Full wwPDB X-ray Structure Validation Report (i)

Nov 1, 2023 – 02:21 AM EDT

PDB ID	:	3Q2H
Title	:	Adamts1 in complex with N-hydroxyformamide inhibitors of ADAM-TS4
Authors	:	Gerhardt, S.; Hargreaves, D.
Deposited on	:	2010-12-20
Resolution	:	2.33 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:

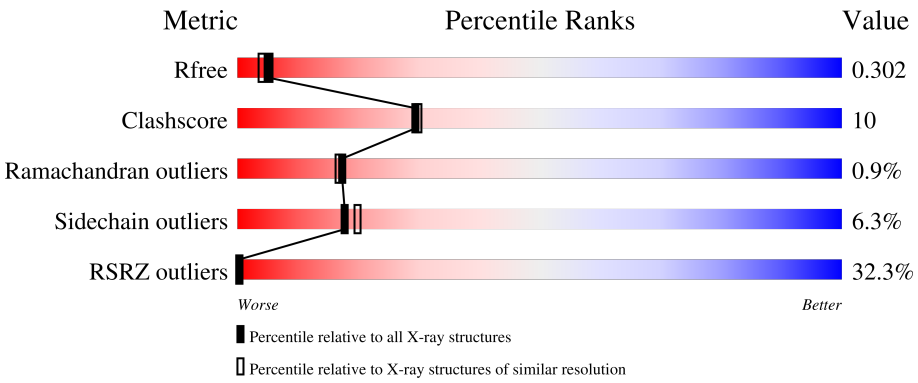
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.33 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	2096 (2.36-2.32)
Clashscore	141614	2193 (2.36-2.32)
Ramachandran outliers	138981	2159 (2.36-2.32)
Sidechain outliers	138945	2160 (2.36-2.32)
RSRZ outliers	127900	2067 (2.36-2.32)

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	297	21% 83% 10% • •
1	B	297	41% 65% 26% • 5%

2 Entry composition (i)

There are 8 unique types of molecules in this entry. The entry contains 4545 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 A disintegrin and metalloproteinase with thrombospondin motifs 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	284	2181	1354	379	423	25	0	0	0
1	B	282	2169	1346	380	418	25	0	0	0

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	297	LEU	-	expression tag	UNP Q9UHI8
A	298	VAL	-	expression tag	UNP Q9UHI8
A	299	PRO	-	expression tag	UNP Q9UHI8
A	300	ARG	-	expression tag	UNP Q9UHI8
B	297	LEU	-	expression tag	UNP Q9UHI8
B	298	VAL	-	expression tag	UNP Q9UHI8
B	299	PRO	-	expression tag	UNP Q9UHI8
B	300	ARG	-	expression tag	UNP Q9UHI8

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Zn		
2	A	1	1	1	0	0
2	B	1	1	1	0	0

- Molecule 3 is CADMIUM ION (three-letter code: CD) (formula: Cd).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Cd		
3	A	3	3	3	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Cd		
3	B	1	1	1	0	0

- Molecule 4 is NICKEL (II) ION (three-letter code: NI) (formula: Ni).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Ni		
4	A	9	9	9	0	0
			Total	Ni		
4	B	5	5	5	0	0

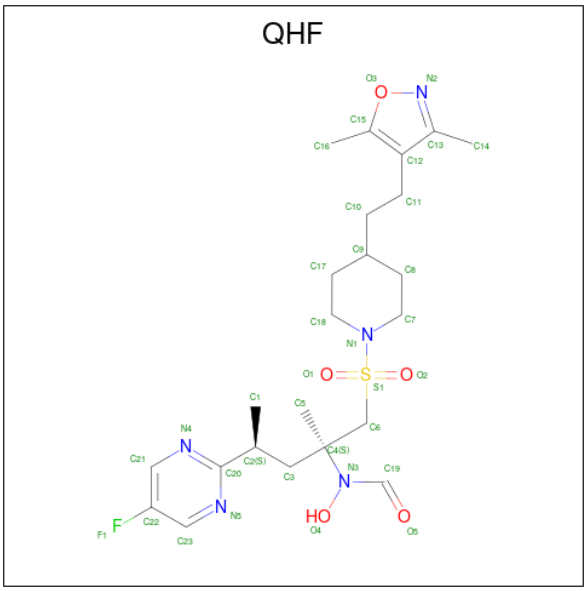
- Molecule 5 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mg		
5	A	2	2	2	0	0
			Total	Mg		
5	B	1	1	1	0	0

- Molecule 6 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Na		
6	A	2	2	2	0	0
			Total	Na		
6	B	2	2	2	0	0

- Molecule 7 is N-[(2S,4S)-1-({4-[2-(3,5-dimethyl-1,2-oxazol-4-yl)ethyl]piperidin-1-yl}sulfonyl)-4-(5-fluoropyrimidin-2-yl)-2-methylpentan-2-yl]-N-hydroxyformamide (three-letter code: QHF) (formula: $C_{23}H_{34}FN_5O_5S$).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
			Total	C	F	N	O	S		
7	A	1	35	23	1	5	5	1	0	0
			Total	C	F	N	O	S		
7	B	1	35	23	1	5	5	1	0	0

- Molecule 8 is water.

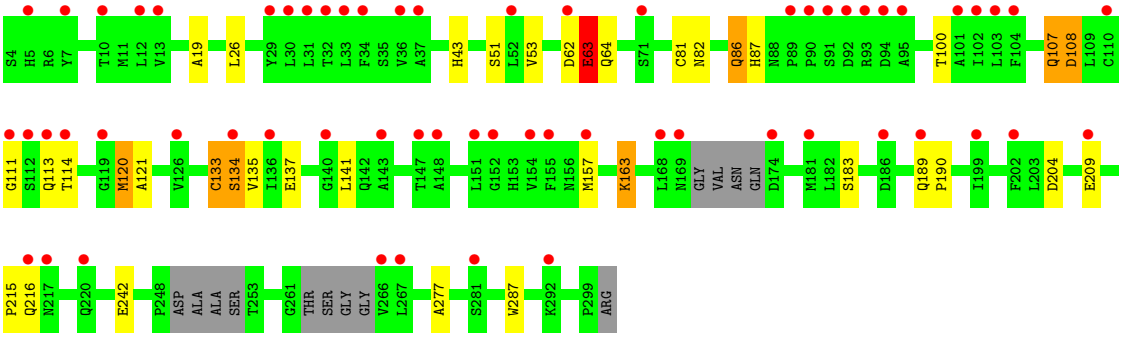
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
8	A	66	66	66	0	0
			Total	O		
8	B	32	32	32	0	0

3 Residue-property plots (i)

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

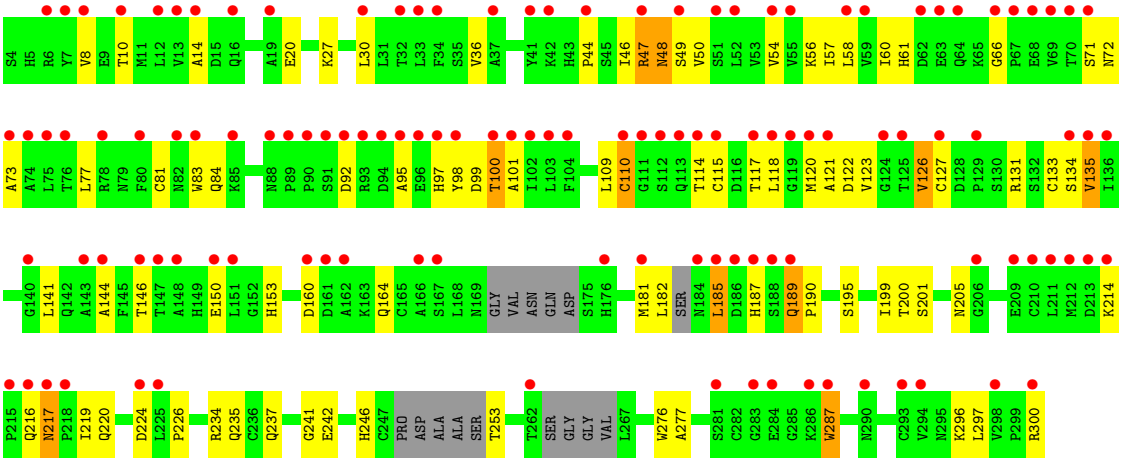
• Molecule 1: A disintegrin and metalloproteinase with thrombospondin motifs 1

Chain A:



• Molecule 1: A disintegrin and metalloproteinase with thrombospondin motifs 1

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	50.86Å 63.33Å 110.84Å 90.00° 91.24° 90.00°	Depositor
Resolution (Å)	27.70 – 2.33 27.70 – 2.33	Depositor EDS
% Data completeness (in resolution range)	98.6 (27.70-2.33) 98.7 (27.70-2.33)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.74 (at 2.34Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.236 , 0.297 0.249 , 0.302	Depositor DCC
R_{free} test set	1514 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å^2)	52.6	Xtriage
Anisotropy	0.315	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.38 , 84.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	0.021 for h,-k,-l	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	4545	wwPDB-VP
Average B, all atoms (Å^2)	84.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.01% of the height of the origin peak. No significant pseudotranslation is detected.*

[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: ZN, NA, CD, QHF, MG, NI

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	0.75	2/2233 (0.1%)	0.77	3/3032 (0.1%)
1	B	0.58	1/2219 (0.0%)	0.66	1/3009 (0.0%)
All	All	0.67	3/4452 (0.1%)	0.72	4/6041 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	63	GLU	CB-CG	8.56	1.68	1.52
1	A	133	CYS	CB-SG	-6.84	1.70	1.82
1	B	99	ASP	CG-OD1	5.60	1.38	1.25

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	108	ASP	CB-CG-OD1	9.57	126.91	118.30
1	A	108	ASP	CB-CG-OD2	-6.12	112.80	118.30
1	A	157	MET	CG-SD-CE	5.42	108.87	100.20
1	B	234	ARG	NE-CZ-NH1	5.08	122.84	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	48	ASN	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	2181	0	2050	22	1
1	B	2169	0	2039	59	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	3	0	0	0	0
3	B	1	0	0	0	0
4	A	9	0	0	0	0
4	B	5	0	0	0	0
5	A	2	0	0	0	0
5	B	1	0	0	0	0
6	A	2	0	0	0	0
6	B	2	0	0	0	0
7	A	35	0	33	0	0
7	B	35	0	33	4	0
8	A	66	0	0	1	0
8	B	32	0	0	2	0
All	All	4545	0	4155	79	1

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 10.

All (79) 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:B:81:CYS:HG	1:B:133:CYS:HG	0.97	0.95
1:B:120:MET:HB3	1:B:135:VAL:HG13	1.58	0.83
1:B:77:LEU:HD22	1:B:120:MET:HG3	1.60	0.83
1:A:242:GLU:O	1:B:27:LYS:NZ	2.20	0.74
1:A:137:GLU:OE1	8:A:327:HOH:O	2.06	0.73
1:A:86:GLN:HG2	1:A:87:HIS:CD2	2.26	0.71
1:A:242:GLU:OE2	1:B:61:HIS:NE2	2.26	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:48:ASN:ND2	1:B:200:THR:OG1	2.25	0.67
1:B:8:VAL:CG2	1:B:50:VAL:CG1	2.73	0.66
1:B:181:MET:SD	1:B:182:LEU:N	2.70	0.64
1:B:242:GLU:OE2	8:B:311:HOH:O	2.15	0.64
1:B:141:LEU:HD12	1:B:277:ALA:HB2	1.79	0.64
1:B:235:GLN:HE22	1:B:277:ALA:H	1.43	0.63
1:B:44:PRO:O	1:B:47:ARG:N	2.30	0.60
1:B:77:LEU:HD13	1:B:135:VAL:HG12	1.83	0.60
1:B:54:VAL:HG11	1:B:57:ILE:HD11	1.84	0.59
1:B:14:ALA:HB2	1:B:30:LEU:HD11	1.83	0.59
1:B:126:VAL:HG13	1:B:127:CYS:H	1.66	0.59
1:B:46:ILE:HG23	1:B:48:ASN:H	1.69	0.58
1:B:8:VAL:HG23	1:B:50:VAL:HG12	1.87	0.57
1:B:98:TYR:CE2	1:B:101:ALA:HB2	2.40	0.57
1:B:8:VAL:CG2	1:B:50:VAL:HG12	2.37	0.55
1:A:120:MET:HB3	1:A:135:VAL:HG22	1.89	0.54
1:B:141:LEU:HD12	1:B:277:ALA:CB	2.38	0.54
1:B:160:ASP:OD1	8:B:304:HOH:O	2.18	0.54
1:B:182:LEU:HD21	7:B:2:QHF:C13	2.39	0.53
1:B:185:LEU:HD12	1:B:187:HIS:CD2	2.43	0.53
1:B:60:ILE:HG22	1:B:60:ILE:O	2.07	0.53
1:B:95:ALA:HB2	1:B:216:GLN:NE2	2.24	0.52
1:B:60:ILE:HD13	1:B:66:GLY:HA3	1.92	0.52
1:A:43:HIS:CE1	1:A:190:PRO:HD2	2.46	0.51
1:B:36:VAL:CG2	1:B:226:PRO:HG3	2.40	0.51
1:B:54:VAL:HG12	1:B:219:ILE:HD12	1.93	0.51
1:A:242:GLU:OE2	1:B:61:HIS:CE1	2.64	0.50
1:B:8:VAL:HG23	1:B:50:VAL:CG1	2.40	0.50
1:A:111:GLY:HA3	1:A:113:GLN:HE22	1.78	0.49
1:A:81:CYS:HG	1:A:133:CYS:HG	1.59	0.49
1:B:73:ALA:HB2	1:B:109:LEU:HB3	1.95	0.48
1:B:126:VAL:HG13	1:B:127:CYS:N	2.26	0.48
1:B:92:ASP:OD1	1:B:97:HIS:ND1	2.45	0.48
1:B:77:LEU:HD13	1:B:135:VAL:CG1	2.43	0.48
1:A:81:CYS:HA	1:A:133:CYS:HG	1.78	0.48
1:B:36:VAL:HB	1:B:144:ALA:HB1	1.96	0.48
1:A:19:ALA:HA	1:A:26:LEU:HD22	1.94	0.47
1:B:8:VAL:HG21	1:B:50:VAL:CG1	2.45	0.47
1:B:36:VAL:HG22	1:B:226:PRO:HG3	1.95	0.47
1:B:121:ALA:O	7:B:2:QHF:H21	2.15	0.46
1:B:77:LEU:O	1:B:81:CYS:HB2	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:118:LEU:HD12	7:B:2:QHF:H17A	1.97	0.46
1:B:246:HIS:NE2	1:B:276:TRP:CZ2	2.84	0.45
1:A:113:GLN:NE2	1:A:114:THR:H	2.15	0.45
1:B:10:THR:HA	1:B:100:THR:O	2.16	0.45
1:A:62:ASP:O	1:A:63:GLU:C	2.55	0.44
1:B:71:SER:HB2	1:B:110:CYS:SG	2.57	0.44
1:B:201:SER:O	1:B:205:ASN:ND2	2.50	0.44
1:B:216:GLN:O	1:B:217:ASN:C	2.55	0.44
1:B:287:TRP:CE3	1:B:296:LYS:HD2	2.53	0.44
1:A:141:LEU:HD12	1:A:277:ALA:HB2	1.99	0.43
1:B:237:GLN:HA	1:B:241:GLY:O	2.18	0.43
1:B:49:SER:O	1:B:49:SER:OG	2.29	0.43
1:A:163:LYS:HA	1:A:163:LYS:HD2	1.79	0.43
1:B:195:SER:O	1:B:199:ILE:HG22	2.19	0.43
7:B:2:QHF:H5B	7:B:2:QHF:H2	1.53	0.43
1:A:121:ALA:HB2	1:A:134:SER:HB3	2.02	0.42
1:B:123:VAL:HA	1:B:153:HIS:O	2.19	0.42
1:A:81:CYS:SG	1:A:133:CYS:SG	3.17	0.42
1:A:108:ASP:OD1	1:A:137:GLU:OE1	2.38	0.42
1:B:56:LYS:HE2	1:B:58:LEU:HD11	2.01	0.41
1:A:81:CYS:SG	1:A:133:CYS:HB2	2.60	0.41
1:A:108:ASP:HA	1:A:137:GLU:CD	2.41	0.41
1:B:189:GLN:HE21	1:B:189:GLN:HA	1.84	0.41
1:B:121:ALA:HB2	1:B:150:GLU:HB3	2.01	0.41
1:B:92:ASP:CG	1:B:97:HIS:HD1	2.24	0.41
1:A:53:VAL:HG21	1:A:215:PRO:HG3	2.02	0.41
1:A:107:GLN:O	1:A:137:GLU:HG3	2.21	0.41
1:B:146:THR:O	1:B:150:GLU:HG2	2.21	0.41
1:B:83:TRP:CE3	1:B:84:GLN:HA	2.56	0.40
1:B:185:LEU:HD11	1:B:190:PRO:HB3	2.02	0.40
1:B:122:ASP:HB3	1:B:131:ARG:HH21	1.87	0.40

All (1) 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:82:ASN:ND2	1:A:204:ASP:O[2_655]	2.18	0.02

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	276/297 (93%)	267 (97%)	8 (3%)	1 (0%)	34 38
1	B	272/297 (92%)	243 (89%)	25 (9%)	4 (2%)	10 7
All	All	548/594 (92%)	510 (93%)	33 (6%)	5 (1%)	17 17

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	114	THR
1	A	209	GLU
1	B	220	GLN
1	B	126	VAL
1	B	217	ASN

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	247/256 (96%)	234 (95%)	13 (5%)	22 27
1	B	244/256 (95%)	226 (93%)	18 (7%)	13 14
All	All	491/512 (96%)	460 (94%)	31 (6%)	18 20

All (31) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	51	SER

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Mol	Chain	Res	Type
1	A	63	GLU
1	A	64	GLN
1	A	86	GLN
1	A	100	THR
1	A	107	GLN
1	A	120	MET
1	A	134	SER
1	A	163	LYS
1	A	183	SER
1	A	189	GLN
1	A	216	GLN
1	A	287	TRP
1	B	20	GLU
1	B	47	ARG
1	B	72	ASN
1	B	100	THR
1	B	110	CYS
1	B	115	CYS
1	B	117	THR
1	B	134	SER
1	B	135	VAL
1	B	164	GLN
1	B	185	LEU
1	B	189	GLN
1	B	214	LYS
1	B	224	ASP
1	B	253	THR
1	B	287	TRP
1	B	297	LEU
1	B	300	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	5	HIS
1	A	16	GLN
1	A	113	GLN
1	A	189	GLN
1	A	205	ASN
1	A	216	GLN
1	B	156	ASN
1	B	189	GLN

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Mol	Chain	Res	Type
1	B	216	GLN
1	B	235	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 29 ligands modelled in this entry, 27 are monoatomic - leaving 2 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	$\#\|Z\| > 2$
7	QHF	A	1	2	31,37,37	1.53	6 (19%)	37,54,54	2.51	12 (32%)
7	QHF	B	2	2	31,37,37	2.15	7 (22%)	37,54,54	1.67	7 (18%)

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
7	QHF	A	1	2	-	7/25/44/44	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	QHF	B	2	2	-	7/25/44/44	0/3/3/3

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	B	2	QHF	S1-N1	7.63	1.73	1.63
7	B	2	QHF	C4-N3	-5.41	1.43	1.51
7	A	1	QHF	S1-N1	4.81	1.69	1.63
7	B	2	QHF	C3-C4	-3.39	1.51	1.54
7	B	2	QHF	C11-C12	-3.32	1.47	1.52
7	A	1	QHF	C4-N3	-3.29	1.46	1.51
7	A	1	QHF	C12-C13	2.70	1.44	1.39
7	B	2	QHF	C3-C2	-2.41	1.50	1.54
7	B	2	QHF	O1-S1	2.24	1.45	1.43
7	A	1	QHF	C18-N1	2.17	1.50	1.47
7	A	1	QHF	C5-C4	-2.06	1.50	1.53
7	B	2	QHF	C6-S1	2.01	1.81	1.78
7	A	1	QHF	C14-C13	-2.00	1.47	1.50

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	A	1	QHF	C18-N1-C7	7.73	120.72	112.17
7	A	1	QHF	O4-N3-C4	5.99	118.53	107.30
7	A	1	QHF	C11-C12-C13	5.94	131.47	127.30
7	B	2	QHF	O4-N3-C4	4.60	115.93	107.30
7	A	1	QHF	C17-C18-N1	4.24	115.21	109.43
7	B	2	QHF	O1-S1-N1	4.06	110.66	107.23
7	A	1	QHF	C7-N1-S1	-3.24	112.52	118.61
7	B	2	QHF	C11-C10-C9	-3.16	110.42	114.47
7	B	2	QHF	C11-C12-C13	2.86	129.31	127.30
7	A	1	QHF	C6-S1-N1	-2.75	103.15	106.04
7	A	1	QHF	C2-C20-N4	-2.64	113.42	117.03
7	B	2	QHF	C16-C15-C12	2.47	134.89	126.51
7	A	1	QHF	C10-C9-C8	-2.43	106.30	112.11
7	A	1	QHF	C22-C21-N4	-2.39	120.02	121.46
7	A	1	QHF	C1-C2-C20	-2.38	104.73	112.36
7	A	1	QHF	C16-C15-C12	2.23	134.08	126.51
7	B	2	QHF	C6-S1-N1	-2.20	103.72	106.04
7	A	1	QHF	C13-C12-C15	-2.12	103.08	106.62
7	B	2	QHF	O2-S1-O1	2.00	121.03	118.98

There are no chirality outliers.

All (14) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	A	1	QHF	C18-N1-S1-O2
7	A	1	QHF	C18-N1-S1-C6
7	B	2	QHF	C20-C2-C3-C4
7	B	2	QHF	C18-N1-S1-O2
7	B	2	QHF	C4-C6-S1-O2
7	A	1	QHF	C4-C6-S1-N1
7	A	1	QHF	C4-C6-S1-O2
7	B	2	QHF	C18-N1-S1-C6
7	A	1	QHF	C1-C2-C20-N4
7	B	2	QHF	C4-C6-S1-N1
7	B	2	QHF	C11-C10-C9-C17
7	A	1	QHF	C18-N1-S1-O1
7	B	2	QHF	C18-N1-S1-O1
7	A	1	QHF	C7-N1-S1-O2

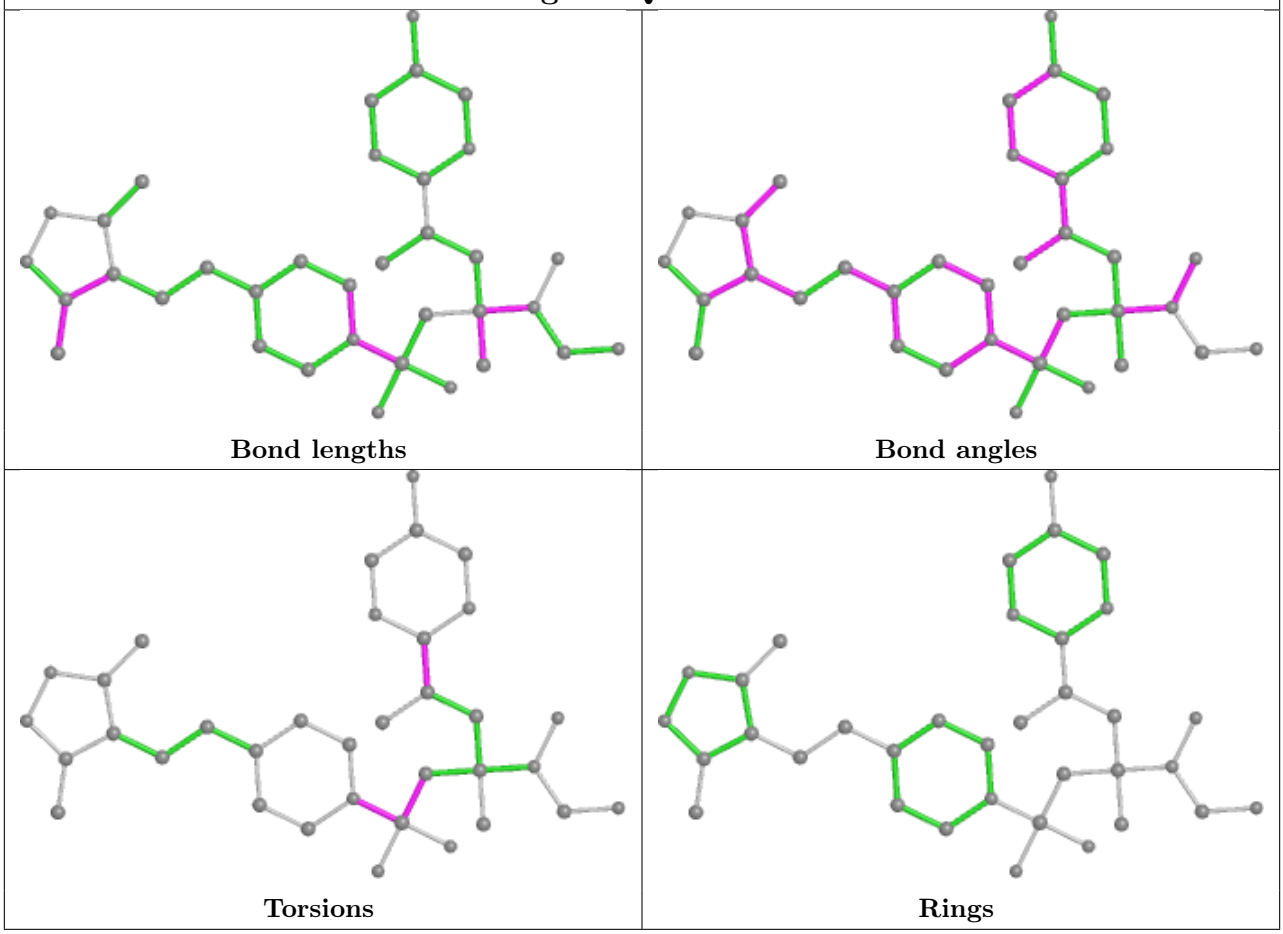
There are no ring outliers.

1 monomer is involved in 4 short contacts:

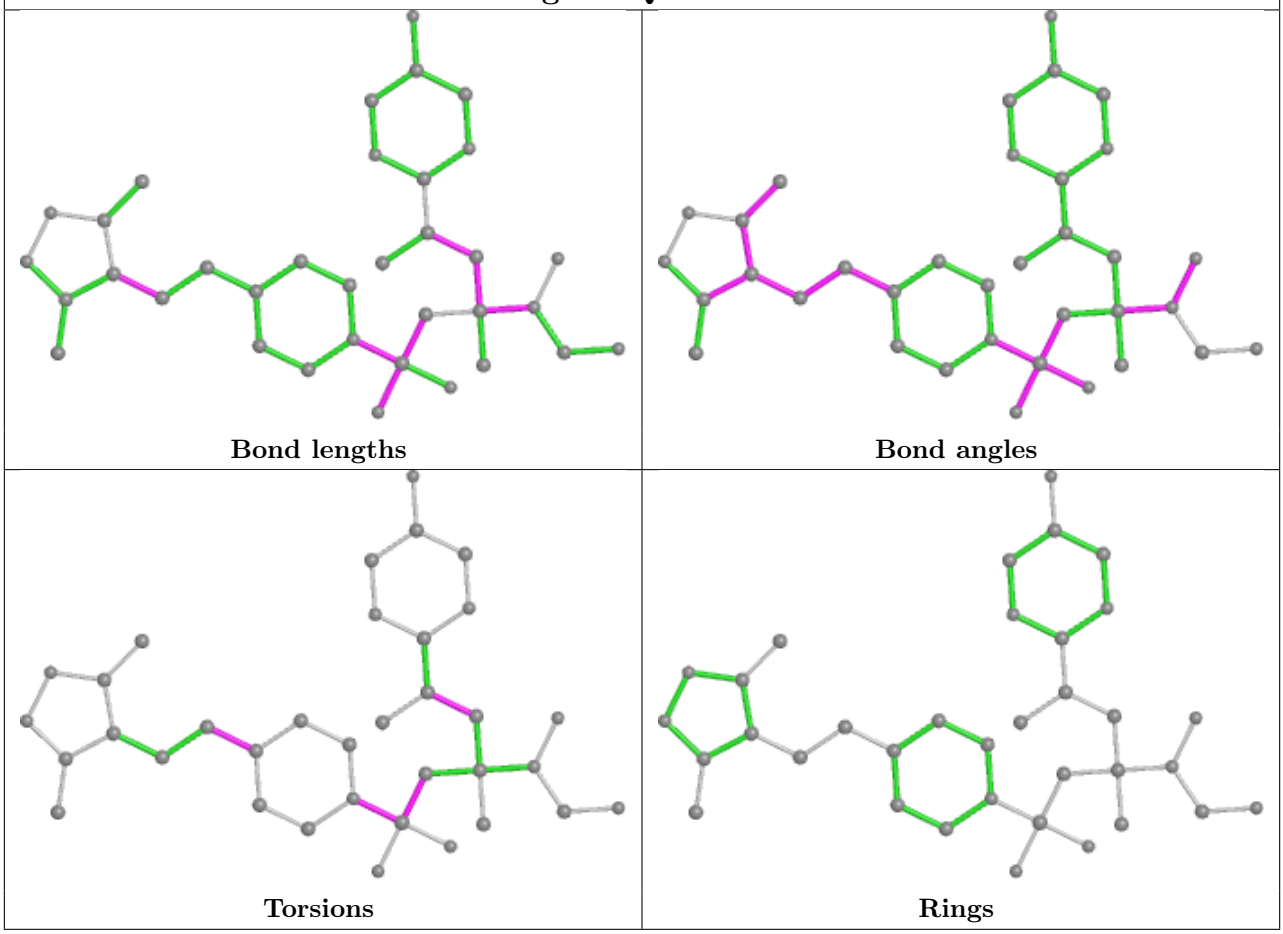
Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	B	2	QHF	4	0

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 QHF A 1



Ligand QHF B 2



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	284/297 (95%)	1.19	61 (21%)	0	1	49, 72, 96, 116	0
1	B	282/297 (94%)	2.23	122 (43%)	0	0	62, 100, 125, 137	0
All	All	566/594 (95%)	1.71	183 (32%)	0	0	49, 83, 119, 137	0

All (183) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	114	THR	11.9
1	B	68	GLU	9.9
1	B	90	PRO	9.5
1	B	111	GLY	8.4
1	B	89	PRO	8.1
1	B	102	ILE	7.9
1	B	55	VAL	7.6
1	B	75	LEU	7.3
1	B	214	LYS	7.0
1	B	112	SER	6.9
1	B	115	CYS	6.9
1	B	91	SER	6.9
1	A	266	VAL	6.6
1	A	90	PRO	6.5
1	B	136	ILE	6.4
1	B	103	LEU	6.2
1	B	88	ASN	6.1
1	B	104	PHE	6.1
1	B	93	ARG	6.1
1	B	8	VAL	5.8
1	B	92	ASP	5.6
1	B	113	GLN	5.6
1	A	111	GLY	5.5
1	B	96	GLU	5.3

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Mol	Chain	Res	Type	RSRZ
1	B	30	LEU	5.2
1	B	212	MET	5.2
1	B	186	ASP	5.2
1	B	215	PRO	5.1
1	A	93	ARG	5.1
1	B	7	TYR	5.1
1	A	91	SER	5.0
1	A	151	LEU	5.0
1	B	209	GLU	4.9
1	A	169	ASN	4.9
1	A	102	ILE	4.8
1	B	147	THR	4.8
1	B	187	HIS	4.7
1	B	210	CYS	4.7
1	A	89	PRO	4.7
1	B	262	THR	4.7
1	B	62	ASP	4.7
1	B	49	SER	4.6
1	A	216	GLN	4.6
1	A	136	ILE	4.5
1	B	70	THR	4.5
1	B	146	THR	4.4
1	B	216	GLN	4.4
1	A	33	LEU	4.4
1	B	33	LEU	4.4
1	B	82	ASN	4.4
1	B	47	ARG	4.4
1	B	188	SER	4.4
1	B	284	GLU	4.4
1	B	110	CYS	4.2
1	B	120	MET	4.2
1	B	151	LEU	4.2
1	A	113	GLN	4.2
1	A	114	THR	4.1
1	B	118	LEU	4.1
1	B	66	GLY	4.1
1	A	209	GLU	4.0
1	B	185	LEU	3.9
1	B	83	TRP	3.9
1	B	134	SER	3.8
1	B	37	ALA	3.8
1	B	121	ALA	3.8

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Mol	Chain	Res	Type	RSRZ
1	B	293	CYS	3.7
1	A	155	PHE	3.7
1	A	154	VAL	3.7
1	B	12	LEU	3.6
1	B	218	PRO	3.6
1	A	147	THR	3.6
1	B	217	ASN	3.6
1	A	112	SER	3.6
1	B	162	ALA	3.5
1	B	52	LEU	3.5
1	B	143	ALA	3.5
1	B	34	PHE	3.5
1	B	67	PRO	3.5
1	A	104	PHE	3.5
1	A	94	ASP	3.5
1	A	143	ALA	3.4
1	B	124	GLY	3.4
1	B	63	GLU	3.4
1	B	298	VAL	3.4
1	B	189	GLN	3.4
1	A	13	VAL	3.4
1	B	44	PRO	3.4
1	B	69	VAL	3.3
1	B	94	ASP	3.3
1	A	148	ALA	3.3
1	B	101	ALA	3.3
1	B	13	VAL	3.3
1	B	181	MET	3.3
1	B	78	ARG	3.3
1	B	184	ASN	3.3
1	A	95	ALA	3.2
1	B	54	VAL	3.2
1	B	14	ALA	3.2
1	B	125	THR	3.2
1	B	160	ASP	3.1
1	B	144	ALA	3.1
1	A	29	TYR	3.1
1	A	92	ASP	3.1
1	B	166	ALA	3.0
1	A	267	LEU	3.0
1	A	5	HIS	3.0
1	B	97	HIS	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	37	ALA	3.0
1	B	51	SER	3.0
1	B	150	GLU	3.0
1	B	135	VAL	3.0
1	A	103	LEU	3.0
1	A	34	PHE	2.9
1	B	58	LEU	2.9
1	B	211	LEU	2.9
1	B	59	VAL	2.9
1	A	168	LEU	2.9
1	A	292	LYS	2.9
1	B	41	TYR	2.9
1	B	6	ARG	2.8
1	B	71	SER	2.8
1	A	10	THR	2.8
1	A	12	LEU	2.8
1	A	217	ASN	2.8
1	B	290	ASN	2.8
1	B	140	GLY	2.7
1	A	181	MET	2.7
1	B	76	THR	2.7
1	B	16	GLN	2.7
1	B	206	GLY	2.7
1	A	202	PHE	2.7
1	A	71	SER	2.7
1	B	161	ASP	2.7
1	A	32	THR	2.7
1	B	74	ALA	2.6
1	B	148	ALA	2.6
1	A	189	GLN	2.6
1	A	157	MET	2.6
1	B	287	TRP	2.5
1	B	80	PHE	2.5
1	B	98	TYR	2.5
1	B	73	ALA	2.5
1	A	186	ASP	2.5
1	B	213	ASP	2.5
1	A	36	VAL	2.4
1	B	176	HIS	2.4
1	B	281	SER	2.4
1	B	300	ARG	2.4
1	B	19	ALA	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	95	ALA	2.4
1	A	62	ASP	2.4
1	A	134	SER	2.4
1	B	294	VAL	2.4
1	A	101	ALA	2.4
1	A	140	GLY	2.4
1	A	152	GLY	2.3
1	B	224	ASP	2.3
1	A	281	SER	2.3
1	B	32	THR	2.3
1	B	286	LYS	2.3
1	B	42	LYS	2.3
1	A	220	GLN	2.3
1	B	225	LEU	2.2
1	B	64	GLN	2.2
1	B	129	PRO	2.2
1	B	127	CYS	2.2
1	B	283	GLY	2.2
1	A	30	LEU	2.2
1	B	117	THR	2.2
1	A	126	VAL	2.2
1	B	85	LYS	2.2
1	A	7	TYR	2.1
1	A	110	CYS	2.1
1	B	10	THR	2.1
1	A	119	GLY	2.1
1	A	31	LEU	2.1
1	A	199	ILE	2.1
1	A	174	ASP	2.0
1	B	167	SER	2.0
1	A	52	LEU	2.0
1	B	119	GLY	2.0
1	B	100	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)

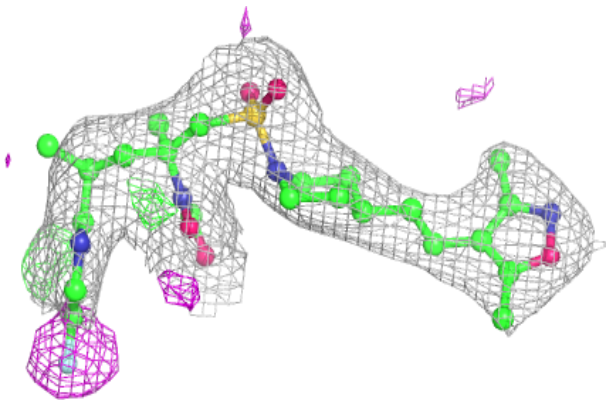
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

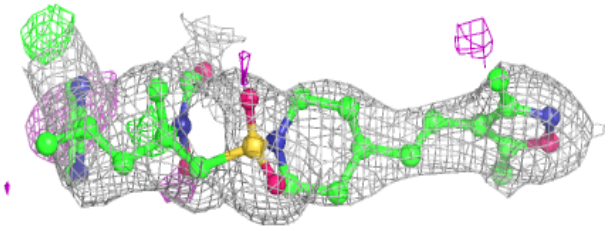
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
6	NA	A	701	1/1	0.62	0.18	76,76,76,76	0
5	MG	B	616	1/1	0.74	0.16	70,70,70,70	0
6	NA	B	702	1/1	0.75	0.29	101,101,101,101	0
4	NI	B	619	1/1	0.78	0.17	118,118,118,118	0
6	NA	A	703	1/1	0.80	0.22	66,66,66,66	0
4	NI	A	613	1/1	0.80	0.12	91,91,91,91	0
4	NI	B	618	1/1	0.81	0.20	118,118,118,118	0
3	CD	B	605	1/1	0.85	0.12	107,107,107,107	0
7	QHF	B	2	35/35	0.87	0.21	68,78,83,84	0
4	NI	A	609	1/1	0.88	0.25	83,83,83,83	0
4	NI	A	615	1/1	0.88	0.09	100,100,100,100	0
4	NI	A	612	1/1	0.88	0.18	85,85,85,85	0
4	NI	B	604	1/1	0.89	0.17	87,87,87,87	0
7	QHF	A	1	35/35	0.91	0.18	59,66,70,73	0
6	NA	B	704	1/1	0.91	0.33	71,71,71,71	0
4	NI	B	617	1/1	0.92	0.15	73,73,73,73	0
4	NI	A	503	1/1	0.92	0.12	99,99,99,99	0
5	MG	A	610	1/1	0.94	0.42	75,75,75,75	0
5	MG	A	621	1/1	0.94	0.46	79,79,79,79	0
4	NI	B	606	1/1	0.94	0.07	88,88,88,88	0
4	NI	A	611	1/1	0.95	0.12	61,61,61,61	0
4	NI	A	607	1/1	0.96	0.18	88,88,88,88	0
3	CD	A	502	1/1	0.96	0.15	87,87,87,87	0
2	ZN	B	402	1/1	0.96	0.05	73,73,73,73	0
3	CD	A	501	1/1	0.96	0.10	80,80,80,80	0
3	CD	A	602	1/1	0.97	0.11	89,89,89,89	0
4	NI	A	601	1/1	0.98	0.18	53,53,53,53	0
2	ZN	A	401	1/1	0.98	0.17	61,61,61,61	0
4	NI	A	504	1/1	0.98	0.31	60,60,60,60	0

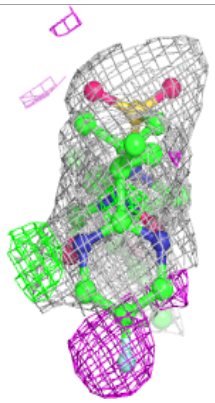
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around QHF B 2:

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

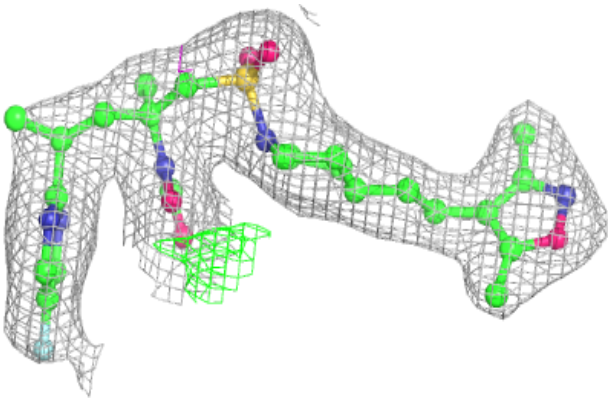


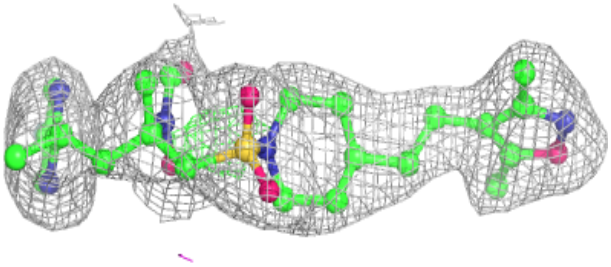


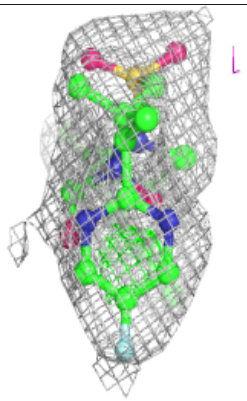


Electron density around QHF A 1:

$2mF_o$-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.