



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 21, 2024 – 09:05 am BST

PDB ID : 4AQ3
Title : HUMAN BCL-2 WITH PHENYLACYLSULFONAMIDE INHIBITOR
Authors : Bertrand, J.A.; Fasolini, M.; Modugno, M.
Deposited on : 2012-04-12
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 ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

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

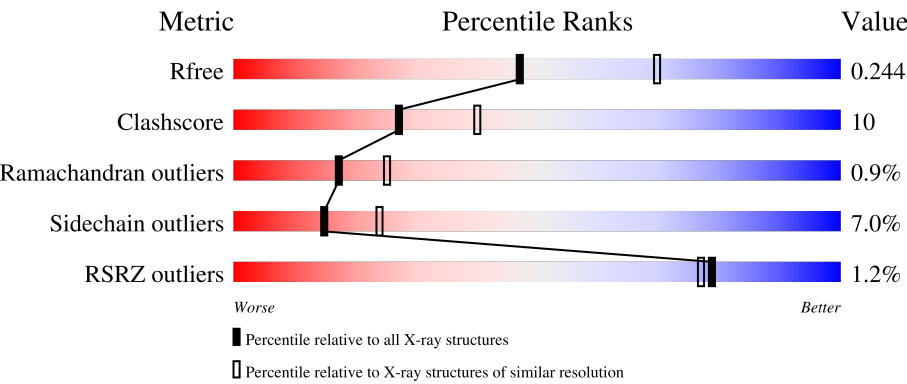
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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.



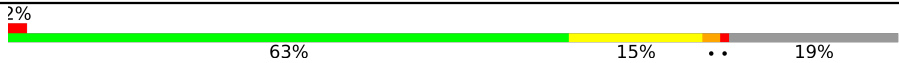
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (2.40-2.40)

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 $\leq 5\%$. 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	169	
1	B	169	
1	C	169	
1	D	169	
1	E	169	

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Mol	Chain	Length	Quality of chain
1	F	169	 A horizontal bar chart showing the quality of chain F. The bar is divided into four segments: a small red segment at the beginning labeled '2%', a large green segment labeled '63%', a yellow segment labeled '15%', and a small red segment at the end labeled '19%'. There are two small black dots between the yellow and red segments.

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 7096 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 APOPTOSIS REGULATOR BCL-2, BCL-2-LIKE PROTEIN 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	135	Total	C	N	O	S	0	0	0
			1126	721	198	201	6			
1	B	135	Total	C	N	O	S	0	0	0
			1126	721	198	201	6			
1	C	135	Total	C	N	O	S	0	0	0
			1126	721	198	201	6			
1	D	137	Total	C	N	O	S	0	0	0
			1141	729	200	206	6			
1	E	135	Total	C	N	O	S	0	0	0
			1119	715	198	200	6			
1	F	137	Total	C	N	O	S	0	0	0
			1140	729	200	205	6			

There are 36 discrepancies between the modelled and reference sequences:

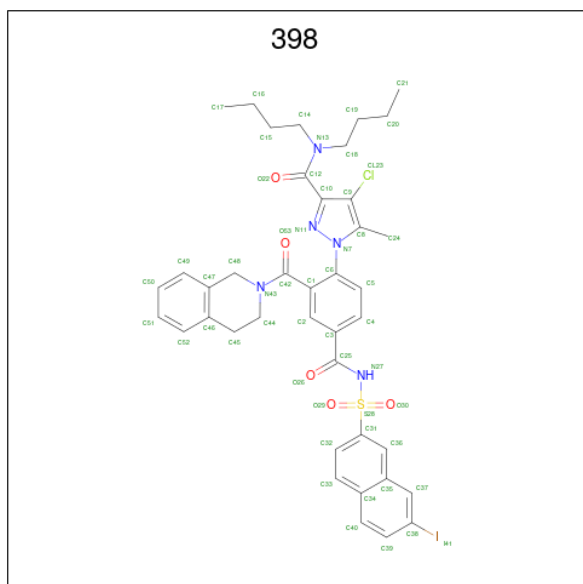
Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	GLY	-	expression tag	UNP P10415
A	-1	SER	-	expression tag	UNP P10415
A	0	HIS	-	expression tag	UNP P10415
A	34	ASP	-	expression tag	UNP P10415
A	55	ALA	THR	variant	UNP P10415
A	69	GLY	ARG	variant	UNP P10415
B	-2	GLY	-	expression tag	UNP P10415
B	-1	SER	-	expression tag	UNP P10415
B	0	HIS	-	expression tag	UNP P10415
B	34	ASP	-	expression tag	UNP P10415
B	55	ALA	THR	variant	UNP P10415
B	69	GLY	ARG	variant	UNP P10415
C	-2	GLY	-	expression tag	UNP P10415
C	-1	SER	-	expression tag	UNP P10415
C	0	HIS	-	expression tag	UNP P10415
C	34	ASP	-	expression tag	UNP P10415

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Chain	Residue	Modelled	Actual	Comment	Reference
C	55	ALA	THR	variant	UNP P10415
C	69	GLY	ARG	variant	UNP P10415
D	-2	GLY	-	expression tag	UNP P10415
D	-1	SER	-	expression tag	UNP P10415
D	0	HIS	-	expression tag	UNP P10415
D	34	ASP	-	expression tag	UNP P10415
D	55	ALA	THR	variant	UNP P10415
D	69	GLY	ARG	variant	UNP P10415
E	-2	GLY	-	expression tag	UNP P10415
E	-1	SER	-	expression tag	UNP P10415
E	0	HIS	-	expression tag	UNP P10415
E	34	ASP	-	expression tag	UNP P10415
E	55	ALA	THR	variant	UNP P10415
E	69	GLY	ARG	variant	UNP P10415
F	-2	GLY	-	expression tag	UNP P10415
F	-1	SER	-	expression tag	UNP P10415
F	0	HIS	-	expression tag	UNP P10415
F	34	ASP	-	expression tag	UNP P10415
F	55	ALA	THR	variant	UNP P10415
F	69	GLY	ARG	variant	UNP P10415

- Molecule 2 is N,N-dibutyl-4-chloranyl-1-[2-(3,4-dihydro-1H-isoquinolin-2-ylcarbonyl)-4-(7-iodanaphthalen-2-yl)sulfonylcarbamoyl]phenyl]-5-methyl-pyrazole-3-carboxamide (three-letter code: 398) (formula: C₄₀H₄₁ClIN₅O₅S).

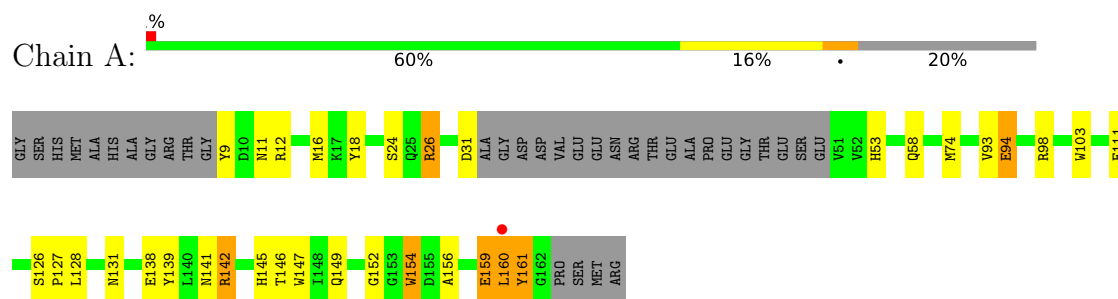


Mol	Chain	Residues	Atoms							ZeroOcc	AltConf
2	A	1	Total 53	C 40	Cl 1	I 1	N 5	O 5	S 1	0	0
2	B	1	Total 53	C 40	Cl 1	I 1	N 5	O 5	S 1	0	0
2	C	1	Total 53	C 40	Cl 1	I 1	N 5	O 5	S 1	0	0
2	D	1	Total 53	C 40	Cl 1	I 1	N 5	O 5	S 1	0	0
2	E	1	Total 53	C 40	Cl 1	I 1	N 5	O 5	S 1	0	0
2	F	1	Total 53	C 40	Cl 1	I 1	N 5	O 5	S 1	0	0

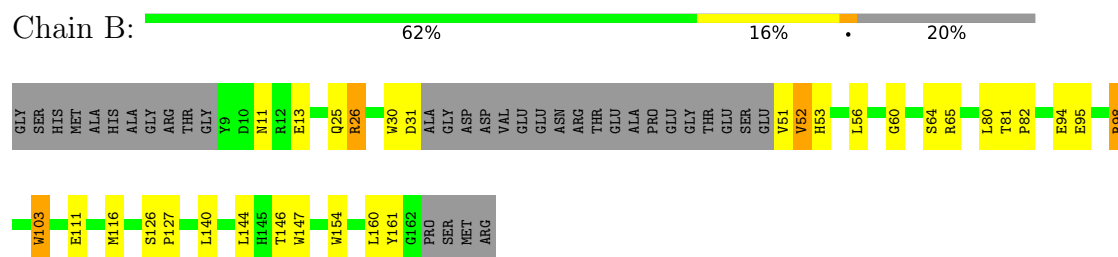
3 Residue-property plots [i](#)

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.

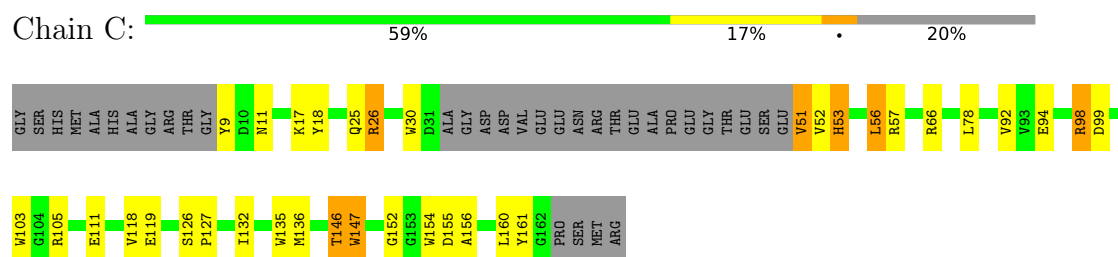
• Molecule 1: APOPTOSIS REGULATOR BCL-2, BCL-2-LIKE PROTEIN 1



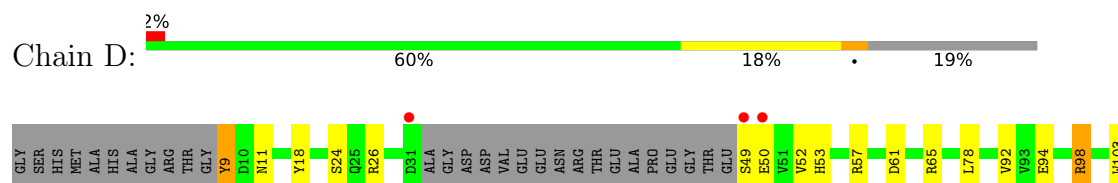
• Molecule 1: APOPTOSIS REGULATOR BCL-2, BCL-2-LIKE PROTEIN 1



• Molecule 1: APOPTOSIS REGULATOR BCL-2, BCL-2-LIKE PROTEIN 1

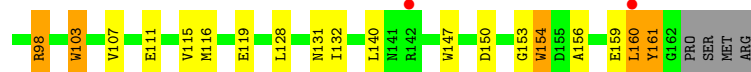
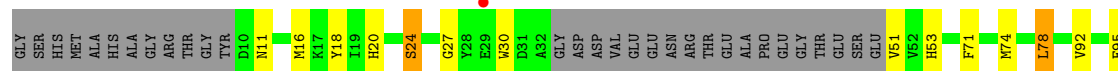


• Molecule 1: APOPTOSIS REGULATOR BCL-2, BCL-2-LIKE PROTEIN 1

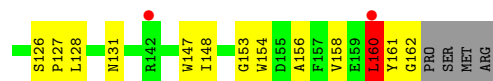
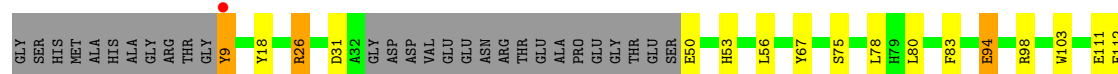




- Molecule 1: APOPTOSIS REGULATOR BCL-2, BCL-2-LIKE PROTEIN 1



- Molecule 1: APOPTOSIS REGULATOR BCL-2, BCL-2-LIKE PROTEIN 1



4 Data and refinement statistics

Property	Value	Source
Space group	P 32	Depositor
Cell constants a, b, c, α , β , γ	115.21Å 115.21Å 102.32Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	100.00 – 2.40 38.25 – 2.40	Depositor EDS
% Data completeness (in resolution range)	97.8 (100.00-2.40) 97.8 (38.25-2.40)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.94 (at 2.39Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.201 , 0.245 0.199 , 0.244	Depositor DCC
R_{free} test set	2926 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	55.4	Xtriage
Anisotropy	0.052	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 30.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.25$	Xtriage
Estimated twinning fraction	0.188 for -h,-k,l 0.067 for h,-h-k,-l 0.059 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	7096	wwPDB-VP
Average B, all atoms (Å ²)	57.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 11.15% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: 398

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	0.88	4/1157 (0.3%)	0.80	0/1564
1	B	0.85	3/1157 (0.3%)	0.79	0/1564
1	C	0.86	4/1157 (0.3%)	0.86	2/1564 (0.1%)
1	D	0.83	1/1172 (0.1%)	0.80	1/1584 (0.1%)
1	E	0.81	3/1149 (0.3%)	0.79	0/1553
1	F	0.80	3/1171 (0.3%)	0.82	1/1583 (0.1%)
All	All	0.84	18/6963 (0.3%)	0.81	4/9412 (0.0%)

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	D	0	1
1	F	0	1
All	All	0	2

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	147	TRP	CD2-CE2	6.08	1.48	1.41
1	B	103	TRP	CD2-CE2	5.92	1.48	1.41
1	C	135	TRP	CD2-CE2	5.89	1.48	1.41
1	F	147	TRP	CD2-CE2	5.87	1.48	1.41
1	A	154	TRP	CD2-CE2	5.68	1.48	1.41
1	C	103	TRP	CD2-CE2	5.57	1.48	1.41
1	E	103	TRP	CD2-CE2	5.55	1.48	1.41
1	E	147	TRP	CD2-CE2	5.50	1.48	1.41
1	F	103	TRP	CD2-CE2	5.45	1.47	1.41
1	A	103	TRP	CD2-CE2	5.34	1.47	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	30	TRP	CD2-CE2	5.33	1.47	1.41
1	F	154	TRP	CD2-CE2	5.21	1.47	1.41
1	E	154	TRP	CD2-CE2	5.18	1.47	1.41
1	B	147	TRP	CD2-CE2	5.17	1.47	1.41
1	C	147	TRP	CD2-CE2	5.12	1.47	1.41
1	A	161	TYR	CE1-CZ	5.09	1.45	1.38
1	C	30	TRP	CD2-CE2	5.03	1.47	1.41
1	D	135	TRP	CD2-CE2	5.01	1.47	1.41

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	66	ARG	NE-CZ-NH2	6.45	123.53	120.30
1	D	61	ASP	CB-CG-OD1	6.36	124.02	118.30
1	F	160	LEU	CA-CB-CG	5.44	127.82	115.30
1	C	66	ARG	NE-CZ-NH1	-5.01	117.79	120.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	9	TYR	Peptide
1	F	9	TYR	Peptide

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1126	0	1059	26	0
1	B	1126	0	1059	21	0
1	C	1126	0	1059	19	0
1	D	1141	0	1070	35	0
1	E	1119	0	1055	21	0
1	F	1140	0	1070	24	0
2	A	53	0	41	3	0
2	B	53	0	41	4	0
2	C	53	0	41	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	53	0	41	2	0
2	E	53	0	41	2	0
2	F	53	0	41	2	0
All	All	7096	0	6618	139	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 10.

All (139) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:26:ARG:HH11	1:F:26:ARG:HG3	1.00	1.12
1:A:160:LEU:HD21	1:E:160:LEU:HD13	1.44	1.00
1:F:158:VAL:O	1:F:162:GLY:HA3	1.61	0.98
1:F:26:ARG:HG3	1:F:26:ARG:NH1	1.72	0.95
1:D:160:LEU:O	1:D:161:TYR:HB2	1.66	0.92
1:D:50:GLU:HA	1:D:53:HIS:HD2	1.33	0.90
1:E:78:LEU:HD23	1:E:119:GLU:HG3	1.53	0.89
1:F:26:ARG:HH11	1:F:26:ARG:CG	1.87	0.86
1:C:18:TYR:OH	1:C:111:GLU:OE2	1.94	0.85
2:B:1163:398:H182	2:B:1163:398:N11	1.92	0.84
1:B:65:ARG:HE	1:D:65:ARG:NH2	1.76	0.82
1:A:58:GLN:HE21	1:A:161:TYR:HD2	1.30	0.79
1:E:18:TYR:OH	1:E:111:GLU:OE2	2.01	0.78
1:A:94:GLU:OE1	1:A:98:ARG:NH2	2.17	0.76
1:F:161:TYR:HB3	1:F:162:GLY:HA2	1.68	0.76
1:E:128:LEU:HA	1:E:131:ASN:HD22	1.50	0.75
1:F:50:GLU:HG2	1:F:53:HIS:HD2	1.53	0.73
1:C:78:LEU:HD23	1:C:119:GLU:HG3	1.72	0.72
1:D:159:GLU:HG2	1:D:160:LEU:HD12	1.72	0.71
1:D:128:LEU:HA	1:D:131:ASN:HD22	1.56	0.70
1:D:50:GLU:HA	1:D:53:HIS:CD2	2.23	0.70
1:F:50:GLU:HG2	1:F:53:HIS:CD2	2.26	0.70
1:F:128:LEU:HA	1:F:131:ASN:HD22	1.56	0.70
1:F:94:GLU:OE1	1:F:98:ARG:NH2	2.24	0.69
1:C:9:TYR:OH	1:C:155:ASP:OD1	2.09	0.69
1:B:65:ARG:HE	1:D:65:ARG:HH21	1.37	0.69
1:F:161:TYR:HB3	1:F:162:GLY:CA	2.23	0.68
1:A:160:LEU:HD21	1:E:160:LEU:CD1	2.22	0.68
1:A:18:TYR:OH	1:A:111:GLU:OE2	2.13	0.66
1:B:60:GLY:HA3	1:B:111:GLU:OE2	1.96	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:11:ASN:HD21	1:A:154:TRP:HE1	1.43	0.66
1:D:160:LEU:O	1:D:161:TYR:CB	2.43	0.64
1:F:112:PHE:HB2	2:F:1163:398:H212	1.81	0.62
1:D:148:ILE:HG22	1:D:153:GLY:HA2	1.82	0.61
1:C:53:HIS:O	1:C:57:ARG:HG2	2.00	0.61
1:E:95:GLU:CD	1:E:98:ARG:HH12	2.03	0.61
1:F:26:ARG:NH1	1:F:26:ARG:CG	2.51	0.61
1:C:51:VAL:N	1:C:53:HIS:CD2	2.69	0.60
1:E:156:ALA:O	1:E:159:GLU:HB3	2.01	0.60
1:C:11:ASN:HD21	1:C:154:TRP:HE1	1.51	0.59
1:D:18:TYR:OH	1:D:111:GLU:OE2	2.18	0.59
1:B:51:VAL:HG23	1:B:52:VAL:H	1.67	0.59
1:D:50:GLU:CA	1:D:53:HIS:HD2	2.12	0.59
1:A:138:GLU:O	1:A:142:ARG:HB2	2.03	0.58
1:A:26:ARG:HH11	1:A:26:ARG:CG	2.17	0.58
1:F:18:TYR:OH	1:F:111:GLU:OE2	2.21	0.57
1:B:103:TRP:HD1	1:D:160:LEU:HG	1.70	0.57
1:E:71:PHE:CD1	1:E:115:VAL:HG21	2.39	0.57
1:D:9:TYR:N	1:D:9:TYR:HD1	2.01	0.57
1:B:26:ARG:NH2	1:E:150:ASP:OD1	2.40	0.55
1:B:65:ARG:NE	1:D:65:ARG:HH21	2.02	0.55
1:B:65:ARG:NE	1:D:65:ARG:NH2	2.51	0.55
1:E:74:MET:HG3	1:F:83:PHE:HZ	1.71	0.55
1:A:128:LEU:HA	1:A:131:ASN:HD22	1.72	0.55
1:E:103:TRP:O	1:E:107:VAL:HG23	2.07	0.55
1:A:74:MET:CE	2:A:1163:398:H152	2.36	0.54
1:D:98:ARG:HG2	1:D:98:ARG:HH11	1.72	0.54
1:A:159:GLU:O	1:A:159:GLU:HG3	2.08	0.54
1:B:95:GLU:OE2	1:B:98:ARG:NH1	2.40	0.54
1:E:16:MET:SD	1:E:30:TRP:HH2	2.31	0.54
1:B:13:GLU:OE2	1:B:53:HIS:HE1	1.92	0.53
1:E:11:ASN:HB3	1:E:140:LEU:HD13	1.91	0.53
1:D:9:TYR:N	1:D:9:TYR:CD1	2.74	0.52
1:B:160:LEU:HD12	1:D:103:TRP:HB2	1.92	0.52
1:A:12:ARG:O	1:A:16:MET:HG2	2.10	0.51
1:D:26:ARG:HH11	1:D:26:ARG:HG2	1.75	0.51
1:B:65:ARG:HH21	1:D:65:ARG:HH21	1.57	0.51
1:E:92:VAL:HG13	2:E:1163:398:H182	1.91	0.51
1:F:161:TYR:CD2	1:F:162:GLY:HA2	2.46	0.51
1:B:11:ASN:HD21	1:B:154:TRP:HE1	1.59	0.51
1:A:9:TYR:CD2	1:A:154:TRP:HB2	2.46	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:128:LEU:HA	1:F:131:ASN:ND2	2.25	0.51
1:D:11:ASN:OD1	1:D:141:ASN:ND2	2.45	0.49
1:D:159:GLU:O	1:D:161:TYR:O	2.30	0.49
1:A:11:ASN:ND2	1:A:154:TRP:HE1	2.10	0.49
1:E:98:ARG:HB2	1:E:98:ARG:CZ	2.39	0.49
1:C:99:ASP:HB2	1:C:105:ARG:HH12	1.77	0.49
1:A:152:GLY:HA3	1:A:156:ALA:HB2	1.94	0.49
1:F:161:TYR:HD2	1:F:162:GLY:HA2	1.77	0.49
1:D:126:SER:N	1:D:127:PRO:CD	2.75	0.48
1:C:146:THR:HG22	1:C:147:TRP:N	2.29	0.48
1:E:20:HIS:O	1:E:24:SER:HB2	2.13	0.48
1:F:161:TYR:CB	1:F:162:GLY:CA	2.92	0.47
1:C:11:ASN:ND2	1:C:154:TRP:HE1	2.13	0.47
1:A:11:ASN:HB2	1:A:141:ASN:HD21	1.80	0.47
1:A:74:MET:HE1	2:A:1163:398:H181	1.95	0.47
1:A:145:HIS:O	1:A:149:GLN:HG2	2.15	0.47
1:F:18:TYR:CD1	1:F:18:TYR:C	2.88	0.47
2:B:1163:398:H36	1:D:161:TYR:HA	1.97	0.47
1:D:9:TYR:HD2	1:D:49:SER:N	2.13	0.47
1:D:92:VAL:HG13	2:D:1163:398:H182	1.98	0.46
1:F:161:TYR:CB	1:F:162:GLY:HA2	2.40	0.46
1:B:81:THR:HB	1:B:82:PRO:HD2	1.97	0.46
1:A:159:GLU:O	1:A:159:GLU:CG	2.64	0.45
1:B:65:ARG:NH2	1:D:65:ARG:HH21	2.14	0.45
1:B:140:LEU:HD23	1:B:144:LEU:HD12	1.98	0.45
1:D:158:VAL:O	1:D:159:GLU:C	2.54	0.45
1:E:16:MET:O	1:E:20:HIS:HB2	2.15	0.45
1:F:148:ILE:HG22	1:F:153:GLY:HA2	1.98	0.45
1:A:93:VAL:CG1	1:A:139:TYR:CE2	2.99	0.45
1:B:51:VAL:HG23	1:B:52:VAL:N	2.30	0.45
1:D:53:HIS:O	1:D:57:ARG:HG2	2.16	0.45
1:A:93:VAL:HG11	1:A:139:TYR:CE2	2.52	0.45
1:A:26:ARG:CG	1:A:26:ARG:NH1	2.80	0.44
1:C:26:ARG:HD2	1:C:118:VAL:HG11	2.00	0.44
1:D:52:VAL:HG22	1:D:158:VAL:CG2	2.48	0.44
1:D:161:TYR:O	1:D:162:GLY:C	2.55	0.44
1:C:17:LYS:HE2	1:C:53:HIS:CE1	2.54	0.43
1:D:159:GLU:HB3	1:D:160:LEU:HD13	2.00	0.43
1:F:67:TYR:CD1	2:F:1163:398:H481	2.53	0.43
1:F:126:SER:N	1:F:127:PRO:CD	2.81	0.43
1:C:92:VAL:HG22	2:C:1163:398:H162	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:26:ARG:CG	1:C:26:ARG:HH11	2.31	0.43
1:C:152:GLY:HA3	1:C:156:ALA:HB2	2.01	0.43
1:D:160:LEU:CD1	1:D:160:LEU:N	2.82	0.43
2:E:1163:398:C42	2:E:1163:398:N11	2.82	0.43
1:C:126:SER:N	1:C:127:PRO:CD	2.82	0.42
1:B:26:ARG:CG	1:B:26:ARG:HH11	2.32	0.42
1:A:26:ARG:HH11	1:A:26:ARG:HG2	1.84	0.42
2:B:1163:398:O22	2:B:1163:398:H152	2.19	0.42
1:F:156:ALA:O	1:F:160:LEU:HD22	2.20	0.42
1:B:95:GLU:O	1:B:98:ARG:HB3	2.20	0.42
1:E:11:ASN:ND2	1:E:154:TRP:HE1	2.18	0.42
1:E:16:MET:SD	1:E:30:TRP:CH2	3.13	0.42
1:B:126:SER:N	1:B:127:PRO:CD	2.83	0.42
1:C:98:ARG:HE	1:C:98:ARG:HB2	1.65	0.41
1:E:116:MET:HB3	1:E:132:ILE:HD13	2.02	0.41
2:B:1163:398:N11	2:B:1163:398:C42	2.83	0.41
1:C:132:ILE:O	1:C:136:MET:HG3	2.20	0.41
1:B:80:LEU:HD11	1:B:116:MET:CE	2.50	0.41
1:D:9:TYR:CE2	1:D:49:SER:HB3	2.55	0.41
1:D:116:MET:HB3	1:D:132:ILE:HD13	2.03	0.41
1:A:74:MET:CE	2:A:1163:398:H181	2.51	0.41
1:C:52:VAL:H	1:C:52:VAL:HG23	1.58	0.41
2:D:1163:398:N11	2:D:1163:398:C42	2.84	0.40
1:C:52:VAL:O	1:C:56:LEU:HB2	2.22	0.40
1:A:126:SER:OG	1:A:127:PRO:HD3	2.22	0.40
1:E:161:TYR:HD1	1:E:161:TYR:O	2.04	0.40
1:A:93:VAL:HG13	1:A:139:TYR:CZ	2.56	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	131/169 (78%)	126 (96%)	4 (3%)	1 (1%)	19	29
1	B	131/169 (78%)	126 (96%)	4 (3%)	1 (1%)	19	29
1	C	131/169 (78%)	126 (96%)	4 (3%)	1 (1%)	19	29
1	D	133/169 (79%)	127 (96%)	5 (4%)	1 (1%)	19	29
1	E	131/169 (78%)	121 (92%)	8 (6%)	2 (2%)	10	14
1	F	133/169 (79%)	128 (96%)	4 (3%)	1 (1%)	19	29
All	All	790/1014 (78%)	754 (95%)	29 (4%)	7 (1%)	17	25

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	161	TYR
1	E	27	GLY
1	E	153	GLY
1	A	159	GLU
1	B	25	GLN
1	C	25	GLN
1	F	31	ASP

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	116/141 (82%)	108 (93%)	8 (7%)	15	25
1	B	116/141 (82%)	107 (92%)	9 (8%)	12	19
1	C	116/141 (82%)	107 (92%)	9 (8%)	12	19
1	D	118/141 (84%)	110 (93%)	8 (7%)	16	25
1	E	115/141 (82%)	108 (94%)	7 (6%)	18	30
1	F	117/141 (83%)	109 (93%)	8 (7%)	16	25
All	All	698/846 (82%)	649 (93%)	49 (7%)	15	24

All (49) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	24	SER
1	A	26	ARG
1	A	31	ASP
1	A	53	HIS
1	A	94	GLU
1	A	142	ARG
1	A	146	THR
1	A	160	LEU
1	B	26	ARG
1	B	31	ASP
1	B	52	VAL
1	B	56	LEU
1	B	64	SER
1	B	94	GLU
1	B	98	ARG
1	B	146	THR
1	B	161	TYR
1	C	26	ARG
1	C	51	VAL
1	C	53	HIS
1	C	56	LEU
1	C	94	GLU
1	C	98	ARG
1	C	146	THR
1	C	160	LEU
1	C	161	TYR
1	D	24	SER
1	D	78	LEU
1	D	94	GLU
1	D	98	ARG
1	D	126	SER
1	D	134	LEU
1	D	155	ASP
1	D	160	LEU
1	E	24	SER
1	E	51	VAL
1	E	53	HIS
1	E	78	LEU
1	E	98	ARG
1	E	160	LEU
1	E	161	TYR
1	F	9	TYR
1	F	26	ARG

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Mol	Chain	Res	Type
1	F	56	LEU
1	F	75	SER
1	F	78	LEU
1	F	80	LEU
1	F	94	GLU
1	F	160	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	11	ASN
1	A	58	GLN
1	A	77	GLN
1	A	131	ASN
1	A	141	ASN
1	A	149	GLN
1	B	11	ASN
1	B	53	HIS
1	B	131	ASN
1	B	141	ASN
1	C	11	ASN
1	C	53	HIS
1	C	58	GLN
1	C	131	ASN
1	C	141	ASN
1	C	149	GLN
1	D	11	ASN
1	D	53	HIS
1	D	131	ASN
1	D	141	ASN
1	E	11	ASN
1	E	131	ASN
1	E	141	ASN
1	F	11	ASN
1	F	53	HIS
1	F	131	ASN
1	F	141	ASN
1	F	145	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

6 ligands 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	$\# Z > 2$
2	398	C	1163	-	55,58,58	2.24	7 (12%)	72,84,84	2.38	20 (27%)
2	398	F	1163	-	55,58,58	2.10	10 (18%)	72,84,84	2.28	20 (27%)
2	398	B	1163	-	55,58,58	2.23	8 (14%)	72,84,84	2.24	16 (22%)
2	398	E	1163	-	55,58,58	1.96	7 (12%)	72,84,84	2.53	23 (31%)
2	398	A	1163	-	55,58,58	2.14	7 (12%)	72,84,84	2.49	19 (26%)
2	398	D	1163	-	55,58,58	2.38	9 (16%)	72,84,84	2.20	14 (19%)

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
2	398	C	1163	-	-	7/39/52/52	0/6/6/6
2	398	F	1163	-	-	10/39/52/52	0/6/6/6

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	398	B	1163	-	-	7/39/52/52	0/6/6/6
2	398	E	1163	-	-	1/39/52/52	0/6/6/6
2	398	A	1163	-	-	7/39/52/52	0/6/6/6
2	398	D	1163	-	-	1/39/52/52	0/6/6/6

All (48) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	1163	398	C31-S28	-9.56	1.61	1.76
2	C	1163	398	C1-C6	9.51	1.52	1.39
2	D	1163	398	C31-S28	-9.27	1.62	1.76
2	D	1163	398	C1-C6	8.81	1.51	1.39
2	B	1163	398	C1-C6	8.65	1.50	1.39
2	B	1163	398	C31-S28	-8.43	1.63	1.76
2	E	1163	398	C31-S28	-8.30	1.63	1.76
2	F	1163	398	C31-S28	-8.17	1.63	1.76
2	A	1163	398	C31-S28	-7.80	1.64	1.76
2	F	1163	398	C1-C6	7.59	1.49	1.39
2	E	1163	398	C1-C6	6.98	1.48	1.39
2	A	1163	398	C1-C6	5.93	1.47	1.39
2	A	1163	398	C46-C47	5.73	1.51	1.40
2	D	1163	398	C9-CL23	5.62	1.85	1.72
2	A	1163	398	C25-N27	-5.52	1.32	1.39
2	B	1163	398	C46-C47	5.37	1.50	1.40
2	E	1163	398	C46-C47	5.27	1.50	1.40
2	A	1163	398	C9-CL23	5.12	1.83	1.72
2	D	1163	398	C25-N27	-5.03	1.33	1.39
2	F	1163	398	C46-C47	4.83	1.49	1.40
2	D	1163	398	C46-C47	4.63	1.49	1.40
2	F	1163	398	C25-N27	-4.58	1.33	1.39
2	F	1163	398	C9-CL23	4.57	1.82	1.72
2	D	1163	398	C9-C8	4.27	1.46	1.38
2	C	1163	398	C46-C47	4.20	1.48	1.40
2	C	1163	398	C9-CL23	4.18	1.81	1.72
2	B	1163	398	C9-CL23	4.14	1.81	1.72
2	A	1163	398	C9-C8	4.02	1.46	1.38
2	B	1163	398	C9-C8	3.87	1.45	1.38
2	B	1163	398	C25-N27	-3.86	1.34	1.39
2	E	1163	398	C25-N27	-3.73	1.34	1.39
2	C	1163	398	C9-C8	3.41	1.44	1.38
2	F	1163	398	C9-C8	3.34	1.44	1.38
2	E	1163	398	C9-CL23	2.95	1.79	1.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	1163	398	C25-N27	-2.94	1.35	1.39
2	E	1163	398	C9-C8	2.55	1.43	1.38
2	F	1163	398	C33-C32	2.54	1.41	1.36
2	D	1163	398	S28-N27	-2.45	1.59	1.64
2	D	1163	398	O29-S28	-2.45	1.40	1.43
2	B	1163	398	C10-N11	-2.40	1.33	1.35
2	D	1163	398	C10-C9	2.38	1.49	1.42
2	F	1163	398	O30-S28	2.34	1.46	1.43
2	B	1163	398	C32-C31	2.33	1.42	1.38
2	A	1163	398	C40-C39	2.32	1.41	1.36
2	C	1163	398	C40-C39	2.19	1.41	1.36
2	E	1163	398	C10-N11	-2.16	1.33	1.35
2	F	1163	398	C40-C39	2.16	1.41	1.36
2	F	1163	398	C36-C31	2.05	1.40	1.36

All (112) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1163	398	C45-C44-N43	-9.29	99.10	110.04
2	E	1163	398	O30-S28-O29	-9.21	108.23	119.55
2	F	1163	398	O30-S28-O29	-8.72	108.83	119.55
2	E	1163	398	C5-C6-C1	-8.45	115.25	122.95
2	C	1163	398	C5-C6-C1	-7.95	115.70	122.95
2	A	1163	398	O30-S28-O29	-7.53	110.29	119.55
2	C	1163	398	C8-C9-CL23	-7.38	117.37	125.92
2	D	1163	398	C5-C6-C1	-7.24	116.35	122.95
2	D	1163	398	C8-C9-CL23	-7.16	117.63	125.92
2	A	1163	398	C5-C6-C1	-6.86	116.70	122.95
2	B	1163	398	C10-C9-CL23	-6.75	120.40	127.50
2	E	1163	398	C8-C9-CL23	-6.67	118.20	125.92
2	F	1163	398	C5-C6-C1	-6.42	117.10	122.95
2	C	1163	398	O30-S28-O29	-6.42	111.66	119.55
2	B	1163	398	C45-C44-N43	-6.29	102.64	110.04
2	E	1163	398	C8-C9-C10	6.15	113.77	105.34
2	B	1163	398	C5-C6-C1	-6.02	117.46	122.95
2	B	1163	398	O30-S28-O29	-5.71	112.53	119.55
2	D	1163	398	O30-S28-O29	-5.62	112.64	119.55
2	C	1163	398	C8-C9-C10	5.57	112.97	105.34
2	D	1163	398	O29-S28-C31	5.34	114.55	107.97
2	A	1163	398	C8-C9-CL23	-5.26	119.83	125.92
2	A	1163	398	C8-N7-N11	5.25	118.92	111.61
2	D	1163	398	C8-N7-N11	5.22	118.87	111.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1163	398	C8-N7-N11	5.14	118.76	111.61
2	C	1163	398	C45-C44-N43	-5.13	104.00	110.04
2	A	1163	398	C8-C9-C10	5.08	112.30	105.34
2	B	1163	398	C8-C9-C10	5.06	112.28	105.34
2	D	1163	398	C1-C42-N43	5.02	126.30	118.28
2	F	1163	398	C8-C9-CL23	-4.67	120.51	125.92
2	A	1163	398	C31-S28-N27	4.67	113.04	105.97
2	F	1163	398	C45-C44-N43	-4.63	104.59	110.04
2	B	1163	398	C25-N27-S28	-4.54	117.50	123.36
2	F	1163	398	C8-N7-N11	4.52	117.90	111.61
2	B	1163	398	C31-S28-N27	4.52	112.82	105.97
2	B	1163	398	C12-C10-N11	4.35	131.89	120.55
2	F	1163	398	C8-C9-C10	4.29	111.22	105.34
2	E	1163	398	C25-N27-S28	-4.24	117.89	123.36
2	E	1163	398	C8-N7-N11	4.23	117.50	111.61
2	D	1163	398	C10-C9-CL23	4.23	131.95	127.50
2	C	1163	398	C8-N7-N11	4.22	117.49	111.61
2	F	1163	398	O26-C25-N27	4.22	126.26	121.08
2	C	1163	398	C1-C42-N43	4.18	124.97	118.28
2	A	1163	398	C47-C48-N43	-4.04	105.36	111.35
2	C	1163	398	C3-C25-N27	3.99	120.92	116.09
2	F	1163	398	C1-C42-N43	3.75	124.28	118.28
2	C	1163	398	C25-N27-S28	-3.73	118.54	123.36
2	B	1163	398	C1-C42-N43	3.72	124.23	118.28
2	D	1163	398	C8-C9-C10	3.71	110.43	105.34
2	E	1163	398	C12-C10-N11	3.71	130.20	120.55
2	E	1163	398	O30-S28-C31	3.67	112.49	107.97
2	E	1163	398	C45-C44-N43	-3.65	105.74	110.04
2	C	1163	398	C39-C38-C37	-3.60	116.80	121.03
2	F	1163	398	C12-C10-N11	3.56	129.83	120.55
2	C	1163	398	O26-C25-C3	-3.55	114.60	120.94
2	D	1163	398	C2-C1-C6	3.51	121.30	117.40
2	E	1163	398	C32-C31-S28	3.47	123.54	119.77
2	A	1163	398	C1-C42-N43	3.41	123.73	118.28
2	F	1163	398	C6-C1-C42	-3.39	116.86	124.08
2	E	1163	398	C2-C1-C6	3.36	121.13	117.40
2	F	1163	398	O30-S28-C31	3.20	111.91	107.97
2	F	1163	398	C32-C31-C36	-3.20	117.13	121.05
2	D	1163	398	C36-C31-S28	3.19	122.72	120.03
2	A	1163	398	C12-C10-N11	3.16	128.77	120.55
2	C	1163	398	O22-C12-N13	-3.01	117.36	122.34
2	E	1163	398	C36-C31-S28	-2.96	117.54	120.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	1163	398	C39-C38-C37	-2.87	117.66	121.03
2	D	1163	398	O53-C42-C1	-2.87	114.27	120.06
2	D	1163	398	C6-C1-C42	-2.87	117.97	124.08
2	F	1163	398	O29-S28-C31	2.86	111.49	107.97
2	A	1163	398	C2-C1-C6	2.86	120.57	117.40
2	B	1163	398	O53-C42-N43	-2.84	117.64	122.34
2	A	1163	398	C15-C14-N13	-2.79	103.70	112.44
2	C	1163	398	O26-C25-N27	2.74	124.45	121.08
2	E	1163	398	C6-C1-C42	-2.73	118.27	124.08
2	C	1163	398	C12-C10-N11	2.72	127.62	120.55
2	A	1163	398	C6-C1-C42	-2.67	118.39	124.08
2	E	1163	398	C40-C39-C38	2.67	123.62	119.98
2	F	1163	398	C37-C38-I41	-2.67	116.40	119.89
2	A	1163	398	O53-C42-C1	-2.66	114.70	120.06
2	D	1163	398	O26-C25-N27	2.64	124.32	121.08
2	F	1163	398	C4-C3-C2	2.62	122.33	119.24
2	E	1163	398	C1-C42-N43	2.60	122.44	118.28
2	C	1163	398	C31-S28-N27	2.60	109.91	105.97
2	F	1163	398	O53-C42-N43	-2.60	118.04	122.34
2	B	1163	398	C2-C1-C6	2.59	120.28	117.40
2	C	1163	398	C2-C1-C6	2.55	120.23	117.40
2	B	1163	398	C4-C3-C2	2.48	122.17	119.24
2	E	1163	398	C15-C14-N13	-2.47	104.70	112.44
2	C	1163	398	O53-C42-C1	-2.39	115.23	120.06
2	F	1163	398	C31-S28-N27	2.39	109.59	105.97
2	F	1163	398	C25-N27-S28	2.35	126.39	123.36
2	F	1163	398	C39-C38-I41	2.35	123.22	119.68
2	E	1163	398	C31-S28-N27	2.31	109.47	105.97
2	C	1163	398	C38-C37-C35	2.28	122.15	119.70
2	A	1163	398	O22-C12-N13	-2.27	118.59	122.34
2	E	1163	398	O26-C25-N27	2.24	123.83	121.08
2	B	1163	398	C6-C1-C42	-2.22	119.34	124.08
2	A	1163	398	C32-C31-C36	-2.21	118.34	121.05
2	A	1163	398	C51-C50-C49	2.20	123.55	120.19
2	E	1163	398	C4-C5-C6	2.19	123.00	119.54
2	B	1163	398	O26-C25-N27	2.16	123.73	121.08
2	E	1163	398	C39-C38-I41	2.15	122.93	119.68
2	F	1163	398	C2-C1-C6	2.14	119.77	117.40
2	B	1163	398	O22-C12-N13	2.13	125.86	122.34
2	E	1163	398	C37-C35-C36	-2.12	117.99	122.16
2	A	1163	398	C39-C38-I41	2.08	122.83	119.68
2	A	1163	398	C39-C38-C37	-2.08	118.59	121.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	1163	398	C36-C31-S28	-2.08	118.29	120.03
2	D	1163	398	C12-C10-N11	2.07	125.95	120.55
2	E	1163	398	C3-C25-N27	2.04	118.56	116.09
2	C	1163	398	C39-C38-I41	2.03	122.75	119.68

There are no chirality outliers.

All (33) torsion outliers are listed below:

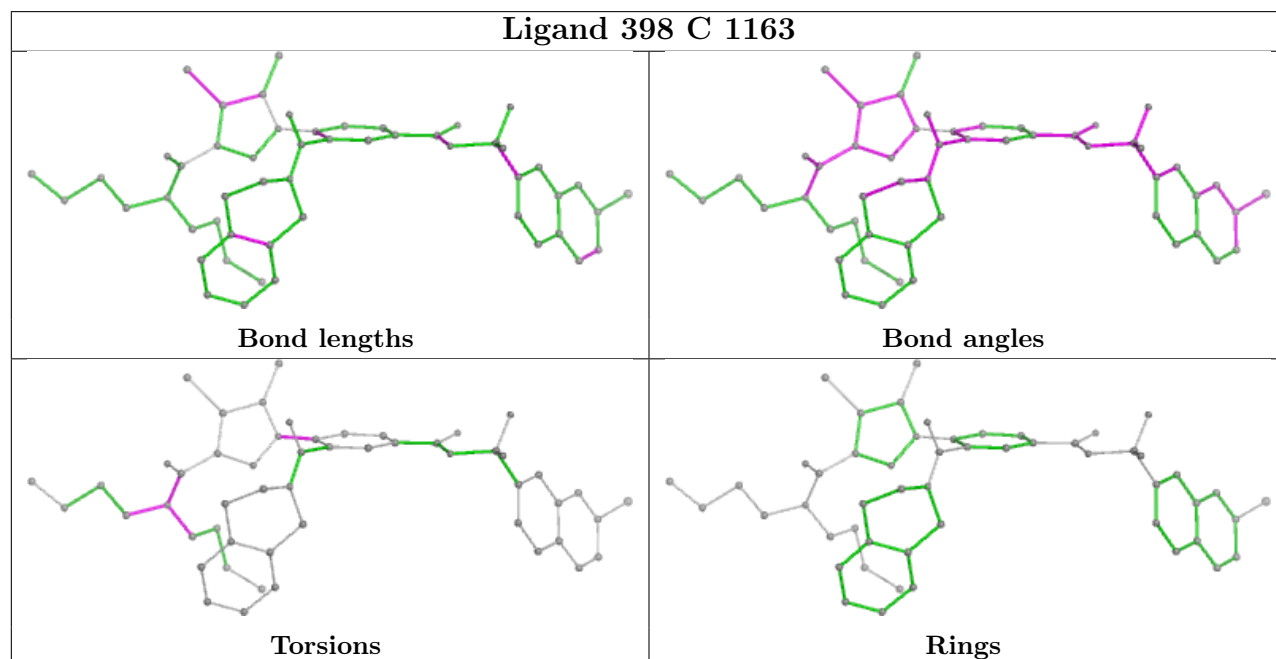
Mol	Chain	Res	Type	Atoms
2	A	1163	398	C10-C12-N13-C18
2	A	1163	398	C10-C12-N13-C14
2	A	1163	398	O22-C12-N13-C18
2	A	1163	398	O22-C12-N13-C14
2	B	1163	398	C15-C14-N13-C12
2	C	1163	398	O22-C12-N13-C18
2	C	1163	398	O22-C12-N13-C14
2	F	1163	398	C10-C12-N13-C18
2	F	1163	398	C10-C12-N13-C14
2	F	1163	398	O22-C12-N13-C18
2	F	1163	398	O22-C12-N13-C14
2	F	1163	398	C15-C14-N13-C12
2	B	1163	398	O22-C12-N13-C18
2	A	1163	398	N13-C18-C19-C20
2	B	1163	398	O22-C12-N13-C14
2	F	1163	398	N13-C18-C19-C20
2	A	1163	398	C14-C15-C16-C17
2	B	1163	398	C15-C14-N13-C18
2	B	1163	398	C19-C18-N13-C12
2	F	1163	398	C14-C15-C16-C17
2	C	1163	398	C10-C12-N13-C18
2	C	1163	398	C15-C14-N13-C18
2	F	1163	398	C15-C14-N13-C18
2	B	1163	398	C19-C18-N13-C14
2	C	1163	398	C15-C14-N13-C12
2	F	1163	398	C18-C19-C20-C21
2	B	1163	398	C1-C6-N7-N11
2	D	1163	398	C1-C6-N7-N11
2	A	1163	398	N13-C14-C15-C16
2	C	1163	398	C1-C6-N7-N11
2	E	1163	398	C1-C6-N7-N11
2	F	1163	398	C1-C6-N7-N11
2	C	1163	398	C19-C18-N13-C14

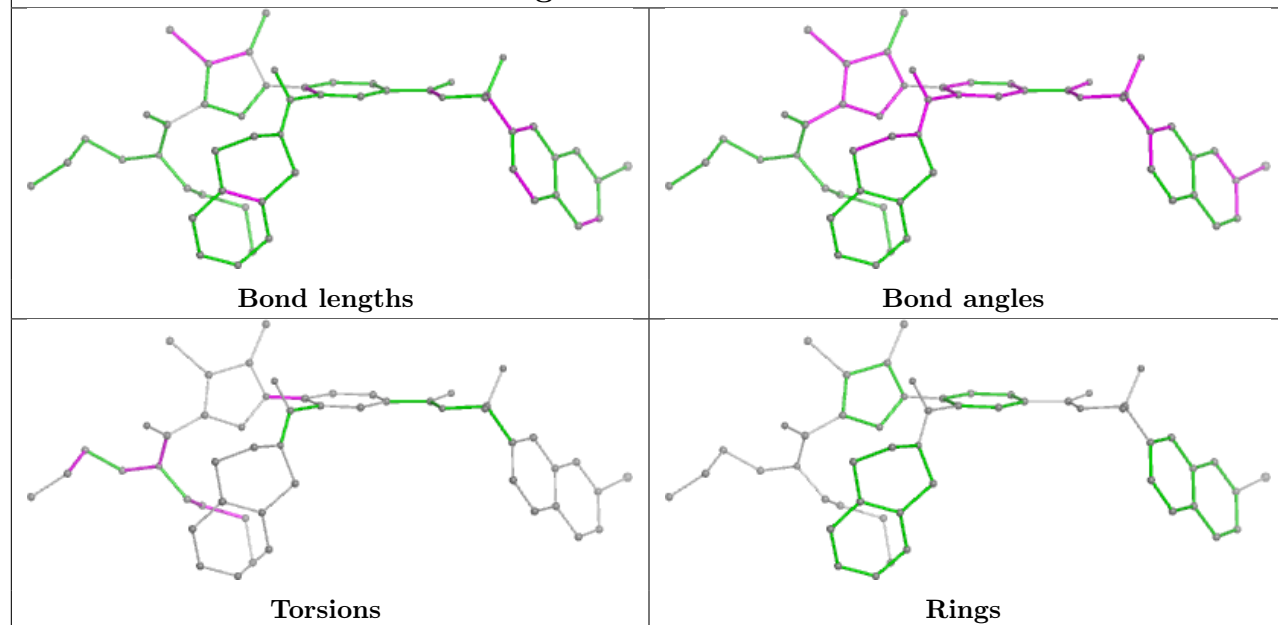
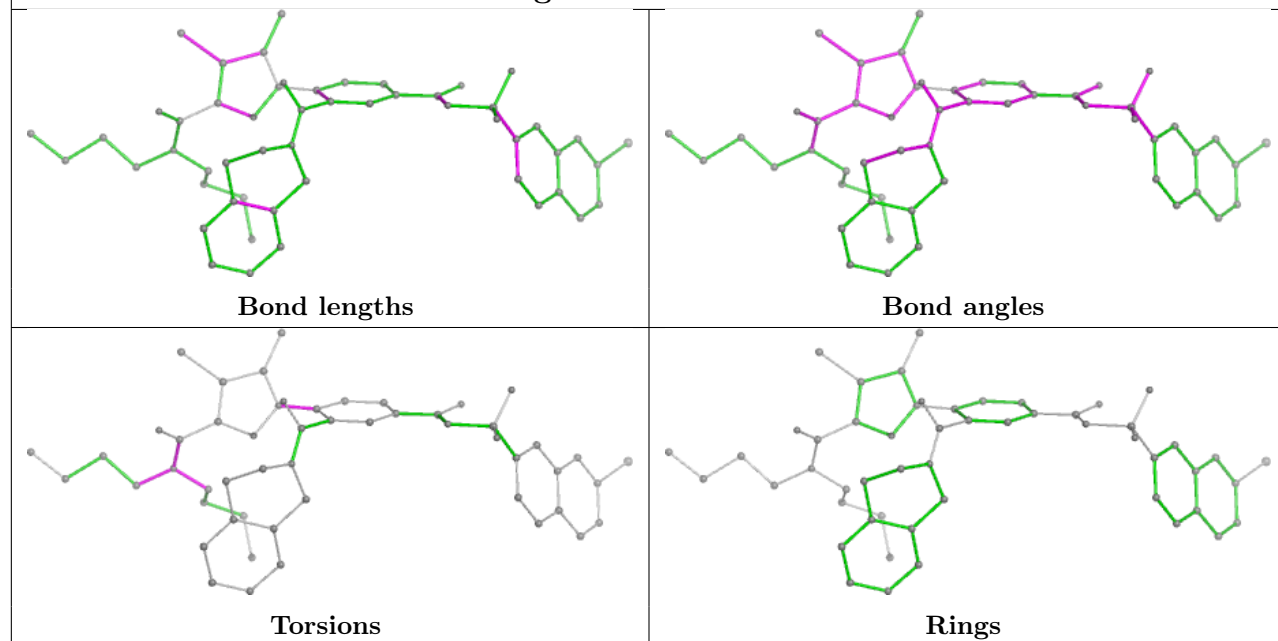
There are no ring outliers.

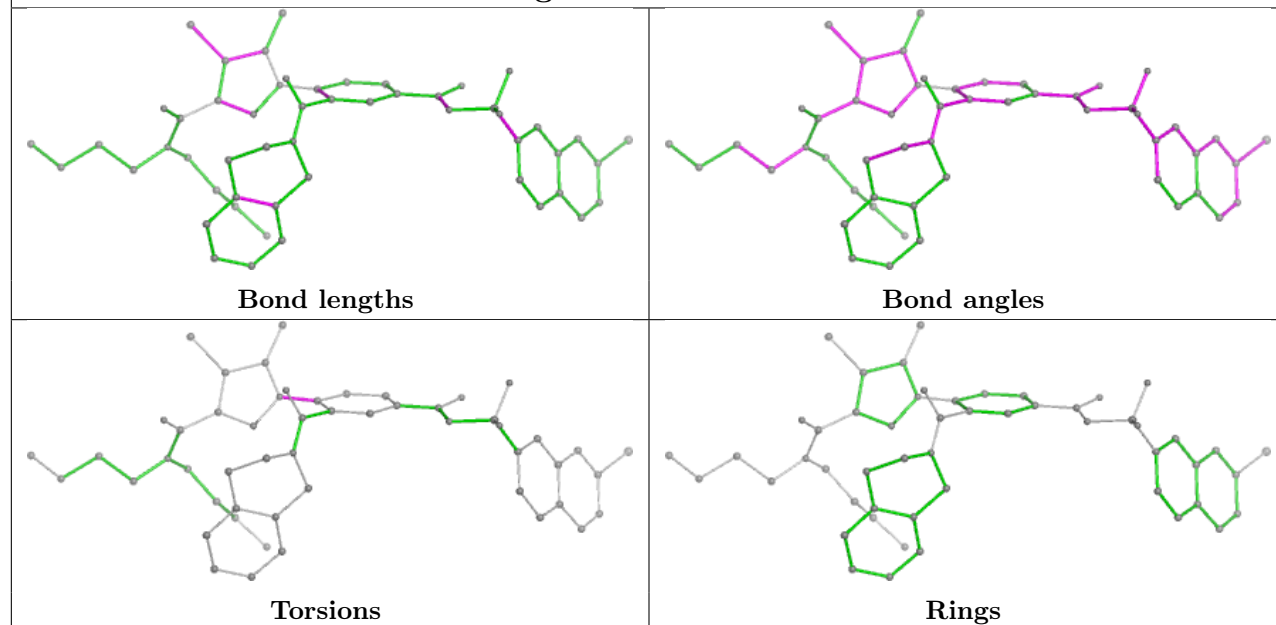
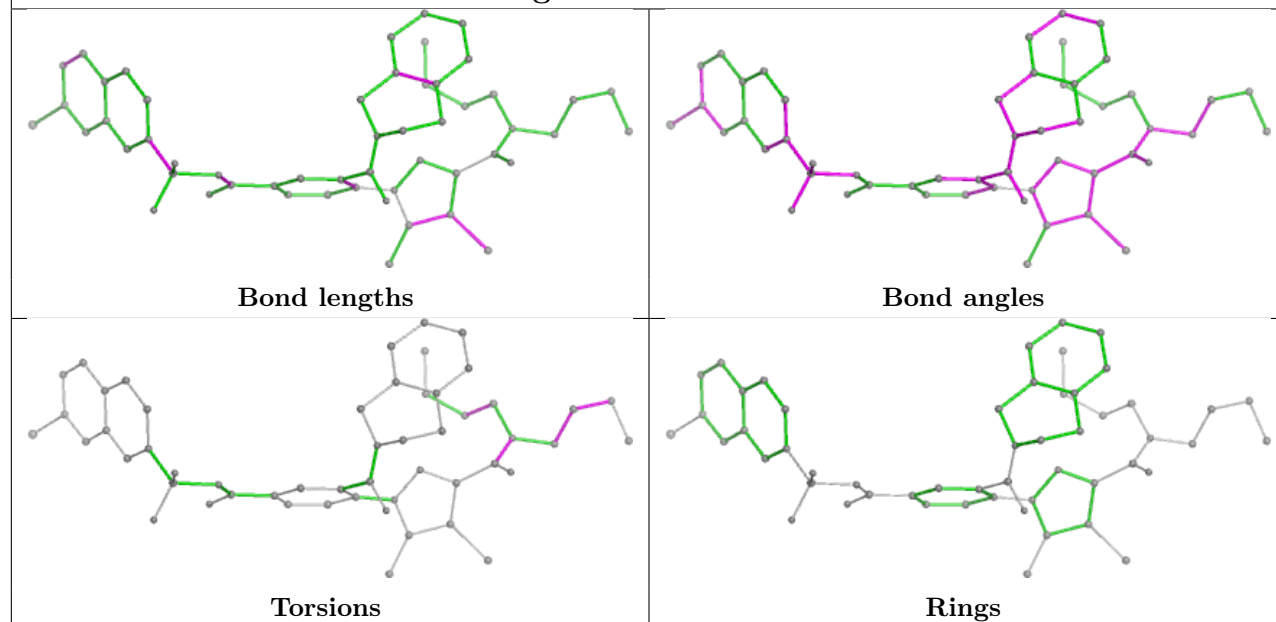
6 monomers are involved in 14 short contacts:

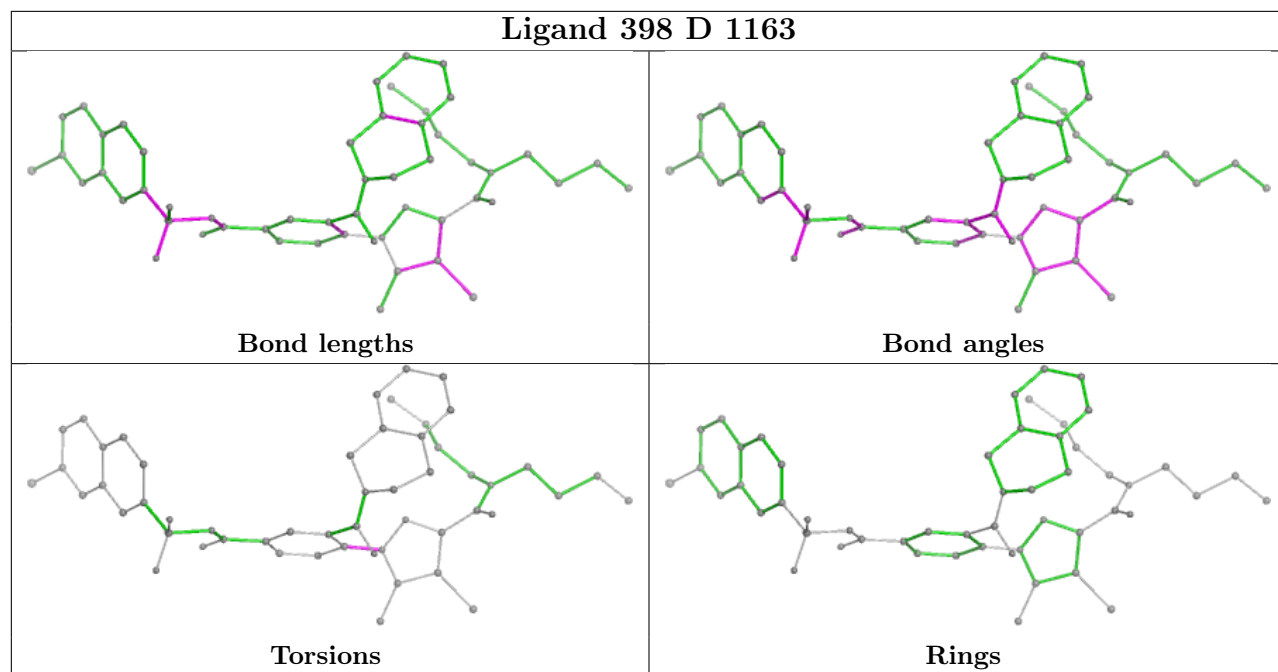
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	1163	398	1	0
2	F	1163	398	2	0
2	B	1163	398	4	0
2	E	1163	398	2	0
2	A	1163	398	3	0
2	D	1163	398	2	0

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



Ligand 398 F 1163**Ligand 398 B 1163**

Ligand 398 E 1163**Ligand 398 A 1163**



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	135/169 (79%)	0.22	1 (0%) 87 86	33, 50, 74, 87	0
1	B	135/169 (79%)	0.22	0 100 100	36, 51, 73, 101	0
1	C	135/169 (79%)	0.26	0 100 100	33, 50, 76, 107	0
1	D	137/169 (81%)	0.29	3 (2%) 62 60	38, 58, 89, 121	0
1	E	135/169 (79%)	0.33	3 (2%) 62 60	37, 59, 92, 113	0
1	F	137/169 (81%)	0.31	3 (2%) 62 60	36, 55, 83, 119	0
All	All	814/1014 (80%)	0.27	10 (1%) 79 77	33, 54, 83, 121	0

All (10) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	9	TYR	8.7
1	D	49	SER	3.3
1	A	160	LEU	2.6
1	D	31	ASP	2.6
1	F	142	ARG	2.5
1	E	142	ARG	2.2
1	D	50	GLU	2.2
1	E	160	LEU	2.1
1	E	29	GLU	2.1
1	F	160	LEU	2.0

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

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](#)

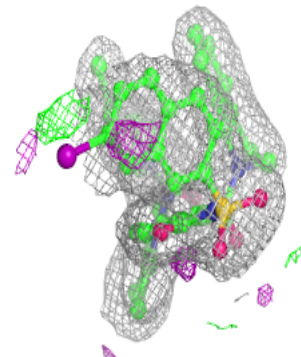
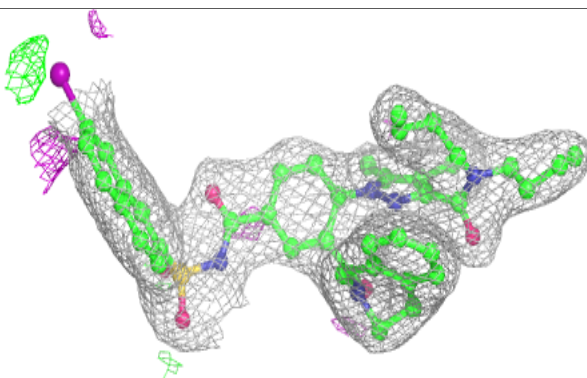
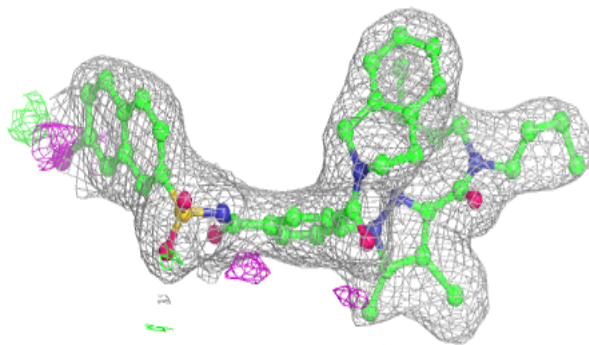
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	398	A	1163	53/53	0.99	0.18	30,43,56,61	0
2	398	B	1163	53/53	0.99	0.16	35,47,61,66	0
2	398	C	1163	53/53	0.99	0.17	32,47,60,64	0
2	398	D	1163	53/53	0.99	0.16	38,49,59,67	0
2	398	E	1163	53/53	0.99	0.17	39,46,59,62	0
2	398	F	1163	53/53	0.99	0.17	38,46,65,72	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.

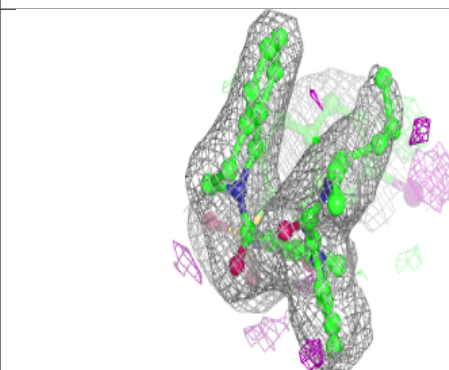
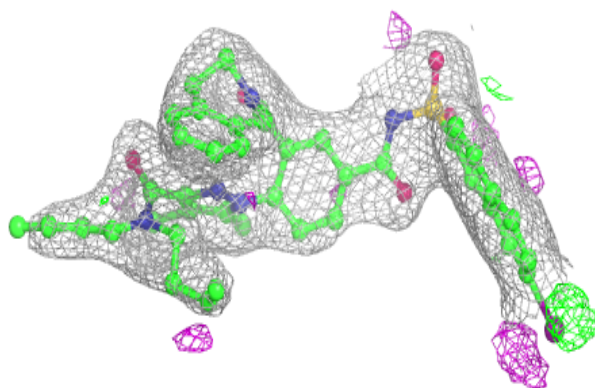
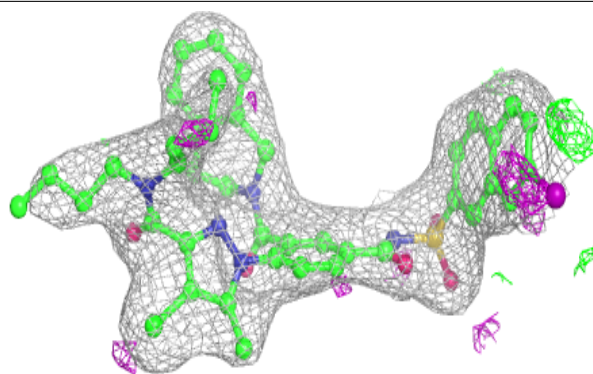
Electron density around 398 A 1163:

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

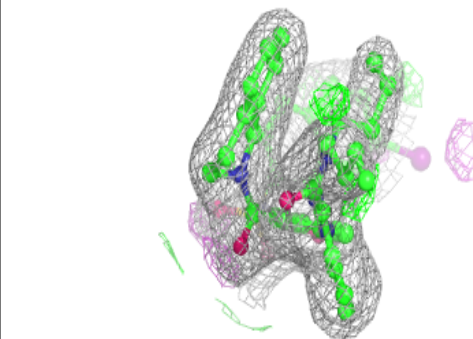
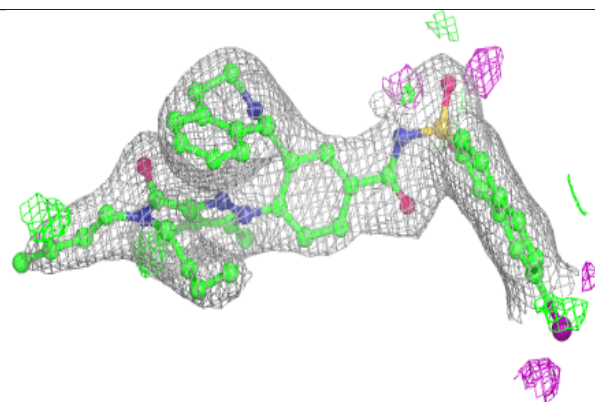
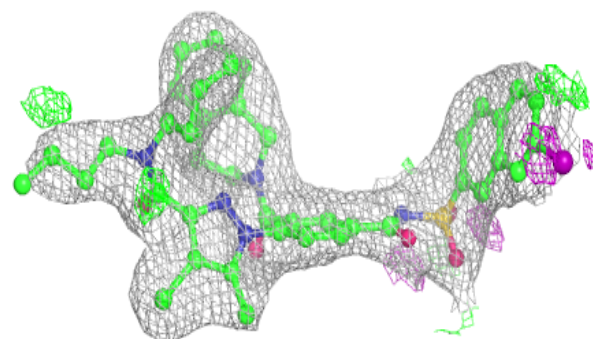


Electron density around 398 B 1163:

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

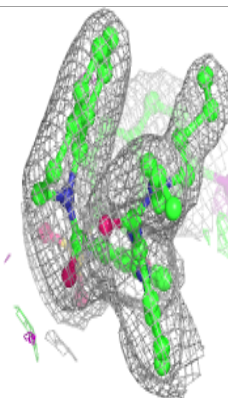
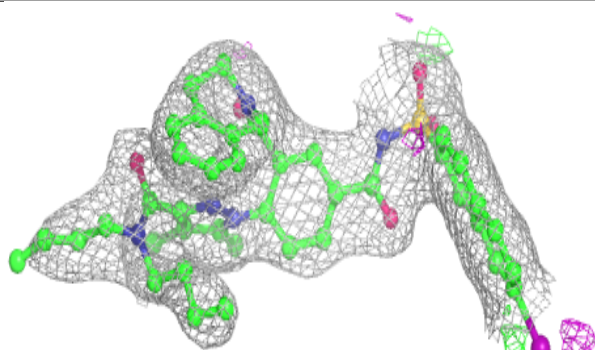
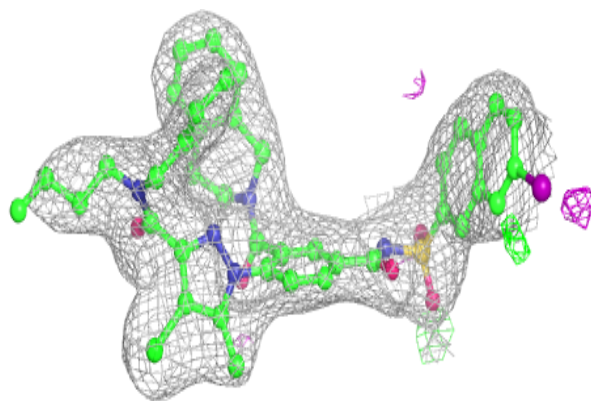
**Electron density around 398 C 1163:**

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

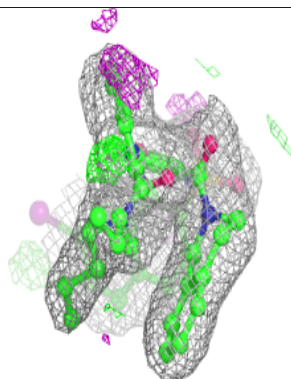
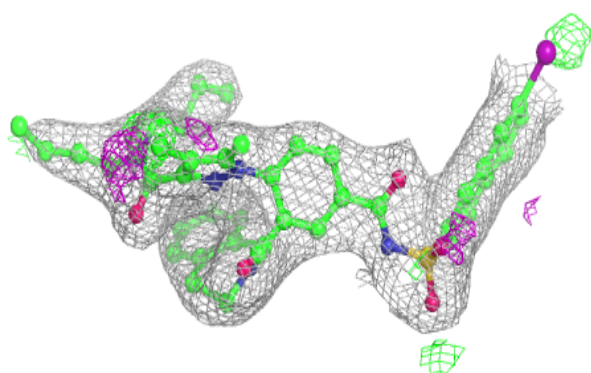
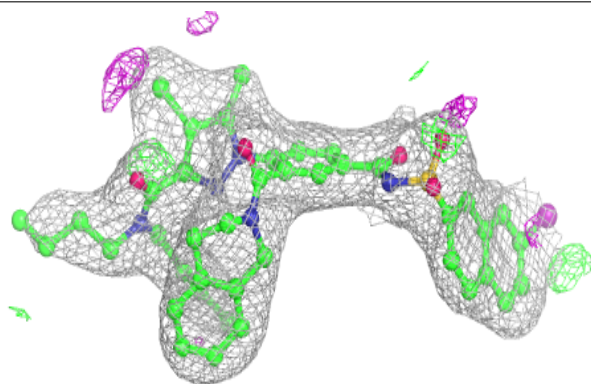


Electron density around 398 D 1163:

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

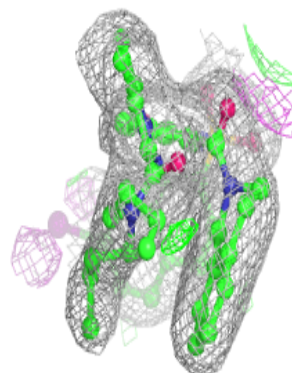
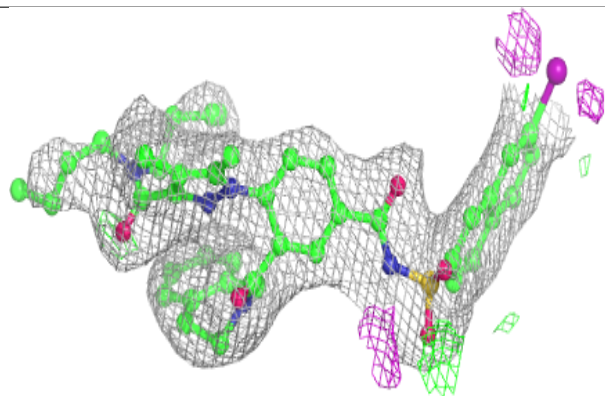
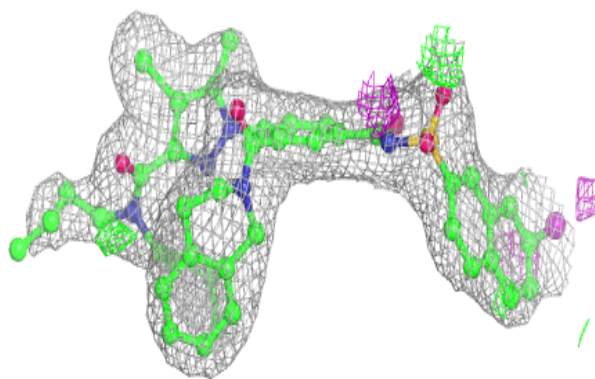
**Electron density around 398 E 1163:**

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



Electron density around 398 F 1163:

$2mF_o - DF_c$ (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.