Full wwPDB X-ray Structure Validation Report (i)

Aug 22, 2023 – 01:10 PM EDT

PDB ID	:	2R9S
Title	:	c-Jun N-terminal Kinase 3 with 3,5-Disubstituted Quinoline inhibitor
Authors	:	Habel, J.
Deposited on	:	2007-09-13
Resolution	:	2.40 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:

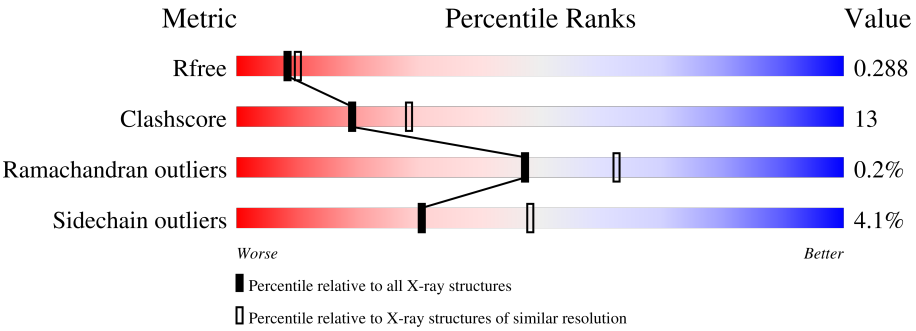
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)

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%

Mol	Chain	Length	Quality of chain
1	A	356	70% 18% · 8%
1	B	356	66% 23% · 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
2	255	A	502	-	-	X	-
2	255	B	501	-	-	X	-

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 5669 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.

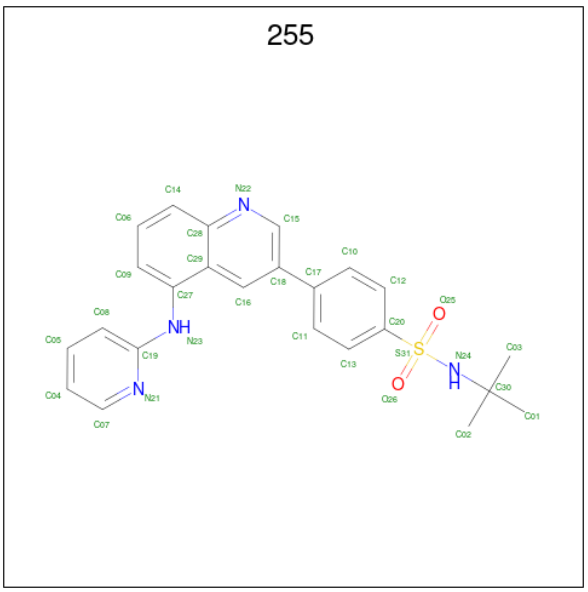
- Molecule 1 is a protein called Mitogen-activated protein kinase 10.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	328	Total	C	N	O	S	0	0	0
			2681	1719	458	485	19			
1	B	328	Total	C	N	O	S	0	0	0
			2681	1719	458	485	19			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	154	OCY	CYS	modified residue	UNP P53779
A	175	OCY	CYS	modified residue	UNP P53779
A	201	OCY	CYS	modified residue	UNP P53779
B	154	OCY	CYS	modified residue	UNP P53779
B	175	OCY	CYS	modified residue	UNP P53779
B	201	OCY	CYS	modified residue	UNP P53779

- Molecule 2 is N-(tert-butyl)-4-[5-(pyridin-2-ylamino)quinolin-3-yl]benzenesulfonamide (three-letter code: 255) (formula: $C_{24}H_{24}N_4O_2S$).

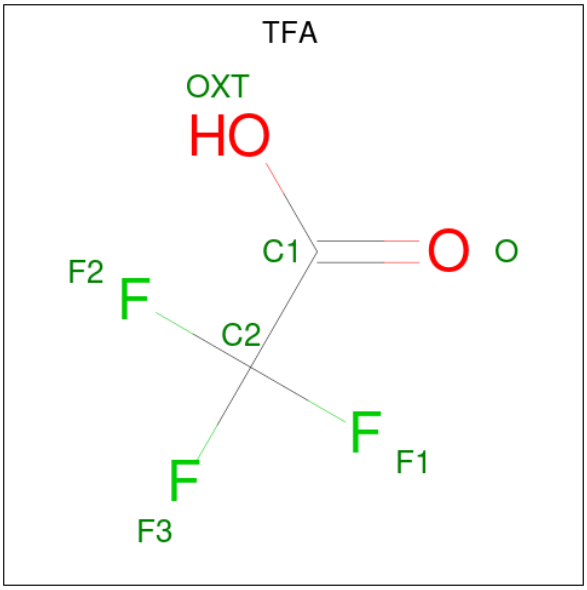


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	S	0	0
			31	24	4	2	1		
2	B	1	Total	C	N	O	S	0	0
			31	24	4	2	1		

- Molecule 3 is UNKNOWN ATOM OR ION (three-letter code: UNX) (formula: X).

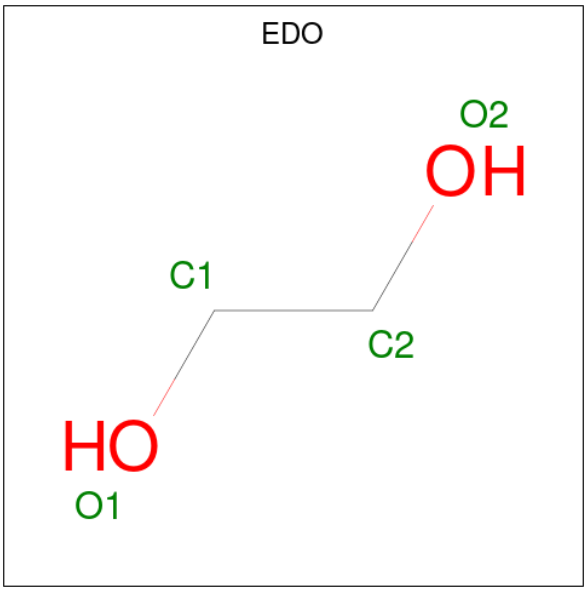
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	17	Total	X	0	0
			17	17		
3	B	10	Total	X	0	0
			10	10		

- Molecule 4 is trifluoroacetic acid (three-letter code: TFA) (formula: $C_2HF_3O_2$).



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

- 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	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

- Molecule 6 is water.

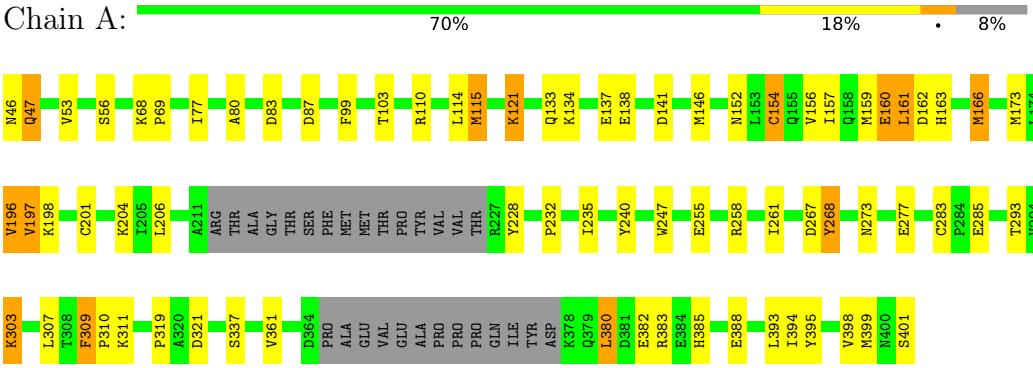
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	119	Total O 119 119	0	0
6	B	63	Total O 63 63	0	0

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. 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. 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.

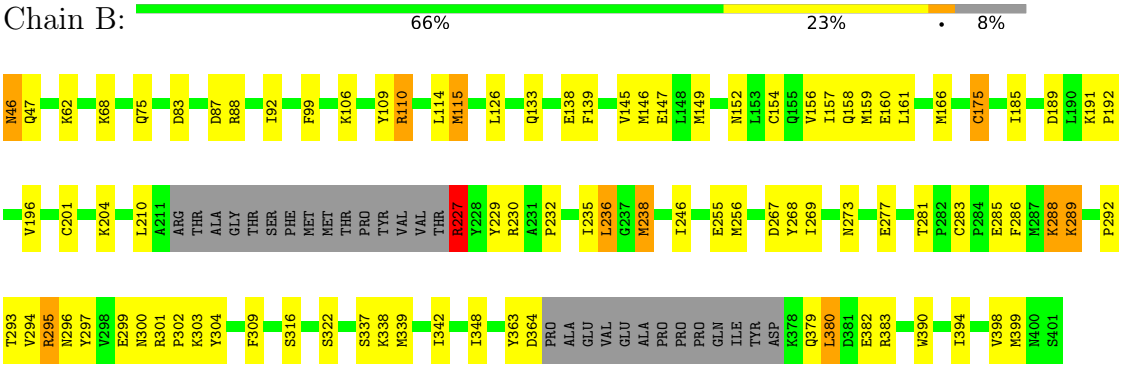
- Molecule 1: Mitogen-activated protein kinase 10

Chain A:



- Molecule 1: Mitogen-activated protein kinase 10

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	68.32Å 81.34Å 123.76Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	38.63 – 2.40 40.67 – 2.27	Depositor EDS
% Data completeness (in resolution range)	99.8 (38.63-2.40) 99.2 (40.67-2.27)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.03 (at 2.27Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.205 , 0.290 0.280 , 0.288	Depositor DCC
R_{free} test set	1637 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å^2)	41.9	Xtriage
Anisotropy	0.267	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 49.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	5669	wwPDB-VP
Average B, all atoms (Å^2)	46.0	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 83.16 % 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 2.3284e-07. 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: TFA, OCY, UNX, EDO, 255

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	1.03	6/2708 (0.2%)	0.92	3/3652 (0.1%)
1	B	1.30	17/2708 (0.6%)	1.06	5/3652 (0.1%)
All	All	1.17	23/5416 (0.4%)	0.99	8/7304 (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 (23) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	295	ARG	CZ-NH2	18.24	1.56	1.33
1	B	288	LYS	CE-NZ	17.88	1.93	1.49
1	B	295	ARG	CZ-NH1	15.67	1.53	1.33
1	B	295	ARG	NE-CZ	13.28	1.50	1.33
1	B	296	ASN	C-O	12.92	1.47	1.23
1	B	288	LYS	CG-CD	12.48	1.94	1.52
1	B	296	ASN	CG-ND2	11.53	1.61	1.32
1	B	300	ASN	CG-OD1	11.30	1.48	1.24
1	B	295	ARG	CD-NE	10.61	1.64	1.46
1	A	303	LYS	CE-NZ	9.08	1.71	1.49
1	B	289	LYS	CE-NZ	8.47	1.70	1.49
1	B	236	LEU	C-O	8.08	1.38	1.23
1	B	296	ASN	C-N	7.26	1.50	1.34
1	A	121	LYS	CE-NZ	6.41	1.65	1.49
1	B	292	PRO	C-N	6.08	1.48	1.34
1	B	300	ASN	CG-ND2	5.80	1.47	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	121	LYS	CD-CE	5.71	1.65	1.51
1	A	47	GLN	CD-OE1	5.54	1.36	1.24
1	A	197	VAL	CB-CG1	-5.44	1.41	1.52
1	B	296	ASN	CG-OD1	5.13	1.35	1.24
1	B	46	ASN	CG-OD1	5.10	1.35	1.24
1	A	309	PHE	CE1-CZ	5.03	1.47	1.37
1	B	236	LEU	C-N	5.02	1.42	1.33

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	295	ARG	NE-CZ-NH2	-31.75	104.42	120.30
1	B	295	ARG	NE-CZ-NH1	10.99	125.80	120.30
1	B	295	ARG	CD-NE-CZ	-10.43	108.99	123.60
1	B	295	ARG	NH1-CZ-NH2	9.43	129.77	119.40
1	A	121	LYS	CD-CE-NZ	6.44	126.51	111.70
1	A	166	MET	CG-SD-CE	5.60	109.15	100.20
1	B	380	LEU	CA-CB-CG	5.58	128.12	115.30
1	A	161	LEU	CA-CB-CG	5.21	127.29	115.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	227	ARG	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	2681	0	2708	62	3
1	B	2681	0	2708	68	3
2	A	31	0	24	12	1
2	B	31	0	24	8	1
3	A	17	0	0	0	0
3	B	10	0	0	0	0
4	A	6	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	6	0	0	1	0
5	A	16	0	24	2	0
5	B	8	0	12	0	0
6	A	119	0	0	2	0
6	B	63	0	0	2	0
All	All	5669	0	5500	143	4

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 13.

All (143) 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:A:303:LYS:CE	1:A:303:LYS:NZ	1.71	1.53
1:B:289:LYS:NZ	1:B:289:LYS:CE	1.70	1.50
1:B:238:MET:SD	1:B:238:MET:CE	2.02	1.48
1:B:288:LYS:CG	1:B:288:LYS:CD	1.94	1.44
1:B:288:LYS:NZ	1:B:288:LYS:CE	1.93	1.32
2:A:502:255:C12	2:A:502:255:H033	1.76	1.16
2:B:501:255:O25	2:B:501:255:H032	1.46	1.15
2:A:502:255:H033	2:A:502:255:C20	1.77	1.15
1:A:47:GLN:O	1:A:47:GLN:HG2	1.64	0.94
2:A:502:255:C20	2:A:502:255:C03	2.49	0.91
1:A:398:VAL:HG12	1:A:399:MET:HE3	1.57	0.86
1:A:152:ASN:OD1	1:A:154:OCY:HB3	1.77	0.85
1:A:283:CYS:HB3	1:A:285:GLU:OE1	1.80	0.82
1:B:152:ASN:OD1	1:B:154:OCY:HB3	1.79	0.81
1:A:115:MET:CE	1:A:146:MET:HG2	2.12	0.79
1:B:238:MET:CE	1:B:289:LYS:HB2	2.13	0.78
1:A:46:ASN:O	1:A:47:GLN:HB3	1.84	0.77
1:A:382:GLU:HG3	1:A:383:ARG:N	2.00	0.76
2:A:502:255:H022	2:A:502:255:H12	1.68	0.75
2:B:501:255:O25	2:B:501:255:C03	2.31	0.75
1:A:115:MET:HE3	1:A:146:MET:HG2	1.69	0.73
1:B:288:LYS:CG	1:B:288:LYS:CE	2.69	0.71
1:B:115:MET:HE3	1:B:146:MET:HG2	1.72	0.71
1:B:238:MET:HE3	1:B:289:LYS:HB2	1.72	0.71
1:A:273:ASN:O	1:A:277:GLU:HG3	1.91	0.71
1:B:46:ASN:O	1:B:47:GLN:HG2	1.92	0.69
1:B:158:GLN:HA	1:B:158:GLN:OE1	1.91	0.69
1:A:382:GLU:HG3	1:A:383:ARG:H	1.58	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:175:OCY:OZ	1:A:175:OCY:HB2	1.94	0.68
1:B:109:TYR:OH	6:B:868:HOH:O	2.12	0.68
1:B:115:MET:CE	1:B:146:MET:HG2	2.23	0.68
1:B:281:THR:HG23	1:B:304:TYR:H	1.60	0.65
1:A:380:LEU:H	1:A:380:LEU:HD13	1.61	0.65
2:B:501:255:C09	2:B:501:255:H08	2.25	0.65
1:B:288:LYS:CD	1:B:288:LYS:CB	2.75	0.65
1:B:289:LYS:NZ	1:B:289:LYS:CD	2.58	0.64
1:B:382:GLU:HG3	1:B:383:ARG:H	1.63	0.63
1:A:204:LYS:NZ	6:A:877:HOH:O	2.21	0.63
1:B:115:MET:HE2	1:B:126:LEU:HB2	1.80	0.62
1:A:398:VAL:HG12	1:A:399:MET:CE	2.28	0.60
1:B:46:ASN:O	1:B:47:GLN:CG	2.50	0.60
1:B:99:PHE:HZ	1:B:139:PHE:CE2	2.19	0.60
1:A:303:LYS:NZ	1:A:303:LYS:CD	2.63	0.59
2:A:502:255:C12	2:A:502:255:C03	2.67	0.59
1:A:115:MET:HE1	1:A:146:MET:HG2	1.83	0.59
1:B:133:GLN:HG2	1:B:138:GLU:O	2.03	0.58
1:A:160:GLU:HG3	1:A:161:LEU:N	2.16	0.58
1:A:53:VAL:HG13	1:A:69:PRO:HG3	1.85	0.58
2:A:502:255:C09	2:A:502:255:H08	2.33	0.58
1:A:240:TYR:H	5:A:701:EDO:H12	1.68	0.57
2:A:502:255:O25	2:A:502:255:H032	2.04	0.57
1:A:99:PHE:HE2	1:A:394:ILE:HD12	1.69	0.57
1:A:156:VAL:HG21	1:A:197:VAL:HG21	1.85	0.57
1:B:269:ILE:HG23	1:B:297:TYR:OH	2.05	0.57
1:A:47:GLN:O	1:A:47:GLN:CG	2.40	0.56
1:B:147:GLU:O	2:B:501:255:H07	2.06	0.56
1:B:382:GLU:HG3	1:B:383:ARG:N	2.20	0.56
1:A:295:ARG:O	1:A:299:GLU:HG2	2.05	0.56
1:B:294:VAL:O	1:B:297:TYR:HB3	2.06	0.56
1:A:196:VAL:HG12	2:A:502:255:H09	1.87	0.56
1:B:149:MET:HG3	1:B:196:VAL:HG23	1.87	0.56
1:B:398:VAL:HG12	1:B:399:MET:CE	2.37	0.55
1:B:196:VAL:HG12	2:B:501:255:H09	1.89	0.55
1:B:273:ASN:OD1	1:B:301:ARG:NH1	2.41	0.54
1:B:75:GLN:O	1:B:75:GLN:HG3	2.08	0.54
1:B:238:MET:HE2	1:B:289:LYS:HB2	1.88	0.54
1:A:382:GLU:OE2	1:A:383:ARG:HG3	2.08	0.53
1:B:156:VAL:O	1:B:159:MET:HG2	2.07	0.53
1:B:99:PHE:HE2	1:B:394:ILE:HD12	1.74	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:141:ASP:OD1	6:A:925:HOH:O	2.19	0.53
1:B:295:ARG:O	1:B:299:GLU:HG2	2.10	0.52
1:B:157:ILE:HG21	1:B:255:GLU:HG2	1.91	0.52
1:B:227:ARG:N	1:B:229:TYR:H	2.08	0.52
1:A:196:VAL:CG1	2:A:502:255:H09	2.41	0.51
1:A:110:ARG:HG3	1:A:114:LEU:HD12	1.93	0.50
1:B:161:LEU:HD12	1:B:166:MET:HB2	1.94	0.50
1:A:235:ILE:HG23	1:A:268:TYR:HE2	1.77	0.49
1:B:297:TYR:O	1:B:301:ARG:HG3	2.12	0.49
1:B:273:ASN:O	1:B:277:GLU:HG3	2.13	0.49
1:A:285:GLU:H	1:A:285:GLU:CD	2.14	0.49
1:B:230:ARG:O	1:B:235:ILE:HD12	2.14	0.48
1:A:157:ILE:HG21	1:A:255:GLU:HG2	1.95	0.48
1:A:175:OCY:OZ	1:A:175:OCY:CB	2.56	0.48
1:B:99:PHE:CZ	1:B:139:PHE:CE2	3.00	0.48
1:B:232:PRO:HG2	1:B:342:ILE:HA	1.96	0.48
1:A:173:MET:O	1:A:177:ILE:HD12	2.14	0.47
1:A:46:ASN:O	1:A:47:GLN:CB	2.56	0.47
1:A:388:GLU:O	1:A:388:GLU:OE2	2.32	0.47
1:B:157:ILE:HG23	1:B:256:MET:HA	1.97	0.47
1:B:236:LEU:HD12	1:B:286:PHE:HZ	1.80	0.47
1:B:398:VAL:HG12	1:B:399:MET:HE3	1.97	0.46
1:B:110:ARG:HG3	1:B:114:LEU:HD12	1.98	0.46
2:A:502:255:C09	2:A:502:255:C08	2.94	0.46
1:B:196:VAL:CG1	2:B:501:255:H09	2.46	0.46
1:A:309:PHE:CE2	1:A:337:SER:HA	2.51	0.46
2:B:501:255:C09	2:B:501:255:C08	2.93	0.46
1:A:206:LEU:HD21	2:A:502:255:C04	2.46	0.46
1:B:175:OCY:HB2	1:B:175:OCY:OZ	2.17	0.45
1:B:288:LYS:CG	1:B:288:LYS:NZ	2.79	0.45
1:B:83:ASP:O	1:B:87:ASP:N	2.49	0.45
1:A:268:TYR:O	1:A:268:TYR:HD2	2.00	0.45
1:A:134:LYS:HD3	1:A:134:LYS:HA	1.42	0.45
1:A:80:ALA:HB1	2:A:502:255:H031	1.98	0.45
1:A:307:LEU:HD22	1:A:311:LYS:HE2	1.99	0.44
1:A:53:VAL:CG1	1:A:77:ILE:HG21	2.47	0.44
1:A:163:HIS:NE2	1:A:319:PRO:HD2	2.32	0.44
2:B:501:255:H08	4:B:602:TFA:F3	2.08	0.44
1:A:395:TYR:O	1:A:399:MET:HG2	2.17	0.44
1:A:56:SER:OG	1:A:77:ILE:HD13	2.18	0.44
1:B:149:MET:HG3	1:B:196:VAL:CG2	2.47	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:110:ARG:HG3	1:A:114:LEU:CD1	2.47	0.43
1:B:204:LYS:NZ	6:B:879:HOH:O	2.47	0.43
1:B:338:LYS:O	1:B:348:ILE:HG22	2.19	0.43
1:A:156:VAL:O	1:A:159:MET:HG2	2.18	0.43
1:B:191:LYS:HB2	1:B:192:PRO:HD2	2.01	0.43
1:B:115:MET:HE2	1:B:126:LEU:CB	2.47	0.43
1:A:382:GLU:CG	1:A:383:ARG:N	2.75	0.43
1:A:228:TYR:CD2	1:A:261:ILE:HD13	2.53	0.43
1:A:380:LEU:HD21	1:A:393:LEU:HD13	1.99	0.43
1:B:189:ASP:HB2	1:B:210:LEU:HD21	2.01	0.42
1:B:302:PRO:HB2	1:B:304:TYR:CE2	2.54	0.42
1:B:246:ILE:HG23	1:B:339:MET:HG2	2.01	0.42
1:A:133:GLN:HG2	1:A:138:GLU:O	2.20	0.42
1:B:99:PHE:HE2	1:B:394:ILE:CD1	2.33	0.42
1:B:398:VAL:HG12	1:B:399:MET:HE2	2.00	0.42
1:A:310:PRO:HG3	5:A:705:EDO:H11	2.02	0.41
1:B:363:TYR:CE2	1:B:364:ASP:HB2	2.55	0.41
1:A:235:ILE:HG23	1:A:268:TYR:CE2	2.56	0.41
1:A:380:LEU:HG	1:A:385:HIS:NE2	2.35	0.41
1:A:121:LYS:O	1:A:204:LYS:HE2	2.19	0.41
1:A:161:LEU:HD21	1:A:166:MET:SD	2.61	0.41
1:B:106:LYS:HG2	1:B:390:TRP:CZ2	2.55	0.41
1:A:283:CYS:CB	1:A:285:GLU:OE1	2.58	0.41
1:A:309:PHE:CZ	1:A:337:SER:HA	2.55	0.41
1:B:309:PHE:CZ	1:B:337:SER:HA	2.56	0.41
1:A:232:PRO:HD3	1:A:247:TRP:CE2	2.55	0.41
1:B:269:ILE:HD12	1:B:297:TYR:CZ	2.56	0.41
1:A:83:ASP:O	1:A:87:ASP:N	2.53	0.41
1:B:92:ILE:HG12	1:B:145:VAL:HG22	2.02	0.41
1:B:115:MET:HE1	1:B:146:MET:HG2	1.99	0.40
1:B:283:CYS:HB3	1:B:285:GLU:OE1	2.21	0.40
1:A:137:GLU:H	1:A:137:GLU:CD	2.24	0.40
1:B:114:LEU:HD22	1:B:185:ILE:HD11	2.03	0.40

All (4) 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:B:68:LYS:NZ	2:A:502:255:O26[3_645]	1.61	0.59
1:A:267:ASP:OD1	1:B:293:THR:OG1[3_645]	1.98	0.22

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:68:LYS:NZ	2:B:501:255:O26[3_655]	2.03	0.17
1:A:293:THR:OG1	1:B:267:ASP:OD1[3_645]	2.05	0.15

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	319/356 (90%)	305 (96%)	13 (4%)	1 (0%)	41 55
1	B	319/356 (90%)	298 (93%)	21 (7%)	0	100 100
All	All	638/712 (90%)	603 (94%)	34 (5%)	1 (0%)	47 62

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	361	VAL

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	294/318 (92%)	283 (96%)	11 (4%)	34 53
1	B	294/318 (92%)	281 (96%)	13 (4%)	28 45
All	All	588/636 (92%)	564 (96%)	24 (4%)	30 48

All (24) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	103	THR
1	A	115	MET
1	A	160	GLU
1	A	162	ASP
1	A	196	VAL
1	A	198	LYS
1	A	258	ARG
1	A	268	TYR
1	A	321	ASP
1	A	380	LEU
1	A	401	SER
1	B	62	LYS
1	B	88	ARG
1	B	110	ARG
1	B	115	MET
1	B	160	GLU
1	B	227	ARG
1	B	238	MET
1	B	268	TYR
1	B	303	LYS
1	B	316	SER
1	B	322	SER
1	B	379	GLN
1	B	380	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

6 non-standard protein/DNA/RNA residues are modelled in this entry.

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	$\#\|Z\|>2$
1	OCY	B	201	1	7,8,9	0.77	0	4,8,10	2.99	2 (50%)
1	OCY	A	201	1	7,8,9	0.79	0	4,8,10	2.11	1 (25%)
1	OCY	B	154	1	7,8,9	0.71	0	4,8,10	1.27	0
1	OCY	B	175	1	7,8,9	0.59	0	4,8,10	3.05	2 (50%)
1	OCY	A	175	1	7,8,9	0.53	0	4,8,10	2.56	1 (25%)
1	OCY	A	154	1	7,8,9	0.75	0	4,8,10	1.55	1 (25%)

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
1	OCY	B	201	1	-	0/5/7/9	-
1	OCY	A	201	1	-	0/5/7/9	-
1	OCY	B	154	1	-	0/5/7/9	-
1	OCY	B	175	1	-	1/5/7/9	-
1	OCY	A	175	1	-	2/5/7/9	-
1	OCY	A	154	1	-	1/5/7/9	-

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	175	OCY	CB-SG-CD	5.46	118.65	102.27
1	B	201	OCY	CB-SG-CD	5.33	118.24	102.27
1	A	175	OCY	CB-SG-CD	4.55	115.91	102.27
1	A	201	OCY	CB-SG-CD	3.39	112.43	102.27
1	B	201	OCY	OZ-CE-CD	2.67	121.37	110.83
1	A	154	OCY	CB-SG-CD	2.61	110.09	102.27
1	B	175	OCY	OZ-CE-CD	-2.21	102.14	110.83

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	B	175	OCY	CE-CD-SG-CB
1	A	175	OCY	SG-CD-CE-OZ
1	A	154	OCY	CA-CB-SG-CD
1	A	175	OCY	CE-CD-SG-CB

There are no ring outliers.

4 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	B	154	OCY	1	0
1	B	175	OCY	1	0
1	A	175	OCY	2	0
1	A	154	OCY	1	0

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 37 ligands modelled in this entry, 27 are unknown - leaving 10 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	TFA	B	602	-	5,5,6	0.93	0	6,7,9	1.23	0
5	EDO	A	702	-	3,3,3	0.43	0	2,2,2	0.46	0
5	EDO	B	703	-	3,3,3	0.47	0	2,2,2	0.43	0
2	255	B	501	-	32,34,34	8.44	29 (90%)	43,50,50	1.77	6 (13%)
5	EDO	A	707	-	3,3,3	0.43	0	2,2,2	0.52	0
4	TFA	A	601	-	5,5,6	0.92	0	6,7,9	1.46	1 (16%)
5	EDO	A	701	-	3,3,3	0.43	0	2,2,2	1.14	0
5	EDO	B	704	-	3,3,3	0.55	0	2,2,2	0.45	0
5	EDO	A	705	-	3,3,3	0.70	0	2,2,2	0.21	0
2	255	A	502	-	32,34,34	8.44	29 (90%)	43,50,50	1.77	6 (13%)

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	TFA	B	602	-	-	0/0/3/6	-
5	EDO	A	702	-	-	1/1/1/1	-
5	EDO	B	703	-	-	0/1/1/1	-
2	255	B	501	-	-	5/16/20/20	0/4/4/4
5	EDO	A	707	-	-	0/1/1/1	-
4	TFA	A	601	-	-	0/0/3/6	-
5	EDO	A	701	-	-	1/1/1/1	-
5	EDO	B	704	-	-	0/1/1/1	-
5	EDO	A	705	-	-	0/1/1/1	-
2	255	A	502	-	-	6/16/20/20	0/4/4/4

All (58) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	502	255	O25-S31	19.97	1.66	1.43
2	B	501	255	O25-S31	19.93	1.66	1.43
2	B	501	255	O26-S31	19.90	1.66	1.43
2	A	502	255	O26-S31	19.80	1.66	1.43
2	A	502	255	C15-N22	17.34	1.51	1.30
2	B	501	255	C15-N22	17.34	1.51	1.30
2	B	501	255	C12-C20	9.63	1.54	1.38
2	A	502	255	C12-C20	9.62	1.54	1.38
2	A	502	255	C13-C20	9.51	1.53	1.38
2	B	501	255	C13-C20	9.49	1.53	1.38
2	A	502	255	C11-C13	8.01	1.53	1.36
2	A	502	255	C06-C14	8.01	1.54	1.36
2	B	501	255	C11-C13	8.00	1.53	1.36
2	B	501	255	C06-C14	8.00	1.54	1.36
2	B	501	255	C10-C12	7.97	1.53	1.36
2	B	501	255	C19-N21	7.95	1.49	1.34
2	A	502	255	C10-C12	7.93	1.53	1.36
2	A	502	255	C19-N21	7.92	1.49	1.34
2	B	501	255	C07-N21	7.87	1.51	1.34
2	A	502	255	C07-N21	7.86	1.51	1.34
2	A	502	255	C06-C09	7.52	1.54	1.38
2	B	501	255	C06-C09	7.52	1.54	1.38
2	A	502	255	S31-N24	7.50	1.72	1.61
2	B	501	255	S31-N24	7.43	1.72	1.61
2	A	502	255	C09-C27	7.25	1.53	1.38
2	A	502	255	C28-N22	7.24	1.50	1.37
2	B	501	255	C09-C27	7.23	1.53	1.38
2	B	501	255	C28-N22	7.21	1.50	1.37
2	B	501	255	C29-C28	7.17	1.54	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	502	255	C14-C28	7.16	1.54	1.41
2	B	501	255	C14-C28	7.16	1.54	1.41
2	A	502	255	C29-C28	7.14	1.54	1.42
2	B	501	255	C16-C29	6.77	1.51	1.40
2	A	502	255	C16-C29	6.73	1.51	1.40
2	B	501	255	C08-C19	6.65	1.54	1.39
2	A	502	255	C08-C19	6.64	1.54	1.39
2	A	502	255	C27-C29	6.07	1.55	1.43
2	B	501	255	C15-C18	6.07	1.54	1.41
2	B	501	255	C27-C29	6.05	1.55	1.43
2	A	502	255	C15-C18	6.03	1.54	1.41
2	A	502	255	C16-C18	5.78	1.50	1.39
2	B	501	255	C16-C18	5.76	1.50	1.39
2	A	502	255	C04-C07	5.52	1.53	1.37
2	B	501	255	C04-C07	5.51	1.53	1.37
2	A	502	255	C05-C08	5.50	1.50	1.38
2	B	501	255	C05-C08	5.45	1.50	1.38
2	B	501	255	C11-C17	4.97	1.54	1.41
2	A	502	255	C11-C17	4.94	1.53	1.41
2	A	502	255	C10-C17	4.90	1.53	1.41
2	B	501	255	C10-C17	4.89	1.53	1.41
2	B	501	255	C05-C04	4.65	1.50	1.38
2	A	502	255	C05-C04	4.64	1.50	1.38
2	B	501	255	C19-N23	4.10	1.45	1.38
2	A	502	255	C19-N23	4.05	1.45	1.38
2	A	502	255	C20-S31	3.76	1.82	1.76
2	B	501	255	C20-S31	3.75	1.82	1.76
2	A	502	255	C27-N23	2.79	1.46	1.38
2	B	501	255	C27-N23	2.78	1.46	1.38

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	501	255	O26-S31-O25	-8.19	109.49	119.55
2	A	502	255	O26-S31-O25	-8.14	109.54	119.55
2	A	502	255	C18-C15-N22	-3.69	120.03	125.05
2	B	501	255	C18-C15-N22	-3.67	120.06	125.05
2	B	501	255	C27-C29-C28	2.99	119.95	118.06
2	A	502	255	C27-C29-C28	2.97	119.94	118.06
2	A	502	255	C29-C28-N22	-2.66	120.00	122.83
4	A	601	TFA	F2-C2-F1	2.66	117.42	105.47
2	B	501	255	C29-C28-N22	-2.66	120.00	122.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	502	255	C27-N23-C19	-2.16	119.88	126.79
2	B	501	255	C27-N23-C19	-2.16	119.88	126.79
2	A	502	255	C04-C07-N21	-2.10	119.99	123.43
2	B	501	255	C04-C07-N21	-2.09	120.02	123.43

There are no chirality outliers.

All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	502	255	C12-C20-S31-N24
2	A	502	255	C13-C20-S31-N24
2	B	501	255	C12-C20-S31-O26
2	B	501	255	C13-C20-S31-O26
2	B	501	255	C12-C20-S31-N24
2	B	501	255	C13-C20-S31-N24
2	A	502	255	C13-C20-S31-O26
5	A	702	EDO	O1-C1-C2-O2
2	A	502	255	C12-C20-S31-O26
2	B	501	255	C02-C30-N24-S31
5	A	701	EDO	O1-C1-C2-O2
2	A	502	255	C01-C30-N24-S31
2	A	502	255	C02-C30-N24-S31

There are no ring outliers.

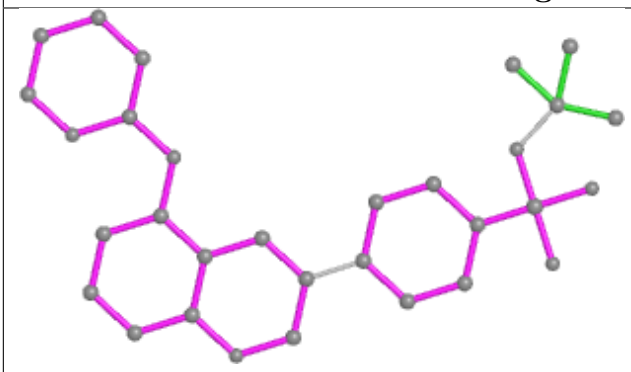
5 monomers are involved in 24 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	602	TFA	1	0
2	B	501	255	8	1
5	A	701	EDO	1	0
5	A	705	EDO	1	0
2	A	502	255	12	1

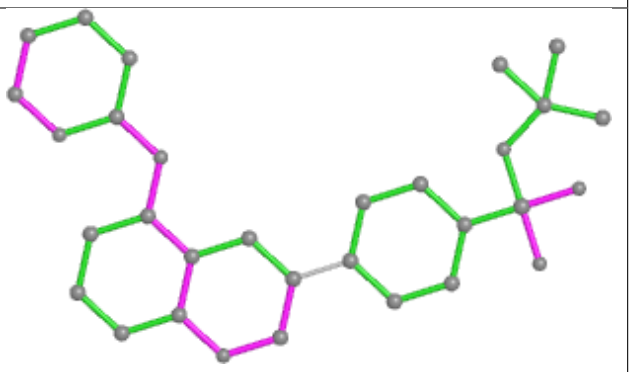
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

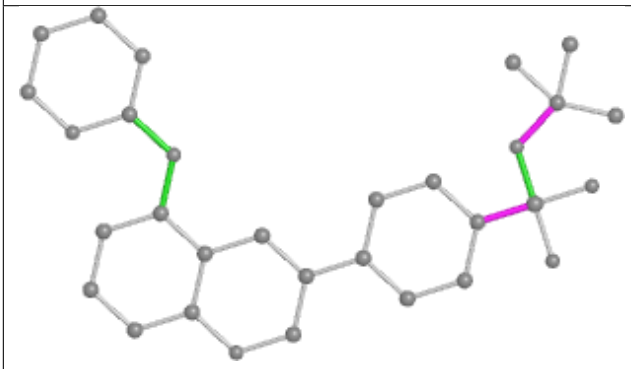
Ligand 255 B 501



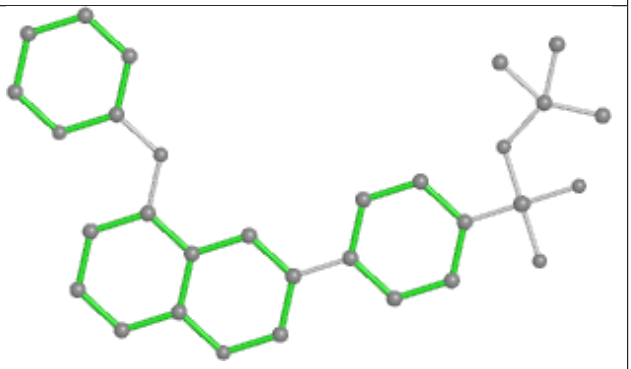
Bond lengths



Bond angles

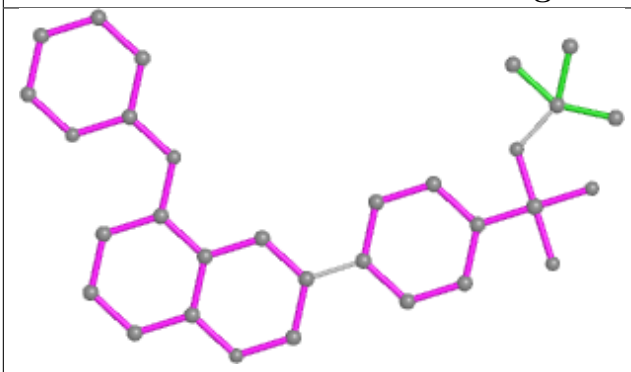


Torsions

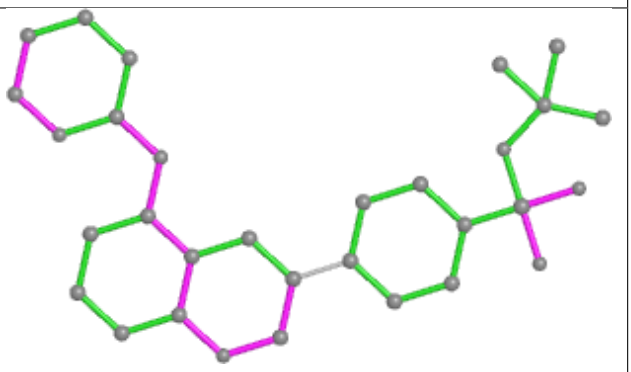


Rings

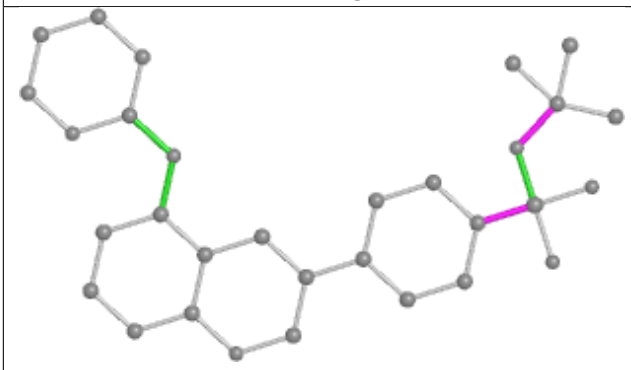
Ligand 255 A 502



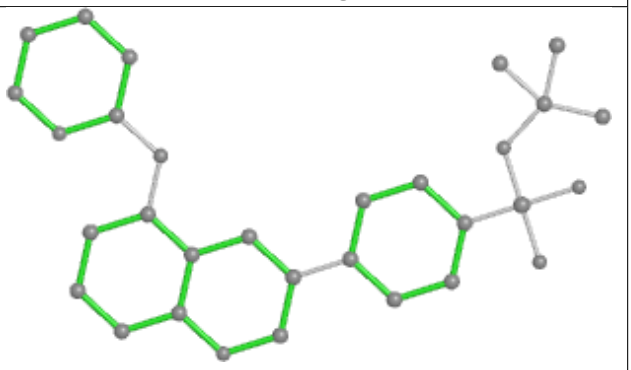
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

Unable to reproduce the depositors R factor - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains

Unable to reproduce the depositors R factor - this section is therefore empty.

6.3 Carbohydrates

Unable to reproduce the depositors R factor - this section is therefore empty.

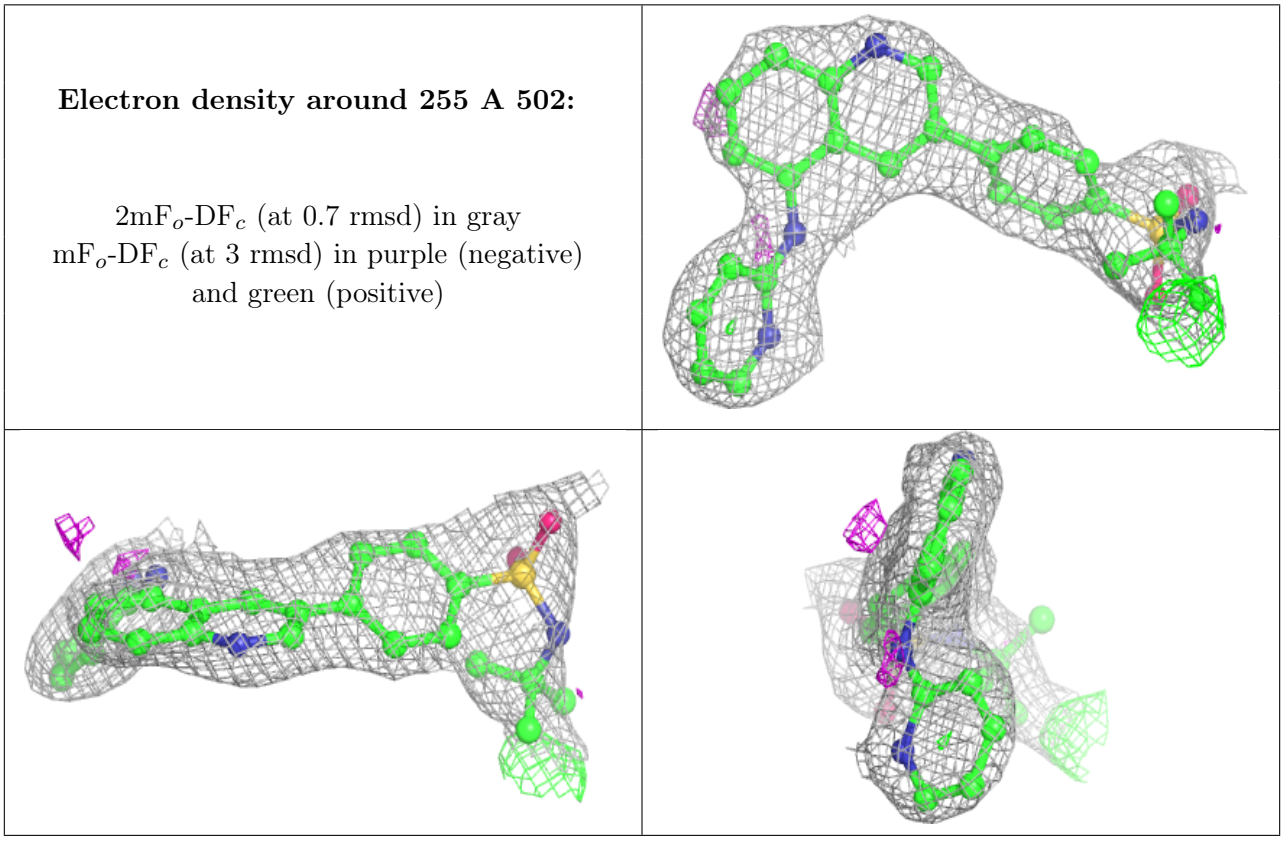
6.4 Ligands

Unable to reproduce the depositors R factor - this section is therefore empty.

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.

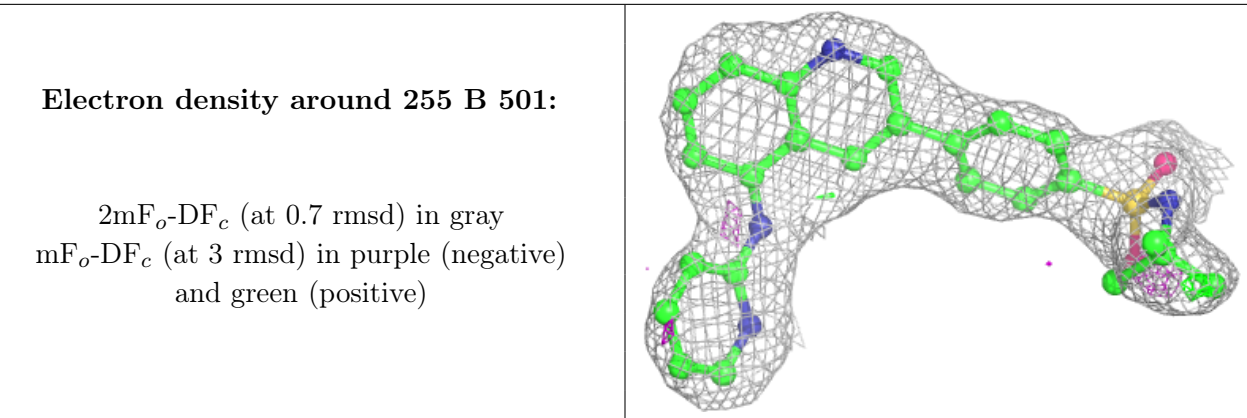
Electron density around 255 A 502:

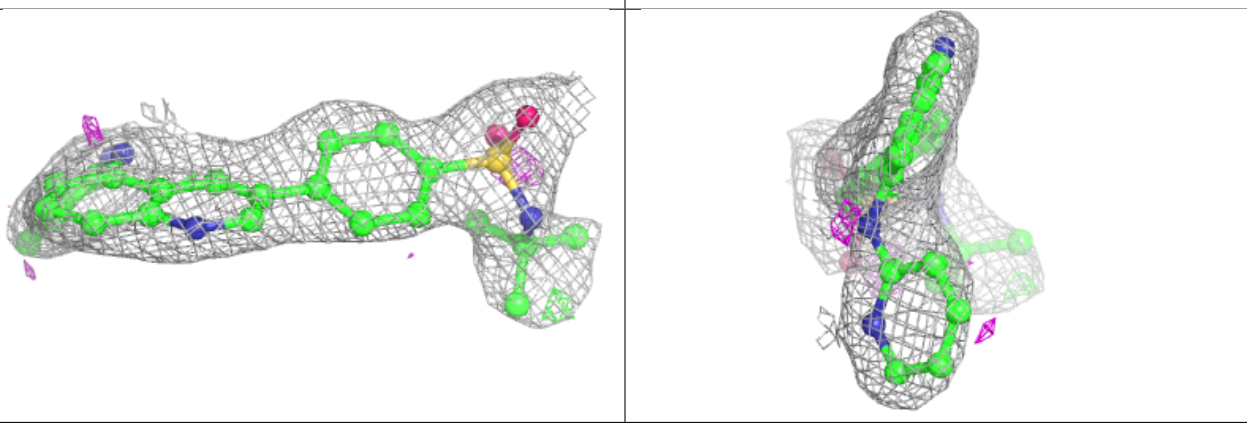
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



Electron density around 255 B 501:

$2mF_o$-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)

Unable to reproduce the depositors R factor - this section is therefore empty.