Full wwPDB X-ray Structure Validation Report (i)

Apr 21, 2024 – 04:52 am BST

PDB ID	:	5OHS
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 (i) 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 (i)) were used in the production of this report:

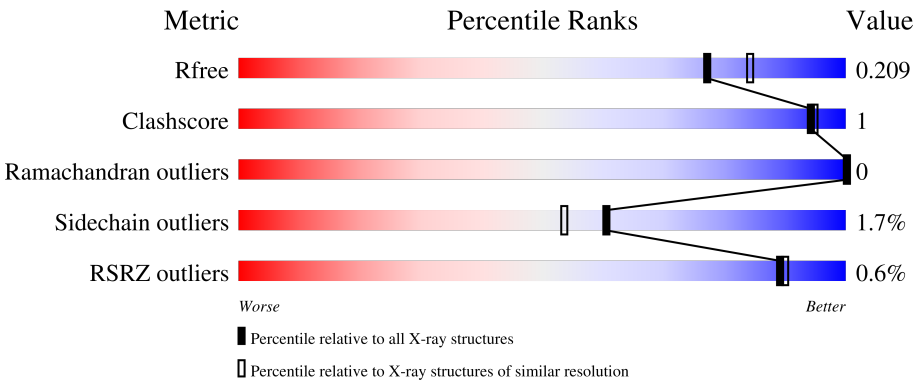
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36.2
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

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}	130704	11647 (2.00-1.96)
Clashscore	141614	1014 (1.98-1.98)
Ramachandran outliers	138981	1006 (1.98-1.98)
Sidechain outliers	138945	1006 (1.98-1.98)
RSRZ outliers	127900	11410 (2.00-1.96)

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

Mol	Chain	Length	Quality of chain
1	A	672	91% 7% • •
1	B	672	% 91% 7% • •
1	C	672	3% 90% 8% • •
1	D	672	90% 7% • •
1	E	672	90% 7% • •

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Mol	Chain	Length	Quality of chain
1	F	672	90% 7%
1	G	672	92% 6%
1	H	672	90% 8%

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 (i)

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

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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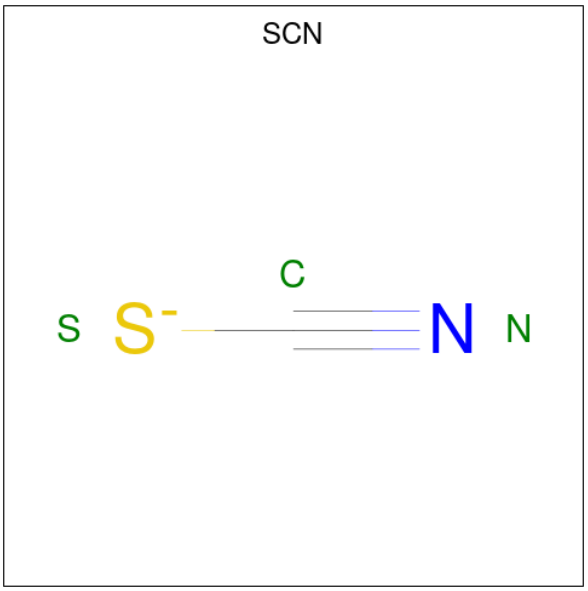
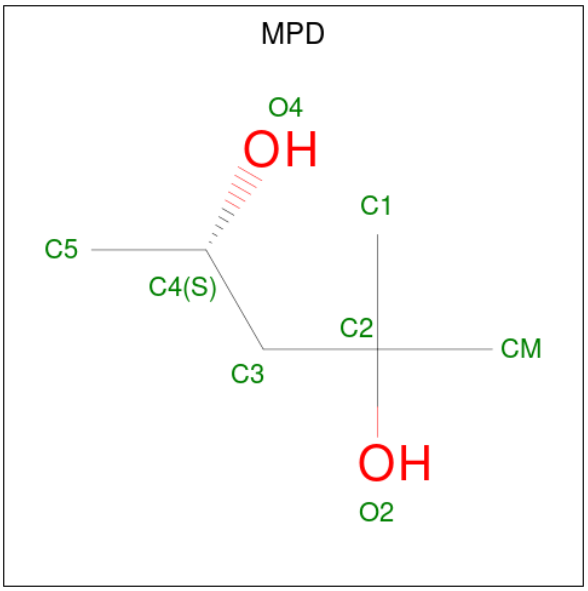
Chain	Residue	Modelled	Actual	Comment	Reference
F	370	ALA	GLU	engineered mutation	UNP A0A083ZKV2
F	371	ALA	GLU	engineered mutation	UNP A0A083ZKV2
F	455	ASN	ASP	engineered mutation	UNP A0A083ZKV2
F	665	LEU	-	expression tag	UNP A0A083ZKV2
F	666	GLU	-	expression tag	UNP A0A083ZKV2
F	667	HIS	-	expression 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 (three-letter code: SCN) (formula: CNS).



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

- Molecule 3 is (4S)-2-METHYL-2,4-PENTANEDIOL (three-letter code: MPD) (formula: $C_6H_{14}O_2$).



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

- Molecule 4 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

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

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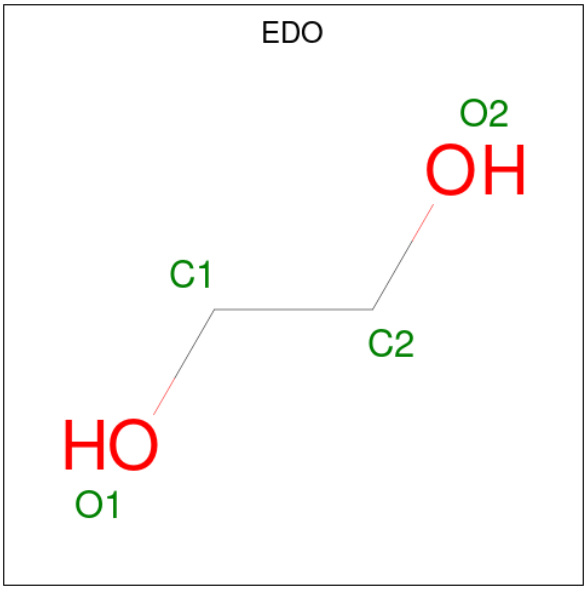
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	F	1	Total Cl 1 1	0	0
4	G	1	Total Cl 1 1	0	0
4	H	1	Total Cl 1 1	0	0

- Molecule 5 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



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

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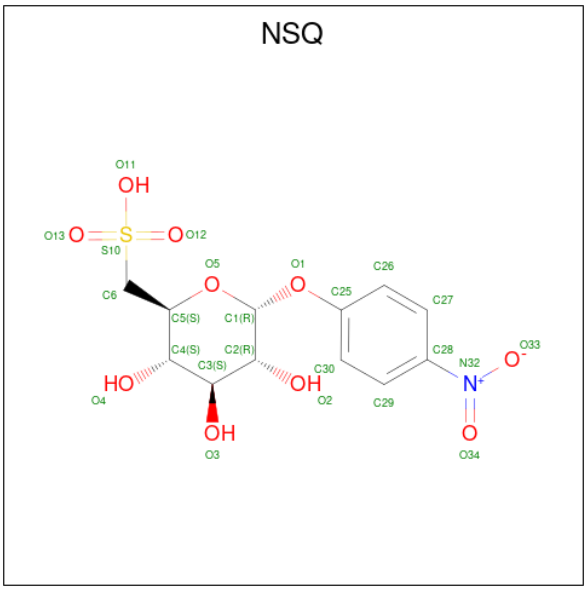
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	O			
5	E	1	4	2	2		0	0
			Total	C	O			
5	F	1	4	2	2		0	0
			Total	C	O			
5	F	1	4	2	2		0	0
			Total	C	O			
5	F	1	4	2	2		0	0
			Total	C	O			
5	F	1	4	2	2		0	0
			Total	C	O			
5	F	1	4	2	2		0	0
			Total	C	O			
5	G	1	4	2	2		0	0
			Total	C	O			
5	G	1	4	2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

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



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

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

- Molecule 7 is POTASSIUM ION (three-letter code: K) (formula: K).

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

- Molecule 8 is water.

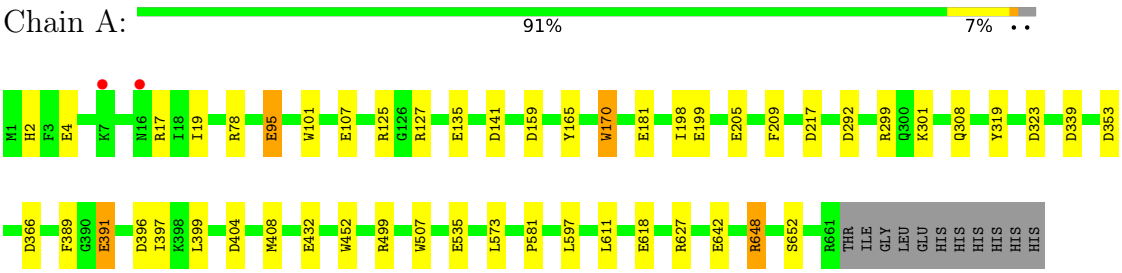
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
8	A	296	298	298	0	2
			Total	O		
8	B	265	265	265	0	0
			Total	O		
8	C	237	238	238	0	1
			Total	O		
8	D	305	307	307	0	2
			Total	O		
8	E	270	272	272	0	2
			Total	O		
8	F	292	294	294	0	2
			Total	O		
8	G	231	231	231	0	0
			Total	O		
8	H	272	273	273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

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.

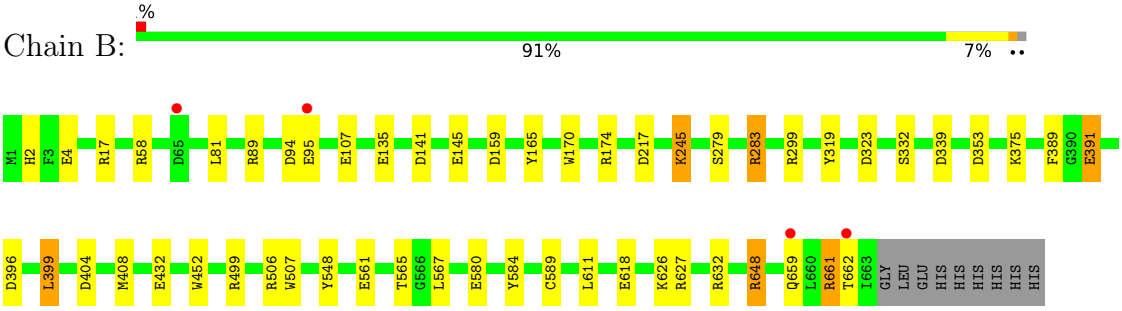
• Molecule 1: Alpha-glucosidase yihQ

Chain A:



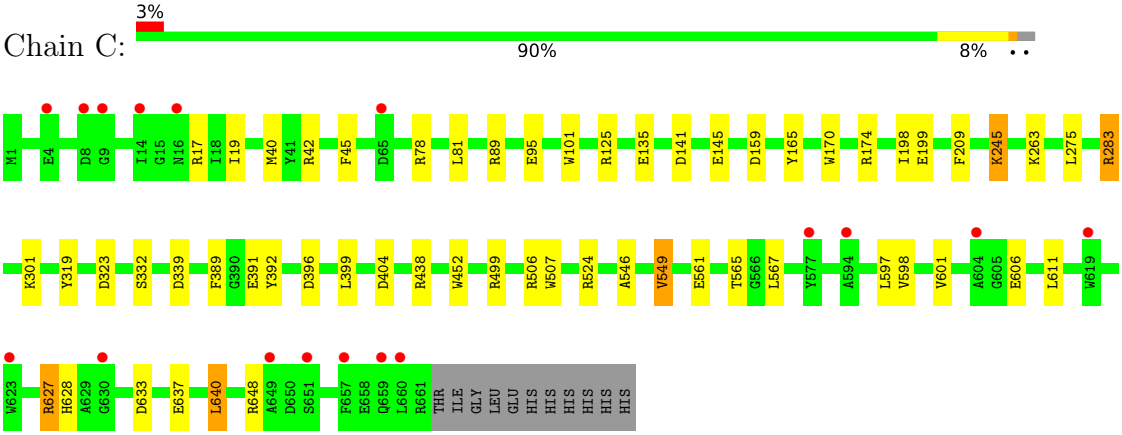
• Molecule 1: Alpha-glucosidase yihQ

Chain B:



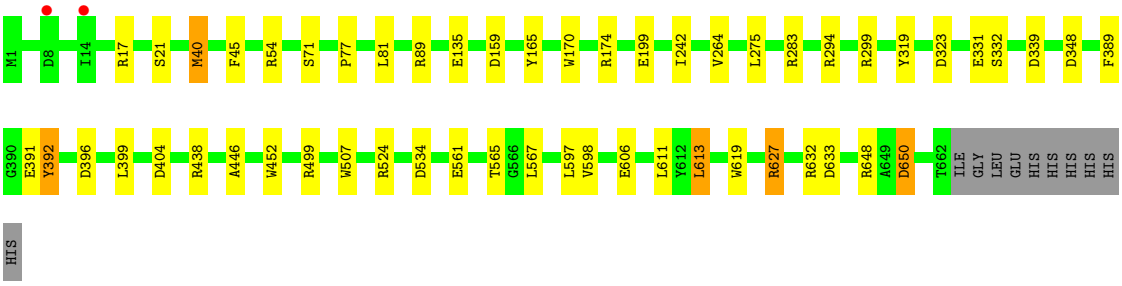
• Molecule 1: Alpha-glucosidase yihQ

Chain C:



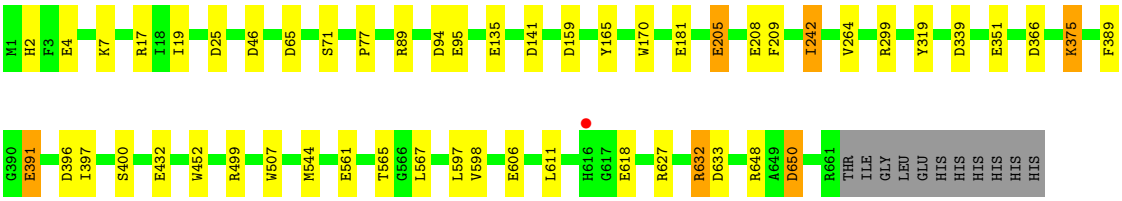
• Molecule 1: Alpha-glucosidase yihQ

Chain D:



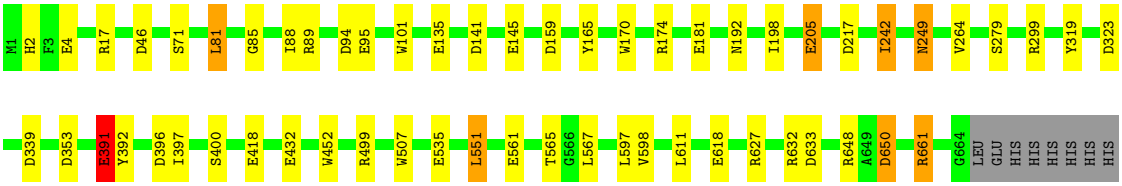
• Molecule 1: Alpha-glucosidase yihQ

Chain E:



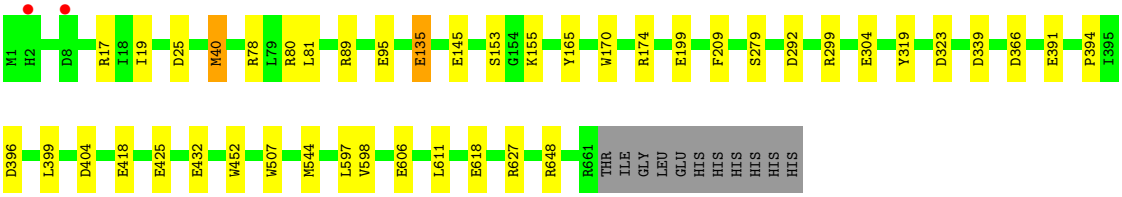
• Molecule 1: Alpha-glucosidase yihQ

Chain F:



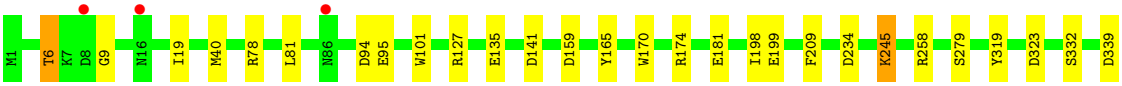
• Molecule 1: Alpha-glucosidase yihQ

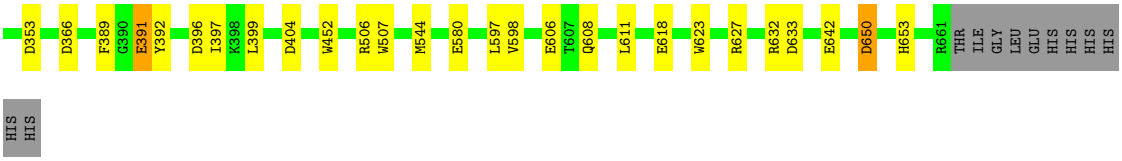
Chain G:



• Molecule 1: Alpha-glucosidase yihQ

Chain H:




D353
D366
F389
G390
E391
Y392
D396
I397
K398
L399
D404
W452
R506
W507
M544
E580
L597
V598
E606
T607
Q608
L611
E618
W623
R627
R632
D633
E642
D650
H653
R661
THR
ILE
GLY
LEU
GLU
HIS
HIS
HIS
HIS
HIS

4 Data and refinement statistics (i)

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
$< I/\sigma(I) >$ [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)	0.35 , 55.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	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	0.96	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.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

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

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	1.00	12/5359 (0.2%)	1.01	25/7286 (0.3%)
1	B	0.98	13/5367 (0.2%)	1.08	31/7299 (0.4%)
1	C	0.97	9/5332 (0.2%)	1.07	43/7251 (0.6%)
1	D	0.99	10/5334 (0.2%)	1.07	40/7254 (0.6%)
1	E	0.96	13/5358 (0.2%)	1.02	28/7284 (0.4%)
1	F	1.00	19/5368 (0.4%)	1.03	29/7300 (0.4%)
1	G	0.93	13/5335 (0.2%)	0.97	26/7257 (0.4%)
1	H	0.95	13/5345 (0.2%)	1.01	29/7268 (0.4%)
All	All	0.97	102/42798 (0.2%)	1.03	251/58199 (0.4%)

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 (102) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	391	GLU	CD-OE1	-12.33	1.12	1.25
1	A	135	GLU	CD-OE1	11.11	1.37	1.25
1	G	391	GLU	CD-OE1	-10.92	1.13	1.25
1	C	245	LYS	CB-CG	-10.82	1.23	1.52
1	H	391	GLU	CD-OE1	-10.77	1.13	1.25
1	G	319	TYR	CZ-OH	9.98	1.54	1.37
1	H	319	TYR	CZ-OH	9.83	1.54	1.37
1	B	319	TYR	CZ-OH	9.69	1.54	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	H	135	GLU	CD-OE1	9.62	1.36	1.25
1	E	135	GLU	CD-OE1	9.29	1.35	1.25
1	A	391	GLU	CD-OE1	-9.01	1.15	1.25
1	E	205	GLU	CD-OE2	8.93	1.35	1.25
1	B	135	GLU	CD-OE1	8.88	1.35	1.25
1	B	245	LYS	CB-CG	-8.83	1.28	1.52
1	G	425	GLU	CG-CD	8.72	1.65	1.51
1	H	650	ASP	CB-CG	-8.50	1.33	1.51
1	A	319	TYR	CZ-OH	8.19	1.51	1.37
1	G	279	SER	CB-OG	-8.16	1.31	1.42
1	D	650	ASP	CB-CG	-8.13	1.34	1.51
1	H	279	SER	CB-OG	-8.04	1.31	1.42
1	F	650	ASP	CB-CG	-8.00	1.34	1.51
1	C	319	TYR	CE2-CZ	7.79	1.48	1.38
1	E	650	ASP	CB-CG	-7.79	1.35	1.51
1	E	4	GLU	CG-CD	7.78	1.63	1.51
1	D	438	ARG	CZ-NH2	7.67	1.43	1.33
1	D	606	GLU	CD-OE1	7.63	1.34	1.25
1	E	319	TYR	CZ-OH	7.40	1.50	1.37
1	E	391	GLU	CD-OE1	-7.35	1.17	1.25
1	A	181	GLU	CG-CD	7.34	1.62	1.51
1	H	135	GLU	CD-OE2	-7.26	1.17	1.25
1	F	319	TYR	CZ-OH	7.21	1.50	1.37
1	H	245	LYS	CD-CE	-7.13	1.33	1.51
1	F	205	GLU	CD-OE2	6.96	1.33	1.25
1	F	400	SER	CB-OG	-6.94	1.33	1.42
1	F	71	SER	CB-OG	6.91	1.51	1.42
1	F	135	GLU	CD-OE1	6.90	1.33	1.25
1	E	400	SER	CB-OG	-6.89	1.33	1.42
1	F	135	GLU	CD-OE2	-6.86	1.18	1.25
1	C	606	GLU	CG-CD	-6.79	1.41	1.51
1	E	181	GLU	CG-CD	6.66	1.61	1.51
1	F	279	SER	CB-OG	-6.64	1.33	1.42
1	F	535	GLU	CD-OE1	6.62	1.32	1.25
1	D	332	SER	CB-OG	-6.52	1.33	1.42
1	D	199	GLU	CD-OE2	-6.45	1.18	1.25
1	C	332	SER	CB-OG	-6.44	1.33	1.42
1	F	391	GLU	CD-OE2	-6.44	1.18	1.25
1	C	199	GLU	CD-OE2	-6.41	1.18	1.25
1	C	42	ARG	CZ-NH1	6.32	1.41	1.33
1	H	580	GLU	CD-OE2	-6.25	1.18	1.25
1	F	205	GLU	CG-CD	6.21	1.61	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	392	TYR	CE2-CZ	6.19	1.46	1.38
1	D	319	TYR	CE2-CZ	6.18	1.46	1.38
1	H	332	SER	CB-OG	-6.12	1.34	1.42
1	D	71	SER	CB-OG	6.11	1.50	1.42
1	E	208	GLU	CG-CD	6.08	1.61	1.51
1	E	205	GLU	CG-CD	6.08	1.61	1.51
1	G	135	GLU	CD-OE1	6.07	1.32	1.25
1	G	606	GLU	CD-OE1	-5.94	1.19	1.25
1	F	249	ASN	CB-CG	-5.94	1.37	1.51
1	A	135	GLU	CD-OE2	-5.90	1.19	1.25
1	A	535	GLU	CD-OE2	5.87	1.32	1.25
1	A	205	GLU	CD-OE2	5.87	1.32	1.25
1	E	71	SER	CB-OG	5.87	1.49	1.42
1	A	648	ARG	CD-NE	-5.83	1.36	1.46
1	B	332	SER	CB-OG	-5.80	1.34	1.42
1	A	432	GLU	CD-OE1	5.77	1.31	1.25
1	F	432	GLU	CD-OE1	5.73	1.31	1.25
1	B	279	SER	CB-OG	-5.68	1.34	1.42
1	G	135	GLU	CD-OE2	-5.67	1.19	1.25
1	G	418	GLU	CD-OE1	5.66	1.31	1.25
1	A	199	GLU	CD-OE2	-5.65	1.19	1.25
1	A	95	GLU	CG-CD	5.63	1.60	1.51
1	D	21	SER	CB-OG	-5.60	1.34	1.42
1	H	606	GLU	CG-CD	5.60	1.60	1.51
1	B	135	GLU	CD-OE2	-5.59	1.19	1.25
1	G	199	GLU	CD-OE2	-5.58	1.19	1.25
1	E	432	GLU	CD-OE1	5.50	1.31	1.25
1	B	432	GLU	CD-OE1	5.49	1.31	1.25
1	D	606	GLU	CG-CD	-5.47	1.43	1.51
1	B	107	GLU	CD-OE2	-5.46	1.19	1.25
1	F	418	GLU	CD-OE2	5.46	1.31	1.25
1	E	606	GLU	CG-CD	-5.35	1.44	1.51
1	G	432	GLU	CD-OE1	5.29	1.31	1.25
1	G	153	SER	CB-OG	-5.28	1.35	1.42
1	C	438	ARG	CZ-NH2	5.28	1.40	1.33
1	H	199	GLU	CD-OE1	-5.22	1.20	1.25
1	G	425	GLU	CD-OE2	5.22	1.31	1.25
1	F	85	GLY	C-O	-5.20	1.15	1.23
1	B	580	GLU	CD-OE1	-5.18	1.20	1.25
1	H	199	GLU	CD-OE2	-5.15	1.20	1.25
1	D	331	GLU	CD-OE1	-5.14	1.20	1.25
1	B	283	ARG	CZ-NH1	-5.10	1.26	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	145	GLU	CD-OE1	5.08	1.31	1.25
1	B	548	TYR	CG-CD1	5.08	1.45	1.39
1	H	606	GLU	CD-OE1	5.08	1.31	1.25
1	F	392	TYR	CE1-CZ	5.05	1.45	1.38
1	B	283	ARG	CD-NE	-5.04	1.37	1.46
1	F	145	GLU	CD-OE1	5.03	1.31	1.25
1	F	249	ASN	CG-OD1	5.02	1.34	1.24
1	A	170	TRP	CZ3-CH2	5.02	1.48	1.40
1	F	249	ASN	CG-ND2	5.02	1.45	1.32
1	G	304	GLU	CD-OE2	5.01	1.31	1.25

All (251) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	283	ARG	NE-CZ-NH2	23.38	131.99	120.30
1	B	283	ARG	NE-CZ-NH1	-22.20	109.20	120.30
1	F	17	ARG	NE-CZ-NH1	14.73	127.67	120.30
1	B	661	ARG	NE-CZ-NH1	13.58	127.09	120.30
1	D	319	TYR	CB-CG-CD1	-13.00	113.20	121.00
1	C	319	TYR	CB-CG-CD1	-12.38	113.57	121.00
1	H	650	ASP	CB-CG-OD2	12.27	129.34	118.30
1	A	366	ASP	CB-CG-OD2	11.83	128.95	118.30
1	F	650	ASP	CB-CG-OD1	-10.70	108.67	118.30
1	D	438	ARG	NE-CZ-NH1	10.52	125.56	120.30
1	E	650	ASP	CB-CG-OD1	-10.47	108.88	118.30
1	C	245	LYS	N-CA-CB	-10.40	91.88	110.60
1	E	650	ASP	CB-CG-OD2	10.22	127.50	118.30
1	B	245	LYS	N-CA-CB	-10.13	92.36	110.60
1	E	17	ARG	NE-CZ-NH1	10.09	125.34	120.30
1	F	650	ASP	CB-CG-OD2	10.02	127.32	118.30
1	C	438	ARG	NE-CZ-NH1	10.00	125.30	120.30
1	A	366	ASP	CB-CG-OD1	-9.96	109.33	118.30
1	F	633	ASP	CB-CG-OD1	9.79	127.11	118.30
1	H	650	ASP	CB-CG-OD1	-9.62	109.65	118.30
1	C	125	ARG	NE-CZ-NH2	9.59	125.09	120.30
1	C	135	GLU	OE1-CD-OE2	9.51	134.72	123.30
1	H	633	ASP	CB-CG-OD1	-9.51	109.74	118.30
1	A	17	ARG	NE-CZ-NH2	-9.37	115.61	120.30
1	B	159	ASP	CB-CG-OD2	-9.08	110.12	118.30
1	F	551	LEU	CA-CB-CG	8.64	135.18	115.30
1	D	524	ARG	NE-CZ-NH2	-8.62	115.99	120.30
1	D	396	ASP	CB-CG-OD1	8.54	125.99	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	89	ARG	NE-CZ-NH1	8.54	124.57	120.30
1	D	283	ARG	NE-CZ-NH2	-8.50	116.05	120.30
1	A	292	ASP	CB-CG-OD1	8.42	125.88	118.30
1	C	319	TYR	CB-CG-CD2	8.37	126.02	121.00
1	D	524	ARG	NE-CZ-NH1	8.29	124.44	120.30
1	H	650	ASP	CB-CA-C	-8.27	93.85	110.40
1	C	396	ASP	CB-CG-OD1	8.24	125.72	118.30
1	D	319	TYR	CB-CG-CD2	8.07	125.84	121.00
1	D	135	GLU	OE1-CD-OE2	8.04	132.94	123.30
1	D	392	TYR	CA-CB-CG	7.94	128.49	113.40
1	C	392	TYR	CA-CB-CG	7.93	128.46	113.40
1	D	17	ARG	NE-CZ-NH1	7.92	124.26	120.30
1	B	141	ASP	CB-CG-OD2	-7.79	111.29	118.30
1	B	81	LEU	CB-CG-CD2	-7.78	97.78	111.00
1	F	650	ASP	CB-CA-C	-7.78	94.85	110.40
1	E	650	ASP	CB-CA-C	-7.77	94.85	110.40
1	H	633	ASP	CB-CG-OD2	7.72	125.25	118.30
1	D	606	GLU	OE1-CD-OE2	7.72	132.56	123.30
1	G	544	MET	CG-SD-CE	-7.72	87.85	100.20
1	H	181	GLU	OE1-CD-OE2	-7.71	114.05	123.30
1	D	650	ASP	CB-CA-C	-7.69	95.03	110.40
1	D	40	MET	CG-SD-CE	-7.66	87.95	100.20
1	F	145	GLU	OE1-CD-OE2	7.64	132.47	123.30
1	E	391	GLU	OE1-CD-OE2	-7.53	114.27	123.30
1	H	632	ARG	CB-CA-C	-7.50	95.40	110.40
1	D	633	ASP	CB-CG-OD1	7.49	125.04	118.30
1	C	633	ASP	CB-CG-OD1	7.41	124.96	118.30
1	A	107	GLU	OE1-CD-OE2	-7.33	114.50	123.30
1	G	425	GLU	CA-CB-CG	7.28	129.41	113.40
1	B	391	GLU	OE1-CD-OE2	-7.22	114.64	123.30
1	G	606	GLU	OE1-CD-OE2	-7.16	114.70	123.30
1	C	174	ARG	NE-CZ-NH1	7.16	123.88	120.30
1	D	348	ASP	CB-CG-OD1	7.13	124.72	118.30
1	C	549	VAL	CA-CB-CG1	7.10	121.55	110.90
1	H	632	ARG	CA-CB-CG	7.08	128.97	113.40
1	E	17	ARG	NE-CZ-NH2	-7.07	116.76	120.30
1	C	275	LEU	CA-CB-CG	7.07	131.55	115.30
1	B	89	ARG	NE-CZ-NH1	7.05	123.83	120.30
1	D	404	ASP	CB-CG-OD1	7.04	124.64	118.30
1	E	648	ARG	NE-CZ-NH2	-7.04	116.78	120.30
1	C	524	ARG	NE-CZ-NH2	-6.99	116.81	120.30
1	E	159	ASP	CB-CG-OD2	-6.98	112.01	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	H	506	ARG	NE-CZ-NH1	6.95	123.78	120.30
1	A	391	GLU	OE1-CD-OE2	-6.93	114.98	123.30
1	E	544	MET	CG-SD-CE	-6.90	89.16	100.20
1	E	396	ASP	CB-CG-OD1	6.89	124.50	118.30
1	B	174	ARG	NE-CZ-NH1	6.88	123.74	120.30
1	D	648	ARG	NE-CZ-NH2	-6.87	116.87	120.30
1	F	81	LEU	CA-CB-CG	6.83	131.01	115.30
1	C	89	ARG	NE-CZ-NH1	6.83	123.71	120.30
1	A	125	ARG	NE-CZ-NH2	6.81	123.71	120.30
1	G	145	GLU	OE1-CD-OE2	6.79	131.45	123.30
1	F	396	ASP	CB-CG-OD1	6.78	124.41	118.30
1	B	396	ASP	CB-CG-OD1	6.74	124.37	118.30
1	H	544	MET	CG-SD-CE	-6.72	89.44	100.20
1	H	396	ASP	CB-CG-OD1	6.70	124.33	118.30
1	G	391	GLU	OE1-CD-OE2	-6.68	115.28	123.30
1	A	396	ASP	CB-CG-OD1	6.58	124.22	118.30
1	G	396	ASP	CB-CG-OD1	6.57	124.21	118.30
1	C	648	ARG	NE-CZ-NH2	-6.57	117.02	120.30
1	B	661	ARG	CD-NE-CZ	6.55	132.78	123.60
1	E	633	ASP	CB-CG-OD1	6.50	124.14	118.30
1	D	81	LEU	CB-CG-CD1	-6.47	100.01	111.00
1	C	17	ARG	NE-CZ-NH1	6.43	123.51	120.30
1	G	648	ARG	NE-CZ-NH2	-6.42	117.09	120.30
1	E	375	LYS	CA-CB-CG	6.39	127.46	113.40
1	G	17	ARG	NE-CZ-NH2	-6.35	117.13	120.30
1	H	78	ARG	NE-CZ-NH1	6.34	123.47	120.30
1	E	632	ARG	NE-CZ-NH1	-6.32	117.14	120.30
1	F	353	ASP	CB-CG-OD1	6.30	123.97	118.30
1	C	40[A]	MET	CA-CB-CG	6.28	123.98	113.30
1	C	40[B]	MET	CA-CB-CG	6.28	123.98	113.30
1	E	351	GLU	OE1-CD-OE2	-6.28	115.76	123.30
1	A	499	ARG	NE-CZ-NH1	6.28	123.44	120.30
1	D	319	TYR	OH-CZ-CE2	6.27	137.03	120.10
1	A	95	GLU	OE1-CD-OE2	-6.24	115.81	123.30
1	H	234	ASP	CB-CG-OD1	6.17	123.85	118.30
1	G	78	ARG	NE-CZ-NH1	6.16	123.38	120.30
1	C	319	TYR	OH-CZ-CE2	6.16	136.73	120.10
1	B	323	ASP	CB-CG-OD1	6.15	123.83	118.30
1	E	94	ASP	CB-CG-OD1	6.14	123.83	118.30
1	B	648	ARG	NE-CZ-NH2	-6.11	117.24	120.30
1	A	159	ASP	CB-CG-OD1	6.10	123.79	118.30
1	D	627	ARG	CG-CD-NE	-6.10	98.99	111.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	H	141	ASP	CB-CG-OD2	-6.10	112.81	118.30
1	C	627	ARG	CG-CD-NE	-6.08	99.04	111.80
1	E	65	ASP	CB-CG-OD2	6.07	123.76	118.30
1	F	141	ASP	CB-CG-OD2	-6.05	112.85	118.30
1	H	339	ASP	CB-CG-OD1	6.05	123.74	118.30
1	E	25	ASP	CB-CG-OD1	6.05	123.74	118.30
1	H	391	GLU	OE1-CD-OE2	-6.05	116.05	123.30
1	B	499	ARG	NE-CZ-NH1	6.03	123.32	120.30
1	C	339	ASP	CB-CG-OD1	6.03	123.73	118.30
1	E	339	ASP	CB-CG-OD1	6.01	123.71	118.30
1	C	524	ARG	NE-CZ-NH1	6.00	123.30	120.30
1	B	404	ASP	CB-CG-OD1	6.00	123.70	118.30
1	C	283	ARG	NE-CZ-NH1	-6.00	117.30	120.30
1	G	425	GLU	OE1-CD-OE2	-6.00	116.10	123.30
1	D	294	ARG	NE-CZ-NH1	-5.99	117.31	120.30
1	A	353	ASP	CB-CG-OD1	5.98	123.68	118.30
1	B	339	ASP	CB-CG-OD1	5.97	123.67	118.30
1	D	613	LEU	CA-CB-CG	5.96	129.01	115.30
1	H	506	ARG	NE-CZ-NH2	-5.93	117.33	120.30
1	E	4	GLU	OE1-CD-OE2	-5.93	116.18	123.30
1	G	81	LEU	CB-CG-CD1	-5.91	100.96	111.00
1	F	339	ASP	CB-CG-OD1	5.90	123.61	118.30
1	A	141	ASP	CB-CG-OD2	-5.89	112.99	118.30
1	B	17	ARG	NE-CZ-NH1	5.89	123.25	120.30
1	D	632	ARG	CG-CD-NE	-5.88	99.44	111.80
1	G	339	ASP	CB-CG-OD1	5.88	123.60	118.30
1	A	78	ARG	NE-CZ-NH1	5.87	123.23	120.30
1	C	506	ARG	NE-CZ-NH2	-5.87	117.36	120.30
1	F	499	ARG	NE-CZ-NH1	5.85	123.22	120.30
1	B	145	GLU	OE1-CD-OE2	5.84	130.31	123.30
1	A	339	ASP	CB-CG-OD1	5.82	123.54	118.30
1	D	89	ARG	NE-CZ-NH2	-5.81	117.40	120.30
1	B	299	ARG	NE-CZ-NH2	-5.80	117.40	120.30
1	C	283	ARG	NE-CZ-NH2	-5.80	117.40	120.30
1	C	404	ASP	CB-CG-OD1	5.78	123.50	118.30
1	D	323	ASP	CB-CG-OD1	5.73	123.46	118.30
1	H	323	ASP	CB-CG-OD1	5.73	123.46	118.30
1	F	89	ARG	NE-CZ-NH1	5.72	123.16	120.30
1	F	159	ASP	CB-CG-OD2	-5.72	113.15	118.30
1	F	418	GLU	OE1-CD-OE2	5.71	130.15	123.30
1	G	25	ASP	CB-CG-OD1	5.70	123.43	118.30
1	F	94	ASP	CB-CG-OD1	5.68	123.41	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	650	ASP	N-CA-CB	-5.67	100.39	110.60
1	D	174	ARG	NE-CZ-NH1	5.65	123.13	120.30
1	A	499	ARG	NE-CZ-NH2	-5.62	117.49	120.30
1	E	366	ASP	CB-CG-OD1	5.62	123.35	118.30
1	C	81	LEU	CB-CG-CD1	-5.61	101.46	111.00
1	D	348	ASP	CB-CG-OD2	-5.61	113.25	118.30
1	C	323	ASP	CB-CG-OD1	5.61	123.34	118.30
1	A	323	ASP	CB-CG-OD1	5.60	123.34	118.30
1	C	89	ARG	NE-CZ-NH2	-5.59	117.51	120.30
1	A	642	GLU	OE1-CD-OE2	-5.58	116.60	123.30
1	E	2	HIS	N-CA-CB	5.58	120.65	110.60
1	D	339	ASP	CB-CG-OD1	5.58	123.32	118.30
1	H	174	ARG	NE-CZ-NH1	5.55	123.07	120.30
1	C	40[A]	MET	CG-SD-CE	-5.54	91.33	100.20
1	C	40[B]	MET	CG-SD-CE	-5.54	91.33	100.20
1	C	301	LYS	CD-CE-NZ	-5.54	98.95	111.70
1	H	40	MET	CB-CG-SD	5.52	128.97	112.40
1	A	301	LYS	CD-CE-NZ	-5.52	99.01	111.70
1	B	17	ARG	NE-CZ-NH2	-5.52	117.54	120.30
1	G	299	ARG	CG-CD-NE	5.51	123.37	111.80
1	F	299	ARG	NE-CZ-NH2	-5.51	117.55	120.30
1	D	54	ARG	NE-CZ-NH2	-5.50	117.55	120.30
1	C	606	GLU	OE1-CD-OE2	5.49	129.88	123.30
1	E	499	ARG	NE-CZ-NH1	5.49	123.04	120.30
1	B	626	LYS	CA-CB-CG	5.48	125.45	113.40
1	F	633	ASP	CB-CG-OD2	-5.47	113.38	118.30
1	C	640	LEU	CA-CB-CG	5.46	127.86	115.30
1	G	17	ARG	NE-CZ-NH1	5.46	123.03	120.30
1	D	399	LEU	CA-CB-CG	-5.45	102.76	115.30
1	D	499	ARG	NE-CZ-NH1	5.44	123.02	120.30
1	C	141	ASP	CB-CG-OD2	-5.42	113.42	118.30
1	G	279	SER	CB-CA-C	-5.41	99.82	110.10
1	A	159	ASP	CB-CG-OD2	-5.41	113.43	118.30
1	C	399	LEU	CA-CB-CG	-5.41	102.87	115.30
1	H	399	LEU	CA-CB-CG	-5.39	102.90	115.30
1	F	499	ARG	NE-CZ-NH2	-5.38	117.61	120.30
1	B	632	ARG	CG-CD-NE	-5.35	100.56	111.80
1	C	627	ARG	NE-CZ-NH2	-5.35	117.62	120.30
1	B	217	ASP	CB-CG-OD1	5.34	123.11	118.30
1	C	125	ARG	NE-CZ-NH1	-5.34	117.63	120.30
1	F	217	ASP	CB-CG-OD1	5.34	123.10	118.30
1	G	323	ASP	CB-CG-OD1	5.34	123.10	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	275	LEU	CA-CB-CG	5.32	127.54	115.30
1	F	661	ARG	CG-CD-NE	5.32	122.97	111.80
1	D	299	ARG	NE-CZ-NH2	-5.32	117.64	120.30
1	F	650	ASP	N-CA-CB	-5.31	101.04	110.60
1	F	174	ARG	NE-CZ-NH1	5.29	122.94	120.30
1	G	40	MET	CB-CG-SD	5.26	128.19	112.40
1	B	58	ARG	NE-CZ-NH2	-5.26	117.67	120.30
1	A	648	ARG	NE-CZ-NH1	5.24	122.92	120.30
1	G	404	ASP	CB-CG-OD1	5.24	123.02	118.30
1	D	627	ARG	NE-CZ-NH1	5.24	122.92	120.30
1	B	661	ARG	CG-CD-NE	5.24	122.80	111.80
1	C	499	ARG	NE-CZ-NH1	5.23	122.92	120.30
1	H	404	ASP	CB-CG-OD1	5.23	123.01	118.30
1	G	174	ARG	NE-CZ-NH1	5.23	122.92	120.30
1	A	217	ASP	CB-CG-OD1	5.23	123.00	118.30
1	A	127	ARG	NE-CZ-NH1	5.21	122.91	120.30
1	H	159	ASP	CB-CG-OD2	-5.21	113.61	118.30
1	A	299	ARG	CG-CD-NE	5.20	122.72	111.80
1	E	141	ASP	CB-CG-OD2	-5.20	113.62	118.30
1	E	46	ASP	CB-CG-OD2	-5.19	113.62	118.30
1	B	584	TYR	CB-CG-CD1	5.18	124.11	121.00
1	G	366	ASP	CB-CG-OD1	5.18	122.96	118.30
1	B	506	ARG	NE-CZ-NH1	5.17	122.89	120.30
1	E	299	ARG	NE-CZ-NH1	5.16	122.88	120.30
1	G	174	ARG	NE-CZ-NH2	-5.16	117.72	120.30
1	C	145	GLU	OE1-CD-OE2	5.15	129.48	123.30
1	G	292	ASP	CB-CG-OD1	5.15	122.93	118.30
1	H	127	ARG	NE-CZ-NH1	5.14	122.87	120.30
1	B	399	LEU	CA-CB-CG	-5.13	103.49	115.30
1	H	392	TYR	CB-CG-CD1	-5.13	117.92	121.00
1	E	650	ASP	N-CA-CB	-5.12	101.38	110.60
1	H	94	ASP	CB-CG-OD2	-5.12	113.69	118.30
1	D	159	ASP	CB-CG-OD2	-5.12	113.69	118.30
1	F	181	GLU	CG-CD-OE1	5.12	128.54	118.30
1	E	242	ILE	CB-CG1-CD1	-5.11	99.60	113.90
1	F	242	ILE	CB-CG1-CD1	-5.11	99.60	113.90
1	D	534	ASP	CB-CG-OD2	-5.10	113.71	118.30
1	F	323	ASP	CB-CG-OD1	5.09	122.88	118.30
1	B	94	ASP	CB-CG-OD1	5.08	122.88	118.30
1	F	46	ASP	CB-CG-OD2	-5.08	113.73	118.30
1	G	80	ARG	NE-CZ-NH2	-5.07	117.76	120.30
1	C	78	ARG	NE-CZ-NH1	5.07	122.83	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	323	ASP	CB-CG-OD2	-5.06	113.75	118.30
1	D	319	TYR	CE1-CZ-OH	-5.06	106.45	120.10
1	B	353	ASP	CB-CG-OD1	5.05	122.85	118.30
1	C	319	TYR	CE1-CZ-OH	-5.05	106.46	120.10
1	G	89	ARG	NE-CZ-NH2	-5.05	117.78	120.30
1	F	648	ARG	NE-CZ-NH2	-5.04	117.78	120.30
1	A	404	ASP	CB-CG-OD1	5.03	122.83	118.30
1	D	392	TYR	CB-CG-CD1	-5.03	117.98	121.00
1	G	399	LEU	CA-CB-CG	-5.03	103.73	115.30
1	C	159	ASP	CB-CG-OD2	-5.03	113.78	118.30
1	H	366	ASP	CB-CG-OD1	5.02	122.82	118.30
1	H	81	LEU	CB-CG-CD1	-5.02	102.47	111.00
1	H	353	ASP	CB-CG-OD1	5.00	122.80	118.30

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 (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5207	0	4962	19	0
1	B	5215	0	4965	11	0
1	C	5183	0	4933	18	0
1	D	5187	0	4931	14	0
1	E	5206	0	4964	9	0
1	F	5219	0	4967	17	0
1	G	5186	0	4918	6	0
1	H	5197	0	4945	18	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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
8	D	307	0	0	1	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	102	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 (102) 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
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:263:LYS:HG3	1:C:549:VAL:CG1	2.37	0.53
1:F:81:LEU:HD12	1:F:88:ILE:HG23	1.90	0.53
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: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:581:PRO:HB3	3:A:704:MPD:H13	1.92	0.50
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:B:283:ARG:HD2	6:B:705:NSQ:S10	2.54	0.47
1:C:565:THR:HG23	1:C:567:LEU:H	1.79	0.47
1:D:565:THR:HG23	1:D:567:LEU:H	1.80	0.46
1:E:565:THR:HG23	1:E:567:LEU:H	1.80	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: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:E:597:LEU:HD23	1:E:598:VAL:N	2.34	0.42
1:H:6:THR:HG22	1:H:9:GLY:C	2.39	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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 (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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 (i)

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%)	73	70
1	B	533/545 (98%)	524 (98%)	9 (2%)	60	53
1	C	528/545 (97%)	519 (98%)	9 (2%)	60	53
1	D	527/545 (97%)	520 (99%)	7 (1%)	69	64
1	E	532/545 (98%)	521 (98%)	11 (2%)	53	47
1	F	533/545 (98%)	521 (98%)	12 (2%)	50	44
1	G	527/545 (97%)	520 (99%)	7 (1%)	69	64
1	H	530/545 (97%)	521 (98%)	9 (2%)	60	53
All	All	4243/4360 (97%)	4173 (98%)	70 (2%)	60	56

All (70) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	95	GLU
1	A	165	TYR
1	A	170	TRP
1	A	452	TRP
1	A	507	TRP
1	A	611	LEU

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Mol	Chain	Res	Type
1	B	95	GLU
1	B	165	TYR
1	B	170	TRP
1	B	245	LYS
1	B	375	LYS
1	B	452	TRP
1	B	507	TRP
1	B	611	LEU
1	B	661	ARG
1	C	95	GLU
1	C	165	TYR
1	C	170	TRP
1	C	245	LYS
1	C	283	ARG
1	C	452	TRP
1	C	507	TRP
1	C	611	LEU
1	C	640	LEU
1	D	77	PRO
1	D	165	TYR
1	D	170	TRP
1	D	452	TRP
1	D	507	TRP
1	D	611	LEU
1	D	650	ASP
1	E	7	LYS
1	E	77	PRO
1	E	95	GLU
1	E	165	TYR
1	E	170	TRP
1	E	375	LYS
1	E	452	TRP
1	E	507	TRP
1	E	611	LEU
1	E	632	ARG
1	E	650	ASP
1	F	95	GLU
1	F	165	TYR
1	F	170	TRP
1	F	249	ASN
1	F	391	GLU
1	F	452	TRP

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Mol	Chain	Res	Type
1	F	507	TRP
1	F	551	LEU
1	F	611	LEU
1	F	632	ARG
1	F	650	ASP
1	F	661	ARG
1	G	95	GLU
1	G	155	LYS
1	G	165	TYR
1	G	170	TRP
1	G	452	TRP
1	G	507	TRP
1	G	611	LEU
1	H	6	THR
1	H	95	GLU
1	H	165	TYR
1	H	170	TRP
1	H	245	LYS
1	H	452	TRP
1	H	507	TRP
1	H	611	LEU
1	H	650	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	D	300	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

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	$\#\|Z\| > 2$
3	MPD	F	703	-	7,7,7	0.47	0	9,10,10	0.38	0
5	EDO	E	704	-	3,3,3	0.47	0	2,2,2	0.43	0
3	MPD	E	702	-	7,7,7	0.29	0	9,10,10	0.71	0
5	EDO	D	705	-	3,3,3	0.30	0	2,2,2	0.37	0
6	NSQ	G	706	-	23,25,25	1.04	1 (4%)	32,37,37	1.46	5 (15%)
5	EDO	D	707	-	3,3,3	0.88	0	2,2,2	0.99	0
6	NSQ	A	709	-	23,25,25	1.51	6 (26%)	32,37,37	2.01	7 (21%)
2	SCN	A	701	-	1,2,2	0.23	0	0,1,1	-	-
2	SCN	E	701	-	1,2,2	0.43	0	0,1,1	-	-
6	NSQ	B	705	-	23,25,25	1.44	4 (17%)	32,37,37	1.45	5 (15%)
2	SCN	A	702	-	1,2,2	0.49	0	0,1,1	-	-
3	MPD	D	704	-	7,7,7	0.56	0	9,10,10	1.05	0
5	EDO	C	702	-	3,3,3	0.52	0	2,2,2	0.36	0
5	EDO	A	707	-	3,3,3	0.53	0	2,2,2	0.29	0
5	EDO	B	704	-	3,3,3	1.05	0	2,2,2	0.31	0
5	EDO	F	707	-	3,3,3	0.71	0	2,2,2	0.10	0
5	EDO	F	710	-	3,3,3	0.56	0	2,2,2	0.42	0
3	MPD	F	704	-	7,7,7	0.48	0	9,10,10	0.60	0
5	EDO	G	703	-	3,3,3	0.51	0	2,2,2	0.20	0
3	MPD	A	703	-	7,7,7	0.45	0	9,10,10	0.79	0
5	EDO	F	708	-	3,3,3	0.62	0	2,2,2	0.17	0
6	NSQ	C	703	-	23,25,25	1.49	4 (17%)	32,37,37	2.18	6 (18%)
5	EDO	F	709	-	3,3,3	1.01	0	2,2,2	0.64	0
2	SCN	D	702	-	1,2,2	0.25	0	0,1,1	-	-
5	EDO	H	703	-	3,3,3	0.99	0	2,2,2	0.47	0
6	NSQ	H	704	-	23,25,25	1.09	3 (13%)	32,37,37	1.35	4 (12%)
3	MPD	D	703	-	7,7,7	0.33	0	9,10,10	0.54	0
6	NSQ	D	708	-	23,25,25	1.46	5 (21%)	32,37,37	1.82	8 (25%)
5	EDO	F	706	-	3,3,3	0.43	0	2,2,2	0.75	0
5	EDO	D	706	-	3,3,3	0.87	0	2,2,2	0.72	0
2	SCN	G	701	-	1,2,2	0.09	0	0,1,1	-	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
6	NSQ	E	705	-	23,25,25	1.16	2 (8%)	32,37,37	1.69	5 (15%)
3	MPD	B	701	-	7,7,7	0.57	0	9,10,10	1.21	1 (11%)
3	MPD	A	705	-	7,7,7	0.68	0	9,10,10	1.00	1 (11%)
5	EDO	G	705	-	3,3,3	0.43	0	2,2,2	0.37	0
5	EDO	B	703	-	3,3,3	0.54	0	2,2,2	0.69	0
6	NSQ	F	711	-	23,25,25	1.31	4 (17%)	32,37,37	1.26	2 (6%)
2	SCN	H	701	-	1,2,2	0.48	0	0,1,1	-	-
5	EDO	G	704	-	3,3,3	0.52	0	2,2,2	0.57	0
3	MPD	A	704	-	7,7,7	0.76	0	9,10,10	1.27	2 (22%)
2	SCN	F	701	-	1,2,2	0.01	0	0,1,1	-	-
2	SCN	F	702	-	1,2,2	0.09	0	0,1,1	-	-
5	EDO	A	708	-	3,3,3	0.89	0	2,2,2	0.32	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
3	MPD	F	703	-	-	0/5/5/5	-
5	EDO	E	704	-	-	1/1/1/1	-
3	MPD	E	702	-	-	1/5/5/5	-
5	EDO	D	705	-	-	1/1/1/1	-
6	NSQ	G	706	-	-	2/11/33/33	0/2/2/2
5	EDO	D	707	-	-	0/1/1/1	-
6	NSQ	A	709	-	-	2/11/33/33	0/2/2/2
6	NSQ	B	705	-	-	2/11/33/33	0/2/2/2
3	MPD	D	704	-	-	3/5/5/5	-
5	EDO	C	702	-	-	0/1/1/1	-
5	EDO	A	707	-	-	1/1/1/1	-
5	EDO	B	704	-	-	1/1/1/1	-
5	EDO	F	707	-	-	0/1/1/1	-
5	EDO	F	710	-	-	1/1/1/1	-
3	MPD	F	704	-	-	1/5/5/5	-
5	EDO	G	703	-	-	0/1/1/1	-
3	MPD	A	703	-	-	0/5/5/5	-
5	EDO	F	708	-	-	0/1/1/1	-
6	NSQ	C	703	-	-	4/11/33/33	0/2/2/2
5	EDO	F	709	-	-	1/1/1/1	-
5	EDO	H	703	-	-	1/1/1/1	-

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

All (29) 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
6	D	708	NSQ	O34-N32	3.67	1.29	1.22
6	C	703	NSQ	O34-N32	3.24	1.28	1.22
6	B	705	NSQ	O34-N32	3.13	1.28	1.22
6	D	708	NSQ	C6-S10	-3.02	1.66	1.77
6	F	711	NSQ	O1-C25	-2.90	1.32	1.38
6	E	705	NSQ	C6-S10	-2.73	1.67	1.77
6	D	708	NSQ	O1-C1	2.71	1.45	1.41
6	A	709	NSQ	C6-S10	-2.70	1.67	1.77
6	E	705	NSQ	C28-N32	-2.67	1.38	1.45
6	C	703	NSQ	C4-C5	2.62	1.58	1.53
6	G	706	NSQ	C28-N32	-2.47	1.39	1.45
6	F	711	NSQ	C6-S10	-2.46	1.68	1.77
6	B	705	NSQ	C6-S10	-2.44	1.68	1.77
6	A	709	NSQ	C28-N32	-2.38	1.39	1.45
6	F	711	NSQ	O1-C1	2.32	1.44	1.41
6	F	711	NSQ	O34-N32	2.31	1.26	1.22
6	H	704	NSQ	C28-N32	-2.21	1.39	1.45
6	D	708	NSQ	O13-S10	2.21	1.51	1.45
6	H	704	NSQ	O34-N32	2.19	1.26	1.22
6	H	704	NSQ	O12-S10	2.14	1.51	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	C	703	NSQ	C6-S10	-2.11	1.69	1.77
6	A	709	NSQ	O34-N32	2.10	1.26	1.22
6	A	709	NSQ	O13-S10	2.09	1.51	1.45
6	D	708	NSQ	C4-C5	2.05	1.57	1.53
6	A	709	NSQ	O1-C25	-2.01	1.34	1.38
6	B	705	NSQ	O13-S10	2.01	1.51	1.45

All (46) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	A	709	NSQ	O12-S10-C6	-6.56	99.14	106.94
6	C	703	NSQ	C29-C28-N32	6.47	124.25	119.38
6	C	703	NSQ	O12-S10-C6	5.98	114.05	106.94
6	E	705	NSQ	O11-S10-C6	5.06	113.81	105.74
6	D	708	NSQ	C27-C28-N32	5.04	123.17	119.38
6	A	709	NSQ	O11-S10-C6	4.76	113.33	105.74
6	F	711	NSQ	O13-S10-C6	4.73	112.56	106.94
6	G	706	NSQ	O11-S10-C6	4.71	113.24	105.74
6	C	703	NSQ	C27-C28-N32	-4.28	116.16	119.38
6	D	708	NSQ	O11-S10-C6	4.27	112.54	105.74
6	E	705	NSQ	C29-C28-N32	4.20	122.53	119.38
6	C	703	NSQ	O1-C1-C2	3.96	112.89	107.14
6	G	706	NSQ	O2-C2-C3	3.68	118.85	110.35
6	E	705	NSQ	C27-C28-N32	-3.66	116.62	119.38
6	B	705	NSQ	O11-S10-O12	3.53	119.90	111.27
6	A	709	NSQ	O13-S10-C6	3.43	111.01	106.94
6	B	705	NSQ	C4-C3-C2	-3.34	105.00	110.82
6	C	703	NSQ	O3-C3-C4	3.30	117.98	110.35
6	A	709	NSQ	O4-C4-C5	3.22	117.30	109.30
6	D	708	NSQ	O1-C1-C2	3.14	111.69	107.14
6	H	704	NSQ	O2-C2-C3	3.13	117.58	110.35
6	B	705	NSQ	O13-S10-O12	-2.96	103.72	113.95
6	E	705	NSQ	O11-S10-O13	-2.94	104.08	111.27
6	A	709	NSQ	O11-S10-O13	-2.77	104.50	111.27
6	D	708	NSQ	O3-C3-C4	2.76	116.74	110.35
6	F	711	NSQ	C4-C3-C2	-2.75	106.03	110.82
6	D	708	NSQ	O12-S10-C6	2.61	110.05	106.94
3	A	705	MPD	O2-C2-C1	-2.53	99.95	108.08
6	D	708	NSQ	C4-C3-C2	-2.51	106.44	110.82
6	A	709	NSQ	O11-S10-O12	2.49	117.36	111.27
6	H	704	NSQ	C29-C28-N32	2.48	121.24	119.38
6	H	704	NSQ	O13-S10-O12	-2.48	105.38	113.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	E	705	NSQ	C25-O1-C1	2.38	121.29	117.79
6	G	706	NSQ	O13-S10-O12	-2.37	105.74	113.95
6	G	706	NSQ	C1-O5-C5	2.29	118.19	113.69
3	A	704	MPD	O2-C2-CM	2.24	115.28	108.08
6	D	708	NSQ	C29-C28-N32	-2.22	117.71	119.38
6	B	705	NSQ	C3-C4-C5	2.22	114.19	110.24
6	D	708	NSQ	O13-S10-O12	-2.13	106.57	113.95
3	A	704	MPD	O4-C4-C5	2.11	118.52	109.38
6	H	704	NSQ	O11-S10-C6	2.09	109.07	105.74
6	G	706	NSQ	O12-S10-C6	2.06	109.39	106.94
6	B	705	NSQ	O11-S10-C6	-2.06	102.46	105.74
6	C	703	NSQ	O3-C3-C2	-2.04	105.63	110.35
6	A	709	NSQ	C4-C3-C2	-2.03	107.28	110.82
3	B	701	MPD	O2-C2-C1	-2.03	101.58	108.08

There are no chirality outliers.

All (42) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	D	704	MPD	C2-C3-C4-O4
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	D	705	EDO	O1-C1-C2-O2
5	E	704	EDO	O1-C1-C2-O2
5	G	705	EDO	O1-C1-C2-O2
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
6	C	703	NSQ	C30-C25-O1-C1
6	E	705	NSQ	C26-C25-O1-C1
3	E	702	MPD	O2-C2-C3-C4
6	E	705	NSQ	C30-C25-O1-C1

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Mol	Chain	Res	Type	Atoms
6	D	708	NSQ	C26-C25-O1-C1
6	D	708	NSQ	C30-C25-O1-C1
3	A	704	MPD	C2-C3-C4-C5
3	A	705	MPD	C2-C3-C4-C5
5	A	708	EDO	O1-C1-C2-O2
3	D	703	MPD	CM-C2-C3-C4
3	D	704	MPD	C1-C2-C3-C4
3	A	705	MPD	O2-C2-C3-C4
3	D	703	MPD	O2-C2-C3-C4
3	D	704	MPD	O2-C2-C3-C4
5	D	706	EDO	O1-C1-C2-O2
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	B	701	MPD	C2-C3-C4-C5
3	F	704	MPD	C2-C3-C4-C5
5	A	707	EDO	O1-C1-C2-O2
5	B	704	EDO	O1-C1-C2-O2
3	A	705	MPD	C2-C3-C4-O4

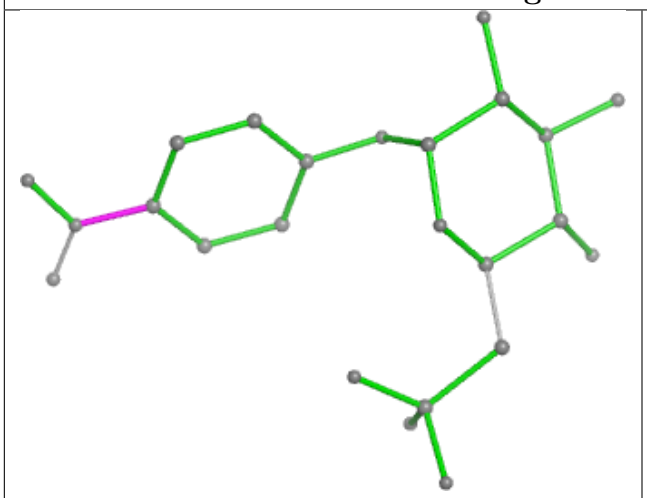
There are no ring outliers.

4 monomers are involved in 10 short contacts:

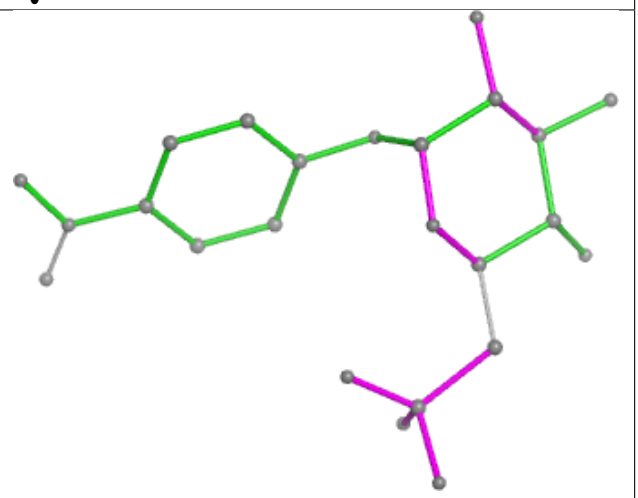
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	D	707	EDO	5	0
6	B	705	NSQ	2	0
5	D	706	EDO	1	0
3	A	704	MPD	2	0

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

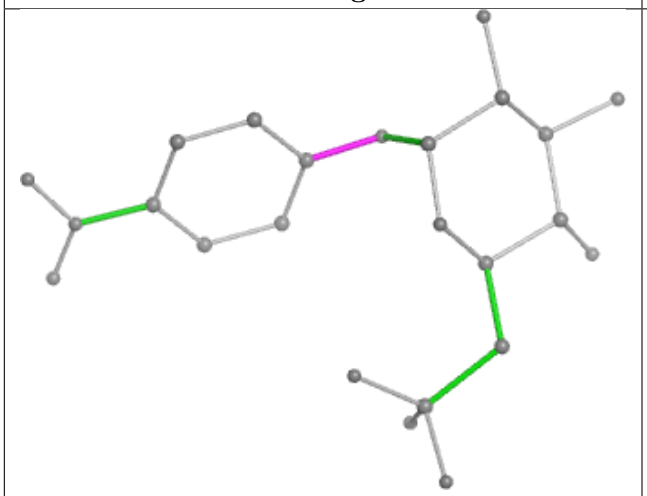
Ligand NSQ G 706



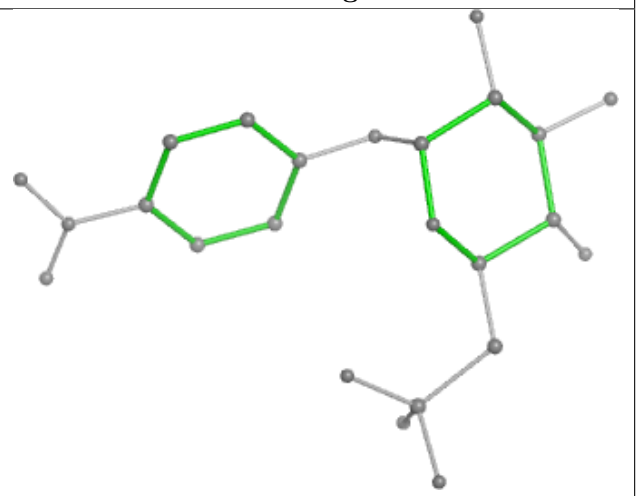
Bond lengths



Bond angles

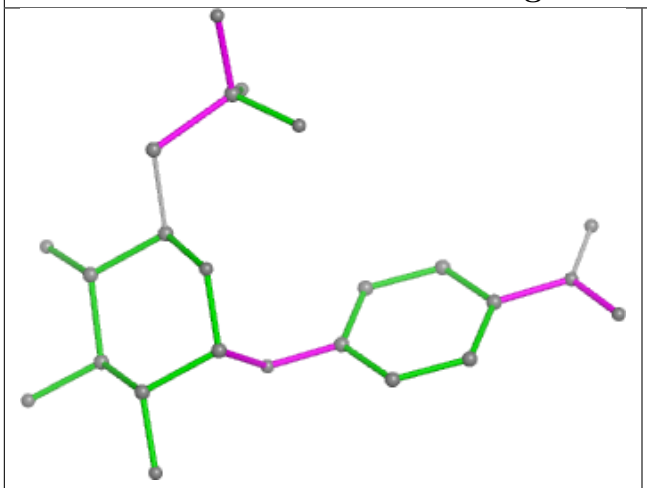


Torsions

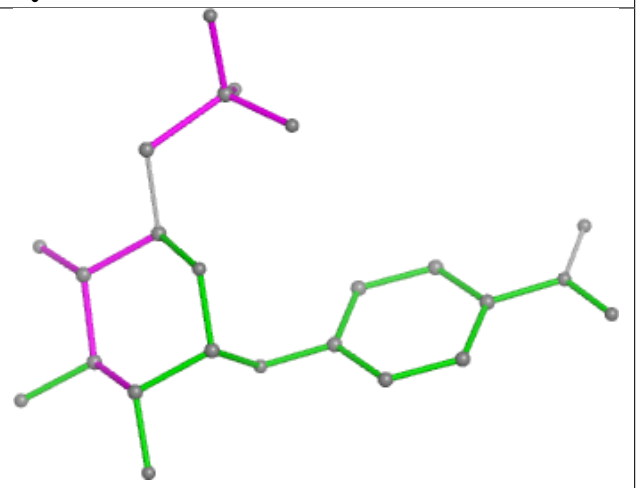


Rings

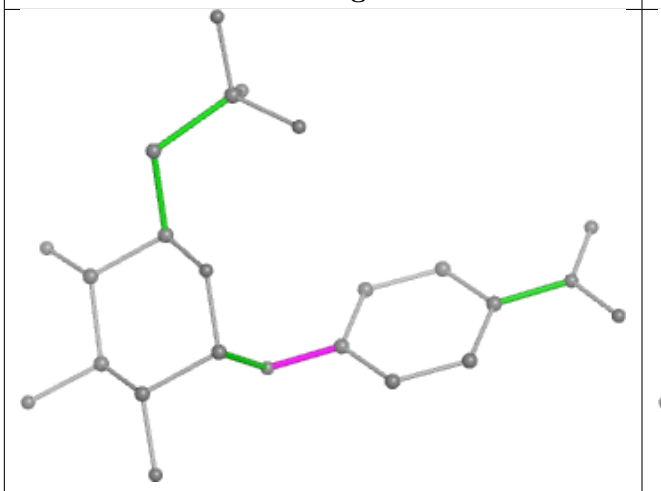
Ligand NSQ A 709



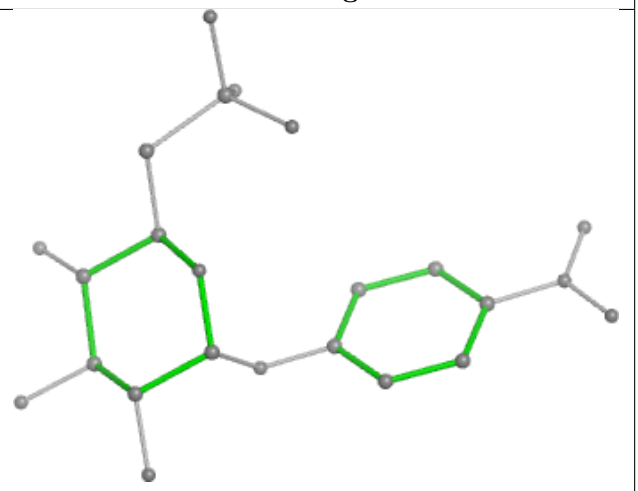
Bond lengths



Bond angles

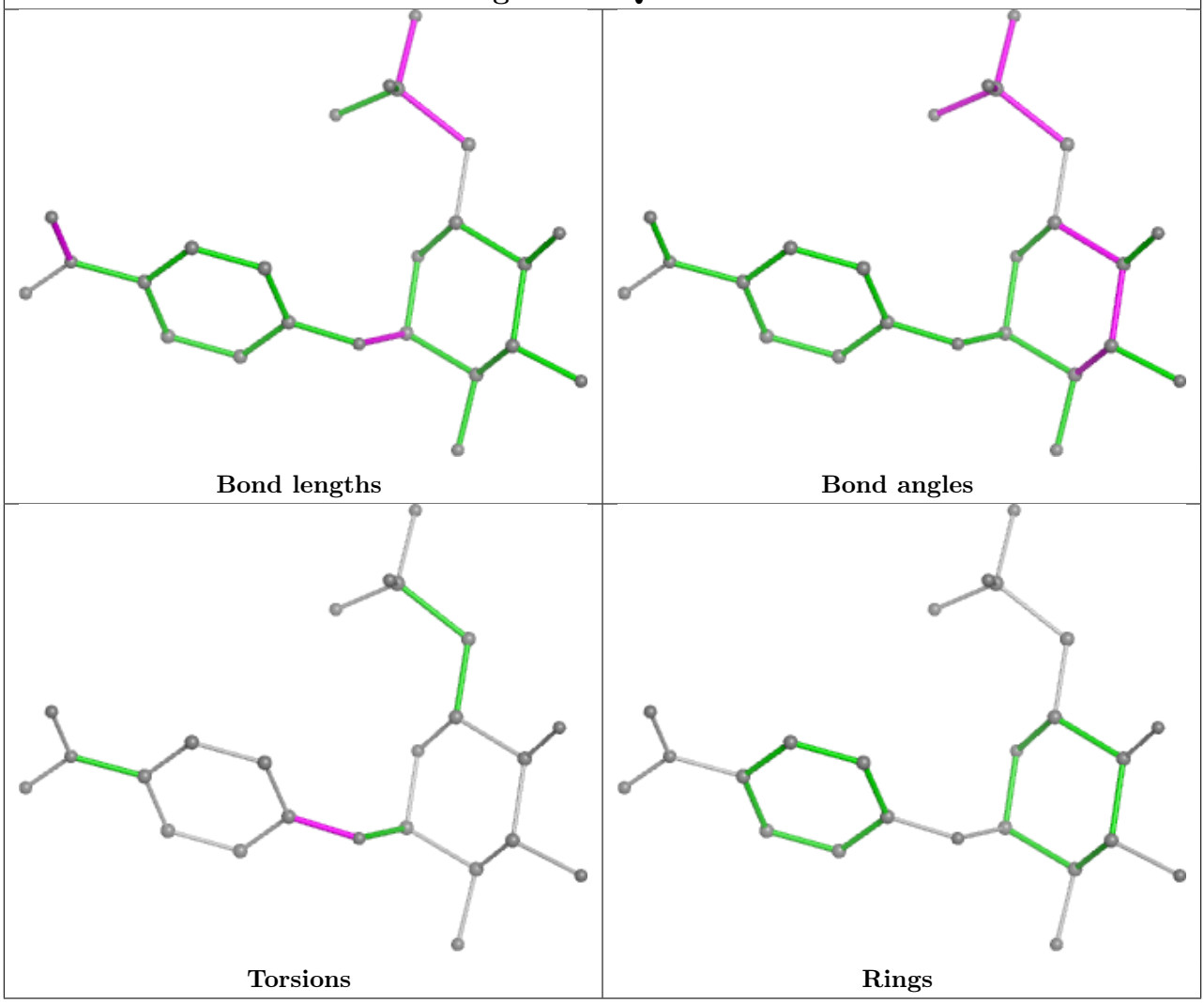


Torsions

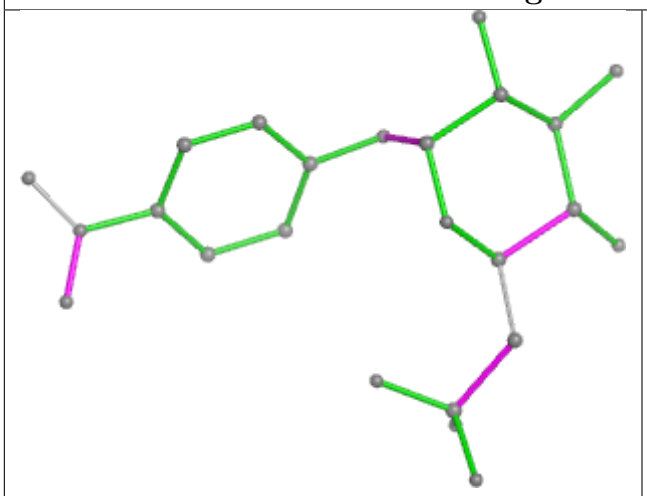


Rings

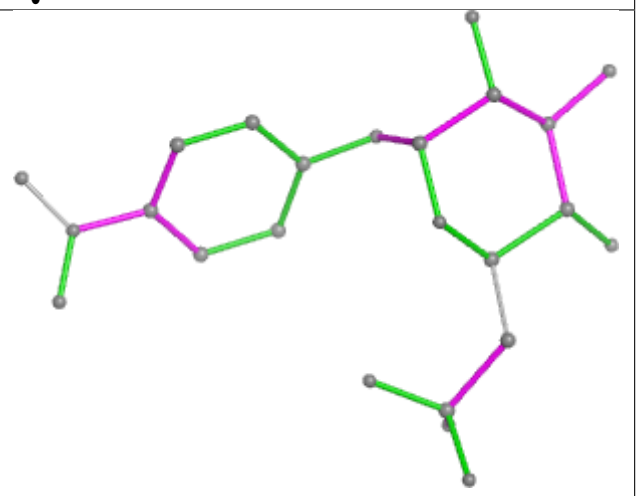
Ligand NSQ B 705



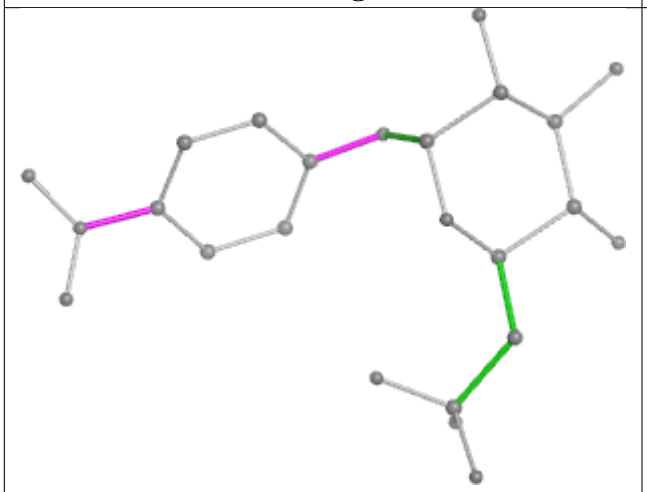
Ligand NSQ C 703



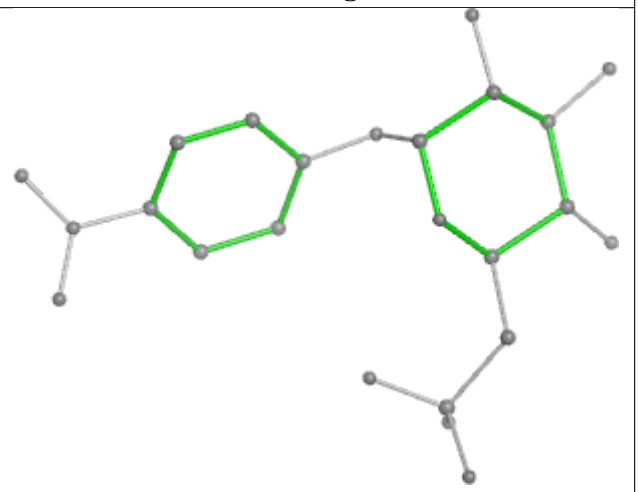
Bond lengths



Bond angles

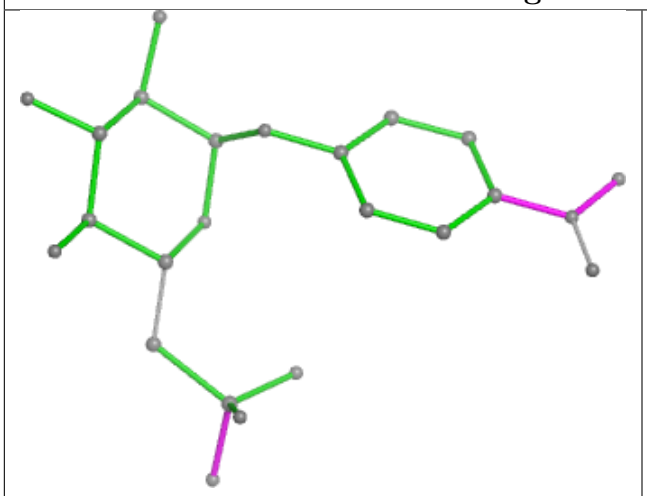


Torsions

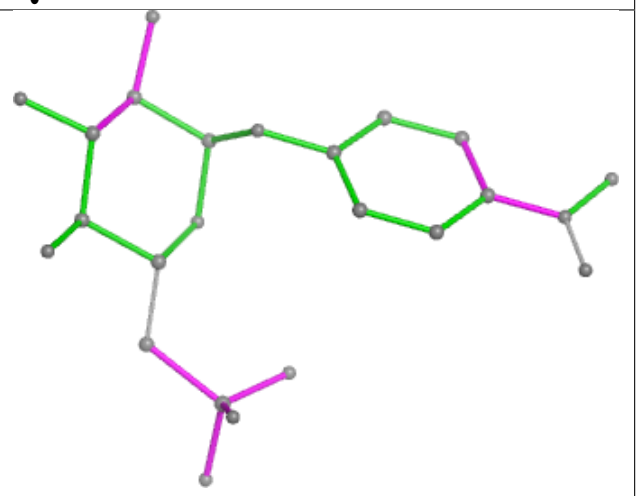


Rings

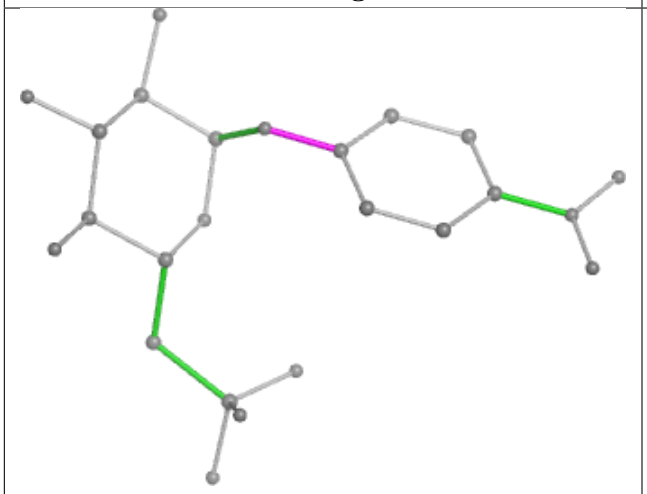
Ligand NSQ H 704



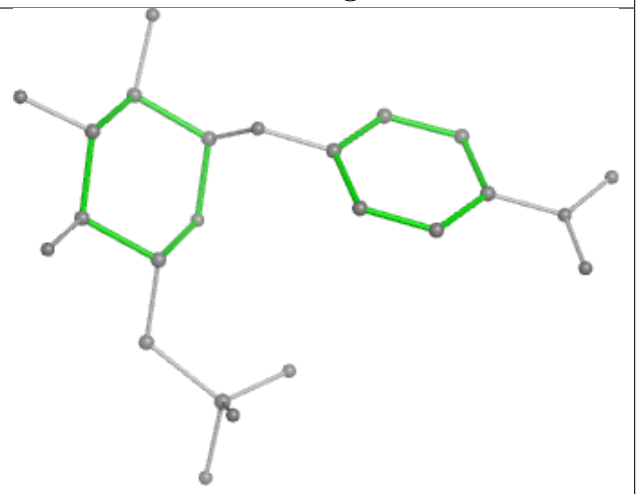
Bond lengths



Bond angles

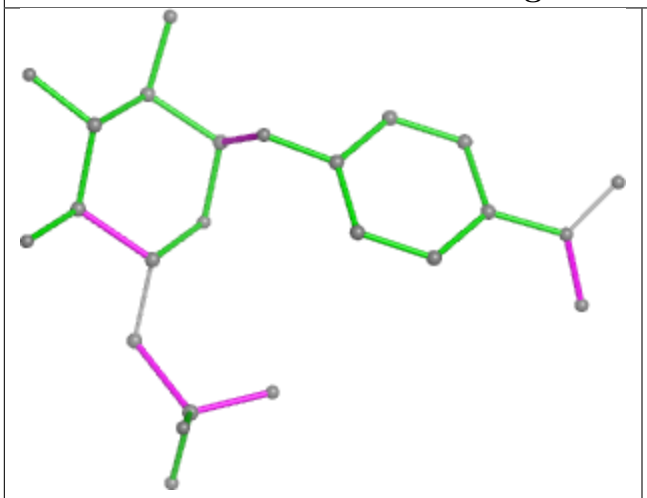


Torsions

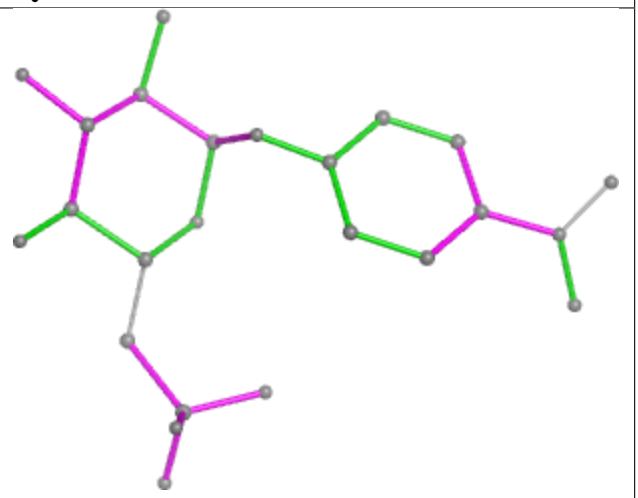


Rings

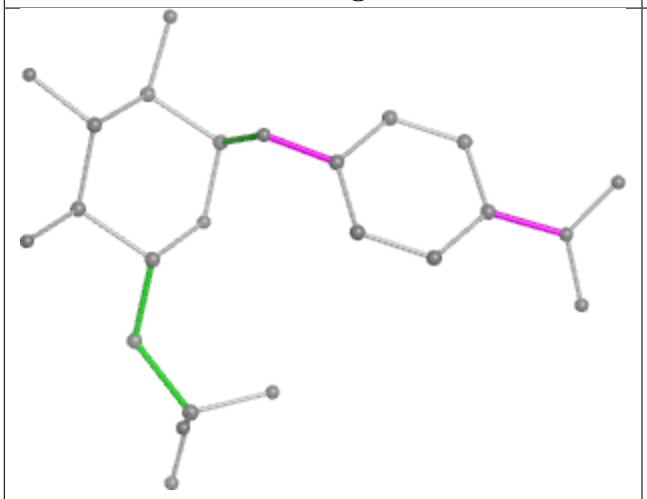
Ligand NSQ D 708



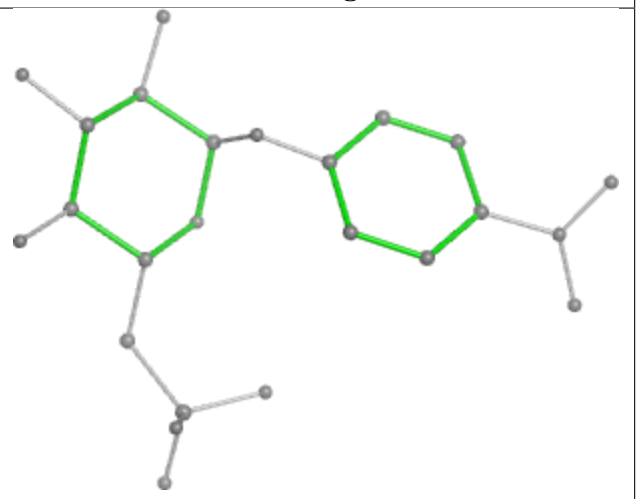
Bond lengths



Bond angles

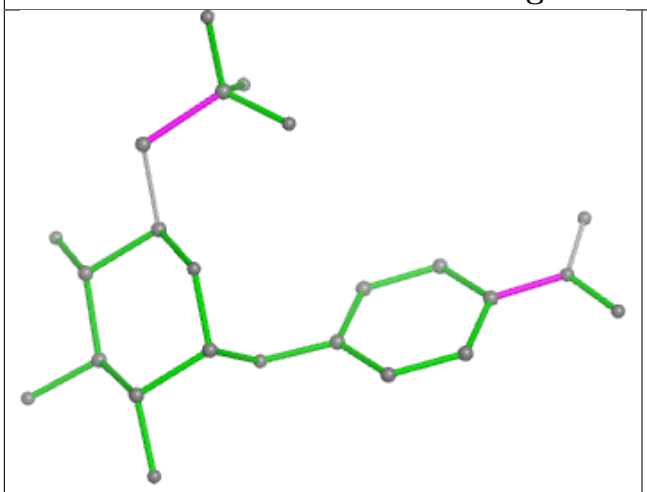


Torsions

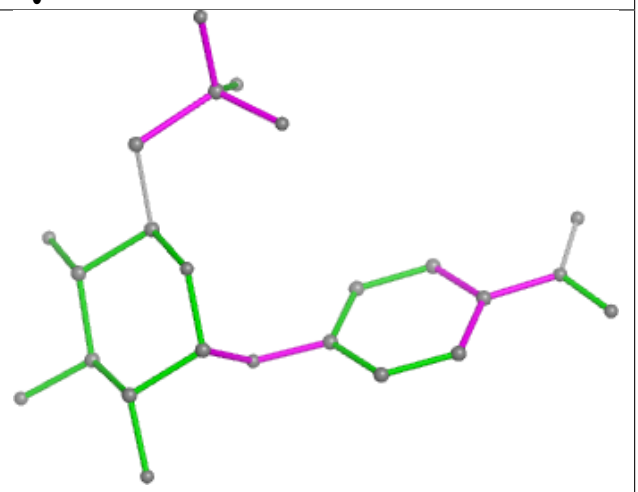


Rings

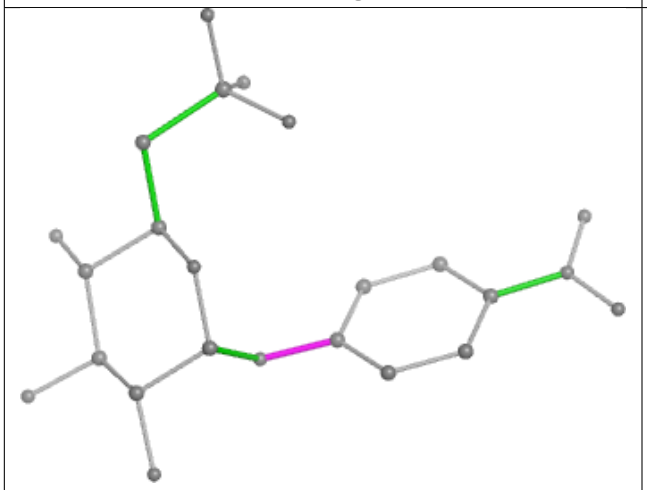
Ligand NSQ E 705



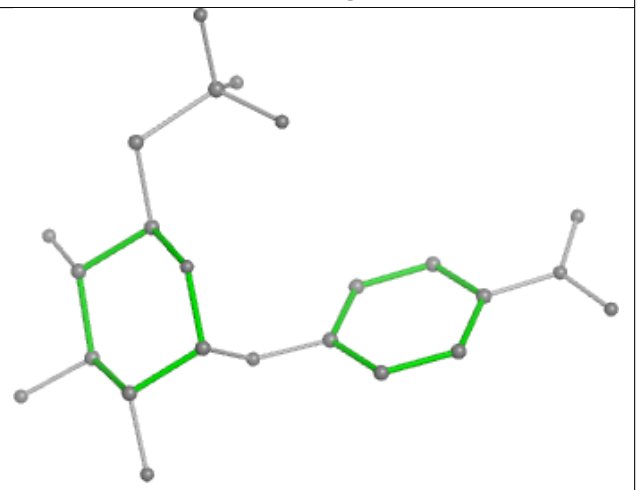
Bond lengths



Bond angles

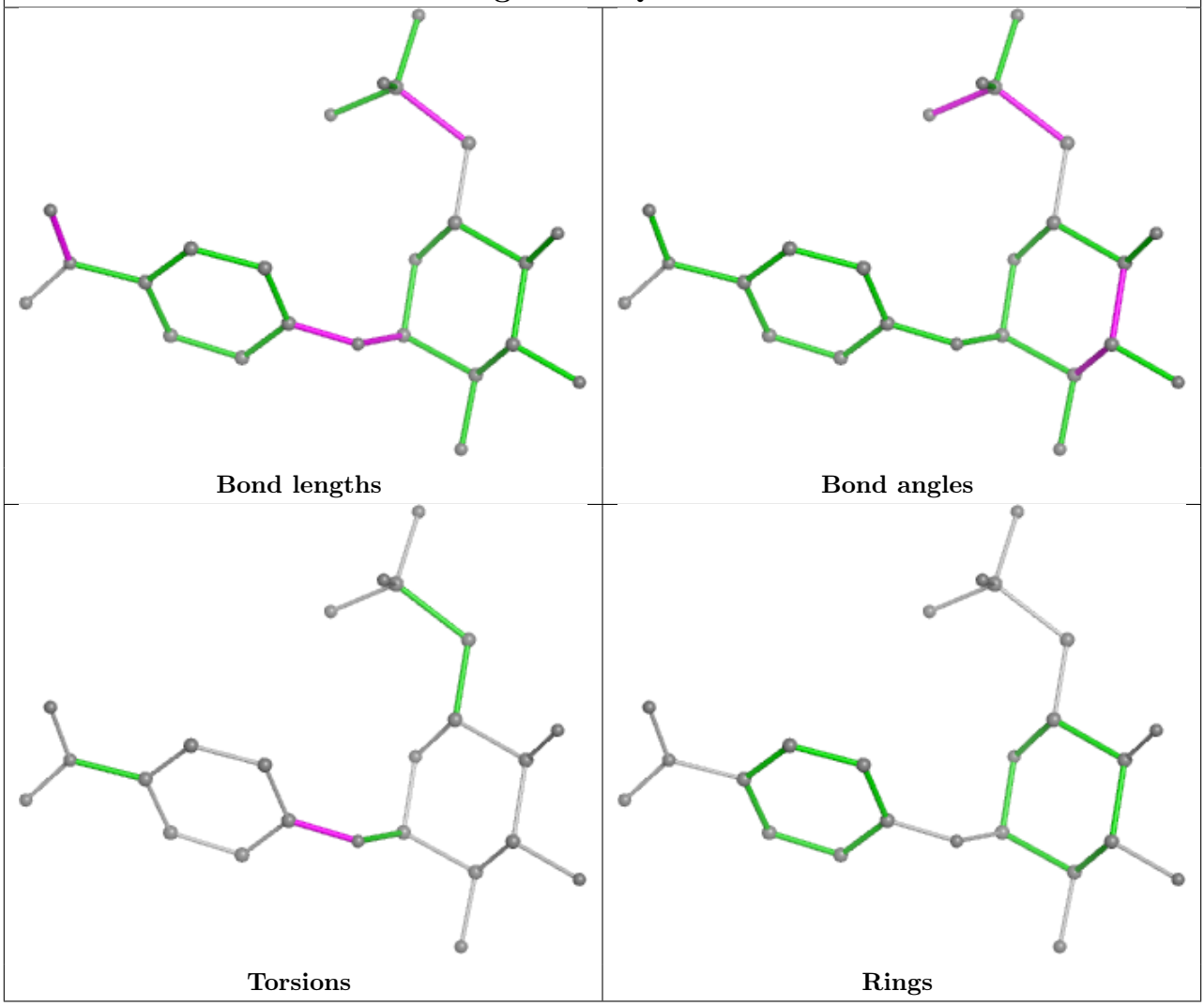


Torsions



Rings

Ligand NSQ F 711



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	661/672 (98%)	-0.27	2 (0%)	94	94	20, 30, 49, 77	0
1	B	663/672 (98%)	-0.23	4 (0%)	89	90	20, 32, 55, 78	0
1	C	661/672 (98%)	0.05	17 (2%)	56	58	22, 38, 69, 92	1 (0%)
1	D	662/672 (98%)	-0.24	2 (0%)	94	94	20, 31, 50, 75	0
1	E	661/672 (98%)	-0.21	1 (0%)	95	95	20, 32, 50, 70	0
1	F	664/672 (98%)	-0.17	0	100	100	19, 28, 47, 70	0
1	G	661/672 (98%)	-0.21	2 (0%)	94	94	21, 36, 59, 89	0
1	H	661/672 (98%)	-0.18	3 (0%)	91	91	20, 33, 58, 93	0
All	All	5294/5376 (98%)	-0.18	31 (0%)	89	90	19, 32, 57, 93	1 (0%)

All (31) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	8	ASP	3.3
1	D	8	ASP	3.1
1	C	660	LEU	3.1
1	C	630	GLY	2.9
1	C	604	ALA	2.8
1	C	4	GLU	2.8
1	C	8	ASP	2.7
1	B	65	ASP	2.7
1	C	9	GLY	2.7
1	G	2	HIS	2.7
1	C	623	TRP	2.7
1	C	14	ILE	2.6
1	C	594	ALA	2.6
1	C	577	TYR	2.5
1	D	14	ILE	2.5
1	C	16	ASN	2.5

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Mol	Chain	Res	Type	RSRZ
1	C	651	SER	2.5
1	A	7	LYS	2.4
1	A	16	ASN	2.3
1	C	649	ALA	2.2
1	H	16	ASN	2.2
1	E	616	HIS	2.2
1	H	8	ASP	2.2
1	B	659	GLN	2.2
1	C	659	GLN	2.2
1	H	86	ASN	2.2
1	C	657	PHE	2.1
1	C	65	ASP	2.1
1	B	95	GLU	2.1
1	C	619	TRP	2.0
1	B	662	THR	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 monosaccharides 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	0.69	0.24	49,51,53,54	0
5	EDO	D	707	4/4	0.76	0.20	39,40,42,43	0
5	EDO	F	707	4/4	0.77	0.20	32,39,41,43	4
3	MPD	D	704	8/8	0.80	0.21	49,56,58,62	0
5	EDO	H	703	4/4	0.80	0.15	40,43,44,46	0
5	EDO	F	708	4/4	0.81	0.17	46,46,49,50	0
3	MPD	A	705	8/8	0.81	0.23	38,43,44,47	8
5	EDO	F	709	4/4	0.83	0.16	41,42,43,48	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	EDO	A	708	4/4	0.85	0.13	38,39,40,44	0
5	EDO	B	703	4/4	0.85	0.14	46,48,49,50	0
3	MPD	B	701	8/8	0.86	0.19	42,48,52,54	0
5	EDO	D	705	4/4	0.87	0.21	40,41,42,44	4
5	EDO	E	704	4/4	0.87	0.19	31,32,32,35	4
5	EDO	G	704	4/4	0.89	0.12	47,49,50,51	0
3	MPD	A	703	8/8	0.89	0.16	39,43,45,58	0
4	CL	H	702	1/1	0.90	0.09	44,44,44,44	1
5	EDO	B	704	4/4	0.91	0.13	39,39,39,41	0
3	MPD	F	704	8/8	0.91	0.15	51,56,58,58	0
3	MPD	E	702	8/8	0.93	0.10	26,29,32,32	0
3	MPD	A	704	8/8	0.93	0.15	32,38,42,45	0
5	EDO	G	705	4/4	0.93	0.14	35,42,46,47	0
2	SCN	A	702	3/3	0.93	0.11	33,33,38,48	3
4	CL	G	702	1/1	0.94	0.11	39,39,39,39	1
3	MPD	F	703	8/8	0.94	0.14	28,35,37,38	0
5	EDO	F	710	4/4	0.94	0.13	43,43,45,46	0
5	EDO	C	702	4/4	0.95	0.10	40,46,47,54	0
5	EDO	G	703	4/4	0.95	0.09	40,42,44,48	0
3	MPD	D	703	8/8	0.95	0.21	41,47,49,52	0
4	CL	E	703	1/1	0.95	0.12	48,48,48,48	1
5	EDO	A	707	4/4	0.95	0.12	41,44,45,47	0
4	CL	F	705	1/1	0.96	0.09	44,44,44,44	0
4	CL	B	702	1/1	0.96	0.09	46,46,46,46	0
2	SCN	F	702	3/3	0.97	0.11	34,34,34,39	3
2	SCN	H	701	3/3	0.97	0.11	35,35,38,41	0
2	SCN	D	702	3/3	0.97	0.10	42,42,45,49	0
6	NSQ	D	708	24/24	0.97	0.10	20,26,60,67	0
2	SCN	E	701	3/3	0.98	0.12	41,41,53,56	0
2	SCN	A	701	3/3	0.98	0.10	33,33,36,40	0
5	EDO	F	706	4/4	0.98	0.06	30,32,33,35	0
6	NSQ	A	709	24/24	0.98	0.08	21,25,36,41	0
6	NSQ	B	705	24/24	0.98	0.09	19,24,37,38	0
6	NSQ	C	703	24/24	0.98	0.10	22,24,64,69	0
4	CL	A	706	1/1	0.98	0.04	48,48,48,48	0
6	NSQ	E	705	24/24	0.98	0.10	22,26,35,42	0
6	NSQ	F	711	24/24	0.98	0.10	19,22,29,34	0
6	NSQ	H	704	24/24	0.98	0.08	17,24,33,35	0
2	SCN	G	701	3/3	0.99	0.10	39,39,43,47	0
6	NSQ	G	706	24/24	0.99	0.07	20,25,29,35	0
2	SCN	F	701	3/3	0.99	0.08	34,34,35,48	0
7	K	C	701	1/1	0.99	0.07	37,37,37,37	0

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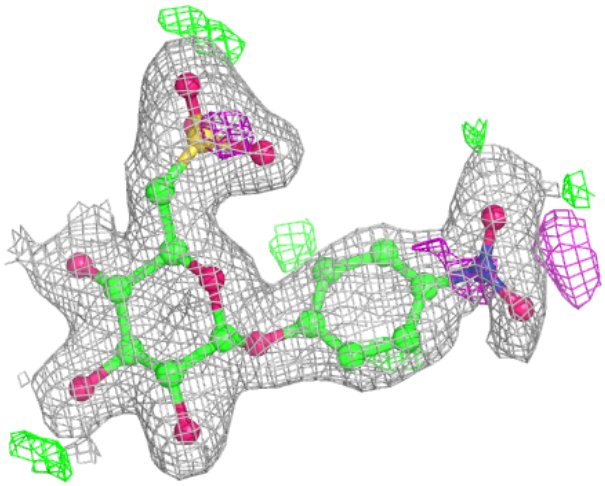
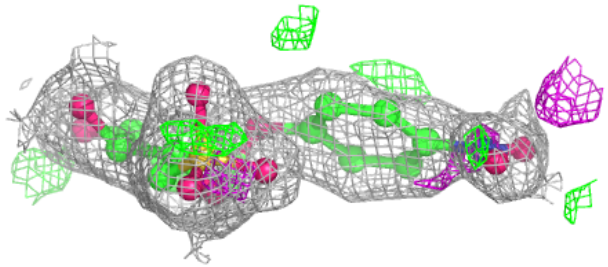
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
7	K	D	701	1/1	0.99	0.06	33,33,33,33	0

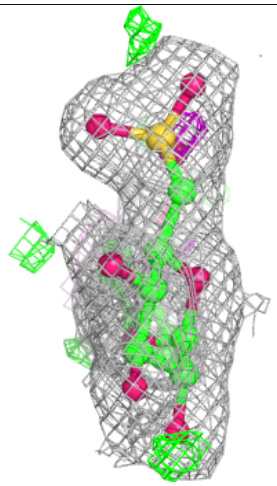
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around NSQ D 708:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative) and green (positive)

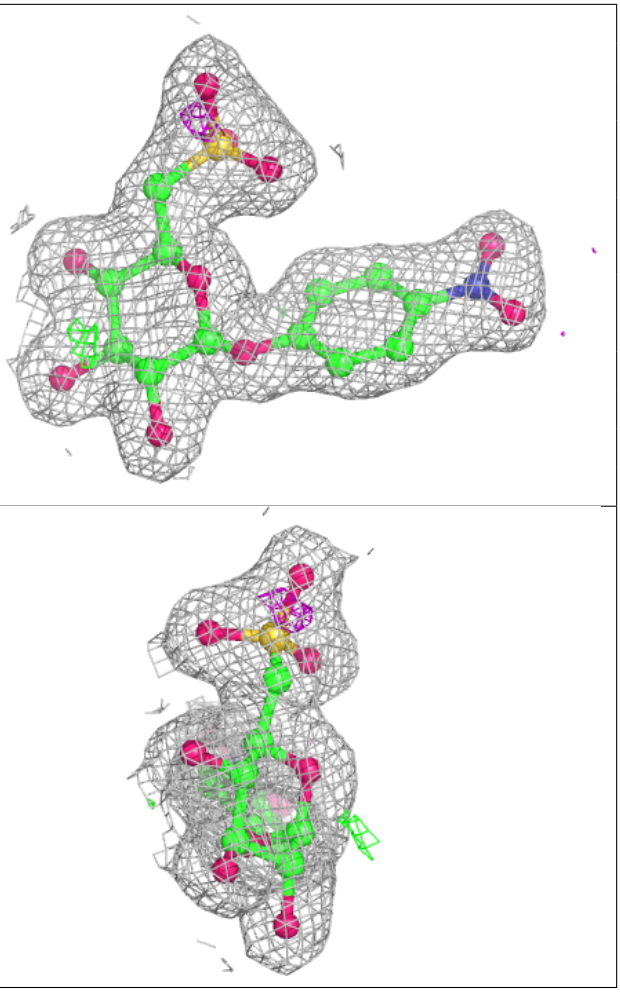






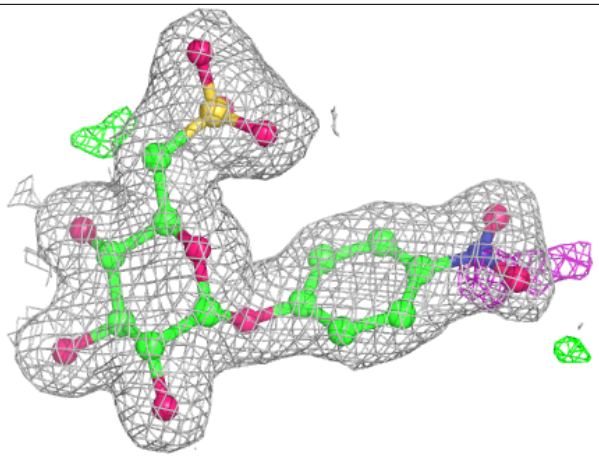
Electron density around NSQ A 709:

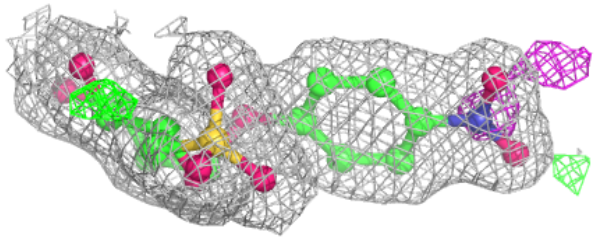
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

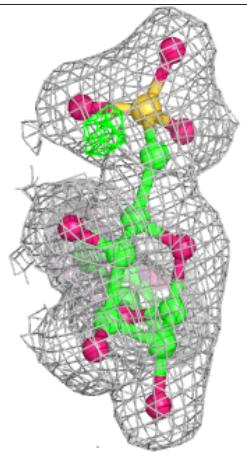


Electron density around NSQ B 705:

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

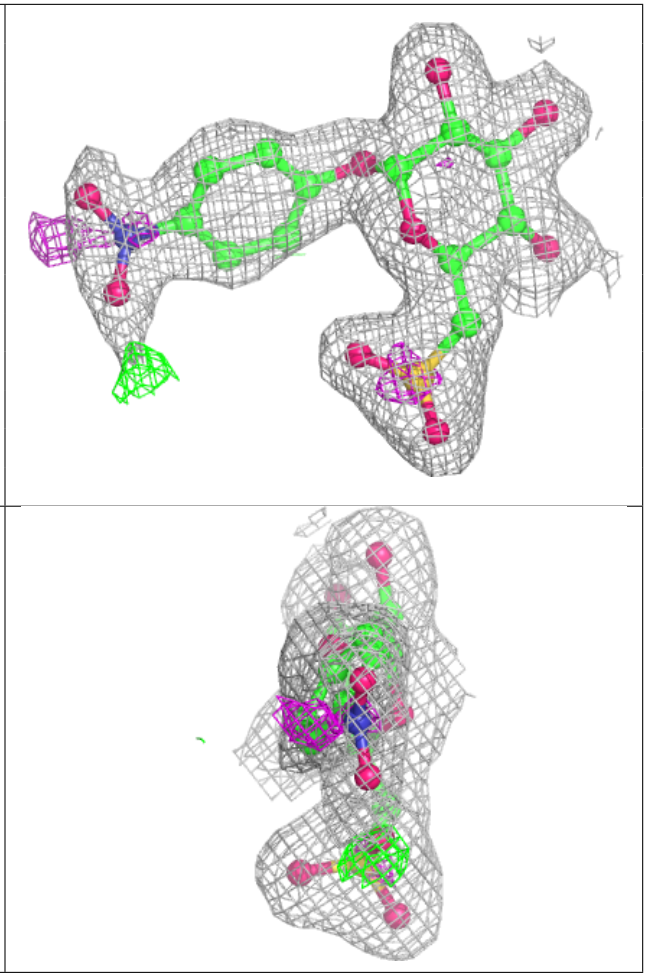






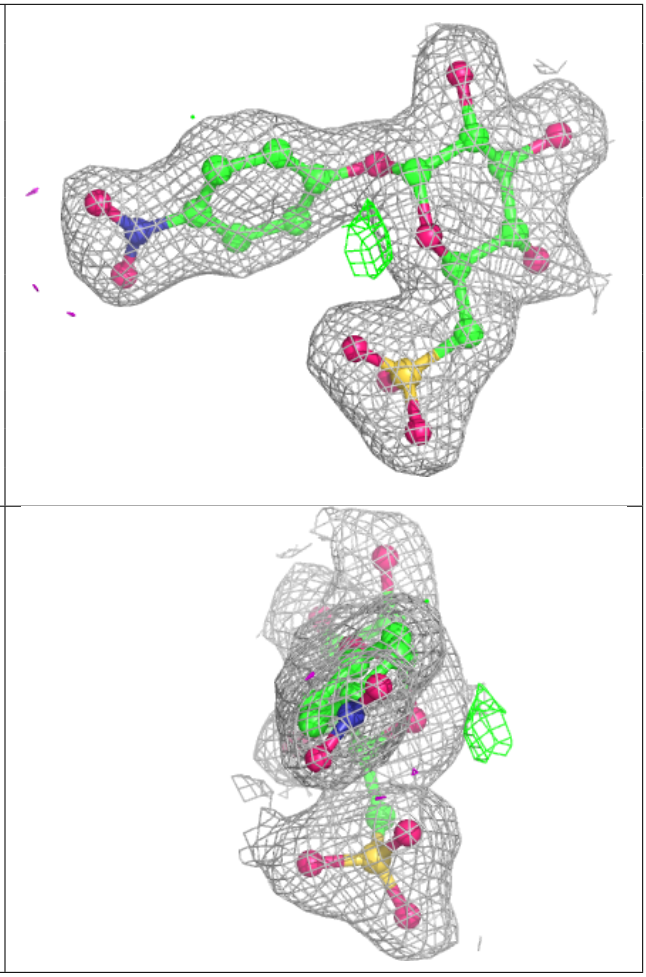
Electron density around NSQ C 703:

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



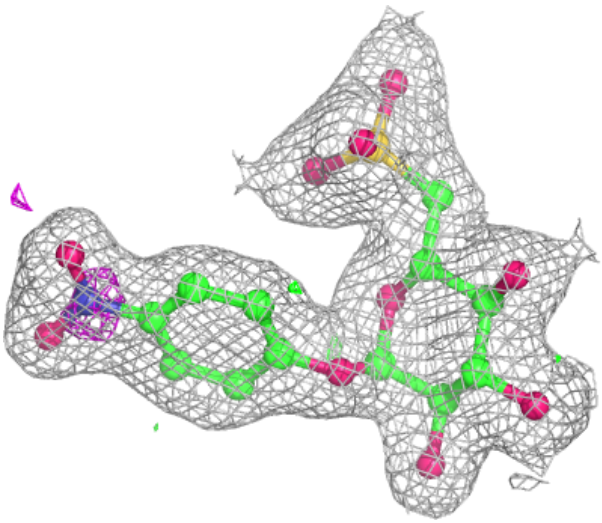
Electron density around NSQ E 705:

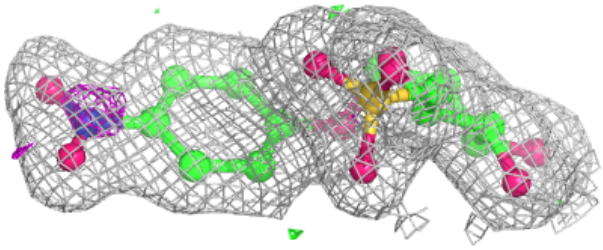
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

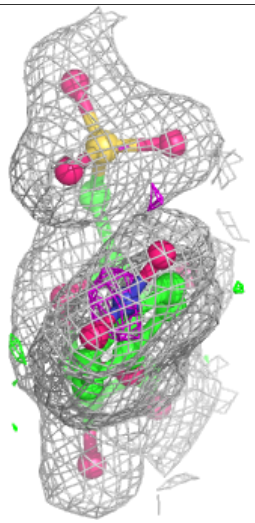


Electron density around NSQ F 711:

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

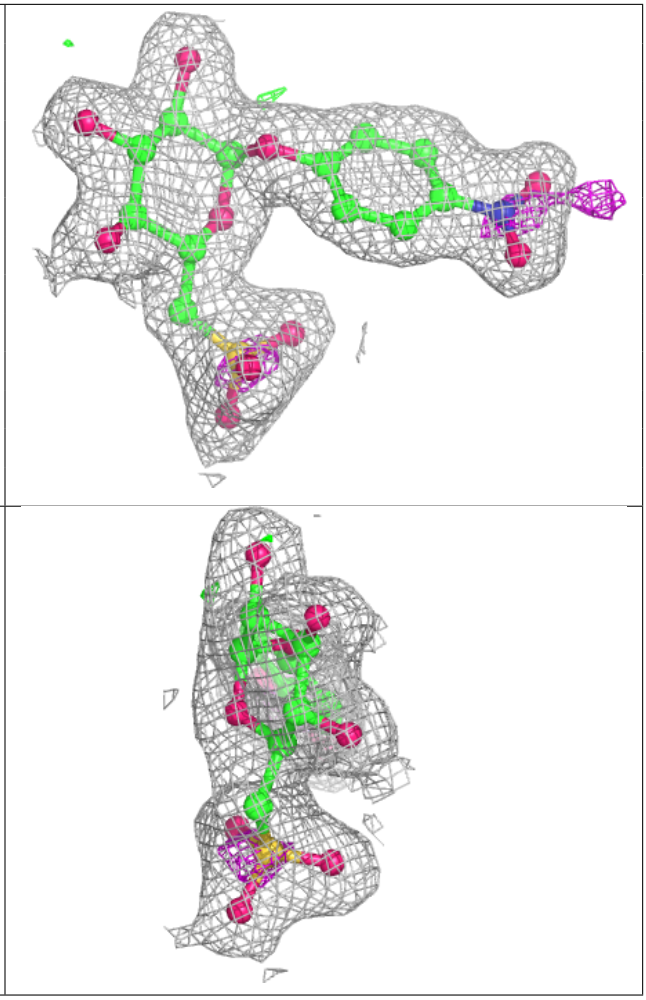






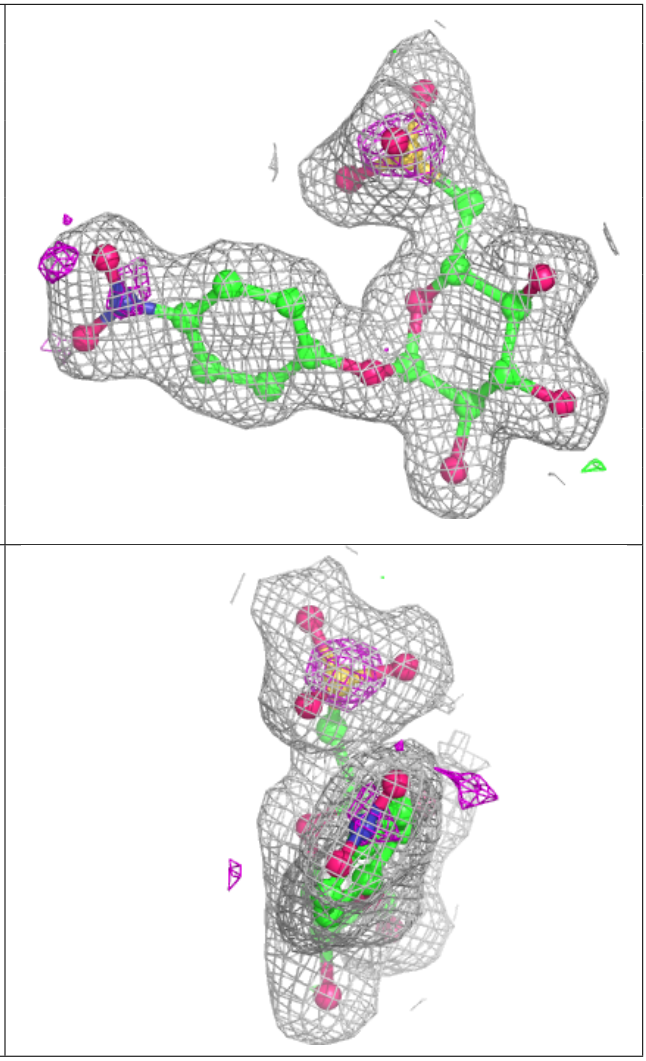
Electron density around NSQ H 704:

$2mF_o$-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 (i)

There are no such residues in this entry.