



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 8, 2023 – 07:16 AM EDT

PDB ID : 1Q3A  
Title : Crystal structure of the catalytic domain of human matrix metalloproteinase 10  
Authors : Calderone, V.; Bertini, I.; Fragai, M.; Luchinat, C.; Mangani, S.; Terni, B.  
Deposited on : 2003-07-29  
Resolution : 2.10 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](mailto: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>.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.35  
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) : 2.35

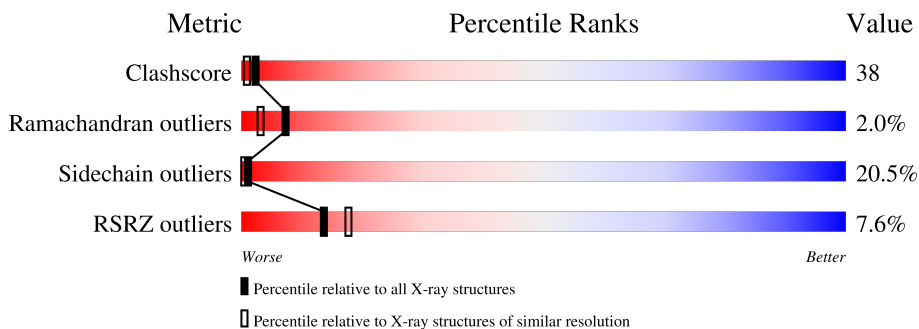
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.10 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))
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (2.10-2.10)

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  $\geq 3$ , 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	165	
1	B	165	
1	C	165	

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
4	NGH	A	480	X	X	-	-
4	NGH	B	479	X	X	-	-
4	NGH	C	481	X	X	X	-

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 4175 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 Stromelysin-2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	156	Total 1241	C 793	N 205	O 240	S 3	0	0	0
1	B	160	Total 1272	C 813	N 209	O 247	S 3	0	0	0
1	C	155	Total 1233	C 788	N 204	O 239	S 2	0	0	0

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	170	ASN	PHE	engineered mutation	UNP P09238
B	170	ASN	PHE	engineered mutation	UNP P09238
C	170	ASN	PHE	engineered mutation	UNP P09238

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	2	Total 2	Zn 2	0	0
2	B	2	Total 2	Zn 2	0	0
2	C	2	Total 2	Zn 2	0	0

- Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca).

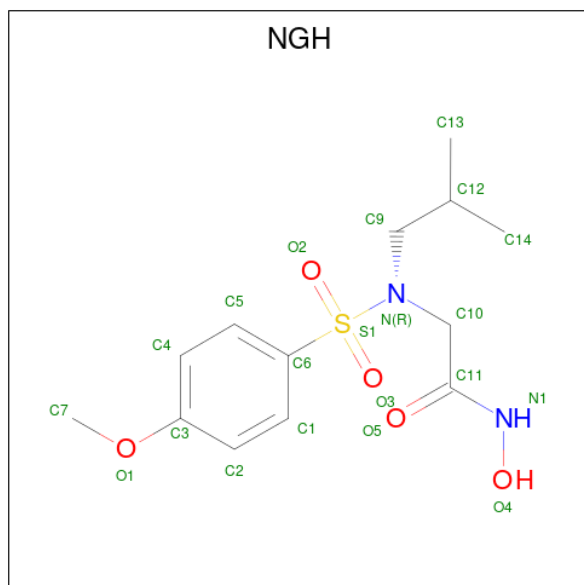
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	3	Total 3	Ca 3	0	0
3	B	3	Total 3	Ca 3	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	C	3	Total Ca 3 3	0	0

- Molecule 4 is N-ISOBUTYL-N-[4-METHOXYPHENYLSULFONYL]GLYCYL HYDROX-AMIC ACID (three-letter code: NGH) (formula: C<sub>13</sub>H<sub>20</sub>N<sub>2</sub>O<sub>5</sub>S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C N O S 21 13 2 5 1	0	0
4	B	1	Total C N O S 21 13 2 5 1	0	0
4	C	1	Total C N O S 21 13 2 5 1	0	0

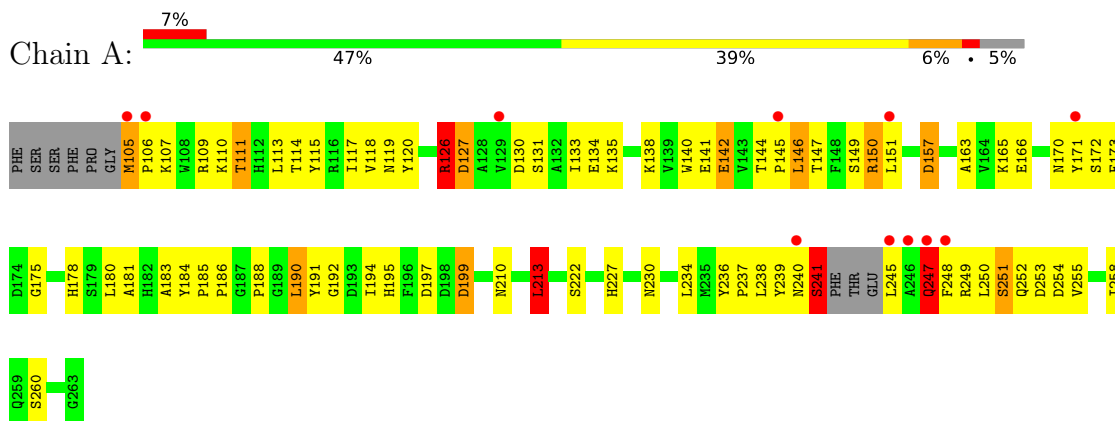
- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	150	Total O 150 150	0	0
5	B	126	Total O 126 126	0	0
5	C	75	Total O 75 75	0	0

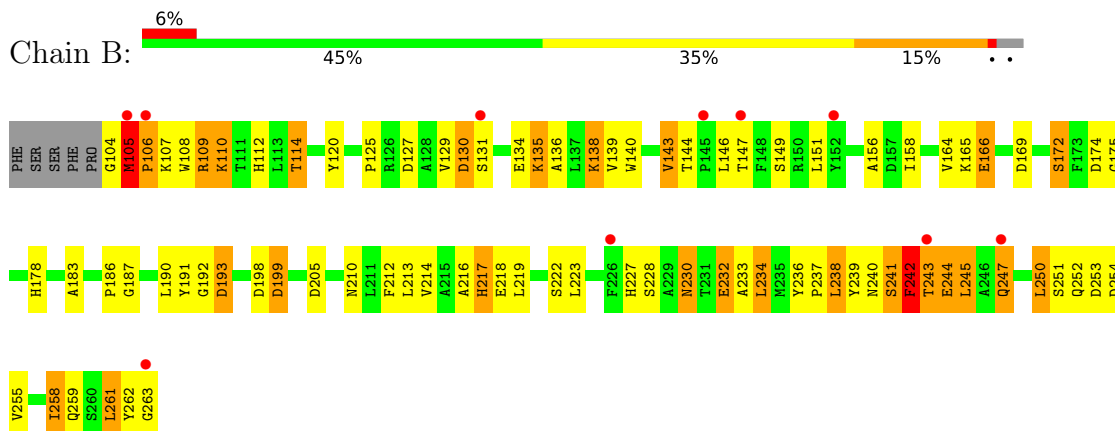
### 3 Residue-property plots

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.

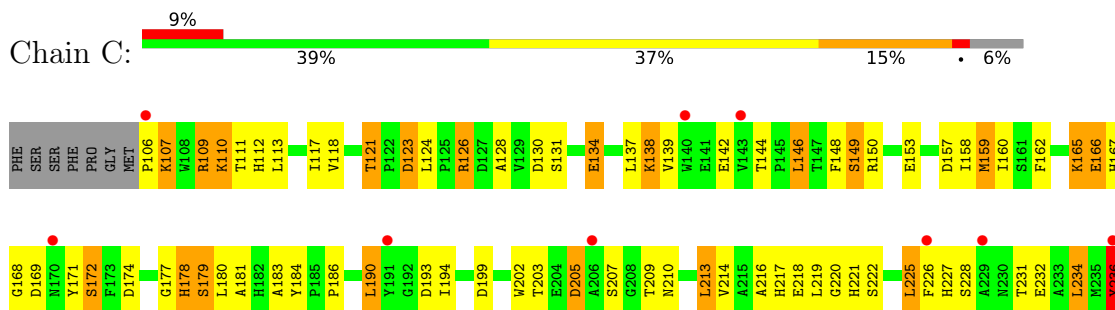
- Molecule 1: Stromelysin-2



- Molecule 1: Stromelysin-2



- Molecule 1: Stromelysin-2





## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	117.15Å 61.14Å 68.59Å 90.00° 108.68° 90.00°	Depositor
Resolution (Å)	51.30 – 2.10 18.88 – 2.10	Depositor EDS
% Data completeness (in resolution range)	100.0 (51.30-2.10) 93.6 (18.88-2.10)	Depositor EDS
$R_{merge}$	0.14	Depositor
$R_{sym}$	0.14	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.64 (at 2.11Å)	Xtrriage
Refinement program	REFMAC 5.1.24, CNS	Depositor
R, $R_{free}$	0.276 , 0.298 0.270 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	24.2	Xtrriage
Anisotropy	0.606	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 67.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.90	EDS
Total number of atoms	4175	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	37.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.32% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: NGH, ZN, CA

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	0.79	1/1278 (0.1%)	1.10	5/1738 (0.3%)
1	B	0.90	3/1311 (0.2%)	1.11	9/1784 (0.5%)
1	C	1.31	3/1270 (0.2%)	1.18	14/1727 (0.8%)
All	All	1.02	7/3859 (0.2%)	1.13	28/5249 (0.5%)

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	B	0	4
1	C	0	4
All	All	0	9

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	236	TYR	C-O	35.08	1.90	1.23
1	C	237	PRO	CG-CD	11.14	1.87	1.50
1	C	237	PRO	N-CD	9.94	1.61	1.47
1	B	244	GLU	N-CA	9.90	1.66	1.46
1	A	241	SER	CB-OG	6.62	1.50	1.42
1	B	104	GLY	N-CA	6.51	1.55	1.46
1	B	106	PRO	N-CD	6.25	1.56	1.47

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	237	PRO	N-CD-CG	-11.02	86.67	103.20
1	C	236	TYR	CA-C-N	10.93	147.69	117.10
1	C	236	TYR	CA-C-O	-10.70	97.63	120.10
1	C	123	ASP	CB-CG-OD2	8.13	125.61	118.30
1	B	253	ASP	CB-CG-OD2	8.05	125.55	118.30
1	A	197	ASP	CB-CG-OD2	7.27	124.84	118.30
1	B	250	LEU	CA-CB-CG	6.98	131.35	115.30
1	A	157	ASP	CB-CG-OD2	6.89	124.50	118.30
1	B	130	ASP	CB-CG-OD2	6.88	124.50	118.30
1	B	199	ASP	CB-CG-OD2	6.71	124.33	118.30
1	B	205	ASP	CB-CG-OD2	6.32	123.99	118.30
1	C	205	ASP	CB-CG-OD2	6.04	123.74	118.30
1	A	199	ASP	CB-CG-OD2	5.96	123.67	118.30
1	A	109	ARG	NE-CZ-NH1	-5.86	117.37	120.30
1	C	157	ASP	CB-CG-OD2	5.85	123.57	118.30
1	B	193	ASP	CB-CG-OD1	5.80	123.52	118.30
1	C	193	ASP	CB-CG-OD2	5.75	123.48	118.30
1	C	174	ASP	CB-CG-OD2	5.70	123.43	118.30
1	C	169	ASP	CB-CG-OD2	5.67	123.40	118.30
1	B	198	ASP	CB-CG-OD2	5.64	123.37	118.30
1	B	169	ASP	C-N-CA	-5.53	107.88	121.70
1	C	238	LEU	CA-CB-CG	5.52	128.00	115.30
1	A	213	LEU	CA-CB-CG	5.50	127.95	115.30
1	C	239	TYR	CB-CG-CD1	-5.48	117.71	121.00
1	C	199	ASP	CB-CG-OD2	5.41	123.17	118.30
1	B	174	ASP	CB-CG-OD2	5.36	123.12	118.30
1	C	254	ASP	CB-CG-OD2	5.34	123.11	118.30
1	C	169	ASP	C-N-CA	-5.27	108.53	121.70

There are no chirality outliers.

All (9) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	247	GLN	Peptide
1	B	105	MET	Peptide
1	B	120	TYR	Peptide
1	B	242	PHE	Peptide
1	B	243	THR	Peptide
1	C	236	TYR	Peptide,Mainchain
1	C	237	PRO	Peptide
1	C	238	LEU	Peptide

## 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	1241	0	1161	58	2
1	B	1272	0	1187	105	0
1	C	1233	0	1153	110	2
2	A	2	0	0	0	0
2	B	2	0	0	0	0
2	C	2	0	0	0	0
3	A	3	0	0	0	0
3	B	3	0	0	0	0
3	C	3	0	0	0	0
4	A	21	0	19	4	0
4	B	21	0	19	7	0
4	C	21	0	20	25	0
5	A	150	0	0	12	0
5	B	126	0	0	28	0
5	C	75	0	0	15	0
All	All	4175	0	3559	284	2

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 38.

All (284) 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)
4:C:481:NGH:N1	4:C:481:NGH:C11	1.68	1.54
1:C:237:PRO:CG	1:C:237:PRO:CD	1.87	1.50
4:C:481:NGH:N	4:C:481:NGH:C9	1.82	1.42
4:B:479:NGH:C7	4:B:479:NGH:O1	1.69	1.39
1:B:143:VAL:HG11	1:B:255:VAL:HG22	1.29	1.10
1:C:236:TYR:O	1:C:236:TYR:C	1.90	1.10
1:C:126:ARG:HG2	1:C:126:ARG:HH11	0.94	1.08
1:B:216:ALA:HB2	5:B:488:HOH:O	1.56	1.05
1:B:109:ARG:C	1:B:109:ARG:HD2	1.76	1.04
1:A:120:TYR:HB2	5:A:516:HOH:O	1.56	1.03
1:C:221:HIS:HB3	5:C:485:HOH:O	1.60	1.02
5:B:499:HOH:O	4:C:481:NGH:H131	1.61	1.00

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:181:ALA:O	4:C:481:NGH:H91	1.63	0.98
1:B:244:GLU:HB3	1:B:247:GLN:NE2	1.79	0.98
1:A:130:ASP:O	1:A:134:GLU:HG3	1.63	0.96
1:B:243:THR:HG23	1:B:244:GLU:HA	1.49	0.94
1:C:236:TYR:CD2	1:C:237:PRO:O	2.19	0.94
1:C:236:TYR:O	1:C:236:TYR:CD1	2.20	0.94
1:B:243:THR:CG2	1:C:171:TYR:HE2	1.80	0.92
1:C:126:ARG:HG2	1:C:126:ARG:NH1	1.73	0.92
1:A:126:ARG:HG2	1:A:126:ARG:HH21	1.32	0.92
1:A:119:ASN:HA	5:A:629:HOH:O	1.72	0.90
1:C:239:TYR:H	4:C:481:NGH:H2	1.35	0.90
1:C:138:LYS:O	1:C:142:GLU:HG3	1.70	0.89
1:B:143:VAL:HG11	1:B:255:VAL:CG2	2.01	0.89
1:C:139:VAL:HG11	1:C:248:PHE:HE2	1.36	0.89
4:C:481:NGH:C9	5:C:544:HOH:O	2.21	0.88
5:B:535:HOH:O	4:C:481:NGH:H142	1.74	0.88
1:B:243:THR:HG22	1:C:171:TYR:CE2	2.09	0.87
1:B:243:THR:CG2	1:B:244:GLU:HA	2.05	0.86
1:B:239:TYR:HD1	5:B:583:HOH:O	1.59	0.85
5:B:605:HOH:O	4:C:481:NGH:C14	2.24	0.85
1:C:126:ARG:HH11	1:C:126:ARG:CG	1.86	0.83
4:C:481:NGH:H102	5:C:491:HOH:O	1.79	0.83
1:B:243:THR:CG2	1:C:171:TYR:CE2	2.63	0.82
1:A:106:PRO:HD3	5:A:489:HOH:O	1.82	0.80
1:B:243:THR:HG21	1:C:171:TYR:HE2	1.44	0.79
1:C:180:LEU:HD11	1:C:239:TYR:CD1	2.17	0.79
1:B:109:ARG:NH2	1:B:110:LYS:HD2	1.97	0.79
1:B:243:THR:OG1	1:B:244:GLU:HA	1.83	0.79
4:C:481:NGH:H92	5:C:544:HOH:O	1.83	0.78
1:A:126:ARG:HH21	1:A:126:ARG:CG	1.97	0.78
1:B:166:GLU:OE1	1:B:166:GLU:HA	1.83	0.78
1:B:243:THR:HG23	1:B:244:GLU:CA	2.14	0.77
4:C:481:NGH:C11	4:C:481:NGH:O4	2.33	0.77
1:C:236:TYR:CG	1:C:237:PRO:O	2.37	0.76
1:B:216:ALA:HB3	5:B:494:HOH:O	1.85	0.76
1:A:127:ASP:O	1:A:131:SER:HB2	1.85	0.75
1:C:227:HIS:NE2	1:C:237:PRO:HD3	2.01	0.74
1:A:180:LEU:N	4:A:480:NGH:O3	2.17	0.74
1:A:126:ARG:HD3	1:A:126:ARG:H	1.52	0.74
1:B:114:THR:OG1	1:B:151:LEU:HD13	1.88	0.74
1:B:233:ALA:HA	1:B:251:SER:OG	1.88	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:244:GLU:CB	1:B:247:GLN:NE2	2.51	0.73
1:C:109:ARG:O	1:C:109:ARG:HD3	1.89	0.73
1:B:146:LEU:HD21	1:B:262:TYR:CE2	2.24	0.73
1:A:230:ASN:O	1:A:236:TYR:CD2	2.42	0.72
1:A:173:PHE:CE1	5:A:486:HOH:O	2.42	0.72
5:B:605:HOH:O	4:C:481:NGH:H143	1.86	0.72
1:B:214:VAL:O	1:B:218:GLU:HG2	1.90	0.71
1:B:239:TYR:CD1	5:B:583:HOH:O	2.38	0.71
1:B:252:GLN:HB2	5:B:508:HOH:O	1.89	0.71
1:C:153:GLU:HB3	5:C:488:HOH:O	1.89	0.71
1:B:109:ARG:C	1:B:109:ARG:CD	2.55	0.71
1:C:106:PRO:HD2	1:C:186:PRO:HD2	1.71	0.71
4:B:479:NGH:C7	4:B:479:NGH:C3	2.69	0.70
1:B:242:PHE:HZ	1:C:184:TYR:CZ	2.10	0.70
1:A:210:ASN:HD22	1:A:213:LEU:H	1.37	0.70
1:C:236:TYR:C	1:C:237:PRO:O	2.31	0.68
1:B:242:PHE:HZ	1:C:184:TYR:CE2	2.12	0.68
1:B:109:ARG:NH2	1:B:110:LYS:CD	2.56	0.68
1:B:212:PHE:O	5:B:488:HOH:O	2.10	0.68
4:B:479:NGH:O1	5:B:583:HOH:O	2.12	0.68
1:C:227:HIS:CD2	1:C:237:PRO:CD	2.78	0.67
1:B:175:GLY:HA2	1:B:199:ASP:OD2	1.93	0.67
1:A:166:GLU:HG2	5:A:586:HOH:O	1.95	0.67
1:A:105:MET:N	1:A:106:PRO:HD2	2.10	0.66
1:B:244:GLU:HB3	1:B:247:GLN:HE22	1.61	0.66
1:A:240:ASN:ND2	5:A:542:HOH:O	2.28	0.65
1:C:184:TYR:CE1	1:C:190:LEU:HD12	2.31	0.65
1:C:228:SER:O	1:C:236:TYR:HB2	1.95	0.65
1:C:238:LEU:HB3	4:C:481:NGH:C7	2.26	0.65
1:C:179:SER:HB2	4:C:481:NGH:H142	1.79	0.65
1:C:226:PHE:CG	1:C:227:HIS:N	2.65	0.65
1:B:219:LEU:O	1:B:223:LEU:HG	1.97	0.65
1:B:230:ASN:ND2	1:B:232:GLU:HG2	2.12	0.65
1:B:238:LEU:HG	1:C:178:HIS:HA	1.79	0.65
1:B:107:LYS:HD2	1:B:261:LEU:O	1.97	0.65
1:C:239:TYR:N	4:C:481:NGH:H2	2.11	0.65
1:C:210:ASN:HD22	1:C:213:LEU:H	1.45	0.64
1:B:259:GLN:O	1:B:263:GLY:N	2.28	0.64
1:B:243:THR:CB	1:B:244:GLU:HA	2.28	0.64
1:B:140:TRP:NE1	1:B:216:ALA:O	2.27	0.63
1:C:139:VAL:HG11	1:C:248:PHE:CE2	2.26	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:109:ARG:HD2	1:B:110:LYS:N	2.12	0.63
1:B:130:ASP:HB2	5:B:486:HOH:O	1.99	0.62
1:B:216:ALA:N	5:B:488:HOH:O	2.32	0.62
1:C:142:GLU:HB3	5:C:534:HOH:O	1.99	0.62
1:B:127:ASP:HA	5:B:486:HOH:O	2.00	0.62
1:B:213:LEU:HA	5:B:494:HOH:O	1.99	0.62
1:A:105:MET:N	1:A:106:PRO:CD	2.63	0.61
1:B:216:ALA:CB	5:B:488:HOH:O	2.30	0.61
1:C:227:HIS:CD2	1:C:237:PRO:HD2	2.36	0.61
1:A:230:ASN:O	1:A:236:TYR:HD2	1.83	0.61
1:A:247:GLN:HA	1:A:247:GLN:NE2	2.16	0.61
4:C:481:NGH:H133	5:C:504:HOH:O	2.01	0.60
1:B:243:THR:OG1	1:B:244:GLU:CA	2.50	0.60
1:C:138:LYS:O	1:C:142:GLU:CG	2.46	0.60
1:A:173:PHE:CD1	5:A:486:HOH:O	2.55	0.59
1:B:245:LEU:C	1:B:247:GLN:H	2.03	0.59
1:B:109:ARG:HD2	1:B:109:ARG:O	2.03	0.59
1:A:105:MET:HA	5:A:483:HOH:O	2.03	0.59
1:A:210:ASN:ND2	1:A:213:LEU:H	2.00	0.58
1:C:205:ASP:OD1	1:C:207:SER:N	2.30	0.58
1:C:234:LEU:HA	1:C:238:LEU:HD13	1.86	0.58
1:A:126:ARG:HG2	1:A:126:ARG:NH2	2.10	0.58
1:C:227:HIS:NE2	1:C:237:PRO:CD	2.67	0.58
4:C:481:NGH:C9	4:C:481:NGH:C10	2.77	0.57
1:C:227:HIS:CG	1:C:237:PRO:HD2	2.39	0.57
1:C:259:GLN:HB3	1:C:263:GLY:O	2.05	0.57
4:C:481:NGH:N1	4:C:481:NGH:C10	2.65	0.57
1:A:126:ARG:H	1:A:126:ARG:CD	2.17	0.56
1:A:181:ALA:HB1	1:A:195:HIS:O	2.05	0.56
1:B:144:THR:HG21	1:B:258:ILE:HD13	1.87	0.56
1:C:107:LYS:NZ	1:C:109:ARG:NH1	2.52	0.56
1:C:210:ASN:ND2	1:C:213:LEU:H	2.03	0.56
4:A:480:NGH:H92	4:A:480:NGH:O5	2.05	0.56
1:B:147:THR:HA	5:B:561:HOH:O	2.05	0.56
1:C:107:LYS:HZ3	1:C:109:ARG:NH1	2.04	0.55
1:C:165:LYS:HG3	1:C:166:GLU:H	1.70	0.55
1:A:111:THR:HG23	1:A:145:PRO:O	2.06	0.55
1:A:144:THR:OG1	1:A:146:LEU:HB2	2.07	0.55
1:C:183:ALA:C	5:C:485:HOH:O	2.45	0.55
1:B:109:ARG:CD	1:B:109:ARG:O	2.55	0.55
1:A:126:ARG:CD	1:A:126:ARG:N	2.70	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:112:HIS:HB2	5:B:506:HOH:O	2.08	0.54
1:B:114:THR:HG23	1:B:156:ALA:HB1	1.89	0.54
1:B:244:GLU:CB	1:B:247:GLN:HE22	2.18	0.54
1:B:125:PRO:O	1:B:129:VAL:HG23	2.07	0.54
1:C:109:ARG:NH2	1:C:109:ARG:HG2	2.24	0.53
1:A:251:SER:O	1:A:255:VAL:HG23	2.07	0.53
1:C:177:GLY:O	1:C:178:HIS:HB2	2.09	0.53
1:B:164:VAL:O	1:B:165:LYS:C	2.46	0.53
1:C:220:GLY:O	1:C:225:LEU:HB2	2.09	0.52
1:B:243:THR:OG1	1:B:244:GLU:C	2.48	0.52
1:C:210:ASN:HD22	1:C:213:LEU:HB2	1.74	0.52
1:C:112:HIS:C	1:C:112:HIS:CD2	2.83	0.52
1:C:144:THR:OG1	1:C:146:LEU:HB2	2.09	0.52
1:B:108:TRP:CE2	1:B:186:PRO:HB3	2.45	0.52
1:B:166:GLU:OE1	1:B:172:SER:HB3	2.09	0.52
1:A:119:ASN:CB	5:A:629:HOH:O	2.57	0.51
1:A:184:TYR:O	1:A:222:SER:HA	2.10	0.51
1:C:167:HIS:CE1	1:C:171:TYR:O	2.63	0.51
1:B:216:ALA:CA	5:B:488:HOH:O	2.58	0.51
1:B:144:THR:OG1	1:B:146:LEU:HD12	2.10	0.51
5:B:535:HOH:O	1:C:179:SER:HB2	2.09	0.51
1:B:214:VAL:O	1:B:218:GLU:CG	2.57	0.51
1:A:140:TRP:O	1:A:144:THR:HG23	2.11	0.51
1:A:115:TYR:CZ	1:A:150:ARG:HB2	2.46	0.51
1:B:230:ASN:HD22	1:B:232:GLU:H	1.58	0.51
1:C:107:LYS:NZ	1:C:109:ARG:HH11	2.09	0.51
1:C:165:LYS:HG3	1:C:166:GLU:N	2.27	0.50
1:B:250:LEU:HD13	1:B:254:ASP:HB2	1.93	0.50
1:B:135:LYS:O	1:B:139:VAL:HG23	2.10	0.50
1:A:183:ALA:CB	1:A:194:ILE:HG12	2.42	0.50
1:C:130:ASP:O	1:C:134:GLU:HB2	2.12	0.50
1:B:108:TRP:CD2	1:B:186:PRO:HB3	2.47	0.49
1:B:139:VAL:HG12	1:B:250:LEU:HD21	1.94	0.49
1:C:205:ASP:OD1	1:C:207:SER:CB	2.60	0.49
4:C:481:NGH:H143	4:C:481:NGH:H101	1.95	0.49
1:C:121:THR:OG1	1:C:123:ASP:HB2	2.13	0.49
1:C:158:ILE:HG22	1:C:160:ILE:HD11	1.94	0.49
1:A:213:LEU:HD11	1:A:241:SER:HB3	1.95	0.49
1:C:236:TYR:O	1:C:236:TYR:CG	2.64	0.49
1:B:250:LEU:HD12	1:B:255:VAL:HG23	1.95	0.48
1:B:130:ASP:N	1:B:130:ASP:OD1	2.47	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:184:TYR:CE1	1:C:190:LEU:CD1	2.96	0.48
1:C:259:GLN:O	1:C:263:GLY:N	2.46	0.48
1:B:237:PRO:O	4:B:479:NGH:C1	2.62	0.48
1:C:106:PRO:CD	1:C:186:PRO:HD2	2.39	0.48
1:C:106:PRO:HG2	1:C:186:PRO:HD2	1.95	0.48
1:C:107:LYS:HB2	1:C:107:LYS:HE2	1.41	0.48
1:C:112:HIS:NE2	1:C:149:SER:HB2	2.28	0.48
1:C:221:HIS:CB	5:C:485:HOH:O	2.39	0.48
1:B:114:THR:HG23	1:B:156:ALA:CB	2.44	0.48
1:B:230:ASN:O	1:B:236:TYR:CD2	2.66	0.48
5:B:535:HOH:O	1:C:179:SER:CB	2.61	0.48
1:C:203:THR:HG21	1:C:207:SER:OG	2.14	0.47
1:B:187:GLY:C	1:B:191:TYR:HB2	2.34	0.47
1:C:202:TRP:HA	1:C:209:THR:O	2.14	0.47
4:C:481:NGH:N1	4:C:481:NGH:O5	2.43	0.47
1:C:165:LYS:CG	1:C:166:GLU:H	2.26	0.47
1:C:236:TYR:O	1:C:236:TYR:HD1	1.89	0.47
1:A:126:ARG:CG	1:A:126:ARG:NH2	2.65	0.47
1:B:112:HIS:CE1	1:B:149:SER:HB3	2.50	0.47
1:A:118:VAL:HG12	1:A:118:VAL:O	2.13	0.47
1:B:109:ARG:CZ	1:B:110:LYS:HD2	2.45	0.47
1:C:236:TYR:O	1:C:236:TYR:CA	2.60	0.47
1:B:227:HIS:HB2	5:B:586:HOH:O	2.15	0.47
1:C:249:ARG:NH1	5:C:515:HOH:O	2.46	0.47
1:A:114:THR:HA	1:A:149:SER:O	2.15	0.47
1:C:184:TYR:CD1	1:C:190:LEU:HD12	2.49	0.47
1:C:251:SER:O	1:C:254:ASP:HB2	2.14	0.47
1:A:106:PRO:HB2	1:A:186:PRO:HD2	1.96	0.47
1:B:241:SER:O	1:B:243:THR:HB	2.14	0.47
1:A:140:TRP:O	1:A:141:GLU:C	2.53	0.46
1:B:243:THR:HG21	1:C:171:TYR:CE2	2.36	0.46
1:C:109:ARG:HG2	1:C:109:ARG:HH21	1.80	0.46
1:B:242:PHE:CZ	1:C:184:TYR:CZ	2.99	0.46
1:B:237:PRO:O	4:B:479:NGH:H1	2.14	0.46
1:A:250:LEU:HD22	1:A:254:ASP:CB	2.46	0.46
1:B:244:GLU:HB3	1:B:247:GLN:HE21	1.75	0.46
1:C:139:VAL:HG12	1:C:250:LEU:HG	1.98	0.46
1:A:117:ILE:HD13	1:A:133:ILE:HD12	1.97	0.45
1:A:181:ALA:O	4:A:480:NGH:H101	2.15	0.45
1:C:205:ASP:OD1	1:C:207:SER:HB3	2.15	0.45
1:B:210:ASN:HD22	1:B:213:LEU:HB2	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:113:LEU:HA	1:A:157:ASP:OD2	2.16	0.45
1:B:239:TYR:H	1:C:178:HIS:CD2	2.34	0.45
1:B:109:ARG:NH2	1:B:110:LYS:HD3	2.31	0.45
1:C:109:ARG:HH21	1:C:109:ARG:CG	2.30	0.45
1:C:225:LEU:N	5:C:546:HOH:O	2.50	0.45
1:A:241:SER:CB	4:A:480:NGH:H73	2.46	0.45
1:B:217:HIS:HB3	4:B:479:NGH:H72	1.97	0.45
1:B:234:LEU:HD11	5:B:494:HOH:O	2.16	0.45
1:A:170:ASN:C	1:A:171:TYR:CD1	2.91	0.44
1:C:137:LEU:HD22	1:C:148:PHE:CG	2.53	0.44
1:C:124:LEU:HD23	1:C:124:LEU:HA	1.61	0.44
4:C:481:NGH:N	4:C:481:NGH:C12	2.77	0.44
1:C:216:ALA:HB1	1:C:234:LEU:HD21	2.00	0.44
1:B:125:PRO:HA	5:B:504:HOH:O	2.17	0.44
1:C:238:LEU:HB3	4:C:481:NGH:H72	1.96	0.44
1:A:183:ALA:HB1	1:A:194:ILE:HG12	1.99	0.44
1:A:239:TYR:CG	1:A:240:ASN:HA	2.52	0.44
1:B:105:MET:HG3	1:B:187:GLY:HA2	1.98	0.44
1:A:184:TYR:CD1	1:A:190:LEU:HD22	2.53	0.43
1:C:110:LYS:H	1:C:110:LYS:HG2	1.60	0.43
1:A:140:TRP:CZ2	1:A:234:LEU:HD23	2.53	0.43
1:A:238:LEU:HD22	1:B:178:HIS:HD2	1.83	0.43
1:C:112:HIS:HD2	1:C:113:LEU:N	2.17	0.43
1:C:180:LEU:N	5:C:544:HOH:O	2.45	0.43
1:A:163:ALA:HB3	5:A:486:HOH:O	2.17	0.43
1:C:121:THR:HB	1:C:162:PHE:CD2	2.53	0.43
1:A:119:ASN:CA	5:A:629:HOH:O	2.46	0.43
4:B:479:NGH:C7	5:B:583:HOH:O	2.67	0.43
5:B:605:HOH:O	4:C:481:NGH:H142	2.09	0.43
1:A:227:HIS:ND1	1:A:237:PRO:HB3	2.34	0.43
1:C:118:VAL:CG2	1:C:159:MET:HG3	2.49	0.43
1:A:163:ALA:C	5:A:486:HOH:O	2.56	0.43
1:B:158:ILE:HG23	1:B:192:GLY:O	2.19	0.43
1:C:166:GLU:HA	1:C:172:SER:HB3	2.01	0.43
1:B:112:HIS:CD2	1:B:147:THR:HB	2.55	0.42
1:C:217:HIS:NE2	5:C:491:HOH:O	2.36	0.42
1:C:107:LYS:HE3	1:C:261:LEU:O	2.19	0.42
1:C:181:ALA:N	5:C:544:HOH:O	2.25	0.42
1:A:192:GLY:O	1:A:222:SER:HB2	2.19	0.42
1:B:217:HIS:CD2	1:B:217:HIS:C	2.92	0.42
1:B:262:TYR:O	1:B:263:GLY:O	2.38	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:179:SER:HB2	4:C:481:NGH:C14	2.49	0.42
1:C:227:HIS:CD2	1:C:237:PRO:HD3	2.51	0.42
1:A:184:TYR:HA	1:A:185:PRO:HD3	1.81	0.42
1:B:112:HIS:HD2	1:B:147:THR:HB	1.84	0.42
1:B:138:LYS:O	1:B:139:VAL:C	2.57	0.42
1:B:144:THR:HG21	1:B:258:ILE:CD1	2.50	0.42
1:B:230:ASN:HD21	1:B:232:GLU:CD	2.19	0.42
1:B:130:ASP:O	1:B:134:GLU:HB2	2.20	0.41
1:C:106:PRO:CG	1:C:186:PRO:HD2	2.50	0.41
1:C:128:ALA:O	1:C:131:SER:HB2	2.20	0.41
1:B:139:VAL:HG12	1:B:250:LEU:CD2	2.49	0.41
1:B:105:MET:HA	1:B:106:PRO:HD2	1.85	0.41
1:C:214:VAL:O	1:C:218:GLU:HG2	2.21	0.41
1:B:136:ALA:HA	5:B:488:HOH:O	2.20	0.41
1:B:183:ALA:HA	1:B:193:ASP:O	2.20	0.41
1:B:109:ARG:HH22	1:B:110:LYS:HD3	1.85	0.41
1:A:175:GLY:HA2	1:A:199:ASP:OD2	2.20	0.41
1:B:125:PRO:CA	5:B:504:HOH:O	2.69	0.41
1:B:230:ASN:ND2	1:B:232:GLU:CG	2.84	0.41
1:C:117:ILE:HD12	1:C:150:ARG:CZ	2.50	0.41
1:A:188:PRO:O	1:A:191:TYR:HB2	2.21	0.40
1:C:167:HIS:HE1	1:C:171:TYR:O	2.04	0.40
1:C:194:ILE:HD11	1:C:219:LEU:HD23	2.03	0.40
1:B:242:PHE:CZ	1:C:184:TYR:CE2	3.00	0.40
1:C:219:LEU:HA	1:C:222:SER:HB2	2.03	0.40
4:C:481:NGH:C6	5:C:491:HOH:O	2.68	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:166:GLU:OE2	1:C:168:GLY:O[4_556]	2.07	0.13
1:A:166:GLU:OE1	1:C:168:GLY:O[4_556]	2.19	0.01

## 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	152/165 (92%)	133 (88%)	15 (10%)	4 (3%)	5	2
1	B	158/165 (96%)	138 (87%)	20 (13%)	0	100	100
1	C	151/165 (92%)	132 (87%)	14 (9%)	5 (3%)	4	1
All	All	461/495 (93%)	403 (87%)	49 (11%)	9 (2%)	7	3

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	247	GLN
1	C	236	TYR
1	C	237	PRO
1	A	142	GLU
1	A	178	HIS
1	C	178	HIS
1	C	234	LEU
1	C	239	TYR
1	A	126	ARG

### 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	131/139 (94%)	105 (80%)	26 (20%)	1	0
1	B	134/139 (96%)	109 (81%)	25 (19%)	1	0
1	C	130/139 (94%)	100 (77%)	30 (23%)	1	0
All	All	395/417 (95%)	314 (80%)	81 (20%)	1	0

All (81) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	105	MET
1	A	107	LYS
1	A	110	LYS
1	A	111	THR
1	A	126	ARG
1	A	127	ASP
1	A	135	LYS
1	A	138	LYS
1	A	142	GLU
1	A	146	LEU
1	A	147	THR
1	A	150	ARG
1	A	151	LEU
1	A	165	LYS
1	A	172	SER
1	A	190	LEU
1	A	213	LEU
1	A	241	SER
1	A	245	LEU
1	A	248	PHE
1	A	249	ARG
1	A	251	SER
1	A	252	GLN
1	A	253	ASP
1	A	258	ILE
1	A	260	SER
1	B	105	MET
1	B	109	ARG
1	B	110	LYS
1	B	114	THR
1	B	131	SER
1	B	135	LYS
1	B	138	LYS
1	B	143	VAL
1	B	166	GLU
1	B	172	SER
1	B	190	LEU
1	B	217	HIS
1	B	222	SER
1	B	228	SER
1	B	230	ASN
1	B	232	GLU
1	B	234	LEU

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	B	238	LEU
1	B	240	ASN
1	B	241	SER
1	B	242	PHE
1	B	245	LEU
1	B	247	GLN
1	B	258	ILE
1	B	261	LEU
1	C	107	LYS
1	C	109	ARG
1	C	110	LYS
1	C	111	THR
1	C	121	THR
1	C	126	ARG
1	C	134	GLU
1	C	138	LYS
1	C	146	LEU
1	C	149	SER
1	C	159	MET
1	C	165	LYS
1	C	166	GLU
1	C	172	SER
1	C	179	SER
1	C	190	LEU
1	C	213	LEU
1	C	225	LEU
1	C	231	THR
1	C	232	GLU
1	C	236	TYR
1	C	238	LEU
1	C	239	TYR
1	C	240	ASN
1	C	247	GLN
1	C	249	ARG
1	C	251	SER
1	C	252	GLN
1	C	258	ILE
1	C	259	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	210	ASN
1	A	230	ASN
1	A	247	GLN
1	B	112	HIS
1	B	178	HIS
1	B	210	ASN
1	B	230	ASN
1	B	247	GLN
1	B	256	ASN
1	B	259	GLN
1	C	170	ASN
1	C	178	HIS
1	C	210	ASN
1	C	247	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 18 ligands modelled in this entry, 15 are monoatomic - leaving 3 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	$\# Z  > 2$
4	NGH	A	480	2	21,21,21	9.13	15 (71%)	27,29,29	5.04	13 (48%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	NGH	B	479	2	21,21,21	8.46	16 (76%)	27,29,29	3.49	13 (48%)
4	NGH	C	481	2	21,21,21	12.09	17 (80%)	27,29,29	6.33	17 (62%)

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
4	NGH	A	480	2	1/1/4/5	7/24/24/24	0/1/1/1
4	NGH	B	479	2	1/1/4/5	12/24/24/24	0/1/1/1
4	NGH	C	481	2	1/1/4/5	11/24/24/24	0/1/1/1

All (48) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	481	NGH	C11-N1	32.47	1.68	1.32
4	A	480	NGH	O3-S1	20.39	1.66	1.43
4	C	481	NGH	C9-N	19.55	1.82	1.47
4	C	481	NGH	O5-C11	17.47	1.58	1.23
4	C	481	NGH	O3-S1	17.36	1.62	1.43
4	B	479	NGH	C11-N1	16.98	1.50	1.32
4	B	479	NGH	O3-S1	14.95	1.60	1.43
4	A	480	NGH	O2-S1	14.22	1.59	1.43
4	A	480	NGH	C11-N1	14.17	1.47	1.32
4	A	480	NGH	C1-C6	12.39	1.58	1.38
4	B	479	NGH	O2-S1	12.31	1.57	1.43
4	C	481	NGH	O2-S1	12.15	1.57	1.43
4	C	481	NGH	C5-C6	12.07	1.57	1.38
4	C	481	NGH	C5-C4	11.68	1.60	1.38
4	C	481	NGH	C1-C6	11.51	1.56	1.38
4	B	479	NGH	C5-C6	11.41	1.56	1.38
4	B	479	NGH	O5-C11	10.94	1.45	1.23
4	A	480	NGH	C5-C4	10.74	1.58	1.38
4	C	481	NGH	O1-C3	10.67	1.59	1.37
4	C	481	NGH	C2-C1	10.64	1.58	1.38
4	A	480	NGH	C4-C3	10.08	1.58	1.38
4	B	479	NGH	O1-C3	9.99	1.58	1.37
4	A	480	NGH	O5-C11	9.39	1.42	1.23
4	A	480	NGH	C5-C6	9.21	1.53	1.38
4	A	480	NGH	C2-C1	9.21	1.55	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	480	NGH	O1-C3	9.12	1.56	1.37
4	B	479	NGH	O1-C7	8.93	1.69	1.42
4	B	479	NGH	C5-C4	8.76	1.54	1.38
4	C	481	NGH	C2-C3	8.54	1.55	1.38
4	B	479	NGH	C10-N	8.40	1.60	1.47
4	B	479	NGH	C4-C3	8.22	1.55	1.38
4	A	480	NGH	C2-C3	8.04	1.54	1.38
4	B	479	NGH	C1-C6	8.02	1.51	1.38
4	A	480	NGH	C10-C11	7.74	1.64	1.52
4	A	480	NGH	C10-N	7.74	1.59	1.47
4	C	481	NGH	C4-C3	7.42	1.53	1.38
4	B	479	NGH	C2-C1	7.15	1.51	1.38
4	C	481	NGH	C9-C12	6.87	1.71	1.52
4	B	479	NGH	C2-C3	6.46	1.51	1.38
4	B	479	NGH	O4-N1	-4.92	1.27	1.40
4	C	481	NGH	C10-C11	4.66	1.59	1.52
4	A	480	NGH	O4-N1	-4.63	1.28	1.40
4	C	481	NGH	S1-N	-4.03	1.57	1.63
4	C	481	NGH	O4-N1	-3.54	1.31	1.40
4	C	481	NGH	C10-N	-2.88	1.43	1.47
4	A	480	NGH	C9-C12	2.84	1.60	1.52
4	B	479	NGH	C6-S1	-2.59	1.72	1.76
4	B	479	NGH	C10-C11	2.13	1.55	1.52

All (43) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	481	NGH	O5-C11-N1	-21.91	96.37	123.27
4	A	480	NGH	C6-S1-N	15.23	125.45	107.30
4	C	481	NGH	O4-N1-C11	-11.88	102.24	119.79
4	A	480	NGH	O3-S1-O2	-11.60	100.72	119.52
4	C	481	NGH	O2-S1-N	10.55	116.31	106.69
4	B	479	NGH	O2-S1-N	9.65	115.49	106.69
4	A	480	NGH	O3-S1-N	9.30	115.17	106.69
4	A	480	NGH	O5-C11-N1	-9.05	112.16	123.27
4	C	481	NGH	O2-S1-C6	8.08	118.27	108.05
4	B	479	NGH	O5-C11-N1	-7.87	113.61	123.27
4	C	481	NGH	C12-C9-N	-7.71	103.48	112.41
4	B	479	NGH	C1-C6-S1	-6.87	112.52	119.76
4	B	479	NGH	O3-S1-O2	-6.79	108.52	119.52
4	C	481	NGH	C6-S1-N	-6.69	99.33	107.30
4	A	480	NGH	O2-S1-C6	-6.57	99.73	108.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	481	NGH	C5-C6-S1	-6.40	113.01	119.76
4	C	481	NGH	O3-S1-O2	-6.34	109.25	119.52
4	C	481	NGH	C7-O1-C3	-4.73	107.25	117.51
4	A	480	NGH	C5-C6-S1	-4.19	115.35	119.76
4	C	481	NGH	C9-N-S1	3.90	126.07	117.52
4	A	480	NGH	O2-S1-N	-3.75	103.27	106.69
4	A	480	NGH	C10-C11-N1	-3.73	107.04	115.25
4	A	480	NGH	O5-C11-C10	-3.71	114.59	121.08
4	A	480	NGH	C1-C6-S1	-3.35	116.22	119.76
4	C	481	NGH	C4-C5-C6	3.20	122.76	119.45
4	B	479	NGH	C7-O1-C3	-3.16	110.66	117.51
4	B	479	NGH	O4-N1-C11	-3.06	115.27	119.79
4	C	481	NGH	C10-C11-N1	-3.04	108.56	115.25
4	A	480	NGH	C9-N-S1	3.01	124.13	117.52
4	B	479	NGH	C5-C4-C3	-2.98	116.09	119.73
4	B	479	NGH	C10-C11-N1	-2.96	108.74	115.25
4	C	481	NGH	C1-C6-S1	2.88	122.79	119.76
4	C	481	NGH	C5-C6-C1	-2.71	116.66	120.44
4	B	479	NGH	C9-N-S1	2.62	123.27	117.52
4	B	479	NGH	O3-S1-C6	2.56	111.29	108.05
4	B	479	NGH	C10-N-S1	2.38	123.72	117.85
4	B	479	NGH	C4-C3-C2	2.32	123.75	120.18
4	A	480	NGH	C7-O1-C3	-2.29	112.53	117.51
4	A	480	NGH	O1-C3-C2	-2.25	109.04	119.82
4	C	481	NGH	C1-C2-C3	2.21	122.44	119.73
4	B	479	NGH	O1-C3-C2	-2.17	109.43	119.82
4	C	481	NGH	O1-C3-C2	-2.16	109.48	119.82
4	C	481	NGH	O3-S1-N	-2.01	104.86	106.69

All (3) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	A	480	NGH	N
4	B	479	NGH	N
4	C	481	NGH	N

All (30) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	480	NGH	C13-C12-C9-N
4	A	480	NGH	C14-C12-C9-N
4	A	480	NGH	N-C10-C11-N1

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Mol	Chain	Res	Type	Atoms
4	A	480	NGH	C10-C11-N1-O4
4	B	479	NGH	C13-C12-C9-N
4	B	479	NGH	C14-C12-C9-N
4	B	479	NGH	N-C10-C11-N1
4	B	479	NGH	O5-C11-N1-O4
4	C	481	NGH	O5-C11-N1-O4
4	B	479	NGH	C4-C3-O1-C7
4	B	479	NGH	C2-C3-O1-C7
4	A	480	NGH	C4-C3-O1-C7
4	C	481	NGH	C2-C3-O1-C7
4	C	481	NGH	C1-C6-S1-N
4	C	481	NGH	N-C10-C11-O5
4	C	481	NGH	C1-C6-S1-O2
4	C	481	NGH	C9-N-S1-O3
4	A	480	NGH	C1-C6-S1-O3
4	B	479	NGH	C9-N-S1-O2
4	C	481	NGH	C5-C6-S1-O2
4	C	481	NGH	C12-C9-N-C10
4	C	481	NGH	C9-N-S1-C6
4	B	479	NGH	C5-C6-S1-O3
4	A	480	NGH	C9-N-S1-O3
4	C	481	NGH	C9-N-S1-O2
4	B	479	NGH	C11-C10-N-S1
4	B	479	NGH	C5-C6-S1-N
4	C	481	NGH	C10-C11-N1-O4
4	B	479	NGH	C9-N-S1-O3
4	B	479	NGH	C9-N-S1-C6

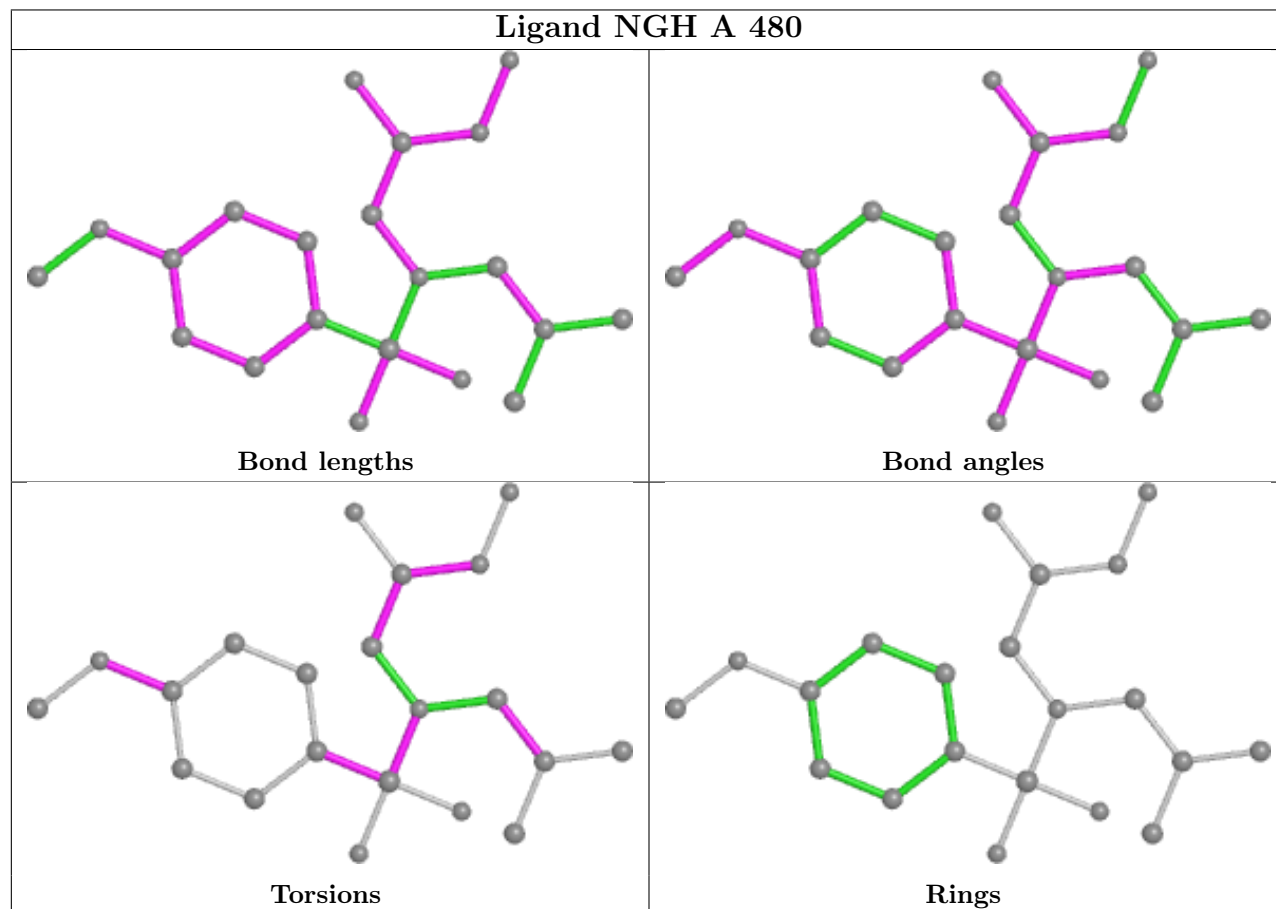
There are no ring outliers.

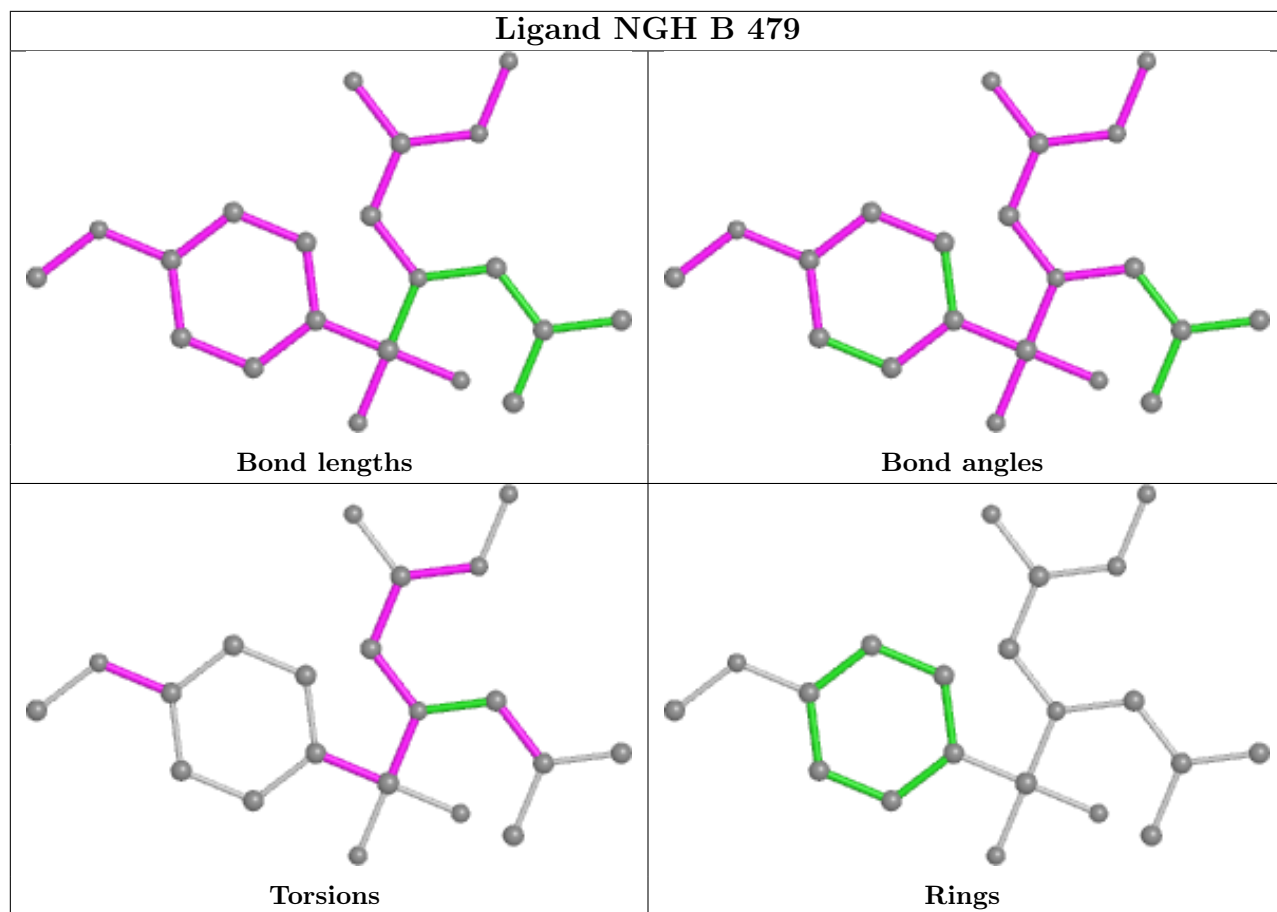
3 monomers are involved in 36 short contacts:

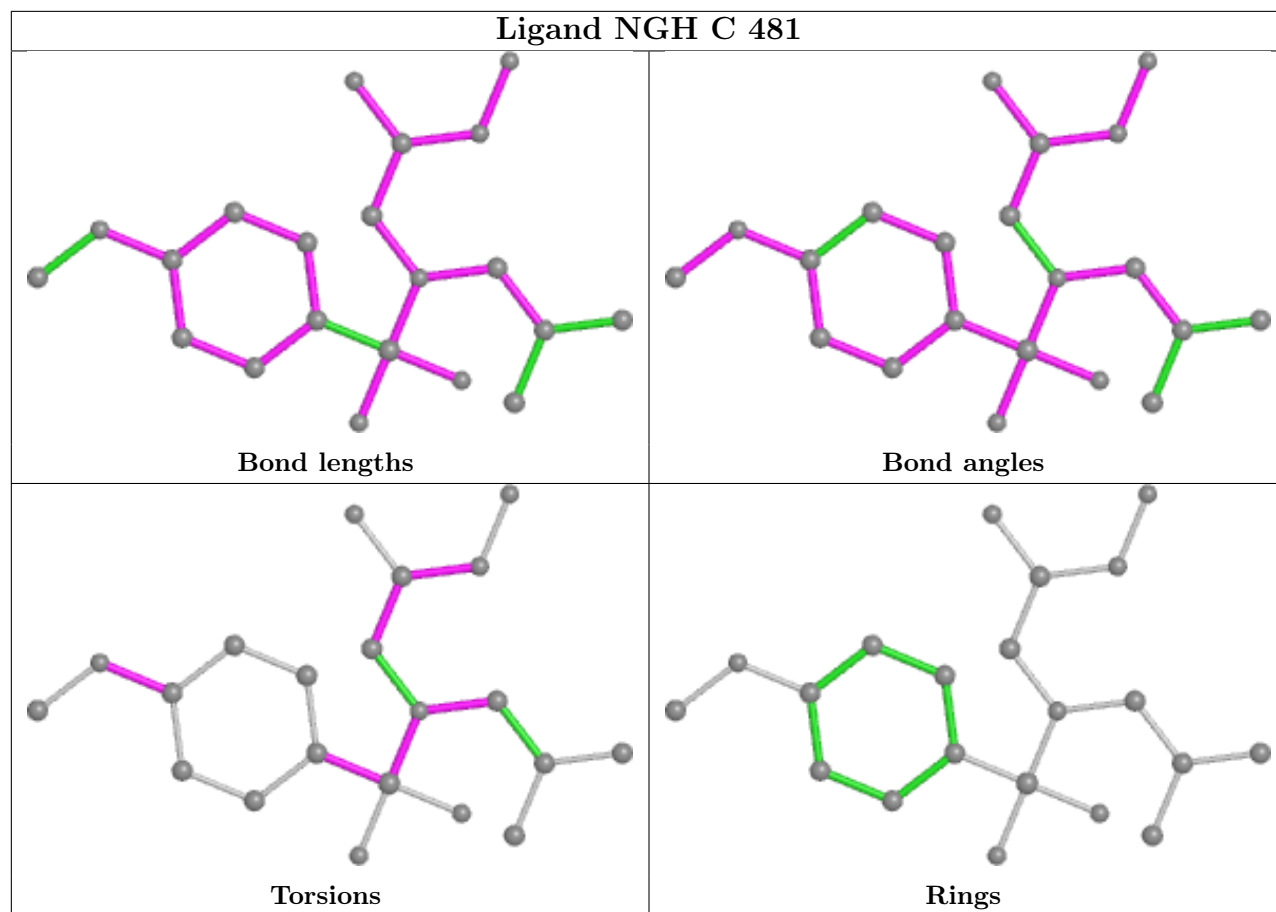
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	480	NGH	4	0
4	B	479	NGH	7	0
4	C	481	NGH	25	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be

highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.







## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	156/165 (94%)	0.62	11 (7%) 16 20	18, 34, 50, 67	0
1	B	160/165 (96%)	0.78	10 (6%) 20 24	23, 36, 50, 60	0
1	C	155/165 (93%)	0.74	15 (9%) 7 10	22, 36, 54, 63	0
All	All	471/495 (95%)	0.72	36 (7%) 13 18	18, 35, 51, 67	0

All (36) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	245	LEU	5.8
1	C	263	GLY	5.2
1	C	239	TYR	4.9
1	C	236	TYR	4.0
1	A	171	TYR	3.9
1	C	229	ALA	3.9
1	A	105	MET	3.5
1	B	263	GLY	3.2
1	B	131	SER	3.1
1	C	226	PHE	2.9
1	C	246	ALA	2.8
1	C	106	PRO	2.8
1	B	152	TYR	2.6
1	A	106	PRO	2.6
1	B	243	THR	2.6
1	C	237	PRO	2.6
1	A	247	GLN	2.6
1	C	206	ALA	2.5
1	B	105	MET	2.5
1	A	129	VAL	2.3
1	A	240	ASN	2.3
1	B	147	THR	2.2
1	C	170	ASN	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	145	PRO	2.2
1	C	245	LEU	2.1
1	B	247	GLN	2.1
1	C	191	TYR	2.1
1	B	106	PRO	2.1
1	B	226	PHE	2.1
1	A	248	PHE	2.1
1	C	140	TRP	2.0
1	A	145	PRO	2.0
1	A	151	LEU	2.0
1	A	246	ALA	2.0
1	C	143	VAL	2.0
1	C	247	GLN	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, 95<sup>th</sup> 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.

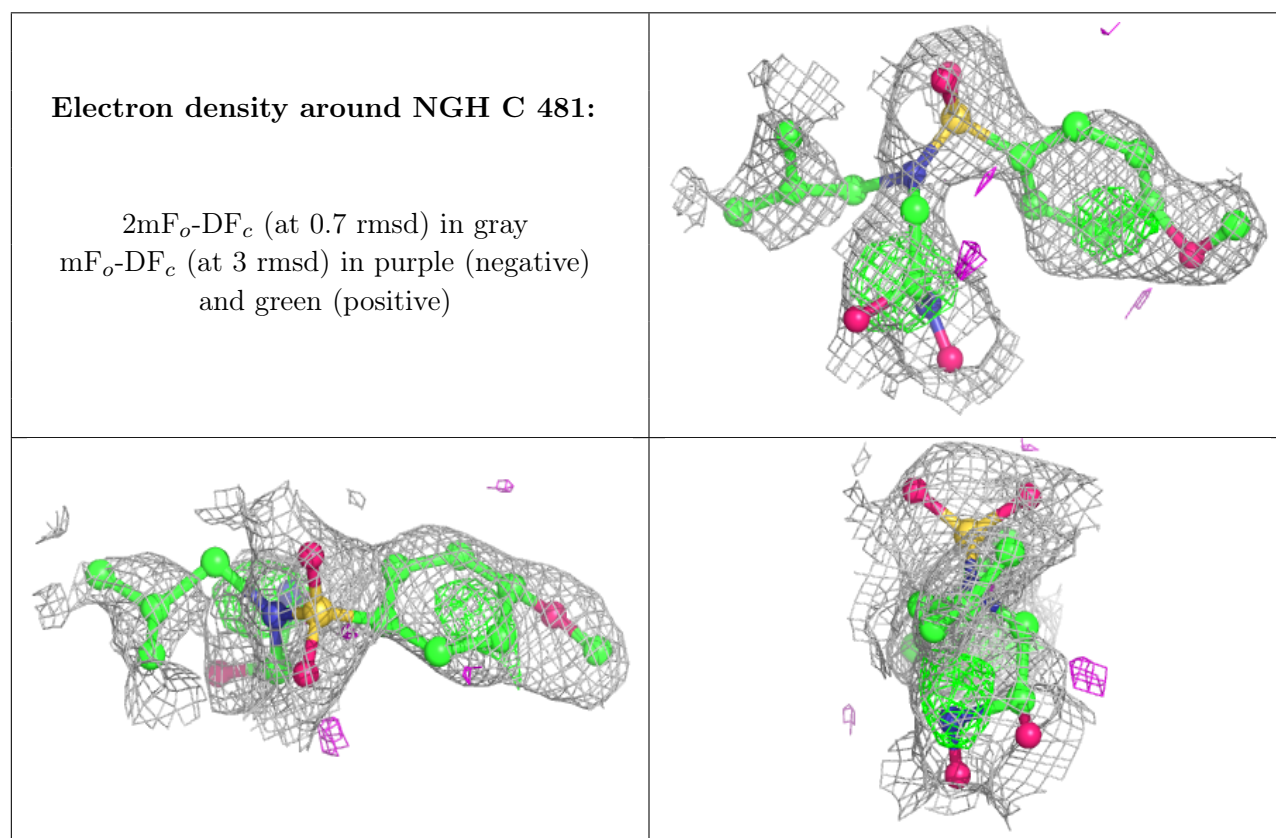
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
4	NGH	C	481	21/21	0.83	0.26	40,46,48,51	0
4	NGH	A	480	21/21	0.87	0.20	35,44,46,47	0
4	NGH	B	479	21/21	0.89	0.19	33,34,37,38	0
3	CA	C	478	1/1	0.94	0.05	44,44,44,44	0
3	CA	C	477	1/1	0.97	0.03	40,40,40,40	0
3	CA	A	466	1/1	0.98	0.06	31,31,31,31	0
3	CA	A	467	1/1	0.98	0.08	31,31,31,31	0
3	CA	B	472	1/1	0.98	0.05	30,30,30,30	0
2	ZN	B	469	1/1	0.98	0.04	33,33,33,33	0
3	CA	C	476	1/1	0.99	0.08	36,36,36,36	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	ZN	C	475	1/1	0.99	0.03	29,29,29,29	0
3	CA	A	468	1/1	0.99	0.05	25,25,25,25	0
3	CA	B	471	1/1	0.99	0.03	26,26,26,26	0
2	ZN	A	464	1/1	0.99	0.03	33,33,33,33	0
3	CA	B	473	1/1	0.99	0.04	34,34,34,34	0
2	ZN	B	470	1/1	1.00	0.03	20,20,20,20	0
2	ZN	C	474	1/1	1.00	0.04	36,36,36,36	0
2	ZN	A	465	1/1	1.00	0.05	29,29,29,29	0

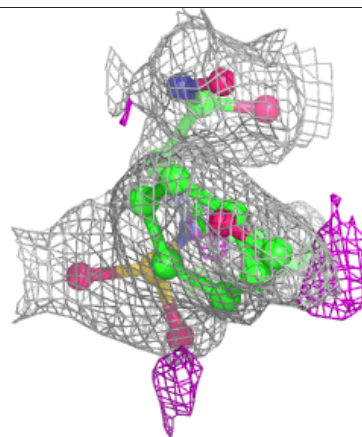
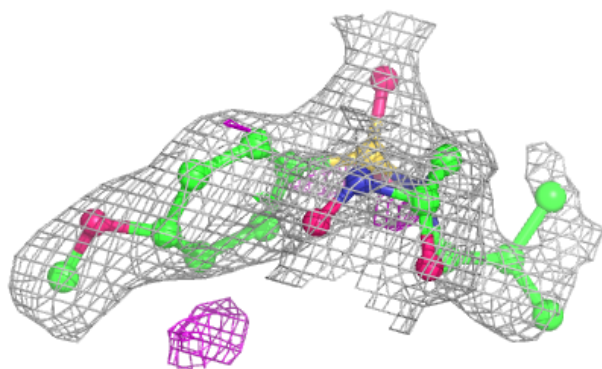
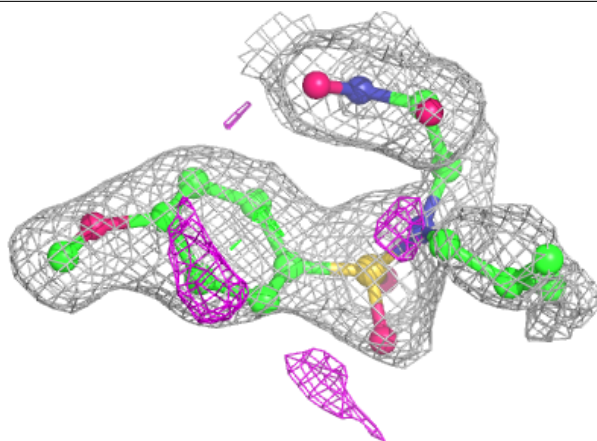
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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



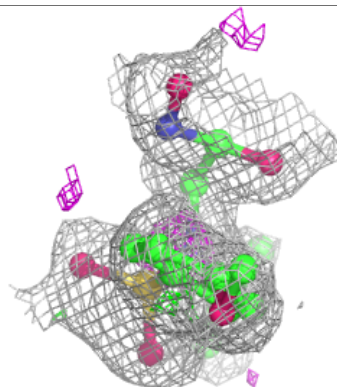
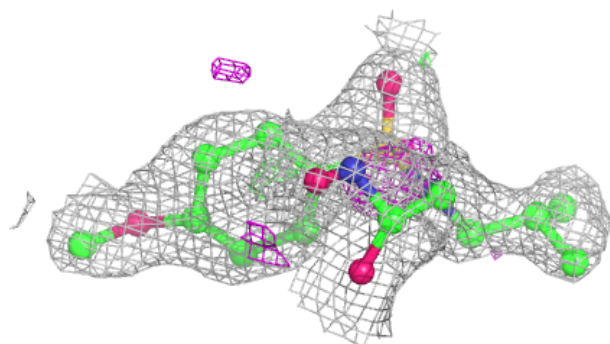
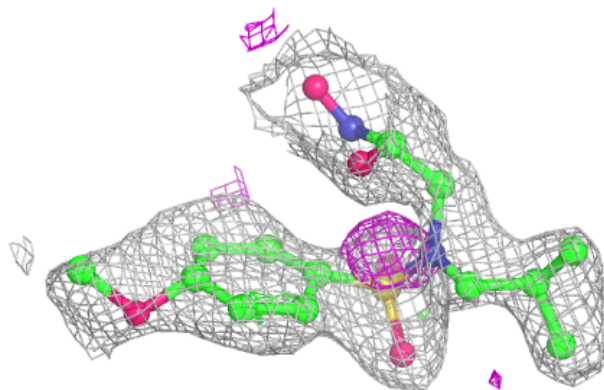


**Electron density around NGH A 480:**

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

**Electron density around NGH B 479:**

$2mF_o-DF_c$  (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.