00
1	H	392	TYR	CB-CA-C	-5.89	101.54	111.02
1	D	40	MET	CG-SD-CE	-5.89	87.95	100.90
1	G	279	SER	CB-CA-C	-5.84	99.82	110.63
1	E	392	TYR	CB-CA-C	-5.83	101.64	111.02
1	C	155	LYS	CG-CD-CE	5.82	124.68	111.30
1	G	392	TYR	CB-CA-C	-5.78	101.72	111.02
1	D	319	TYR	OH-CZ-CE2	5.71	137.03	119.90
1	D	632	ARG	CG-CD-NE	-5.71	99.44	112.00
1	B	626	LYS	CA-CB-CG	5.68	125.45	114.10
1	F	663	ILE	N-CA-C	-5.63	104.88	110.62
1	C	319	TYR	OH-CZ-CE2	5.61	136.73	119.90
1	B	661	ARG	NE-CZ-NH1	5.59	127.09	121.50
1	A	375	LYS	CG-CD-CE	-5.49	98.66	111.30
1	B	283	ARG	CB-CG-CD	-5.49	98.66	111.30
1	B	661	ARG	N-CA-C	-5.47	104.54	111.11
1	C	155	LYS	CB-CG-CD	5.47	123.88	111.30
1	D	650	ASP	N-CA-CB	-5.44	100.39	110.18
1	H	375	LYS	CG-CD-CE	-5.44	98.79	111.30
1	H	40	MET	CB-CG-SD	5.42	128.97	112.70
1	A	392	TYR	CB-CA-C	-5.40	102.33	111.02
1	F	551	LEU	CA-CB-CG	5.39	135.18	116.30
1	F	317	ASN	CB-CA-C	5.39	117.75	110.37
1	H	279	SER	CB-CA-C	-5.35	100.74	110.63
1	E	544	MET	CG-SD-CE	-5.34	89.16	100.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	392	TYR	CB-CA-C	-5.29	102.49	111.02
1	D	661	ARG	N-CA-C	-5.26	104.79	111.11
1	B	375	LYS	CG-CD-CE	5.23	123.33	111.30
1	H	544	MET	CG-SD-CE	-5.21	89.44	100.90
1	H	317	ASN	CB-CA-C	5.20	117.50	110.37
1	B	632	ARG	CG-CD-NE	-5.20	100.56	112.00
1	D	275	LEU	CA-C-O	-5.17	115.16	121.36
1	G	299	ARG	CG-CD-NE	5.17	123.37	112.00
1	G	40	MET	CB-CG-SD	5.16	128.19	112.70
1	A	317	ASN	CB-CA-C	5.15	117.42	110.37
1	B	375	LYS	CB-CG-CD	5.13	123.11	111.30
1	E	317	ASN	CB-CA-C	5.09	117.34	110.37
1	B	317	ASN	CB-CA-C	5.08	117.33	110.37
1	F	650	ASP	N-CA-CB	-5.08	101.04	110.18
1	D	319	TYR	CB-CG-CD1	-5.07	113.20	120.80
1	H	632	ARG	N-CA-CB	-5.06	102.11	111.53
1	E	5	THR	CA-CB-OG1	-5.05	102.02	109.60
1	D	317	ASN	CB-CA-C	5.05	117.29	110.37
1	C	275	LEU	CD1-CG-CD2	5.05	121.91	110.80
1	C	283	ARG	CB-CG-CD	5.02	122.84	111.30
1	A	125	ARG	NE-CZ-NH2	5.01	123.71	119.20

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	308	GLN	Sidechain
1	F	391	GLU	Sidechain

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5207	0	4962	25	0
1	B	5215	0	4965	11	0
1	C	5183	0	4933	22	0
1	D	5187	0	4931	18	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	E	5206	0	4964	9	0
1	F	5219	0	4967	17	0
1	G	5186	0	4918	9	0
1	H	5197	0	4945	22	0
2	A	6	0	0	0	0
2	D	3	0	0	0	0
2	E	3	0	0	0	0
2	F	6	0	0	0	0
2	G	3	0	0	0	0
2	H	3	0	0	0	0
3	A	24	0	42	2	0
3	B	8	0	14	0	0
3	D	16	0	28	0	0
3	E	8	0	14	0	0
3	F	16	0	28	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	E	1	0	0	0	0
4	F	1	0	0	0	0
4	G	1	0	0	0	0
4	H	1	0	0	0	0
5	A	8	0	12	0	0
5	B	8	0	12	0	0
5	C	4	0	6	0	0
5	D	12	0	18	6	0
5	E	4	0	6	0	0
5	F	20	0	30	0	0
5	G	12	0	18	0	0
5	H	4	0	6	0	0
6	A	24	0	5	0	0
6	B	24	0	5	2	0
6	C	24	0	5	0	0
6	D	24	0	4	0	0
6	E	24	0	4	0	0
6	F	24	0	5	0	0
6	G	24	0	5	0	0
6	H	24	0	5	0	0
7	C	1	0	0	0	0
7	D	1	0	0	0	0
8	A	298	0	0	1	0
8	B	265	0	0	1	0
8	C	238	0	0	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	D	307	0	0	2	0
8	E	272	0	0	1	0
8	F	294	0	0	2	0
8	G	231	0	0	3	0
8	H	273	0	0	3	0
All	All	44146	0	39857	121	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 1.

All (121) 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:81:LEU:HD11	1:F:88:ILE:CG2	2.04	0.87
1:F:81:LEU:CD1	1:F:88:ILE:CG2	2.57	0.82
1:H:623:TRP:CD1	1:H:642:GLU:HG3	2.17	0.79
1:C:561:GLU:O	1:C:565:THR:HG22	1.83	0.79
1:E:561:GLU:O	1:E:565:THR:HG22	1.84	0.78
1:B:561:GLU:O	1:B:565:THR:HG22	1.83	0.78
1:F:561:GLU:O	1:F:565:THR:HG22	1.84	0.78
1:D:561:GLU:O	1:D:565:THR:HG22	1.83	0.77
1:D:392:TYR:CE1	5:D:707:EDO:H12	2.21	0.75
1:B:589[A]:CYS:SG	8:B:828:HOH:O	2.46	0.71
1:F:81:LEU:CD1	1:F:88:ILE:HG23	2.20	0.70
1:F:81:LEU:HD11	1:F:88:ILE:HG23	1.75	0.68
1:C:263:LYS:HG3	1:C:549:VAL:HG11	1.78	0.66
1:A:648:ARG:NH2	1:C:627:ARG:NH2	2.44	0.65
1:G:135:GLU:OE1	8:G:801:HOH:O	2.14	0.65
1:F:81:LEU:HD11	1:F:88:ILE:HG21	1.78	0.65
1:F:242:ILE:HD11	1:F:264:VAL:HG22	1.81	0.63
1:C:45:PHE:HE1	8:C:872:HOH:O	1.82	0.63
3:A:704:MPD:H12	8:A:838:HOH:O	1.99	0.61
1:A:2:HIS:NE2	1:A:4:GLU:OE1	2.34	0.60
1:D:446:ALA:O	5:D:706:EDO:H12	2.01	0.59
1:C:637:GLU:O	8:C:801:HOH:O	2.16	0.59
1:D:40:MET:HB2	5:D:707:EDO:O2	2.02	0.59
1:E:242:ILE:HD11	1:E:264:VAL:HG22	1.84	0.58
1:H:623:TRP:HD1	1:H:642:GLU:HG3	1.66	0.58
1:D:242:ILE:HD11	1:D:264:VAL:HG22	1.86	0.58
1:D:392:TYR:CD1	5:D:707:EDO:C1	2.87	0.57
1:F:2:HIS:NE2	1:F:4:GLU:OE1	2.36	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:601:VAL:HG23	8:C:998:HOH:O	2.04	0.57
1:A:652:SER:HB2	1:C:628:HIS:HA	1.87	0.56
1:H:642:GLU:OE1	8:H:801:HOH:O	2.18	0.56
1:D:392:TYR:CE1	5:D:707:EDO:C1	2.88	0.56
1:B:2:HIS:NE2	1:B:4:GLU:OE1	2.34	0.55
1:A:652:SER:HB3	1:C:627:ARG:O	2.07	0.55
1:D:392:TYR:CD1	5:D:707:EDO:H12	2.42	0.55
1:F:205:GLU:HG2	8:F:815:HOH:O	2.07	0.55
1:D:613:LEU:HG	1:D:619:TRP:CD1	2.42	0.54
1:D:45:PHE:HE1	8:D:830:HOH:O	1.91	0.54
1:D:554:TYR:CD2	1:D:596:MET:HE2	2.43	0.54
1:C:546:ALA:HA	1:C:549:VAL:HG12	1.90	0.54
1:E:618:GLU:OE1	1:E:627:ARG:NH1	2.42	0.53
1:C:263:LYS:HG3	1:C:549:VAL:CG1	2.37	0.53
1:C:554:TYR:CD2	1:C:596:MET:HE2	2.44	0.53
1:F:81:LEU:HD12	1:F:88:ILE:HG23	1.90	0.53
1:G:592:TYR:HD2	1:G:596:MET:HE3	1.74	0.52
1:H:554:TYR:CD2	1:H:596:MET:HE2	2.45	0.52
1:D:592:TYR:HD2	1:D:596:MET:HE3	1.74	0.52
1:F:618:GLU:OE1	1:F:627:ARG:NH1	2.42	0.52
1:B:659:GLN:O	1:B:662:THR:HB	2.09	0.51
1:G:554:TYR:CD2	1:G:596:MET:HE2	2.45	0.51
1:H:618:GLU:OE1	1:H:627:ARG:NH1	2.42	0.51
1:A:618:GLU:OE1	1:A:627:ARG:NH1	2.40	0.50
1:G:618:GLU:OE1	1:G:627:ARG:NH1	2.40	0.50
1:A:554:TYR:CD2	1:A:596:MET:HE2	2.47	0.50
1:C:592:TYR:HD2	1:C:596:MET:HE3	1.76	0.50
1:A:581:PRO:HB3	3:A:704:MPD:H13	1.92	0.50
1:A:592:TYR:HD2	1:A:596:MET:HE3	1.76	0.50
1:A:592:TYR:CD2	1:A:596:MET:HE3	2.47	0.50
1:D:592:TYR:CD2	1:D:596:MET:HE3	2.47	0.49
1:B:618:GLU:OE1	1:B:627:ARG:NH1	2.43	0.49
1:A:652:SER:CB	1:C:627:ARG:O	2.61	0.48
1:D:398:LYS:NZ	8:D:812:HOH:O	2.46	0.48
1:B:283:ARG:HD2	6:B:705:NSQ:S10	2.54	0.47
1:H:6:THR:HG22	1:H:9:GLY:C	2.39	0.47
1:H:592:TYR:CD2	1:H:596:MET:HE3	2.48	0.47
1:C:565:THR:HG23	1:C:567:LEU:H	1.79	0.47
1:G:592:TYR:CD2	1:G:596:MET:HE3	2.48	0.47
1:H:592:TYR:HD2	1:H:596:MET:HE3	1.79	0.47
1:D:565:THR:HG23	1:D:567:LEU:H	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:565:THR:HG23	1:E:567:LEU:H	1.80	0.46
1:C:592:TYR:CD2	1:C:596:MET:HE3	2.50	0.46
1:F:192:ASN:ND2	8:F:801:HOH:O	2.04	0.46
1:G:394:PRO:HB3	8:G:1017:HOH:O	2.15	0.46
1:F:565:THR:HG23	1:F:567:LEU:H	1.80	0.46
1:H:19:ILE:HG21	1:H:209:PHE:CE2	2.51	0.46
1:H:258:ARG:NH2	8:H:806:HOH:O	2.47	0.46
1:F:81:LEU:HD12	1:F:88:ILE:CG2	2.43	0.45
1:A:4:GLU:OE1	1:H:608:GLN:CG	2.65	0.45
1:D:389:PHE:HA	1:D:391:GLU:OE1	2.17	0.45
1:B:565:THR:HG23	1:B:567:LEU:H	1.81	0.45
1:A:2:HIS:HE2	1:H:608:GLN:HG2	1.82	0.44
1:E:19:ILE:HG21	1:E:209:PHE:CE2	2.52	0.44
1:G:597:LEU:HD23	1:G:598:VAL:N	2.33	0.44
1:C:389:PHE:HA	1:C:391:GLU:OE1	2.18	0.44
1:H:653:HIS:HD2	8:H:1067:HOH:O	1.99	0.43
1:A:648:ARG:HH21	1:C:627:ARG:NH2	2.17	0.43
1:C:19:ILE:HG21	1:C:209:PHE:CE2	2.54	0.43
1:A:4:GLU:CD	1:H:608:GLN:HG3	2.44	0.43
1:G:40:MET:CB	8:G:1017:HOH:O	2.66	0.43
1:F:597:LEU:HD23	1:F:598:VAL:N	2.33	0.43
1:A:95:GLU:H	1:A:95:GLU:CD	2.27	0.42
1:E:597:LEU:HD23	1:E:598:VAL:N	2.34	0.42
1:H:597:LEU:HD23	1:H:598:VAL:N	2.33	0.42
1:E:389:PHE:HA	1:E:391:GLU:OE1	2.19	0.42
1:G:19:ILE:HG21	1:G:209:PHE:CE2	2.55	0.42
1:D:597:LEU:HD23	1:D:598:VAL:N	2.34	0.42
1:A:397:ILE:HG21	1:A:397:ILE:HD13	1.85	0.42
1:E:397:ILE:HD13	1:E:397:ILE:HG21	1.86	0.42
1:A:652:SER:CB	1:C:628:HIS:HA	2.50	0.41
1:H:101:TRP:HA	1:H:198:ILE:O	2.20	0.41
1:A:101:TRP:HA	1:A:198:ILE:O	2.21	0.41
1:C:597:LEU:HD23	1:C:598:VAL:N	2.35	0.41
1:B:648:ARG:NH2	1:D:627:ARG:NH2	2.68	0.41
1:A:4:GLU:OE1	1:H:608:GLN:HG3	2.20	0.41
1:B:399:LEU:HD13	1:B:408:MET:HG3	2.03	0.41
1:F:101:TRP:HA	1:F:198:ILE:O	2.20	0.41
1:H:389:PHE:HA	1:H:391:GLU:OE1	2.21	0.41
1:E:205:GLU:HG2	8:E:816:HOH:O	2.20	0.41
1:F:397:ILE:HD13	1:F:397:ILE:HG21	1.85	0.41
1:B:389:PHE:HA	1:B:391:GLU:OE1	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:397:ILE:HG21	1:H:397:ILE:HD13	1.88	0.41
1:A:389:PHE:HA	1:A:391:GLU:OE1	2.21	0.41
1:A:2:HIS:NE2	1:H:608:GLN:HG2	2.36	0.40
1:A:19:ILE:HG21	1:A:209:PHE:CE2	2.56	0.40
1:A:652:SER:HB3	1:C:627:ARG:C	2.47	0.40
1:H:6:THR:CG2	1:H:9:GLY:H	2.34	0.40
1:C:101:TRP:HA	1:C:198:ILE:O	2.21	0.40
1:B:283:ARG:HD2	6:B:705:NSQ:O11	2.21	0.40
1:A:573:LEU:HD11	1:A:597:LEU:HD11	2.02	0.40
1:H:642:GLU:O	1:H:642:GLU:HG2	2.21	0.40
1:A:399:LEU:HD13	1:A:408:MET:HG3	2.03	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	660/672 (98%)	640 (97%)	20 (3%)	0	100	100
1	B	662/672 (98%)	641 (97%)	21 (3%)	0	100	100
1	C	660/672 (98%)	642 (97%)	18 (3%)	0	100	100
1	D	660/672 (98%)	637 (96%)	23 (4%)	0	100	100
1	E	660/672 (98%)	639 (97%)	21 (3%)	0	100	100
1	F	662/672 (98%)	642 (97%)	20 (3%)	0	100	100
1	G	659/672 (98%)	639 (97%)	20 (3%)	0	100	100
1	H	659/672 (98%)	638 (97%)	21 (3%)	0	100	100
All	All	5282/5376 (98%)	5118 (97%)	164 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	533/545 (98%)	527 (99%)	6 (1%)	65	61
1	B	533/545 (98%)	522 (98%)	11 (2%)	47	40
1	C	528/545 (97%)	517 (98%)	11 (2%)	47	40
1	D	527/545 (97%)	519 (98%)	8 (2%)	57	52
1	E	532/545 (98%)	522 (98%)	10 (2%)	50	44
1	F	533/545 (98%)	520 (98%)	13 (2%)	43	35
1	G	527/545 (97%)	519 (98%)	8 (2%)	57	52
1	H	530/545 (97%)	522 (98%)	8 (2%)	57	52
All	All	4243/4360 (97%)	4168 (98%)	75 (2%)	51	46

All (75) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	14	ILE
1	A	81	LEU
1	A	104	VAL
1	A	108	THR
1	A	452	TRP
1	A	611	LEU
1	B	14	ILE
1	B	81	LEU
1	B	95	GLU
1	B	104	VAL
1	B	108	THR
1	B	245	LYS
1	B	283	ARG
1	B	375	LYS
1	B	452	TRP
1	B	611	LEU
1	B	661	ARG
1	C	5	THR
1	C	81	LEU

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Mol	Chain	Res	Type
1	C	95	GLU
1	C	104	VAL
1	C	108	THR
1	C	155	LYS
1	C	245	LYS
1	C	283	ARG
1	C	452	TRP
1	C	606	GLU
1	C	640	LEU
1	D	5	THR
1	D	104	VAL
1	D	108	THR
1	D	236	VAL
1	D	242	ILE
1	D	452	TRP
1	D	606	GLU
1	D	650	ASP
1	E	5	THR
1	E	95	GLU
1	E	104	VAL
1	E	108	THR
1	E	236	VAL
1	E	242	ILE
1	E	375	LYS
1	E	452	TRP
1	E	606	GLU
1	E	650	ASP
1	F	75	GLN
1	F	81	LEU
1	F	95	GLU
1	F	104	VAL
1	F	108	THR
1	F	236	VAL
1	F	242	ILE
1	F	249	ASN
1	F	375	LYS
1	F	391	GLU
1	F	452	TRP
1	F	551	LEU
1	F	650	ASP
1	G	75	GLN
1	G	81	LEU

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Mol	Chain	Res	Type
1	G	95	GLU
1	G	104	VAL
1	G	108	THR
1	G	155	LYS
1	G	256	LYS
1	G	452	TRP
1	H	6	THR
1	H	81	LEU
1	H	95	GLU
1	H	104	VAL
1	H	108	THR
1	H	155	LYS
1	H	452	TRP
1	H	650	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	456	GLN
1	A	653	HIS
1	B	297	HIS
1	B	456	GLN
1	B	616	HIS
1	B	628	HIS
1	B	653	HIS
1	C	277	GLN
1	C	297	HIS
1	C	456	GLN
1	C	653	HIS
1	C	659	GLN
1	D	297	HIS
1	D	456	GLN
1	D	653	HIS
1	E	297	HIS
1	E	456	GLN
1	F	297	HIS
1	F	456	GLN
1	G	297	HIS
1	G	456	GLN
1	G	653	HIS
1	H	297	HIS
1	H	456	GLN

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Mol	Chain	Res	Type
1	H	653	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 51 ligands modelled in this entry, 8 are monoatomic - leaving 43 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	$\# Z > 2$
2	SCN	H	701	-	1,2,2	0.47	0	0,1,1	-	-
5	EDO	D	706	-	3,3,3	0.83	0	2,2,2	0.62	0
3	MPD	F	703	-	7,7,7	0.51	0	9,10,10	0.39	0
3	MPD	E	702	-	7,7,7	0.29	0	9,10,10	0.75	0
3	MPD	F	704	-	7,7,7	0.52	0	9,10,10	0.62	0
5	EDO	E	704	-	3,3,3	0.45	0	2,2,2	0.40	0
6	NSQ	E	705	-	23,25,25	1.06	1 (4%)	32,37,37	1.52	5 (15%)
2	SCN	F	701	-	1,2,2	0.02	0	0,1,1	-	-
5	EDO	F	709	-	3,3,3	0.98	0	2,2,2	0.56	0
3	MPD	D	704	-	7,7,7	0.51	0	9,10,10	1.08	0
2	SCN	A	701	-	1,2,2	0.22	0	0,1,1	-	-
6	NSQ	B	705	-	23,25,25	1.37	3 (13%)	32,37,37	1.40	4 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	SCN	D	702	-	1,2,2	0.25	0	0,1,1	-	-
2	SCN	F	702	-	1,2,2	0.09	0	0,1,1	-	-
3	MPD	A	704	-	7,7,7	0.80	0	9,10,10	1.29	2 (22%)
5	EDO	B	703	-	3,3,3	0.51	0	2,2,2	0.70	0
6	NSQ	A	709	-	23,25,25	1.44	5 (21%)	32,37,37	1.76	7 (21%)
3	MPD	A	703	-	7,7,7	0.47	0	9,10,10	0.81	0
5	EDO	G	705	-	3,3,3	0.41	0	2,2,2	0.29	0
2	SCN	E	701	-	1,2,2	0.43	0	0,1,1	-	-
6	NSQ	H	704	-	23,25,25	1.06	3 (13%)	32,37,37	1.31	3 (9%)
5	EDO	G	703	-	3,3,3	0.48	0	2,2,2	0.24	0
6	NSQ	F	711	-	23,25,25	1.23	3 (13%)	32,37,37	1.17	2 (6%)
2	SCN	A	702	-	1,2,2	0.47	0	0,1,1	-	-
5	EDO	A	707	-	3,3,3	0.51	0	2,2,2	0.32	0
3	MPD	A	705	-	7,7,7	0.66	0	9,10,10	1.04	1 (11%)
5	EDO	G	704	-	3,3,3	0.49	0	2,2,2	0.60	0
5	EDO	F	708	-	3,3,3	0.59	0	2,2,2	0.21	0
5	EDO	C	702	-	3,3,3	0.49	0	2,2,2	0.41	0
6	NSQ	C	703	-	23,25,25	1.45	3 (13%)	32,37,37	1.97	6 (18%)
5	EDO	F	710	-	3,3,3	0.52	0	2,2,2	0.43	0
3	MPD	D	703	-	7,7,7	0.35	0	9,10,10	0.58	0
2	SCN	G	701	-	1,2,2	0.10	0	0,1,1	-	-
6	NSQ	G	706	-	23,25,25	1.03	1 (4%)	32,37,37	1.36	4 (12%)
5	EDO	F	707	-	3,3,3	0.66	0	2,2,2	0.15	0
5	EDO	F	706	-	3,3,3	0.40	0	2,2,2	0.75	0
5	EDO	D	705	-	3,3,3	0.28	0	2,2,2	0.40	0
5	EDO	A	708	-	3,3,3	0.86	0	2,2,2	0.32	0
5	EDO	B	704	-	3,3,3	1.02	0	2,2,2	0.24	0
6	NSQ	D	708	-	23,25,25	1.35	4 (17%)	32,37,37	1.67	7 (21%)
3	MPD	B	701	-	7,7,7	0.58	0	9,10,10	1.20	1 (11%)
5	EDO	D	707	-	3,3,3	0.88	0	2,2,2	0.89	0
5	EDO	H	703	-	3,3,3	0.98	0	2,2,2	0.48	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	EDO	D	706	-	-	1/1/1/1	-
3	MPD	F	703	-	-	0/5/5/5	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	MPD	E	702	-	-	3/5/5/5	-
3	MPD	F	704	-	-	0/5/5/5	-
5	EDO	E	704	-	-	1/1/1/1	-
6	NSQ	E	705	-	-	2/11/33/33	0/2/2/2
5	EDO	F	709	-	-	1/1/1/1	-
3	MPD	D	704	-	-	3/5/5/5	-
6	NSQ	B	705	-	-	2/11/33/33	0/2/2/2
3	MPD	A	704	-	-	1/5/5/5	-
5	EDO	B	703	-	-	1/1/1/1	-
6	NSQ	A	709	-	-	2/11/33/33	0/2/2/2
3	MPD	A	703	-	-	1/5/5/5	-
5	EDO	G	705	-	-	1/1/1/1	-
6	NSQ	H	704	-	-	2/11/33/33	0/2/2/2
5	EDO	G	703	-	-	0/1/1/1	-
6	NSQ	F	711	-	-	2/11/33/33	0/2/2/2
5	EDO	A	707	-	-	1/1/1/1	-
3	MPD	A	705	-	-	5/5/5/5	-
5	EDO	G	704	-	-	0/1/1/1	-
5	EDO	F	708	-	-	0/1/1/1	-
5	EDO	C	702	-	-	0/1/1/1	-
6	NSQ	C	703	-	-	4/11/33/33	0/2/2/2
5	EDO	F	710	-	-	1/1/1/1	-
3	MPD	D	703	-	-	2/5/5/5	-
6	NSQ	G	706	-	-	2/11/33/33	0/2/2/2
5	EDO	F	707	-	-	0/1/1/1	-
5	EDO	F	706	-	-	0/1/1/1	-
5	EDO	D	705	-	-	1/1/1/1	-
5	EDO	A	708	-	-	1/1/1/1	-
5	EDO	B	704	-	-	1/1/1/1	-
6	NSQ	D	708	-	-	4/11/33/33	0/2/2/2
3	MPD	B	701	-	-	1/5/5/5	-
5	EDO	D	707	-	-	0/1/1/1	-
5	EDO	H	703	-	-	1/1/1/1	-

All (23) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	709	NSQ	O1-C1	4.30	1.47	1.41
6	C	703	NSQ	O1-C1	4.10	1.47	1.41
6	B	705	NSQ	O1-C1	3.68	1.46	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	D	708	NSQ	O34-N32	3.61	1.29	1.22
6	C	703	NSQ	O34-N32	3.19	1.28	1.22
6	B	705	NSQ	O34-N32	3.08	1.28	1.22
6	F	711	NSQ	O1-C25	-2.91	1.32	1.38
6	E	705	NSQ	C28-N32	-2.73	1.38	1.45
6	D	708	NSQ	O1-C1	2.70	1.45	1.41
6	C	703	NSQ	C4-C5	2.59	1.58	1.53
6	G	706	NSQ	C28-N32	-2.53	1.39	1.45
6	A	709	NSQ	C28-N32	-2.44	1.39	1.45
6	F	711	NSQ	O1-C1	2.31	1.44	1.41
6	D	708	NSQ	O13-S10	2.28	1.51	1.45
6	F	711	NSQ	O34-N32	2.27	1.26	1.22
6	H	704	NSQ	C28-N32	-2.26	1.39	1.45
6	H	704	NSQ	O12-S10	2.20	1.51	1.45
6	H	704	NSQ	O34-N32	2.16	1.26	1.22
6	A	709	NSQ	O13-S10	2.16	1.51	1.45
6	B	705	NSQ	O13-S10	2.07	1.51	1.45
6	A	709	NSQ	O34-N32	2.07	1.26	1.22
6	D	708	NSQ	C4-C5	2.03	1.57	1.53
6	A	709	NSQ	O1-C25	-2.01	1.34	1.38

All (42) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	C	703	NSQ	C29-C28-N32	5.62	124.25	119.34
6	A	709	NSQ	O12-S10-C6	-5.10	99.14	106.76
6	C	703	NSQ	O12-S10-C6	4.88	114.05	106.76
6	D	708	NSQ	C27-C28-N32	4.39	123.17	119.34
6	E	705	NSQ	O11-S10-C6	4.06	113.81	105.97
6	C	703	NSQ	O1-C1-C2	3.93	112.89	107.16
6	F	711	NSQ	O13-S10-C6	3.89	112.56	106.76
6	A	709	NSQ	O11-S10-C6	3.81	113.33	105.97
6	G	706	NSQ	O11-S10-C6	3.76	113.24	105.97
6	E	705	NSQ	C29-C28-N32	3.66	122.53	119.34
6	C	703	NSQ	C27-C28-N32	-3.64	116.16	119.34
6	G	706	NSQ	O2-C2-C3	3.60	118.85	110.38
6	D	708	NSQ	O11-S10-C6	3.40	112.54	105.97
6	B	705	NSQ	O11-S10-O12	3.40	119.90	111.40
6	B	705	NSQ	C4-C3-C2	-3.32	105.00	110.83
6	A	709	NSQ	O4-C4-C5	3.24	117.30	109.32
6	C	703	NSQ	O3-C3-C4	3.23	117.98	110.38
6	E	705	NSQ	C27-C28-N32	-3.11	116.62	119.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	D	708	NSQ	O1-C1-C2	3.11	111.69	107.16
6	B	705	NSQ	O13-S10-O12	-3.11	103.72	113.82
6	H	704	NSQ	O2-C2-C3	3.06	117.58	110.38
6	E	705	NSQ	O11-S10-O13	-2.93	104.08	111.40
6	A	709	NSQ	O13-S10-C6	2.85	111.01	106.76
6	A	709	NSQ	O11-S10-O13	-2.76	104.50	111.40
6	F	711	NSQ	C4-C3-C2	-2.74	106.03	110.83
6	D	708	NSQ	O3-C3-C4	2.70	116.74	110.38
6	H	704	NSQ	O13-S10-O12	-2.60	105.38	113.82
3	A	705	MPD	O2-C2-C1	-2.58	99.95	107.99
6	D	708	NSQ	C4-C3-C2	-2.50	106.44	110.83
6	G	706	NSQ	O13-S10-O12	-2.48	105.74	113.82
6	E	705	NSQ	C25-O1-C1	2.46	121.29	117.82
6	A	709	NSQ	O11-S10-O12	2.38	117.36	111.40
3	A	704	MPD	O2-C2-CM	2.34	115.28	107.99
6	G	706	NSQ	C1-O5-C5	2.29	118.19	113.72
6	D	708	NSQ	O13-S10-O12	-2.23	106.57	113.82
6	D	708	NSQ	O12-S10-C6	2.20	110.05	106.76
6	B	705	NSQ	C3-C4-C5	2.19	114.19	110.23
6	H	704	NSQ	C29-C28-N32	2.18	121.24	119.34
3	A	704	MPD	O4-C4-C5	2.11	118.52	109.45
3	B	701	MPD	O2-C2-C1	-2.06	101.58	107.99
6	A	709	NSQ	C4-C3-C2	-2.02	107.28	110.83
6	C	703	NSQ	O3-C3-C2	-2.01	105.63	110.38

There are no chirality outliers.

All (47) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	704	MPD	C2-C3-C4-C5
3	A	705	MPD	C2-C3-C4-C5
3	B	701	MPD	C2-C3-C4-C5
3	D	704	MPD	C2-C3-C4-O4
3	D	704	MPD	C2-C3-C4-C5
6	C	703	NSQ	C27-C28-N32-O34
6	C	703	NSQ	C29-C28-N32-O34
6	D	708	NSQ	C27-C28-N32-O34
6	D	708	NSQ	C29-C28-N32-O34
6	C	703	NSQ	C26-C25-O1-C1
6	G	706	NSQ	C26-C25-O1-C1
5	E	704	EDO	O1-C1-C2-O2
5	G	705	EDO	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
6	A	709	NSQ	C26-C25-O1-C1
6	A	709	NSQ	C30-C25-O1-C1
6	B	705	NSQ	C26-C25-O1-C1
6	B	705	NSQ	C30-C25-O1-C1
6	F	711	NSQ	C26-C25-O1-C1
6	F	711	NSQ	C30-C25-O1-C1
6	G	706	NSQ	C30-C25-O1-C1
6	H	704	NSQ	C26-C25-O1-C1
6	H	704	NSQ	C30-C25-O1-C1
5	D	705	EDO	O1-C1-C2-O2
6	C	703	NSQ	C30-C25-O1-C1
6	E	705	NSQ	C26-C25-O1-C1
6	E	705	NSQ	C30-C25-O1-C1
6	D	708	NSQ	C26-C25-O1-C1
6	D	708	NSQ	C30-C25-O1-C1
3	D	703	MPD	CM-C2-C3-C4
3	D	704	MPD	C1-C2-C3-C4
5	A	708	EDO	O1-C1-C2-O2
5	A	707	EDO	O1-C1-C2-O2
5	B	704	EDO	O1-C1-C2-O2
5	D	706	EDO	O1-C1-C2-O2
3	A	705	MPD	O2-C2-C3-C4
3	E	702	MPD	O2-C2-C3-C4
3	A	705	MPD	C2-C3-C4-O4
5	F	709	EDO	O1-C1-C2-O2
5	F	710	EDO	O1-C1-C2-O2
5	H	703	EDO	O1-C1-C2-O2
3	A	703	MPD	C1-C2-C3-C4
3	A	705	MPD	C1-C2-C3-C4
3	A	705	MPD	CM-C2-C3-C4
3	D	703	MPD	C1-C2-C3-C4
3	E	702	MPD	C1-C2-C3-C4
3	E	702	MPD	CM-C2-C3-C4
5	B	703	EDO	O1-C1-C2-O2

There are no ring outliers.

4 monomers are involved in 10 short contacts:

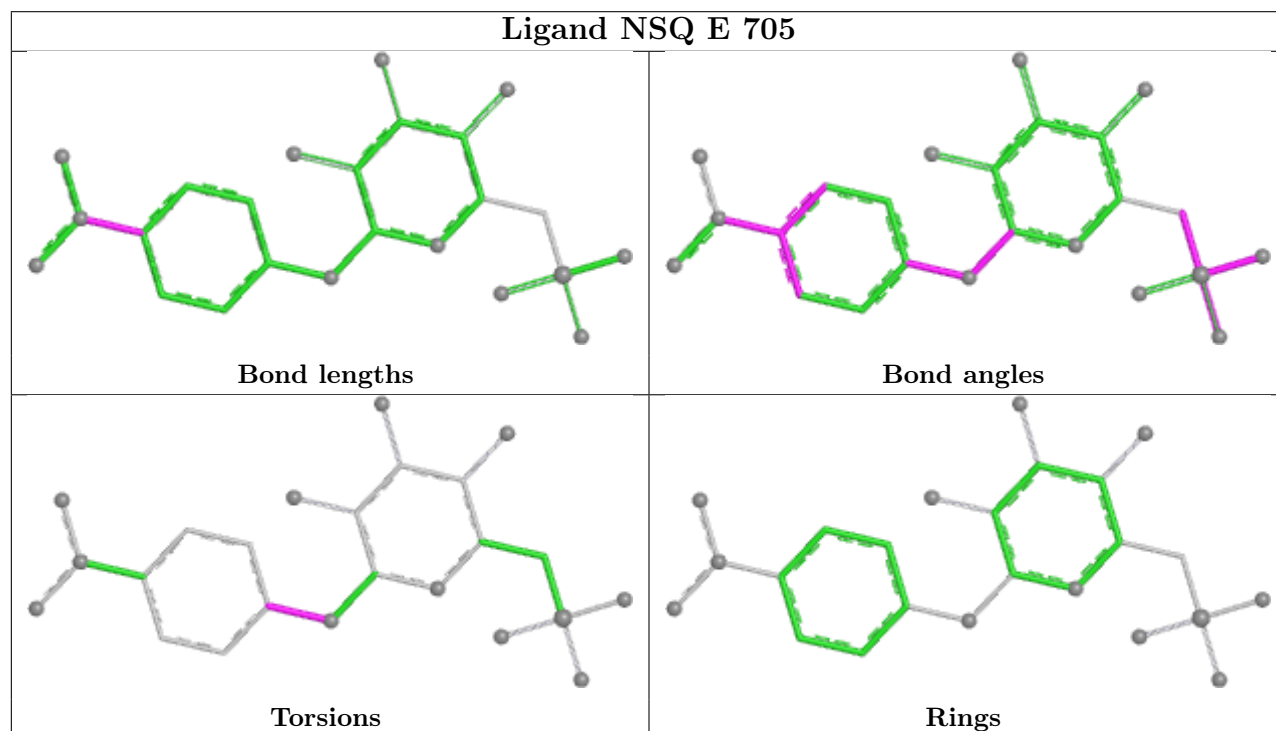
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	D	706	EDO	1	0
6	B	705	NSQ	2	0
3	A	704	MPD	2	0

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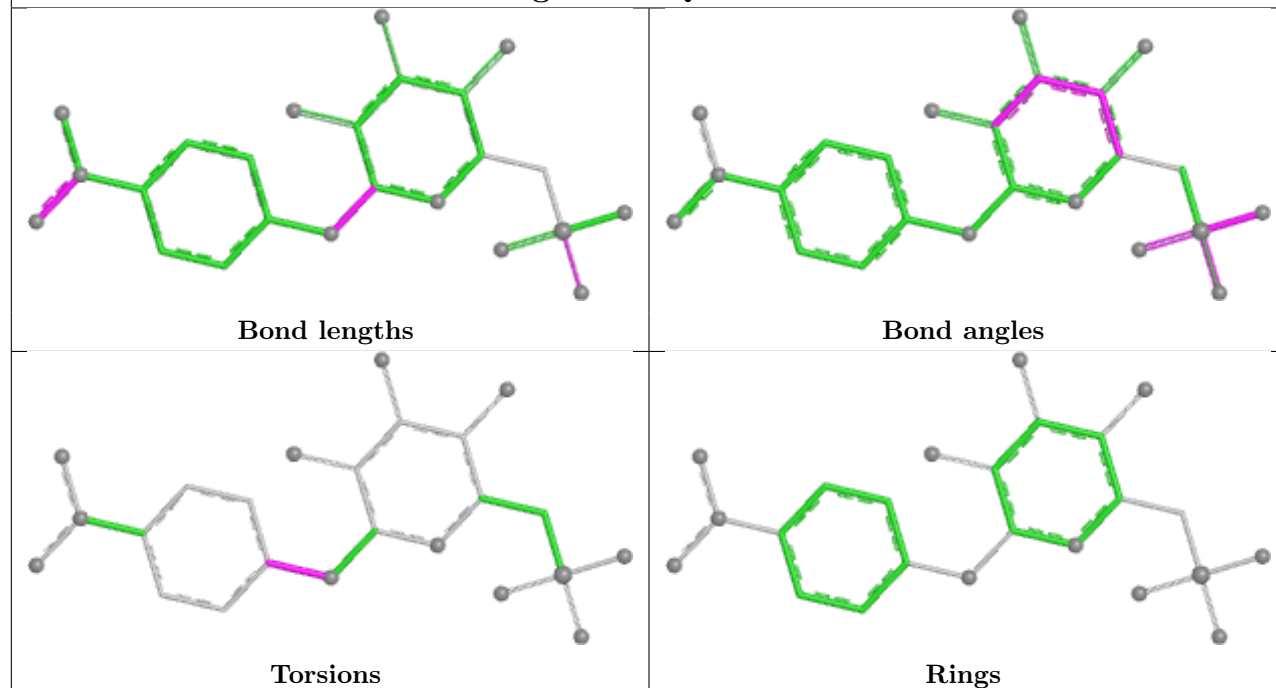
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	D	707	EDO	5	0

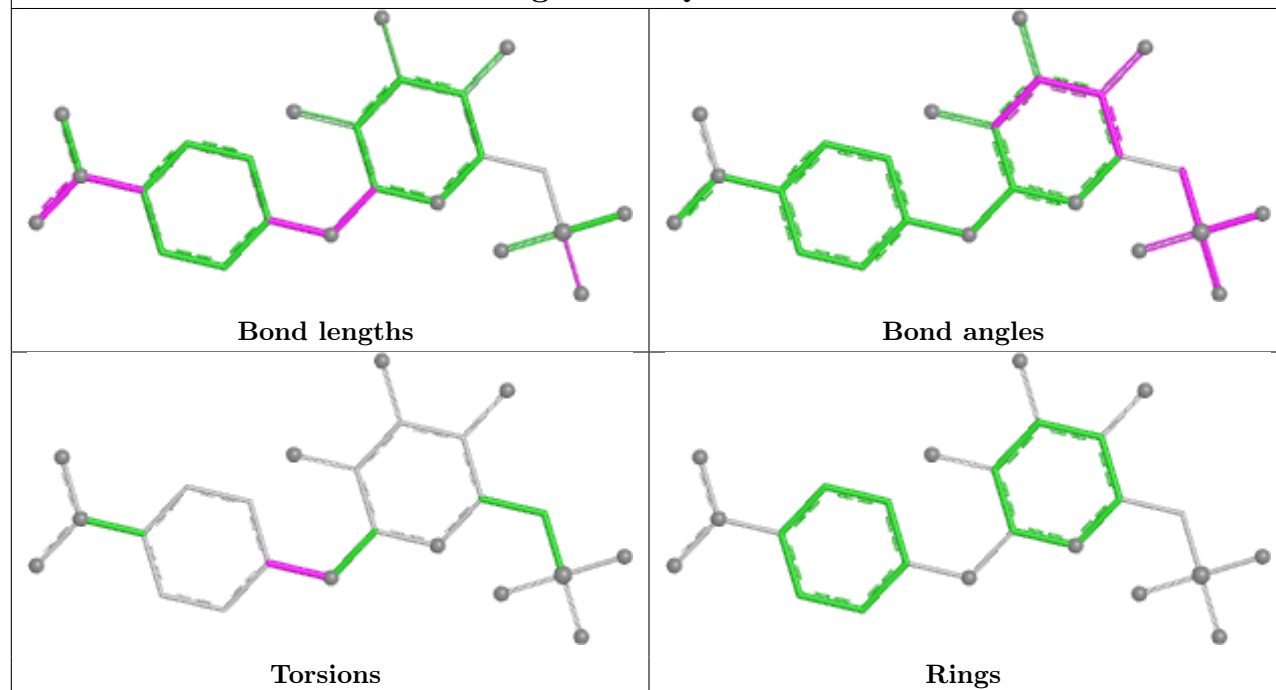
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

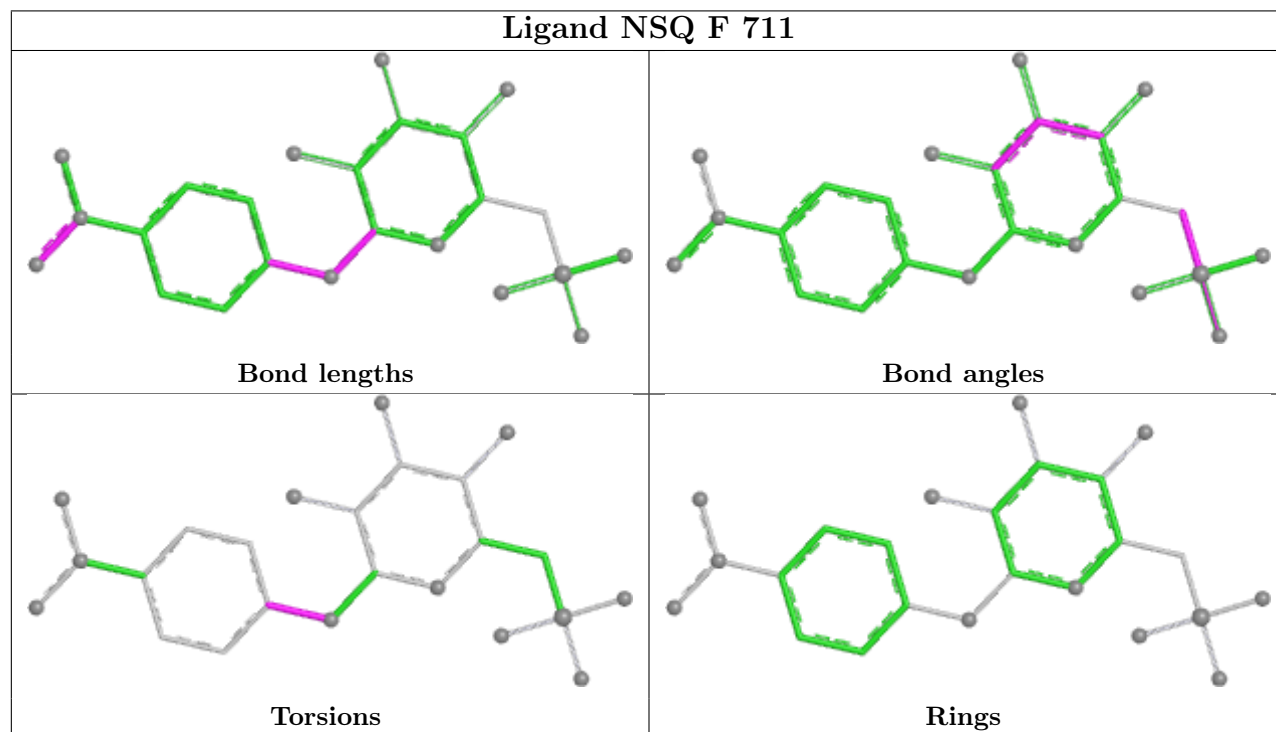
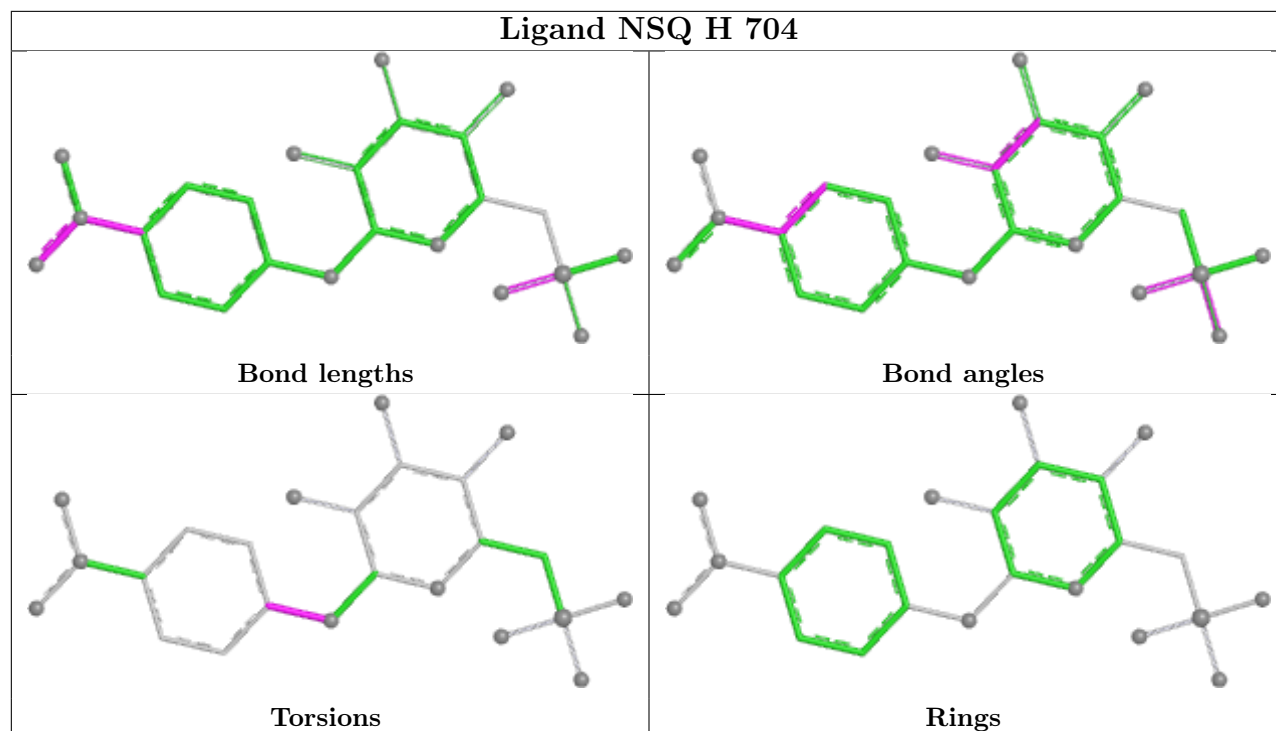


Ligand NSQ B 705

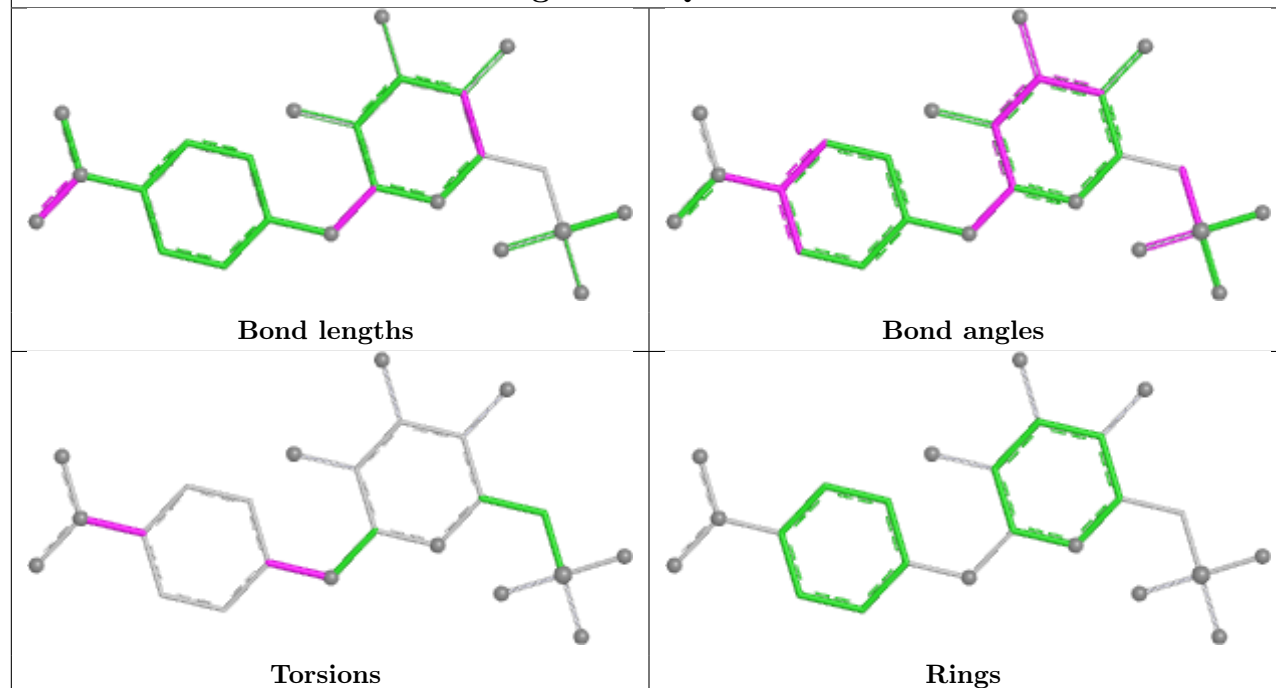


Ligand NSQ A 709

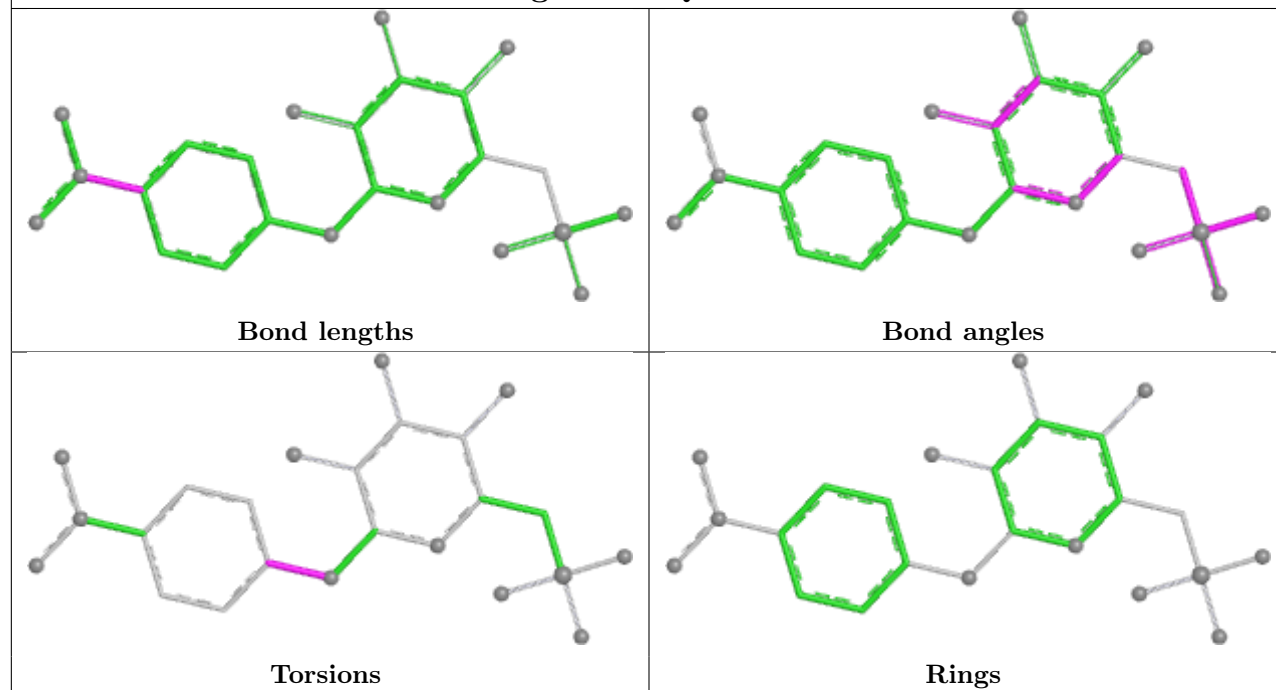


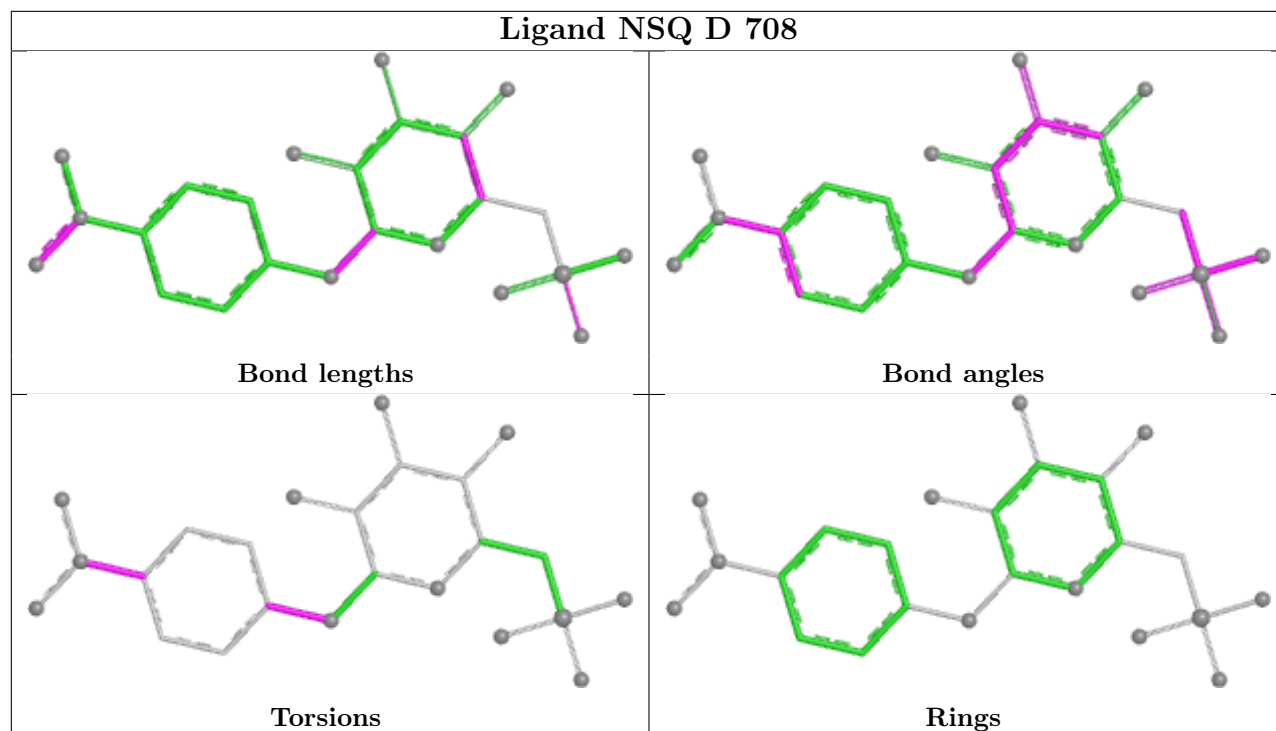


Ligand NSQ C 703



Ligand NSQ G 706





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	661/672 (98%)	-0.16	5 (0%)	82 87	17, 30, 49, 77	1 (0%)
1	B	663/672 (98%)	-0.10	6 (0%)	81 86	19, 32, 55, 78	1 (0%)
1	C	661/672 (98%)	0.30	39 (5%)	28 37	20, 38, 69, 92	2 (0%)
1	D	662/672 (98%)	-0.15	6 (0%)	81 86	20, 31, 50, 75	0
1	E	661/672 (98%)	-0.13	2 (0%)	90 93	14, 32, 50, 70	1 (0%)
1	F	664/672 (98%)	-0.21	4 (0%)	85 90	19, 28, 47, 70	0
1	G	661/672 (98%)	0.04	8 (1%)	76 83	21, 36, 59, 89	0
1	H	661/672 (98%)	-0.05	10 (1%)	72 80	20, 33, 58, 93	0
All	All	5294/5376 (98%)	-0.06	80 (1%)	72 80	14, 32, 57, 93	5 (0%)

All (80) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	3	PHE	3.6
1	C	594	ALA	3.6
1	B	663	ILE	3.5
1	D	662	THR	3.4
1	C	616	HIS	3.4
1	C	565	THR	3.3
1	C	655	ARG	3.3
1	C	4	GLU	3.2
1	C	661	ARG	3.1
1	H	2	HIS	3.0
1	H	3	PHE	3.0
1	C	656	LEU	3.0
1	C	14	ILE	3.0
1	C	651	SER	2.9
1	C	636	VAL	2.9
1	C	629	ALA	2.9

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Mol	Chain	Res	Type	RSRZ
1	D	565	THR	2.8
1	B	340	VAL	2.8
1	C	8	ASP	2.8
1	G	14	ILE	2.8
1	A	62	VAL	2.7
1	D	661	ARG	2.7
1	C	657	PHE	2.7
1	C	632	ARG	2.7
1	G	16	ASN	2.7
1	C	2	HIS	2.7
1	G	2	HIS	2.7
1	C	623	TRP	2.6
1	C	652	SER	2.6
1	C	660	LEU	2.6
1	C	653	HIS	2.6
1	H	1	MET	2.6
1	C	649	ALA	2.6
1	H	62	VAL	2.6
1	C	16	ASN	2.6
1	A	3	PHE	2.5
1	E	616	HIS	2.5
1	C	626	LYS	2.5
1	F	664	GLY	2.5
1	D	14	ILE	2.5
1	C	617	GLY	2.4
1	G	392	TYR	2.4
1	C	634	ILE	2.4
1	A	340	VAL	2.4
1	C	6	THR	2.4
1	G	62	VAL	2.4
1	B	661	ARG	2.3
1	C	15	GLY	2.3
1	C	549	VAL	2.3
1	B	2	HIS	2.3
1	C	7	LYS	2.3
1	C	654	HIS	2.3
1	C	624	SER	2.3
1	C	620	VAL	2.3
1	F	565	THR	2.3
1	F	660	LEU	2.3
1	H	392	TYR	2.2
1	G	332	SER	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	395	ILE	2.2
1	C	18	ILE	2.2
1	H	14	ILE	2.2
1	D	340	VAL	2.2
1	H	64	GLY	2.2
1	A	392	TYR	2.2
1	C	5	THR	2.2
1	H	6	THR	2.2
1	E	660	LEU	2.2
1	H	20	LEU	2.2
1	C	647	TYR	2.1
1	C	628	HIS	2.1
1	F	616	HIS	2.1
1	B	392	TYR	2.1
1	C	11	THR	2.1
1	C	9	GLY	2.1
1	G	85	GLY	2.0
1	H	661	ARG	2.0
1	D	1	MET	2.0
1	A	634	ILE	2.0
1	G	5	THR	2.0
1	C	577	TYR	2.0

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

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

6.3 Carbohydrates [i](#)

There are no 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
5	EDO	D	706	4/4	0.73	0.20	49,51,53,54	0

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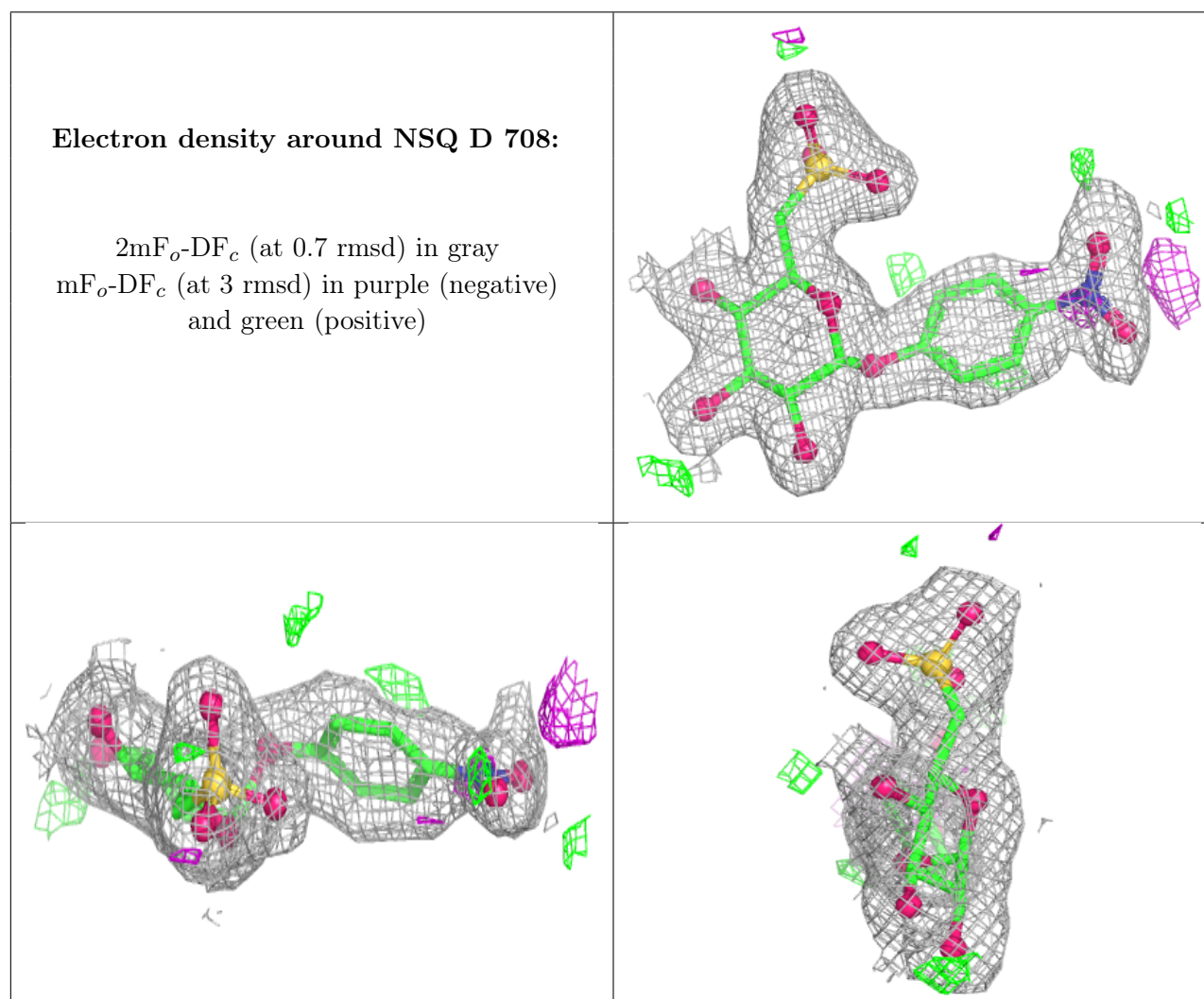
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	MPD	D	704	8/8	0.80	0.21	49,56,58,62	0
5	EDO	D	707	4/4	0.81	0.16	39,40,42,43	0
5	EDO	H	703	4/4	0.81	0.17	40,43,44,46	0
5	EDO	B	703	4/4	0.82	0.16	46,48,49,50	0
5	EDO	F	707	4/4	0.82	0.22	32,39,41,43	4
3	MPD	B	701	8/8	0.82	0.17	42,48,52,54	0
5	EDO	G	704	4/4	0.83	0.18	47,49,50,51	0
5	EDO	F	709	4/4	0.84	0.15	41,42,43,48	0
2	SCN	A	702	3/3	0.84	0.14	33,33,38,48	3
5	EDO	A	708	4/4	0.84	0.14	38,39,40,44	0
5	EDO	E	704	4/4	0.86	0.17	31,32,32,35	4
3	MPD	A	703	8/8	0.86	0.15	39,43,45,58	0
5	EDO	F	708	4/4	0.86	0.19	46,46,49,50	0
5	EDO	D	705	4/4	0.88	0.16	40,41,42,44	4
3	MPD	A	705	8/8	0.88	0.23	38,43,44,47	8
5	EDO	B	704	4/4	0.88	0.12	39,39,39,41	0
3	MPD	F	704	8/8	0.89	0.16	51,56,58,58	0
4	CL	H	702	1/1	0.90	0.13	44,44,44,44	1
5	EDO	C	702	4/4	0.91	0.10	40,46,47,54	0
3	MPD	E	702	8/8	0.91	0.11	26,29,32,32	0
3	MPD	F	703	8/8	0.92	0.11	28,35,37,38	0
5	EDO	G	705	4/4	0.92	0.12	35,42,46,47	0
3	MPD	A	704	8/8	0.92	0.12	32,38,42,45	0
5	EDO	F	710	4/4	0.93	0.09	43,43,45,46	0
5	EDO	G	703	4/4	0.94	0.08	40,42,44,48	0
4	CL	G	702	1/1	0.94	0.09	39,39,39,39	1
3	MPD	D	703	8/8	0.94	0.10	41,47,49,52	0
5	EDO	A	707	4/4	0.94	0.09	41,44,45,47	0
2	SCN	F	702	3/3	0.95	0.15	34,34,34,39	3
4	CL	F	705	1/1	0.96	0.06	44,44,44,44	0
4	CL	E	703	1/1	0.96	0.15	48,48,48,48	1
2	SCN	H	701	3/3	0.97	0.09	35,35,38,41	0
2	SCN	E	701	3/3	0.97	0.08	41,41,53,56	0
4	CL	A	706	1/1	0.97	0.06	48,48,48,48	0
4	CL	B	702	1/1	0.97	0.09	46,46,46,46	0
2	SCN	D	702	3/3	0.97	0.10	42,42,45,49	0
5	EDO	F	706	4/4	0.97	0.05	30,32,33,35	0
2	SCN	G	701	3/3	0.97	0.09	39,39,43,47	0
6	NSQ	D	708	24/24	0.97	0.07	20,26,60,67	0
6	NSQ	E	705	24/24	0.97	0.06	22,26,35,42	0
6	NSQ	A	709	24/24	0.98	0.05	21,25,36,41	0
6	NSQ	B	705	24/24	0.98	0.06	19,24,37,38	0

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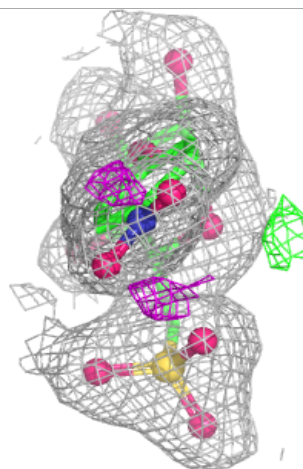
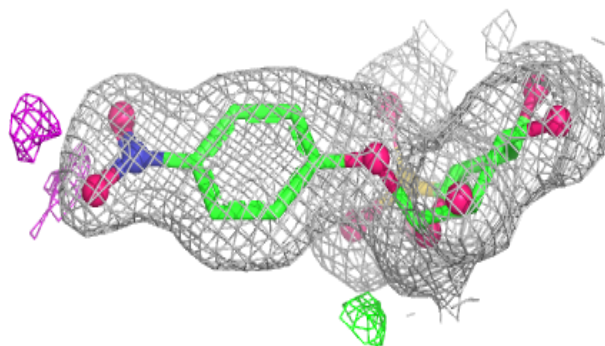
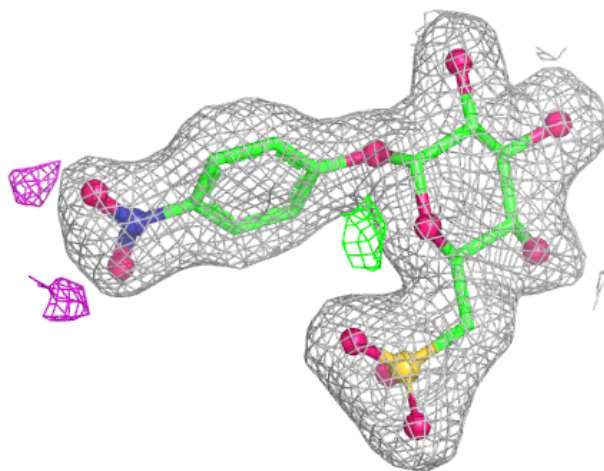
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
6	NSQ	C	703	24/24	0.98	0.07	22,24,64,69	0
2	SCN	A	701	3/3	0.98	0.09	33,33,36,40	0
2	SCN	F	701	3/3	0.98	0.07	34,34,35,48	0
6	NSQ	F	711	24/24	0.98	0.05	19,22,29,34	0
6	NSQ	G	706	24/24	0.98	0.05	20,25,29,35	0
6	NSQ	H	704	24/24	0.98	0.05	17,24,33,35	0
7	K	C	701	1/1	0.99	0.06	37,37,37,37	0
7	K	D	701	1/1	0.99	0.08	33,33,33,33	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.



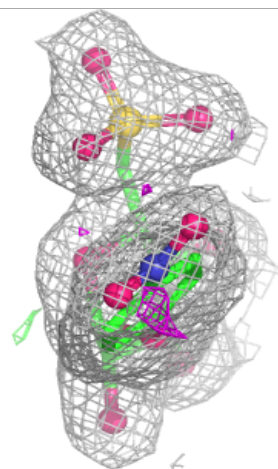
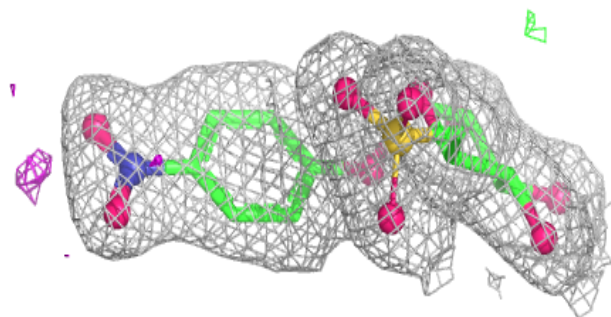
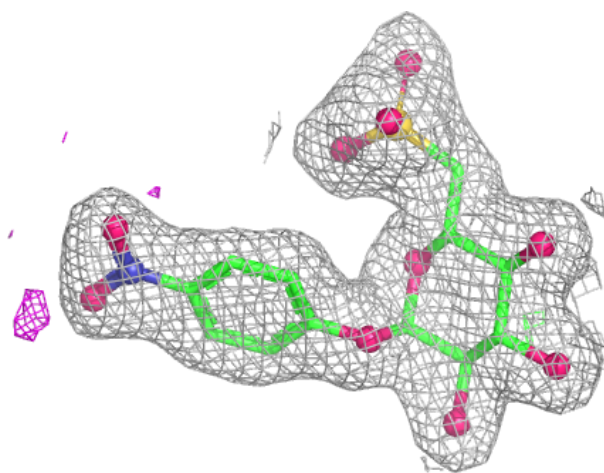
Electron density around NSQ E 705:

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



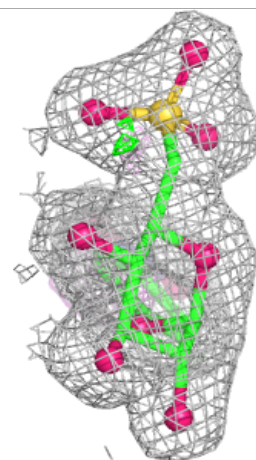
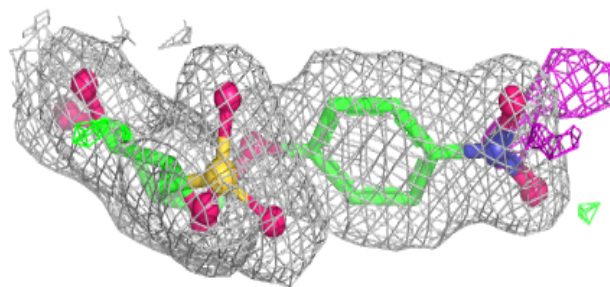
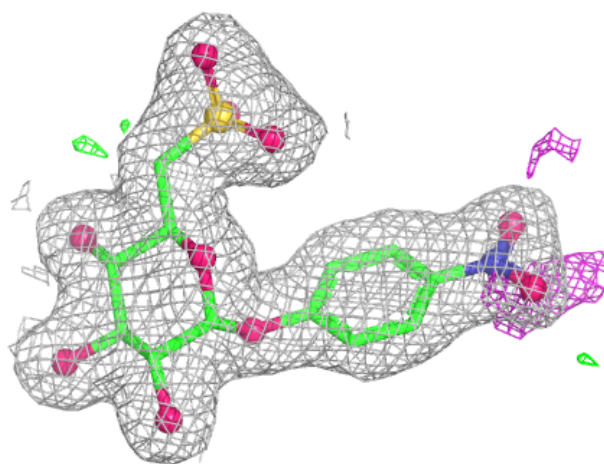
Electron density around NSQ A 709:

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



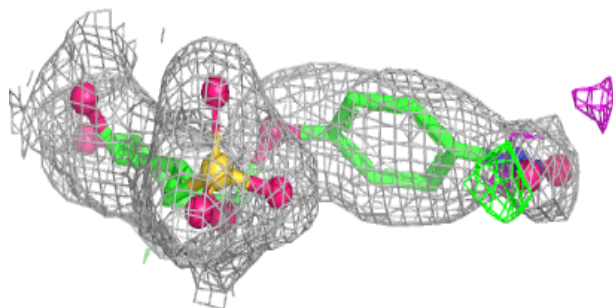
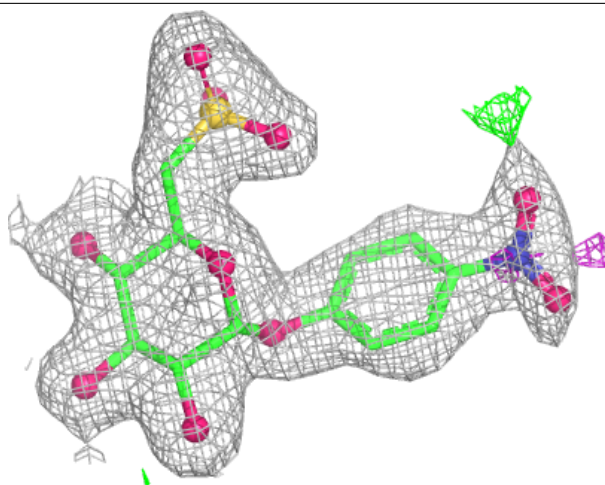
Electron density around NSQ B 705:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



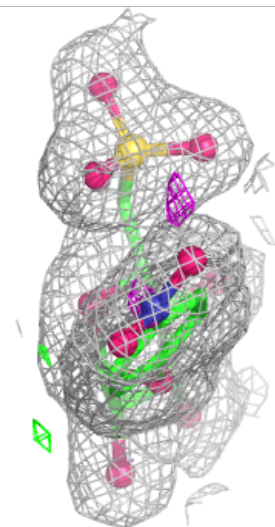
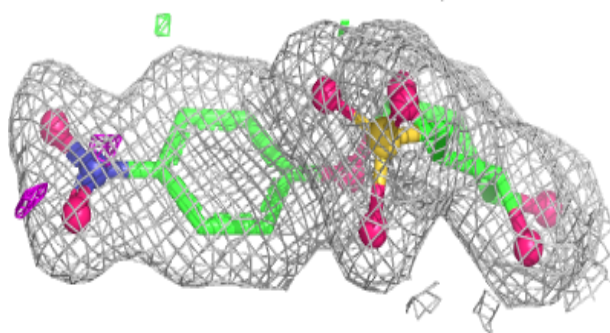
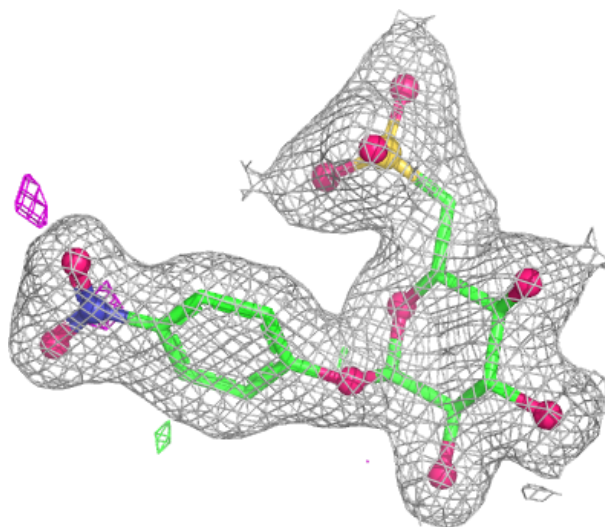
Electron density around NSQ C 703:

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



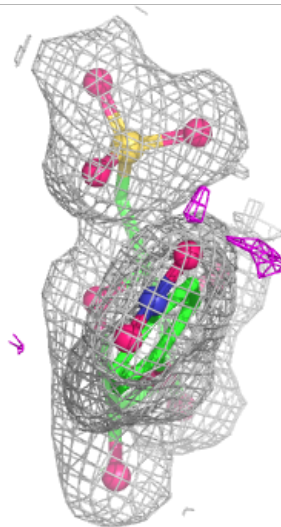
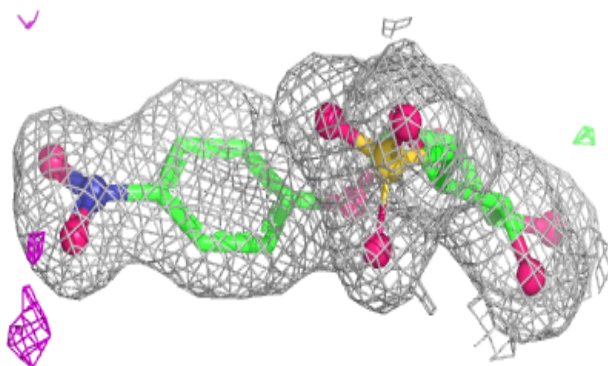
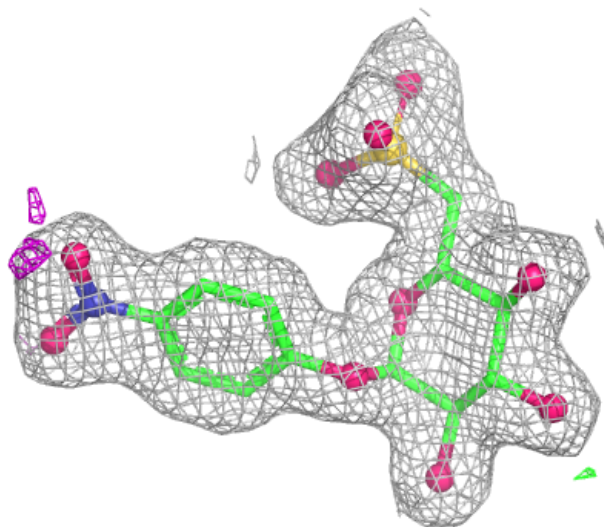
Electron density around NSQ F 711:

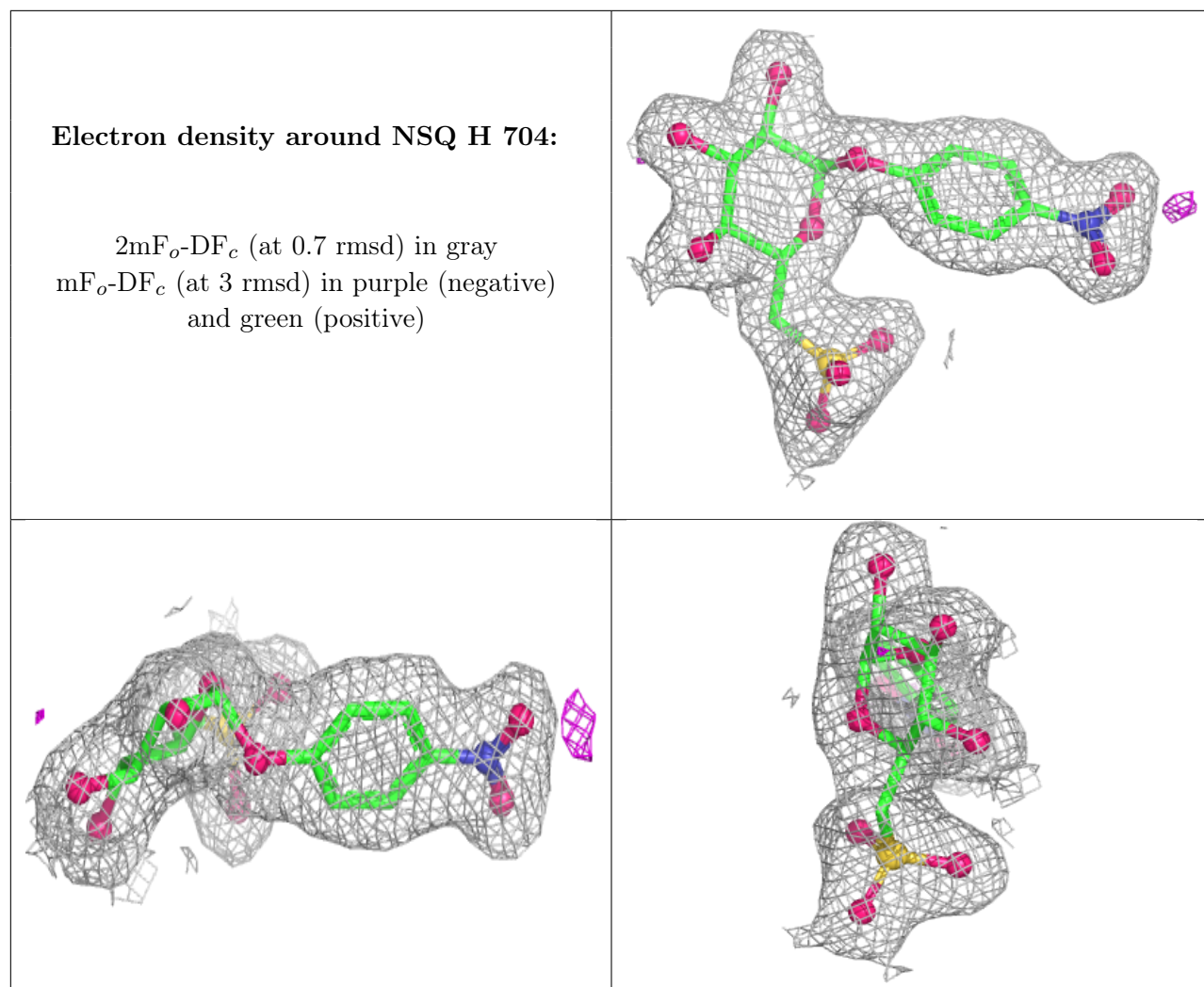
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around NSQ G 706:

$2mF_o-DF_c$ (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.