Full wwPDB X-ray Structure Validation Report ⓘ

Sep 11, 2023 – 01:49 PM EDT

PDB ID	:	4MLP
Title	:	Mammalian cryptochrome in complex with a small molecule competitor of its ubiquitin ligase
Authors	:	Nangle, S.; Xing, W.; Zheng, N.
Deposited on	:	2013-09-06
Resolution	:	1.94 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:

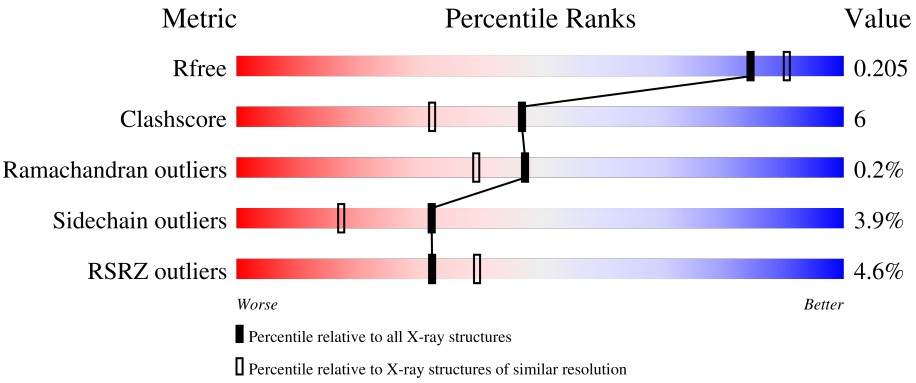
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 1.94 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	4310 (1.96-1.92)
Clashscore	141614	1023 (1.94-1.94)
Ramachandran outliers	138981	1007 (1.94-1.94)
Sidechain outliers	138945	1007 (1.94-1.94)
RSRZ outliers	127900	4250 (1.96-1.92)

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	512	3% 84% 10%
1	B	512	4% 82% 13%
1	C	512	4% 84% 11%
1	D	512	6% 82% 11%

2 Entry composition

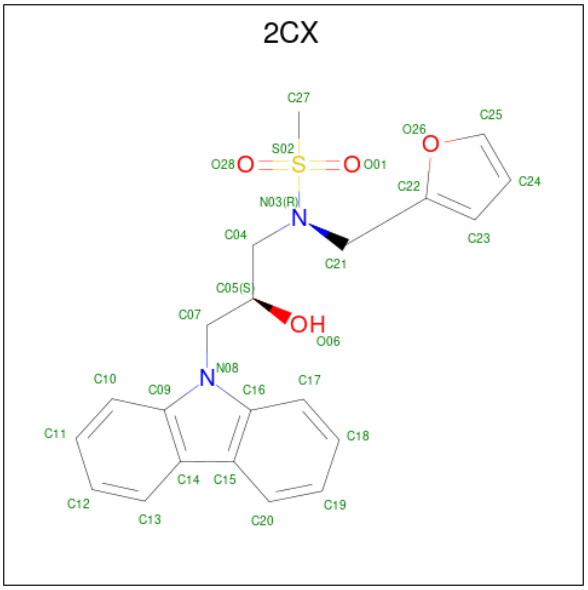
There are 3 unique types of molecules in this entry. The entry contains 17726 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Cryptochrome-2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	C	492	Total	C	N	O	S	0	0	0
			4015	2577	713	705	20			
1	A	492	Total	C	N	O	S	0	0	0
			4015	2577	713	705	20			
1	B	492	Total	C	N	O	S	0	0	0
			4015	2577	713	705	20			
1	D	492	Total	C	N	O	S	0	0	0
			4015	2577	713	705	20			

- Molecule 2 is N-[(2S)-3-(9H-carbazol-9-yl)-2-hydroxypropyl]-N-(furan-2-ylmethyl)methanesulfonamide (three-letter code: 2CX) (formula: $C_{21}H_{22}N_2O_4S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	C	1	Total	C	N	O	S	0	0
			28	21	2	4	1		
2	A	1	Total	C	N	O	S	0	0
			28	21	2	4	1		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	B	1	Total	C	N	O	S	0	0
			28	21	2	4	1		
2	D	1	Total	C	N	O	S	0	0
			28	21	2	4	1		

- Molecule 3 is water.

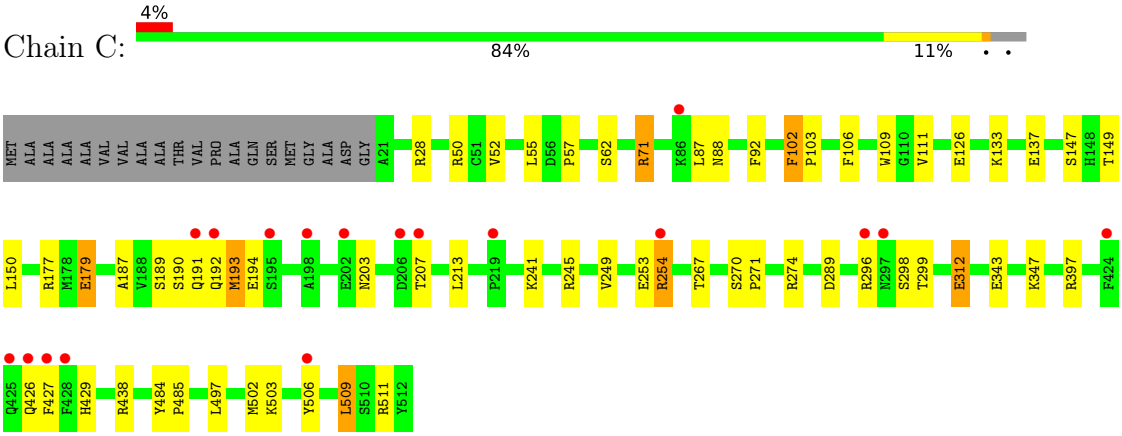
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	C	434	Total	O	0	0
			434	434		
3	A	461	Total	O	0	0
			461	461		
3	B	322	Total	O	0	0
			322	322		
3	D	337	Total	O	0	0
			337	337		

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.

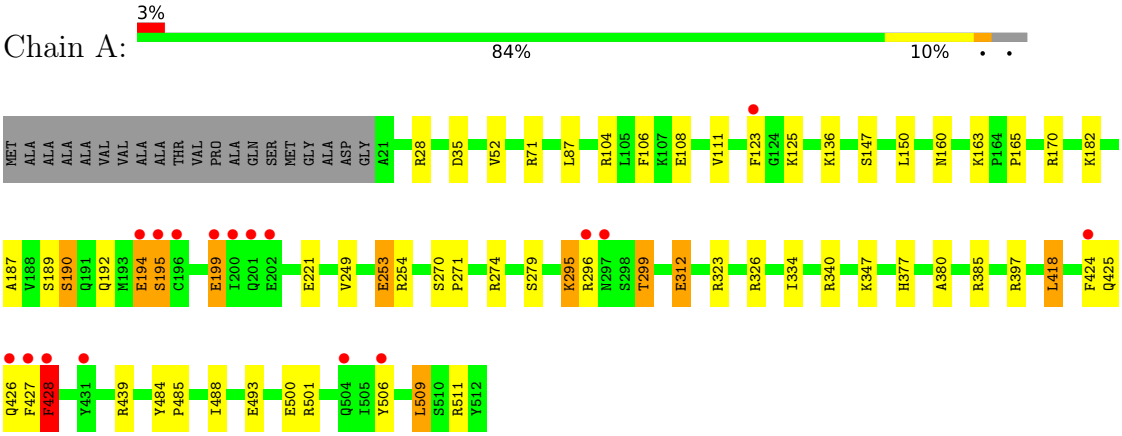
• Molecule 1: Cryptochrome-2

Chain C:



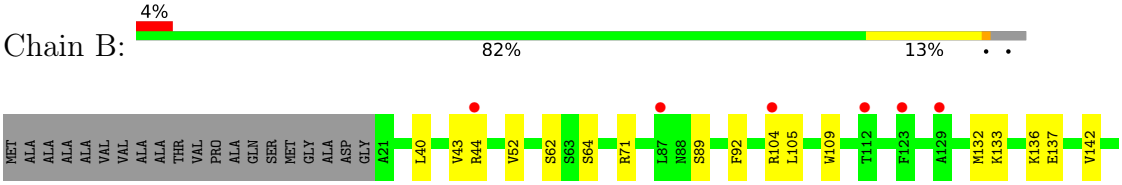
• Molecule 1: Cryptochrome-2

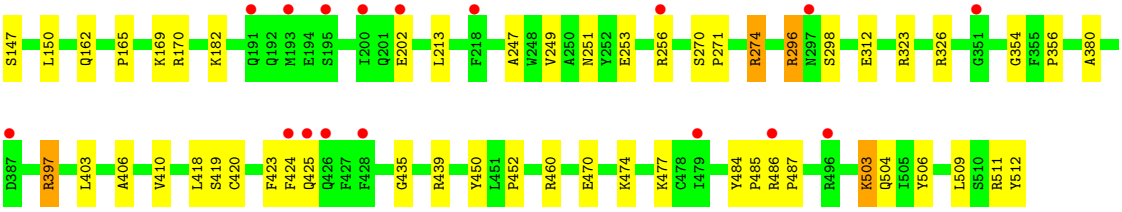
Chain A:



• Molecule 1: Cryptochrome-2

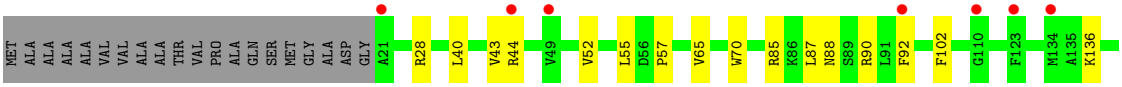
Chain B:

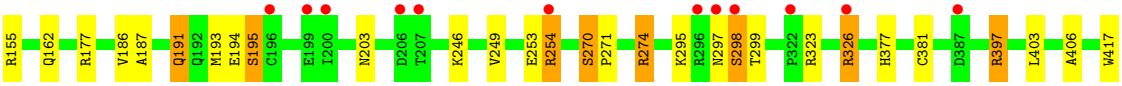


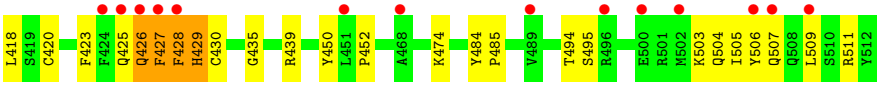


• Molecule 1: Cryptochrome-2

Chain D:







4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	48.21Å 93.65Å 141.18Å 89.94° 90.09° 90.25°	Depositor
Resolution (Å)	44.46 – 1.94 48.21 – 1.94	Depositor EDS
% Data completeness (in resolution range)	(Not available) (44.46-1.94) 93.8 (48.21-1.94)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	4.04 (at 1.94Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.1_1168)	Depositor
R, R_{free}	0.179 , 0.217 0.185 , 0.205	Depositor DCC
R_{free} test set	1530 reflections (0.87%)	wwPDB-VP
Wilson B-factor (Å^2)	26.0	Xtriage
Anisotropy	0.337	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 37.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.109 for h,-k,-l 0.110 for -h,k,-l 0.457 for -h,-k,l	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	17726	wwPDB-VP
Average B, all atoms (Å^2)	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.09% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 2CX

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	1.39	2/4133 (0.0%)	0.76	1/5608 (0.0%)
1	B	1.31	1/4133 (0.0%)	0.76	2/5608 (0.0%)
1	C	1.39	3/4133 (0.1%)	0.79	4/5608 (0.1%)
1	D	1.30	1/4133 (0.0%)	0.76	4/5608 (0.1%)
All	All	1.35	7/16532 (0.0%)	0.77	11/22432 (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	A	0	1
1	C	0	1
All	All	0	2

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	312	GLU	CD-OE2	-5.67	1.19	1.25
1	C	179	GLU	CD-OE1	-5.60	1.19	1.25
1	A	312	GLU	CD-OE2	-5.50	1.19	1.25
1	C	147	SER	CB-OG	-5.46	1.35	1.42
1	B	147	SER	CB-OG	-5.40	1.35	1.42
1	D	270	SER	CB-OG	-5.21	1.35	1.42
1	A	147	SER	CB-OG	-5.04	1.35	1.42

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	397	ARG	NE-CZ-NH2	-9.79	115.41	120.30
1	C	397	ARG	NE-CZ-NH2	-7.11	116.74	120.30
1	D	326	ARG	NE-CZ-NH1	6.56	123.58	120.30
1	D	397	ARG	NE-CZ-NH2	-6.33	117.14	120.30
1	D	326	ARG	O-C-N	-6.00	113.10	122.70
1	D	326	ARG	NE-CZ-NH2	-5.52	117.54	120.30
1	C	289	ASP	CB-CG-OD1	5.49	123.24	118.30
1	C	179	GLU	OE1-CD-OE2	-5.30	116.94	123.30
1	A	397	ARG	NE-CZ-NH2	-5.28	117.66	120.30
1	C	71	ARG	NE-CZ-NH2	-5.25	117.68	120.30
1	B	397	ARG	NE-CZ-NH1	5.15	122.88	120.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	28	ARG	Peptide
1	C	28	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	4015	0	3944	48	0
1	B	4015	0	3944	44	0
1	C	4015	0	3944	45	1
1	D	4015	0	3944	62	0
2	A	28	0	22	1	0
2	B	28	0	22	1	0
2	C	28	0	22	0	0
2	D	28	0	22	0	0
3	A	461	0	0	10	1
3	B	322	0	0	8	0
3	C	434	0	0	9	2
3	D	337	0	0	5	2
All	All	17726	0	15864	197	3

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 6.

All (197) 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:189:SER:OG	1:A:192:GLN:HG3	1.18	1.27
1:B:182:LYS:NZ	3:B:1205:HOH:O	1.75	1.08
1:C:254:ARG:HG3	1:C:254:ARG:HH11	1.24	1.02
1:A:199:GLU:O	3:A:1201:HOH:O	1.83	0.96
1:A:296:ARG:HH11	1:A:296:ARG:HG2	1.31	0.94
1:D:506:TYR:O	1:D:511:ARG:NH2	2.02	0.93
1:A:189:SER:OG	1:A:192:GLN:CG	2.15	0.92
1:D:420:CYS:SG	3:D:1239:HOH:O	2.28	0.91
1:A:439:ARG:NH2	3:A:1339:HOH:O	2.01	0.90
1:C:343:GLU:OE2	3:C:1360:HOH:O	1.88	0.90
1:A:506:TYR:O	1:A:511:ARG:NH2	2.04	0.89
1:A:189:SER:HG	1:A:192:GLN:HG3	1.36	0.88
1:B:296:ARG:HH11	1:B:296:ARG:HG2	1.40	0.86
1:B:503:LYS:HA	1:B:503:LYS:HE2	1.61	0.83
1:D:435:GLY:O	1:D:439:ARG:HG3	1.79	0.82
1:D:423:PHE:O	3:D:1104:HOH:O	1.97	0.81
1:B:506:TYR:O	1:B:511:ARG:NH2	2.14	0.81
1:D:417:TRP:CZ3	1:D:428:PHE:HE2	2.01	0.79
1:D:503:LYS:HE2	1:D:507:GLN:NE2	1.99	0.78
1:A:334:ILE:HD11	1:A:424:PHE:HE1	1.49	0.78
1:B:150:LEU:N	1:B:312:GLU:OE2	2.15	0.77
1:B:133:LYS:O	1:B:137:GLU:HG3	1.85	0.77
1:C:506:TYR:O	1:C:511:ARG:NH2	2.18	0.76
1:C:347:LYS:NZ	3:C:1279:HOH:O	2.12	0.75
1:A:506:TYR:HA	1:A:509:LEU:HD22	1.70	0.74
1:D:507:GLN:C	1:D:511:ARG:HH22	1.91	0.73
1:A:296:ARG:HG2	1:A:296:ARG:NH1	2.00	0.73
1:A:427:PHE:O	1:A:428:PHE:CD2	2.43	0.72
1:B:435:GLY:O	1:B:439:ARG:HG3	1.89	0.72
1:D:417:TRP:CH2	1:D:428:PHE:HE2	2.07	0.72
1:D:426:GLN:HG2	1:D:427:PHE:H	1.56	0.71
1:A:104:ARG:O	1:A:108:GLU:HG2	1.92	0.69
1:A:334:ILE:CD1	1:A:424:PHE:HE1	2.05	0.69
1:C:502:MET:HE1	1:C:506:TYR:HE1	1.57	0.68
1:B:44:ARG:NH1	3:B:1249:HOH:O	2.10	0.66
1:D:191:GLN:O	1:D:195:SER:OG	2.14	0.65
1:B:169:LYS:NZ	3:B:1288:HOH:O	2.29	0.65
1:D:155:ARG:NH1	3:D:1226:HOH:O	2.22	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:511:ARG:NH1	3:A:1388:HOH:O	2.30	0.64
1:B:486:ARG:HB2	1:B:487:PRO:HD2	1.78	0.64
1:C:254:ARG:HG3	1:C:254:ARG:NH1	1.97	0.64
1:B:274:ARG:NH1	1:B:406:ALA:O	2.32	0.63
1:A:323:ARG:HH12	1:A:326:ARG:NH1	1.97	0.62
1:A:150:LEU:N	1:A:312:GLU:OE2	2.25	0.62
1:D:274:ARG:NH1	1:D:406:ALA:O	2.33	0.62
1:B:296:ARG:HH11	1:B:296:ARG:CG	2.10	0.62
1:D:52:VAL:HG12	1:D:92:PHE:HB2	1.81	0.61
1:B:419:SER:O	1:B:420:CYS:HB2	1.99	0.61
1:C:52:VAL:HG12	1:C:92:PHE:HB2	1.83	0.60
1:D:426:GLN:OE1	1:D:426:GLN:N	2.25	0.60
1:A:165:PRO:HB3	1:A:170:ARG:HG3	1.83	0.60
1:B:274:ARG:CZ	1:B:406:ALA:O	2.50	0.60
1:A:334:ILE:HD11	1:A:424:PHE:CE1	2.33	0.60
1:A:123:PHE:HB2	3:A:1346:HOH:O	2.02	0.60
1:D:203:ASN:OD1	1:D:203:ASN:N	2.31	0.59
1:B:323:ARG:CZ	1:B:326:ARG:HD2	2.32	0.59
1:A:500:GLU:OE1	3:A:1397:HOH:O	2.16	0.59
1:C:253:GLU:O	1:C:254:ARG:HD3	2.03	0.59
1:D:377:HIS:HA	1:D:418:LEU:CD1	2.33	0.59
1:B:504:GLN:NE2	3:B:1198:HOH:O	2.36	0.58
1:A:249:VAL:HA	1:A:253:GLU:HG3	1.86	0.58
1:B:64:SER:OG	1:B:397:ARG:NH2	2.36	0.58
1:A:340:ARG:NH2	3:A:1166:HOH:O	2.36	0.57
1:C:106:PHE:HA	1:C:111:VAL:HG13	1.86	0.57
1:D:274:ARG:CZ	1:D:406:ALA:O	2.52	0.57
1:C:177:ARG:NH2	3:C:1209:HOH:O	2.29	0.57
1:A:106:PHE:HA	1:A:111:VAL:HG13	1.87	0.56
1:D:85:ARG:NH2	1:D:90:ARG:NH1	2.53	0.56
1:C:506:TYR:HA	1:C:509:LEU:HD22	1.88	0.56
1:D:323:ARG:NH1	1:D:326:ARG:CD	2.69	0.56
1:B:512:TYR:O	3:B:1229:HOH:O	2.18	0.56
1:C:502:MET:CE	1:C:506:TYR:HE1	2.19	0.56
1:D:427:PHE:CD2	1:D:428:PHE:N	2.69	0.56
1:D:85:ARG:NH2	1:D:90:ARG:CZ	2.69	0.55
1:C:502:MET:CE	1:C:506:TYR:CE1	2.89	0.55
1:B:40:LEU:HB3	1:B:44:ARG:HH12	1.72	0.55
1:C:189:SER:HB3	1:C:192:GLN:HG3	1.88	0.55
1:B:71:ARG:HD3	1:B:213:LEU:HD11	1.89	0.55
1:C:426:GLN:H	1:C:426:GLN:CD	2.11	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:191:GLN:NE2	1:C:194:GLU:OE1	2.40	0.54
1:B:423:PHE:O	1:B:424:PHE:HB2	2.08	0.53
1:D:323:ARG:CZ	1:D:326:ARG:CD	2.86	0.53
1:D:323:ARG:NH1	1:D:326:ARG:NE	2.57	0.53
1:A:182:LYS:NZ	3:A:1376:HOH:O	2.31	0.53
1:C:426:GLN:O	1:C:426:GLN:NE2	2.42	0.53
1:C:187:ALA:HB1	3:C:1266:HOH:O	2.09	0.52
1:C:177:ARG:NE	3:C:1209:HOH:O	2.31	0.52
1:D:417:TRP:CH2	1:D:428:PHE:CE2	2.93	0.52
1:C:50:ARG:HH21	1:C:109:TRP:HB3	1.75	0.52
1:D:507:GLN:CA	1:D:511:ARG:HH22	2.23	0.52
1:A:347:LYS:HE2	3:A:1113:HOH:O	2.09	0.52
1:D:426:GLN:H	1:D:426:GLN:CD	2.09	0.52
1:B:484:TYR:CD2	1:B:485:PRO:HD2	2.44	0.51
1:C:427:PHE:HE1	1:C:429:HIS:CG	2.29	0.51
1:D:504:GLN:NE2	1:D:507:GLN:OE1	2.44	0.51
1:A:190:SER:O	1:A:194:GLU:HG3	2.11	0.51
1:D:187:ALA:HA	3:D:1183:HOH:O	2.11	0.51
1:B:132:MET:HG2	1:B:142:VAL:HG11	1.93	0.50
1:A:71:ARG:HD2	3:A:1434:HOH:O	2.12	0.50
1:D:43:VAL:HG12	1:D:43:VAL:O	2.11	0.50
1:C:347:LYS:NZ	3:C:1321:HOH:O	2.26	0.50
1:D:377:HIS:ND1	1:D:418:LEU:HD12	2.26	0.50
1:C:438:ARG:HD3	3:C:1174:HOH:O	2.11	0.50
1:A:484:TYR:CD1	1:A:485:PRO:HD2	2.47	0.50
1:A:424:PHE:O	1:A:425:GLN:HB2	2.10	0.50
1:D:427:PHE:H	1:D:427:PHE:HD2	1.59	0.49
1:C:189:SER:CB	1:C:192:GLN:HG3	2.42	0.49
1:A:194:GLU:O	1:A:195:SER:CB	2.60	0.49
1:D:249:VAL:HA	1:D:253:GLU:HB2	1.95	0.49
1:D:323:ARG:CZ	1:D:326:ARG:HD3	2.43	0.49
1:B:296:ARG:HG2	1:B:296:ARG:NH1	2.19	0.49
1:B:165:PRO:HB3	1:B:170:ARG:HG3	1.95	0.49
1:C:87:LEU:HD13	1:C:193:MET:HG2	1.94	0.48
1:D:377:HIS:HA	1:D:418:LEU:HD11	1.94	0.48
1:C:179:GLU:H	1:C:179:GLU:CD	2.17	0.48
1:D:270:SER:OG	1:D:271:PRO:HD3	2.14	0.48
1:A:187:ALA:HB2	3:A:1300:HOH:O	2.13	0.48
1:C:484:TYR:CD2	1:C:485:PRO:HD2	2.49	0.48
1:C:502:MET:HE1	1:C:506:TYR:CE1	2.42	0.48
1:B:354:GLY:O	1:B:356:PRO:HD3	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:133:LYS:HE2	1:C:137:GLU:OE2	2.14	0.47
1:A:377:HIS:CE1	2:A:900:2CX:H1	2.49	0.47
1:A:270:SER:OG	1:A:271:PRO:HD3	2.14	0.47
1:B:296:ARG:CG	1:B:296:ARG:NH1	2.73	0.47
1:D:246:LYS:HB2	1:D:246:LYS:HE2	1.63	0.47
1:B:503:LYS:HA	1:B:503:LYS:CE	2.36	0.47
1:D:295:LYS:O	1:D:298:SER:OG	2.33	0.47
1:B:270:SER:OG	1:B:271:PRO:HD3	2.15	0.47
1:D:427:PHE:CG	1:D:428:PHE:N	2.83	0.47
1:D:428:PHE:C	1:D:428:PHE:CD1	2.88	0.47
1:D:503:LYS:HE2	1:D:507:GLN:HE22	1.80	0.46
1:C:150:LEU:N	1:C:312:GLU:OE2	2.35	0.46
1:D:40:LEU:O	1:D:44:ARG:HG3	2.15	0.46
1:A:87:LEU:HD22	1:A:190:SER:HA	1.97	0.46
1:B:450:TYR:C	1:B:452:PRO:HD3	2.37	0.45
1:D:428:PHE:C	1:D:428:PHE:HD1	2.19	0.45
1:D:417:TRP:CZ3	1:D:428:PHE:CE2	2.92	0.45
1:C:241:LYS:HB3	1:C:267:THR:HG22	1.98	0.45
1:C:312:GLU:HG2	3:C:1036:HOH:O	2.17	0.45
1:B:136:LYS:HG3	1:B:137:GLU:N	2.31	0.45
1:C:502:MET:HE3	1:C:506:TYR:CE1	2.52	0.45
1:C:179:GLU:OE1	3:C:1249:HOH:O	2.21	0.45
1:D:254:ARG:HH11	1:D:254:ARG:CG	2.30	0.45
1:C:189:SER:HB3	1:C:192:GLN:H	1.82	0.44
1:B:105:LEU:HD13	1:B:109:TRP:CZ3	2.53	0.44
1:B:425:GLN:NE2	3:B:1227:HOH:O	2.51	0.44
1:B:380:ALA:HB1	1:B:418:LEU:HD22	2.00	0.44
1:C:55:LEU:O	1:C:57:PRO:HD3	2.18	0.44
1:C:270:SER:OG	1:C:271:PRO:HD3	2.17	0.44
1:A:347:LYS:HD3	1:A:488:ILE:HG21	1.99	0.44
1:D:418:LEU:C	1:D:418:LEU:HD23	2.38	0.44
1:D:484:TYR:CG	1:D:485:PRO:HD2	2.52	0.44
1:C:71:ARG:HB2	1:C:213:LEU:HD11	2.00	0.44
1:B:247:ALA:O	1:B:251:ASN:HB2	2.17	0.44
1:D:417:TRP:CE2	1:D:425:GLN:NE2	2.87	0.43
1:D:162:GLN:HA	1:D:162:GLN:OE1	2.19	0.43
1:C:426:GLN:CD	1:C:426:GLN:N	2.72	0.43
1:B:43:VAL:O	1:B:43:VAL:HG12	2.19	0.43
1:D:87:LEU:HD13	1:D:193:MET:CB	2.49	0.43
1:D:507:GLN:C	1:D:511:ARG:NH2	2.68	0.43
1:B:410:VAL:CG1	2:B:900:2CX:H19	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:299:THR:HG21	1:B:62:SER:OG	2.18	0.43
1:D:155:ARG:HG2	1:D:155:ARG:HH11	1.84	0.42
1:A:199:GLU:H	1:A:199:GLU:HG2	1.70	0.42
1:D:270:SER:N	1:D:271:PRO:CD	2.82	0.42
1:C:427:PHE:CE1	1:C:429:HIS:HA	2.55	0.42
1:D:484:TYR:CD1	1:D:485:PRO:HD2	2.54	0.42
1:C:62:SER:OG	1:D:299:THR:HG21	2.19	0.42
1:A:35:ASP:HB3	1:A:279:SER:HB2	2.01	0.42
1:B:484:TYR:CG	1:B:485:PRO:HD2	2.55	0.42
1:D:507:GLN:HA	1:D:511:ARG:HH22	1.83	0.42
1:D:450:TYR:C	1:D:452:PRO:HD3	2.39	0.42
1:D:381:CYS:HG	1:D:430:CYS:HG	1.66	0.42
1:A:509:LEU:HB2	1:A:511:ARG:HH21	1.85	0.41
1:A:380:ALA:HB1	1:A:418:LEU:HD22	2.02	0.41
1:B:477:LYS:NZ	3:B:1295:HOH:O	2.53	0.41
1:A:160:ASN:OD1	1:A:170:ARG:NH1	2.52	0.41
1:B:249:VAL:HA	1:B:253:GLU:HB2	2.02	0.41
1:D:494:THR:HG23	1:D:495:SER:N	2.34	0.41
1:A:295:LYS:O	1:A:296:ARG:C	2.57	0.41
1:A:385:ARG:NH2	1:A:428:PHE:CZ	2.89	0.41
1:A:509:LEU:O	1:A:511:ARG:NH2	2.54	0.41
1:C:149:THR:HB	1:C:312:GLU:OE2	2.21	0.41
1:D:503:LYS:HE2	1:D:507:GLN:HE21	1.78	0.41
1:C:503:LYS:HD2	1:C:503:LYS:HA	1.89	0.41
1:A:323:ARG:CZ	1:A:326:ARG:HD2	2.50	0.41
1:A:296:ARG:NH1	1:A:296:ARG:CG	2.74	0.41
1:B:298:SER:N	3:B:1244:HOH:O	2.54	0.41
1:B:323:ARG:NH1	1:B:326:ARG:HD2	2.36	0.41
1:D:177:ARG:NE	3:D:1261:HOH:O	2.44	0.41
1:C:245:ARG:O	1:C:249:VAL:HG23	2.21	0.41
1:A:380:ALA:CB	1:A:418:LEU:HD22	2.50	0.41
1:D:55:LEU:O	1:D:57:PRO:HD3	2.21	0.40
1:B:52:VAL:HG12	1:B:92:PHE:HB2	2.03	0.40
1:C:102:PHE:N	1:C:103:PRO:CD	2.84	0.40
1:A:87:LEU:O	1:A:194:GLU:HG2	2.22	0.40
1:D:65:VAL:HB	1:D:70:TRP:HE1	1.86	0.40

All (3) 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)
3:C:1335:HOH:O	3:A:1352:HOH:O[1_554]	1.50	0.70
3:C:1414:HOH:O	3:D:1289:HOH:O[1_565]	2.18	0.02
1:C:177:ARG:NH1	3:D:1287:HOH:O[1_565]	2.19	0.01

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	490/512 (96%)	474 (97%)	14 (3%)	2 (0%)	34 24
1	B	490/512 (96%)	480 (98%)	10 (2%)	0	100 100
1	C	490/512 (96%)	480 (98%)	10 (2%)	0	100 100
1	D	490/512 (96%)	478 (98%)	10 (2%)	2 (0%)	34 24
All	All	1960/2048 (96%)	1912 (98%)	44 (2%)	4 (0%)	47 39

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	426	GLN
1	A	195	SER
1	A	428	PHE
1	D	429	HIS

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	424/434 (98%)	405 (96%)	19 (4%)	27 12
1	B	424/434 (98%)	411 (97%)	13 (3%)	40 26
1	C	424/434 (98%)	410 (97%)	14 (3%)	38 24
1	D	424/434 (98%)	404 (95%)	20 (5%)	26 11
All	All	1696/1736 (98%)	1630 (96%)	66 (4%)	32 17

All (66) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	88	ASN
1	C	102	PHE
1	C	126	GLU
1	C	190	SER
1	C	193	MET
1	C	203	ASN
1	C	207	THR
1	C	254	ARG
1	C	274	ARG
1	C	296	ARG
1	C	298	SER
1	C	299	THR
1	C	497	LEU
1	C	509	LEU
1	A	52	VAL
1	A	125	LYS
1	A	136	LYS
1	A	163	LYS
1	A	190	SER
1	A	194	GLU
1	A	199	GLU
1	A	221	GLU
1	A	253	GLU
1	A	254	ARG
1	A	274	ARG
1	A	295	LYS
1	A	299	THR
1	A	418	LEU
1	A	426	GLN
1	A	428	PHE
1	A	493	GLU
1	A	501	ARG
1	A	509	LEU

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Mol	Chain	Res	Type
1	B	89	SER
1	B	104	ARG
1	B	162	GLN
1	B	202	GLU
1	B	256	ARG
1	B	274	ARG
1	B	296	ARG
1	B	403	LEU
1	B	460	ARG
1	B	470	GLU
1	B	474	LYS
1	B	503	LYS
1	B	509	LEU
1	D	28	ARG
1	D	88	ASN
1	D	102	PHE
1	D	136	LYS
1	D	186	VAL
1	D	191	GLN
1	D	194	GLU
1	D	195	SER
1	D	254	ARG
1	D	274	ARG
1	D	297	ASN
1	D	298	SER
1	D	397	ARG
1	D	403	LEU
1	D	427	PHE
1	D	428	PHE
1	D	429	HIS
1	D	474	LYS
1	D	505	ILE
1	D	509	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	307	GLN
1	C	373	HIS
1	C	429	HIS
1	A	297	ASN
1	A	307	GLN

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Mol	Chain	Res	Type
1	A	373	HIS
1	A	508	GLN
1	B	373	HIS
1	B	425	GLN
1	D	373	HIS
1	D	504	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)

4 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	2CX	D	900	-	26,31,31	2.35	11 (42%)	29,45,45	2.95	6 (20%)
2	2CX	C	900	-	26,31,31	2.38	9 (34%)	29,45,45	3.07	6 (20%)
2	2CX	B	900	-	26,31,31	2.31	11 (42%)	29,45,45	2.91	6 (20%)
2	2CX	A	900	-	26,31,31	2.42	9 (34%)	29,45,45	2.97	6 (20%)

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	2CX	D	900	-	-	3/15/18/18	0/4/4/4
2	2CX	C	900	-	-	4/15/18/18	0/4/4/4
2	2CX	B	900	-	-	3/15/18/18	0/4/4/4
2	2CX	A	900	-	-	5/15/18/18	0/4/4/4

All (40) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	900	2CX	O28-S02	5.61	1.52	1.43
2	C	900	2CX	O28-S02	5.50	1.51	1.43
2	A	900	2CX	S02-N03	5.33	1.70	1.63
2	C	900	2CX	S02-N03	5.27	1.70	1.63
2	D	900	2CX	S02-N03	4.83	1.69	1.63
2	D	900	2CX	O28-S02	4.81	1.50	1.43
2	B	900	2CX	O28-S02	4.76	1.50	1.43
2	B	900	2CX	S02-N03	4.60	1.69	1.63
2	D	900	2CX	C13-C14	3.90	1.48	1.41
2	A	900	2CX	C19-C20	3.83	1.45	1.36
2	B	900	2CX	C13-C14	3.80	1.48	1.41
2	C	900	2CX	C13-C14	3.72	1.48	1.41
2	A	900	2CX	C13-C14	3.70	1.48	1.41
2	A	900	2CX	C11-C10	3.57	1.44	1.36
2	D	900	2CX	C11-C10	3.55	1.44	1.36
2	B	900	2CX	C19-C20	3.53	1.44	1.36
2	B	900	2CX	C18-C17	3.51	1.44	1.36
2	D	900	2CX	C19-C20	3.48	1.44	1.36
2	C	900	2CX	C19-C20	3.41	1.44	1.36
2	D	900	2CX	C18-C17	3.40	1.44	1.36
2	D	900	2CX	C04-C05	3.38	1.60	1.52
2	B	900	2CX	C11-C10	3.33	1.44	1.36
2	C	900	2CX	C11-C10	3.28	1.44	1.36
2	C	900	2CX	C18-C17	3.24	1.44	1.36
2	C	900	2CX	C04-C05	3.22	1.59	1.52
2	A	900	2CX	C18-C17	3.17	1.43	1.36
2	A	900	2CX	C04-C05	3.09	1.59	1.52
2	B	900	2CX	C04-C05	2.95	1.59	1.52
2	B	900	2CX	C21-N03	-2.56	1.44	1.48
2	D	900	2CX	C21-N03	-2.56	1.44	1.48
2	D	900	2CX	C27-S02	2.41	1.81	1.75
2	B	900	2CX	C04-N03	-2.34	1.43	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	900	2CX	C27-S02	2.25	1.80	1.75
2	C	900	2CX	C27-S02	2.24	1.80	1.75
2	B	900	2CX	O01-S02	-2.22	1.40	1.43
2	A	900	2CX	C27-S02	2.17	1.80	1.75
2	D	900	2CX	C04-N03	-2.17	1.44	1.47
2	D	900	2CX	O01-S02	-2.11	1.40	1.43
2	A	900	2CX	C04-N03	-2.10	1.44	1.47
2	C	900	2CX	C04-N03	-2.07	1.44	1.47

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	900	2CX	O28-S02-O01	-12.84	100.28	118.59
2	D	900	2CX	O28-S02-O01	-12.14	101.29	118.59
2	A	900	2CX	O28-S02-O01	-11.97	101.53	118.59
2	B	900	2CX	O28-S02-O01	-11.83	101.72	118.59
2	A	900	2CX	O01-S02-N03	6.89	112.82	107.03
2	C	900	2CX	O01-S02-N03	6.08	112.13	107.03
2	B	900	2CX	O01-S02-N03	6.04	112.10	107.03
2	A	900	2CX	C27-S02-N03	5.95	112.51	107.36
2	D	900	2CX	O28-S02-N03	5.82	111.91	107.03
2	C	900	2CX	C27-S02-N03	5.77	112.35	107.36
2	D	900	2CX	O01-S02-N03	5.32	111.50	107.03
2	B	900	2CX	O28-S02-N03	4.99	111.22	107.03
2	C	900	2CX	O28-S02-N03	4.10	110.47	107.03
2	D	900	2CX	C22-C21-N03	-3.28	106.76	112.69
2	B	900	2CX	C27-S02-N03	3.03	109.98	107.36
2	B	900	2CX	O28-S02-C27	3.00	112.48	108.44
2	D	900	2CX	O28-S02-C27	2.88	112.31	108.44
2	D	900	2CX	C27-S02-N03	2.86	109.84	107.36
2	A	900	2CX	O28-S02-N03	2.69	109.29	107.03
2	B	900	2CX	C22-C21-N03	-2.55	108.08	112.69
2	C	900	2CX	C21-N03-C04	-2.13	113.75	117.61
2	A	900	2CX	O28-S02-C27	2.12	111.29	108.44
2	C	900	2CX	C22-C21-N03	2.10	116.48	112.69
2	A	900	2CX	C22-C21-N03	2.08	116.44	112.69

There are no chirality outliers.

All (15) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	900	2CX	C21-N03-S02-C27

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Mol	Chain	Res	Type	Atoms
2	C	900	2CX	C21-N03-S02-O28
2	C	900	2CX	C05-C04-N03-C21
2	A	900	2CX	C21-N03-S02-C27
2	A	900	2CX	C21-N03-S02-O28
2	A	900	2CX	C05-C04-N03-C21
2	B	900	2CX	N03-C21-C22-C23
2	B	900	2CX	C04-N03-S02-C27
2	B	900	2CX	C04-N03-S02-O28
2	D	900	2CX	N03-C21-C22-C23
2	D	900	2CX	C04-N03-S02-O28
2	C	900	2CX	C22-C21-N03-S02
2	A	900	2CX	C22-C21-N03-S02
2	A	900	2CX	C04-N03-S02-O28
2	D	900	2CX	C04-N03-S02-C27

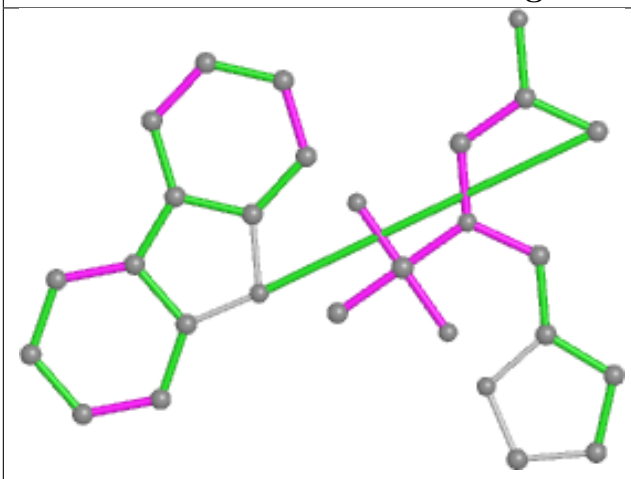
There are no ring outliers.

2 monomers are involved in 2 short contacts:

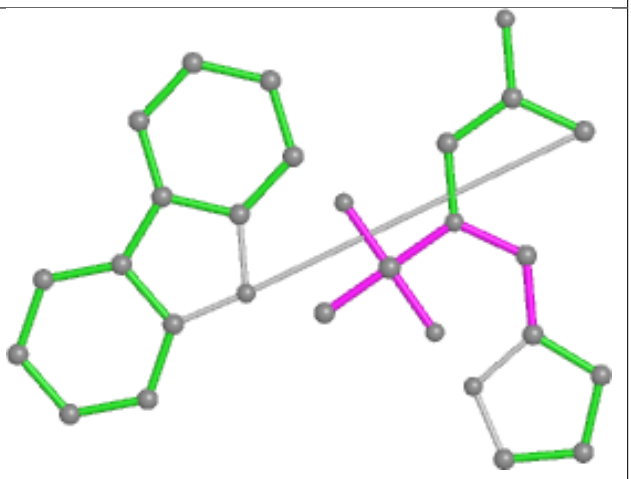
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	900	2CX	1	0
2	A	900	2CX	1	0

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.

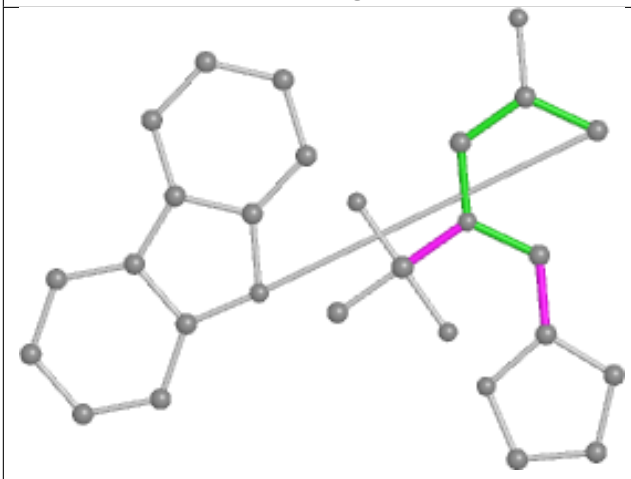
Ligand 2CX D 900



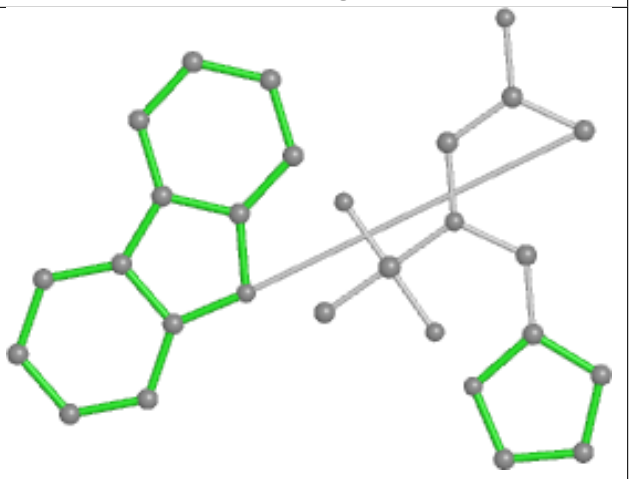
Bond lengths



Bond angles

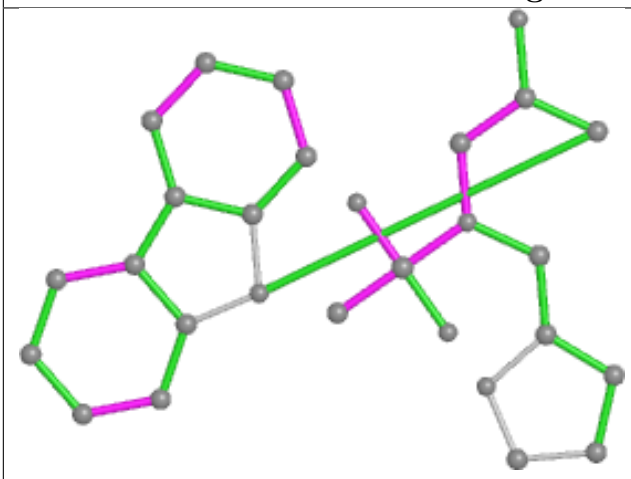


Torsions

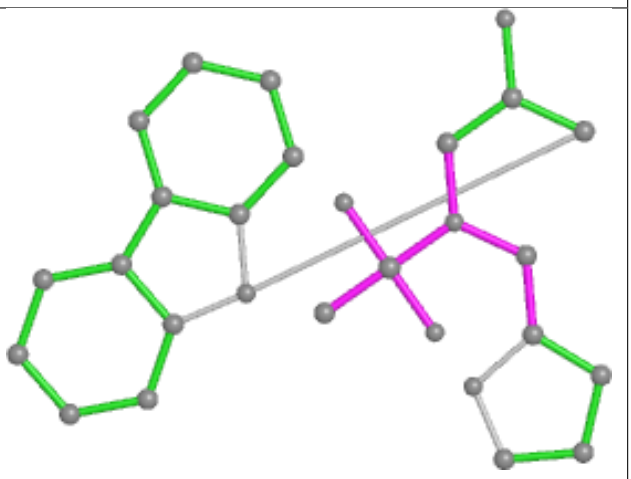


Rings

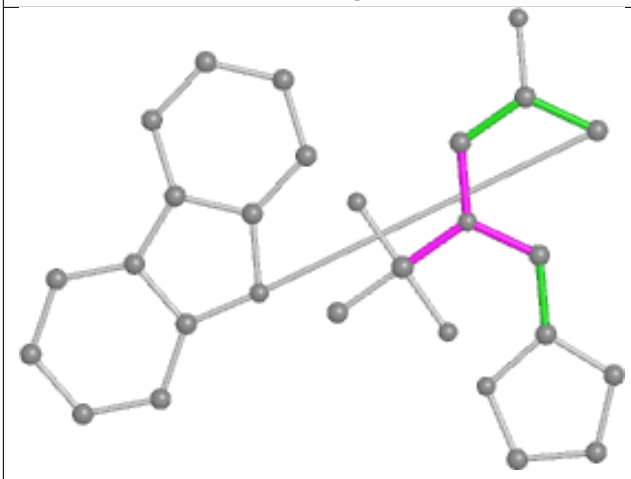
Ligand 2CX C 900



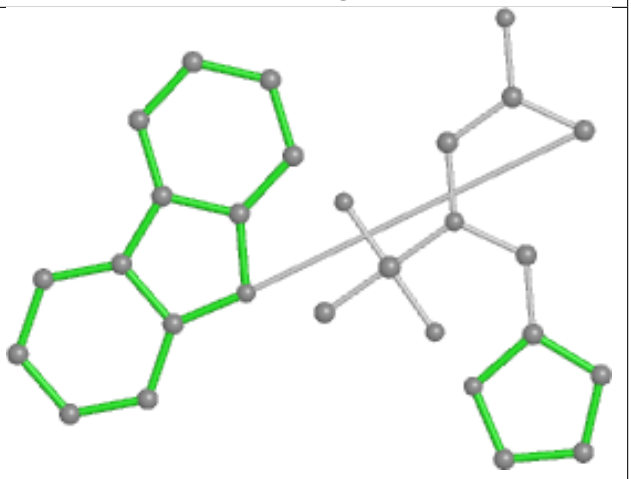
Bond lengths



Bond angles

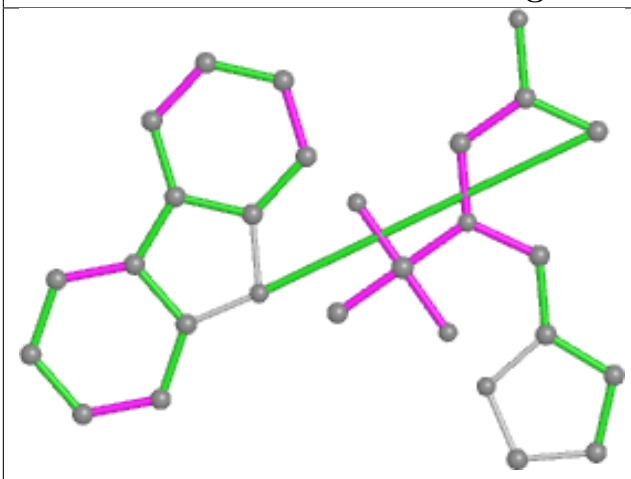


Torsions

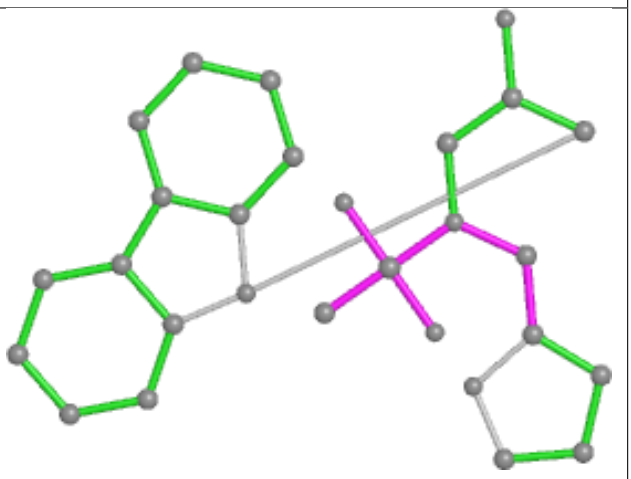


Rings

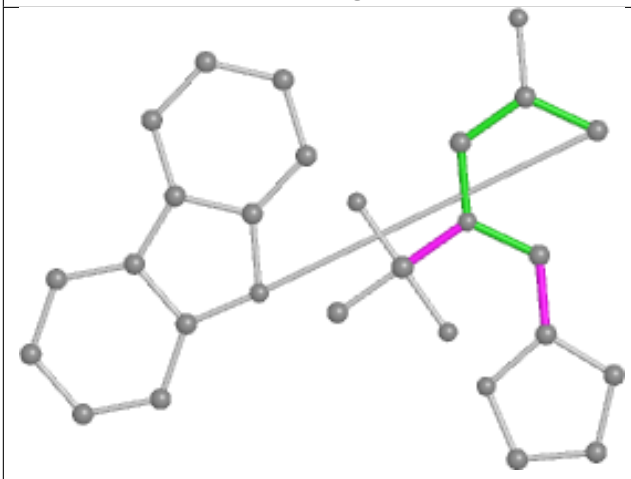
Ligand 2CX B 900



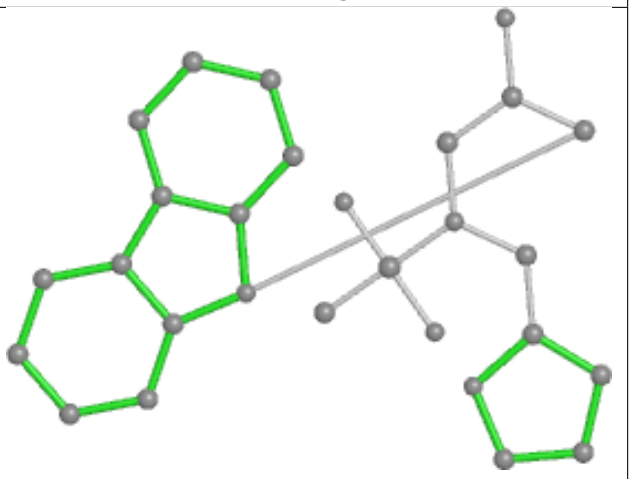
Bond lengths



Bond angles

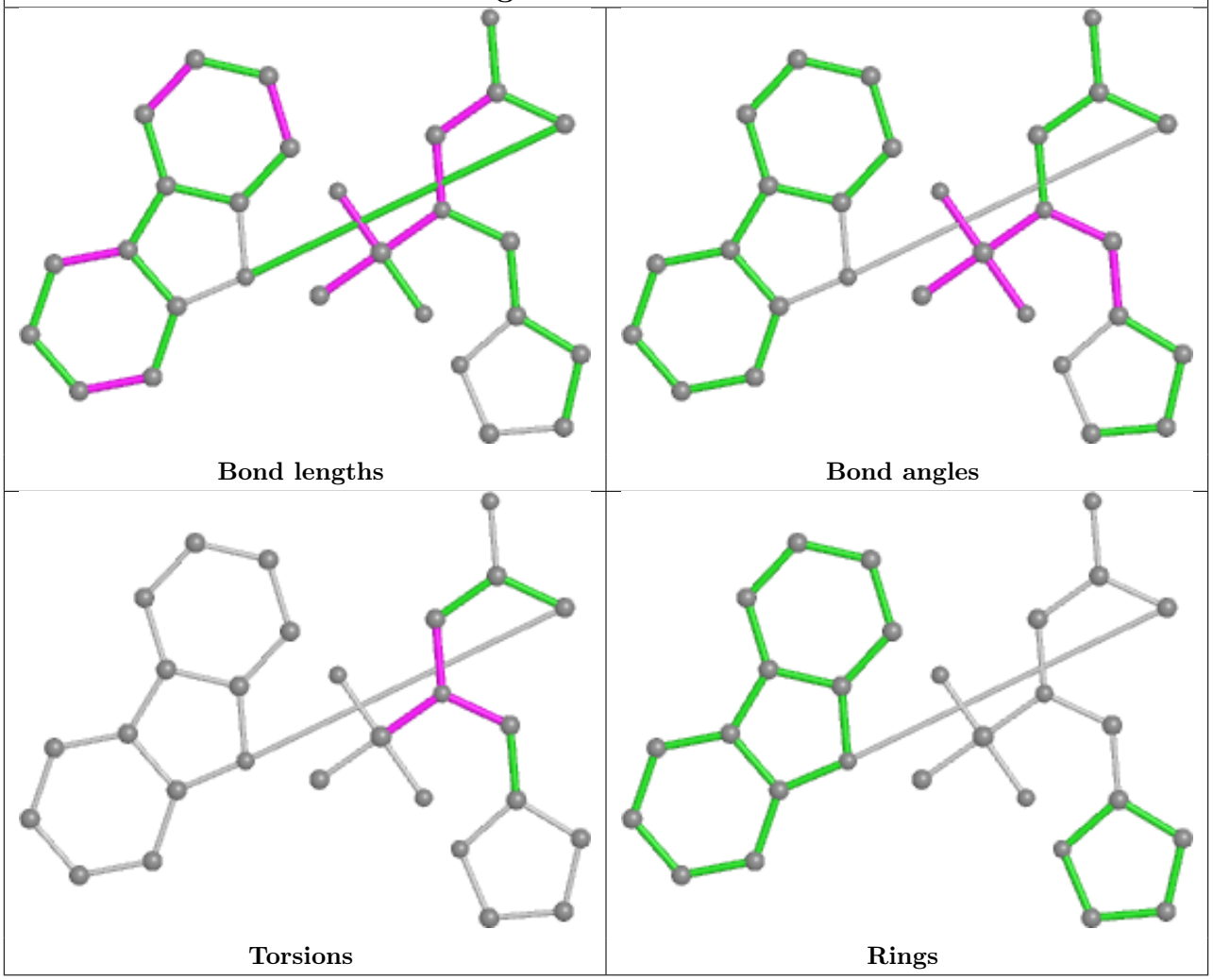


Torsions



Rings

Ligand 2CX A 900



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} 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	492/512 (96%)	0.43	17 (3%)	44	51	15, 26, 50, 74	0
1	B	492/512 (96%)	0.60	23 (4%)	31	39	19, 33, 54, 75	0
1	C	492/512 (96%)	0.41	18 (3%)	41	49	15, 26, 48, 71	0
1	D	492/512 (96%)	0.62	33 (6%)	17	24	19, 33, 54, 81	0
All	All	1968/2048 (96%)	0.52	91 (4%)	32	39	15, 29, 53, 81	0

All (91) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	427	PHE	8.5
1	D	428	PHE	7.5
1	D	297	ASN	5.3
1	C	426	GLN	5.0
1	A	428	PHE	4.9
1	C	425	GLN	4.7
1	D	196	CYS	4.5
1	B	424	PHE	4.4
1	C	202	GLU	4.3
1	B	202	GLU	4.0
1	D	424	PHE	3.9
1	C	195	SER	3.9
1	D	200	ILE	3.9
1	B	425	GLN	3.8
1	D	426	GLN	3.7
1	D	506	TYR	3.7
1	C	296	ARG	3.7
1	C	428	PHE	3.5
1	D	44	ARG	3.4
1	B	256	ARG	3.4
1	C	219	PRO	3.4

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Mol	Chain	Res	Type	RSRZ
1	A	297	ASN	3.3
1	D	468	ALA	3.3
1	B	193	MET	3.2
1	B	297	ASN	3.1
1	C	297	ASN	3.1
1	C	192	GLN	3.1
1	D	199	GLU	3.0
1	D	134	MET	3.0
1	A	200	ILE	3.0
1	B	123	PHE	3.0
1	A	424	PHE	2.9
1	C	206	ASP	2.9
1	D	123	PHE	2.9
1	A	123	PHE	2.9
1	B	191	GLN	2.8
1	C	254	ARG	2.8
1	D	110	GLY	2.7
1	D	326	ARG	2.7
1	B	129	ALA	2.7
1	A	196	CYS	2.7
1	A	431	TYR	2.7
1	D	502	MET	2.6
1	A	296	ARG	2.6
1	C	506	TYR	2.6
1	A	506	TYR	2.6
1	D	296	ARG	2.6
1	B	486	ARG	2.5
1	B	496	ARG	2.5
1	B	44	ARG	2.5
1	B	479	ILE	2.5
1	B	428	PHE	2.5
1	C	207	THR	2.5
1	A	201	GLN	2.5
1	A	427	PHE	2.5
1	D	298	SER	2.5
1	D	451	LEU	2.4
1	D	496	ARG	2.4
1	A	504	GLN	2.4
1	C	424	PHE	2.4
1	B	426	GLN	2.4
1	B	195	SER	2.4
1	C	427	PHE	2.3

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Mol	Chain	Res	Type	RSRZ
1	D	206	ASP	2.3
1	A	199	GLU	2.3
1	A	202	GLU	2.3
1	D	254	ARG	2.3
1	A	194	GLU	2.2
1	C	198	ALA	2.2
1	A	195	SER	2.2
1	A	426	GLN	2.2
1	B	387	ASP	2.2
1	B	218	PHE	2.2
1	B	351	GLY	2.1
1	C	191	GLN	2.1
1	B	112	THR	2.1
1	D	507	GLN	2.1
1	D	500	GLU	2.1
1	D	509	LEU	2.1
1	D	92	PHE	2.1
1	D	207	THR	2.1
1	D	387	ASP	2.1
1	D	322	PRO	2.1
1	B	104	ARG	2.1
1	B	200	ILE	2.1
1	B	87	LEU	2.1
1	D	425	GLN	2.0
1	C	86	LYS	2.0
1	D	21	ALA	2.0
1	D	49	VAL	2.0
1	D	489	VAL	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum,

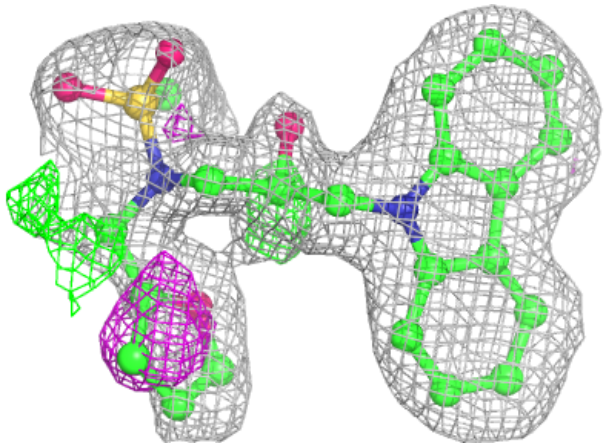
median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

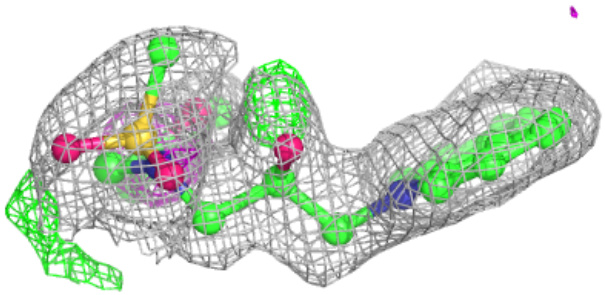
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	2CX	D	900	28/28	0.86	0.19	25,32,44,47	0
2	2CX	C	900	28/28	0.87	0.18	22,28,41,43	0
2	2CX	B	900	28/28	0.91	0.16	24,31,42,43	0
2	2CX	A	900	28/28	0.91	0.15	20,27,40,41	0

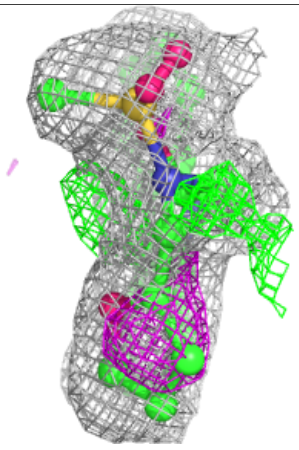
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around 2CX D 900:

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

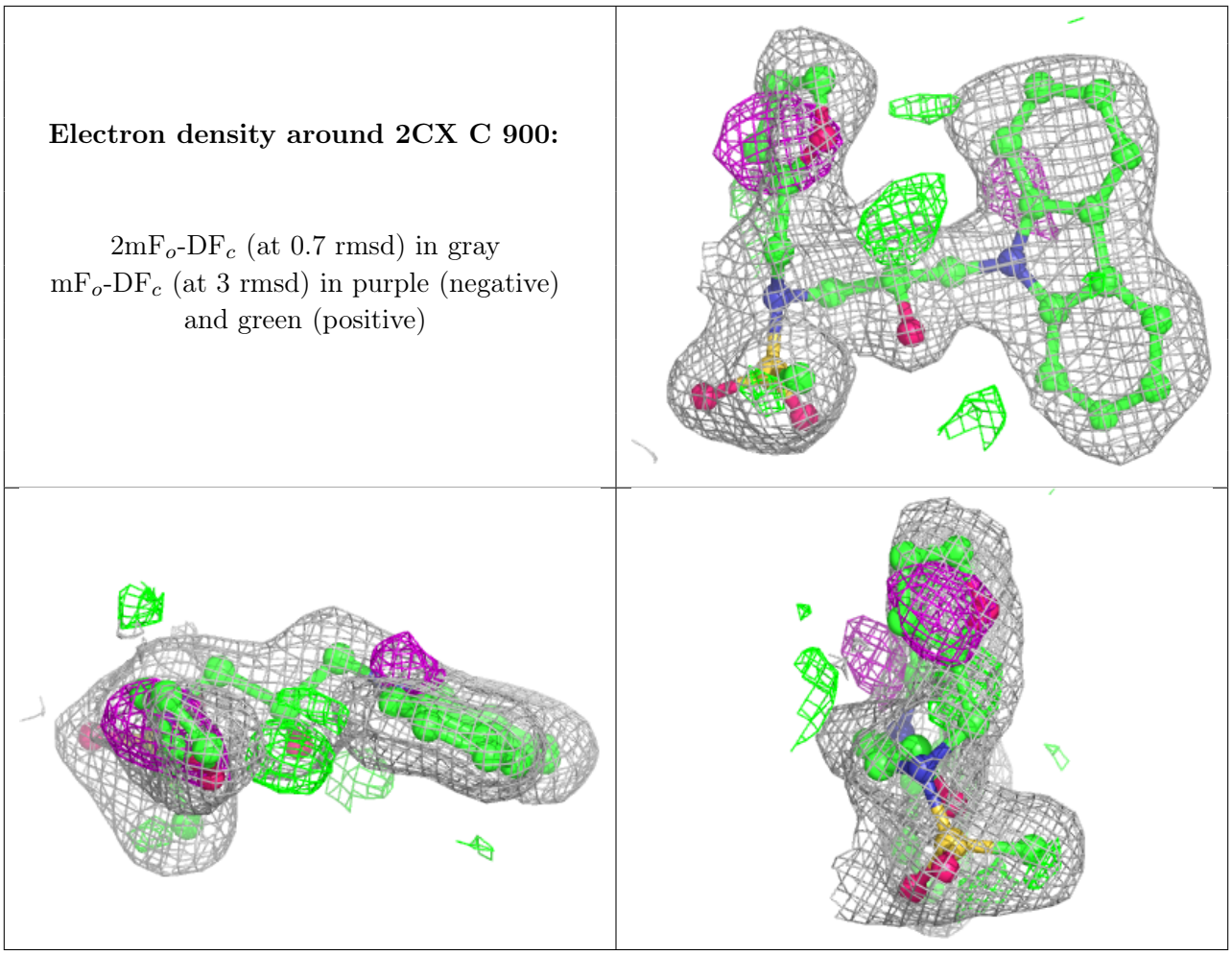






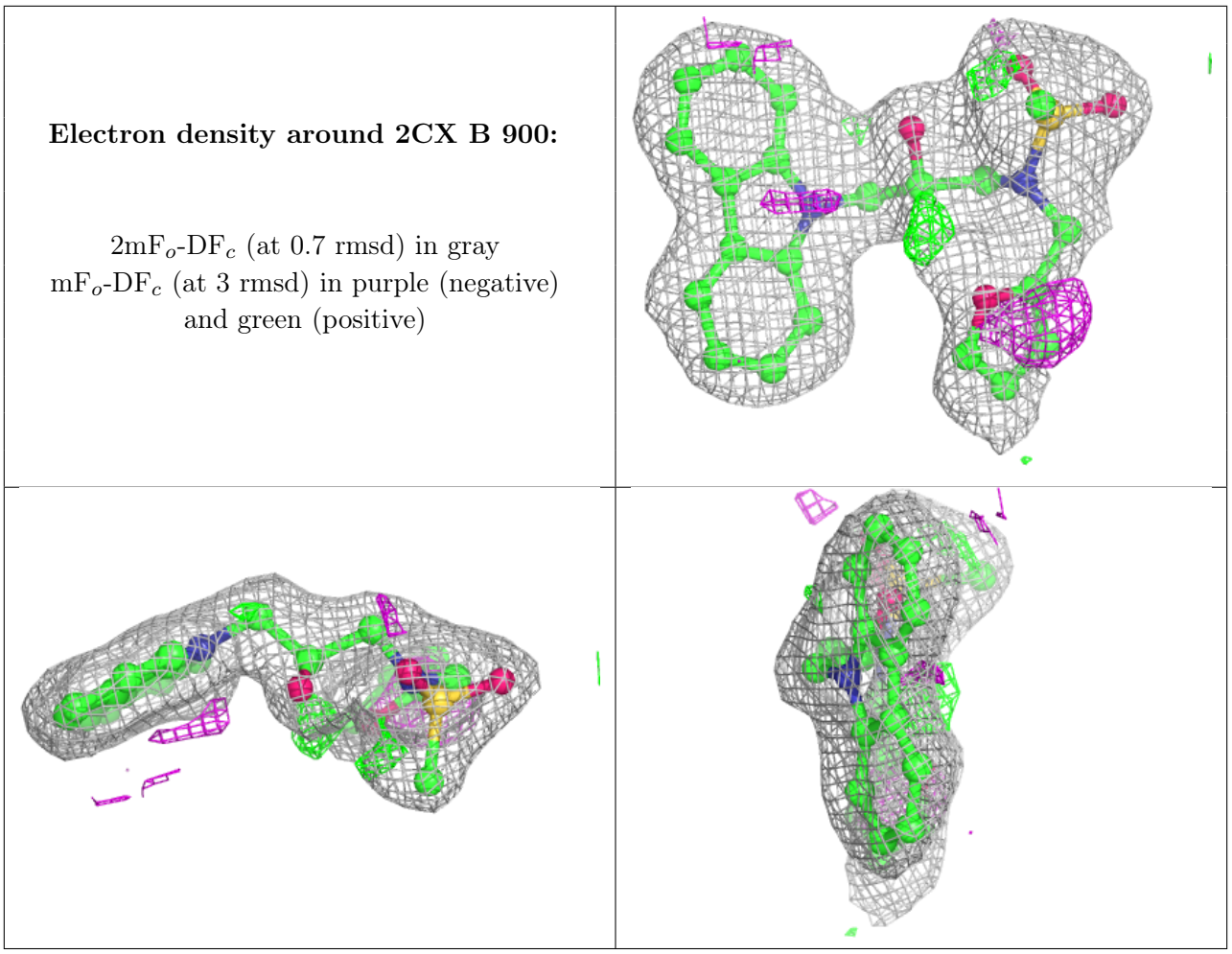
Electron density around 2CX C 900:

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



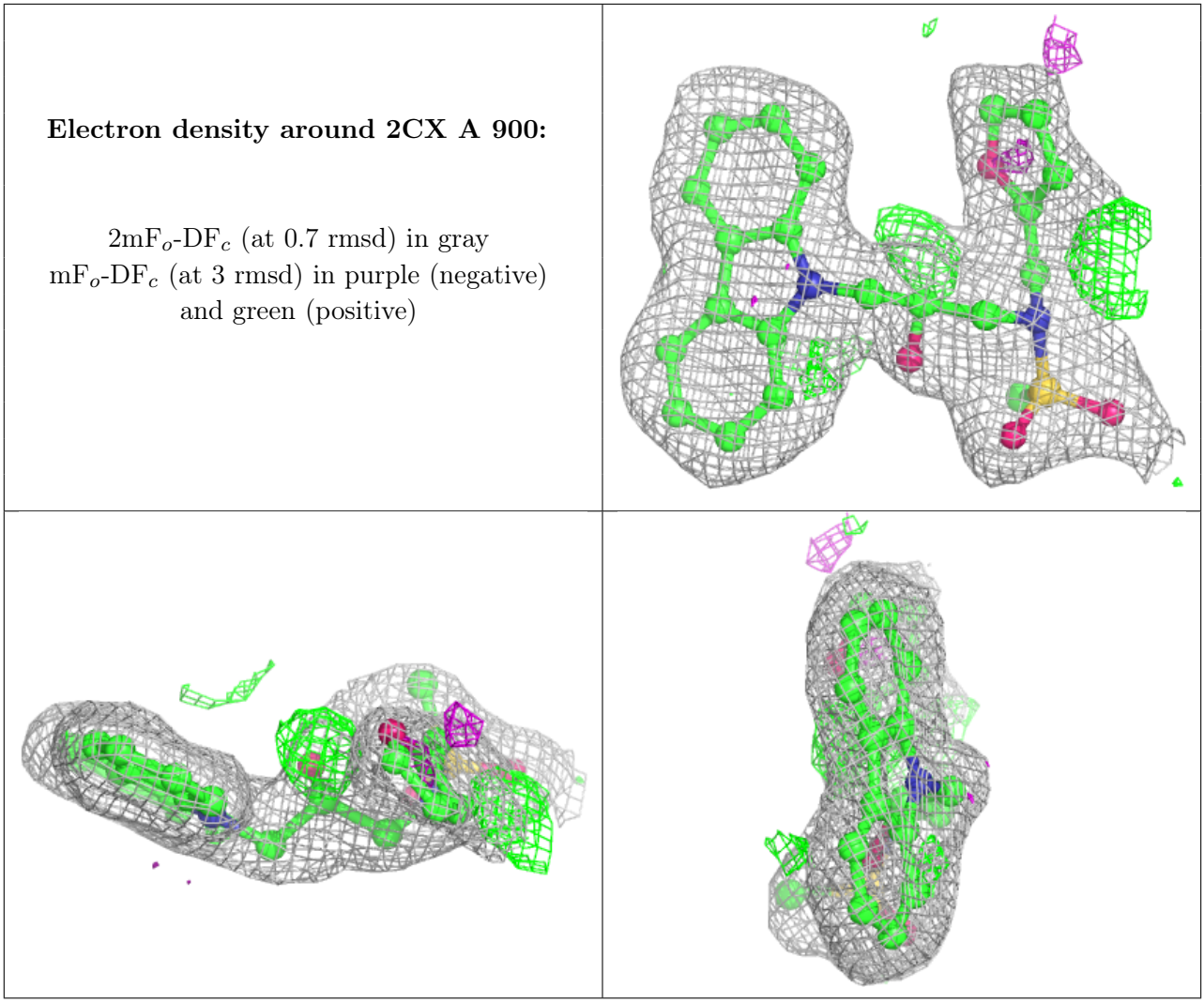
Electron density around 2CX B 900:

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



Electron density around 2CX A 900:

$2mF_o$-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.