Full wwPDB X-ray Structure Validation Report (i)

Jun 19, 2024 – 05:54 AM EDT

PDB ID	:	4MPU
Title	:	Human beta-tryptase co-crystal structure with (6S,8R)-N,N'-bis[3-({4-[3-(aminomethyl)phenyl]piperidin-1-yl}carbonyl)phenyl]-8-hydroxy-6-(1-hydroxycyclobutyl)-5,7-dioxaspiro[3.4]octane-6,8-dicarboxamide
Authors	:	White, A.; Stein, A.J.; Suto, R.K.
Deposited on	:	2013-09-13
Resolution	:	1.65 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:

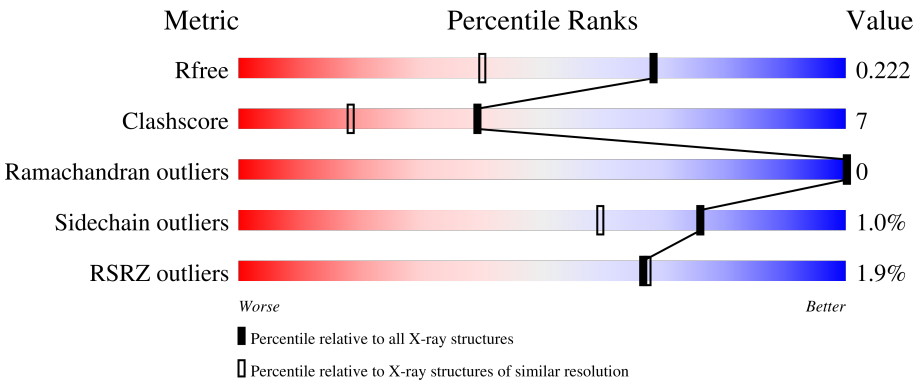
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.37.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

1 Overall quality at a glance (i)

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

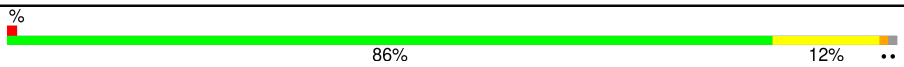
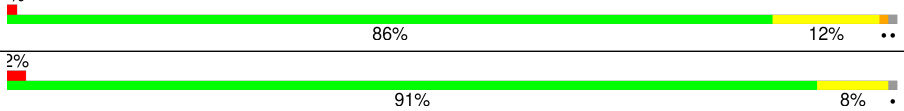
The reported resolution of this entry is 1.65 Å.

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	3122 (1.66-1.62)
Clashscore	141614	3268 (1.66-1.62)
Ramachandran outliers	138981	3215 (1.66-1.62)
Sidechain outliers	138945	3215 (1.66-1.62)
RSRZ outliers	127900	3079 (1.66-1.62)

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	245	
1	B	245	

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
5	X2A	B	301[C]	X	-	-	-
5	X2A	B	301[D]	X	-	-	-

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 4793 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.

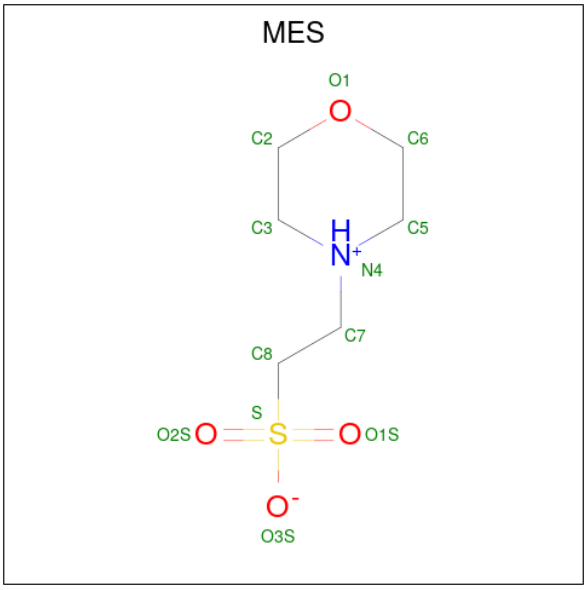
- Molecule 1 is a protein called Tryptase alpha/beta-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	243	1999	1278	353	356	12	0	10	0
1	B	243	1953	1250	346	345	12	0	5	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	132	LYS	ASN	SEE REMARK 999	UNP Q15661
B	132	LYS	ASN	SEE REMARK 999	UNP Q15661

- Molecule 2 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (three-letter code: MES) (formula: $C_6H_{13}NO_4S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	S		
2	A	1	12	6	1	4	1	0	0

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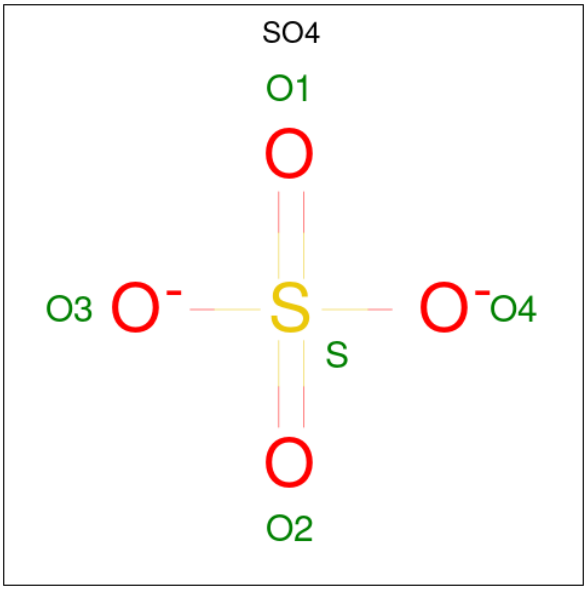
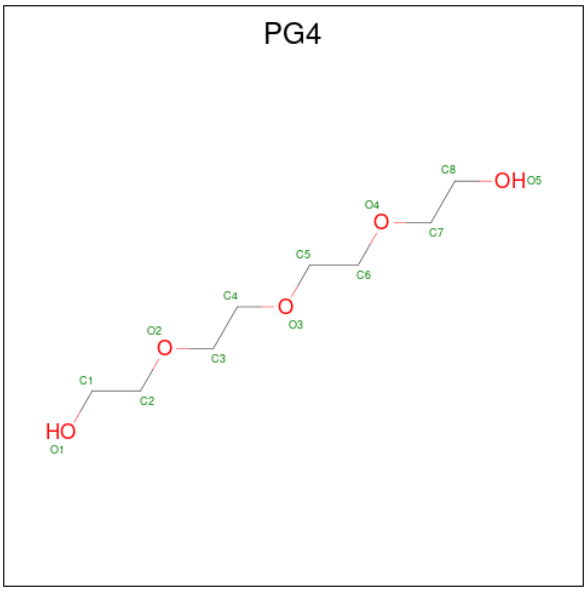
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	S		
2	B	1	12	6	1	4	1	0	0

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



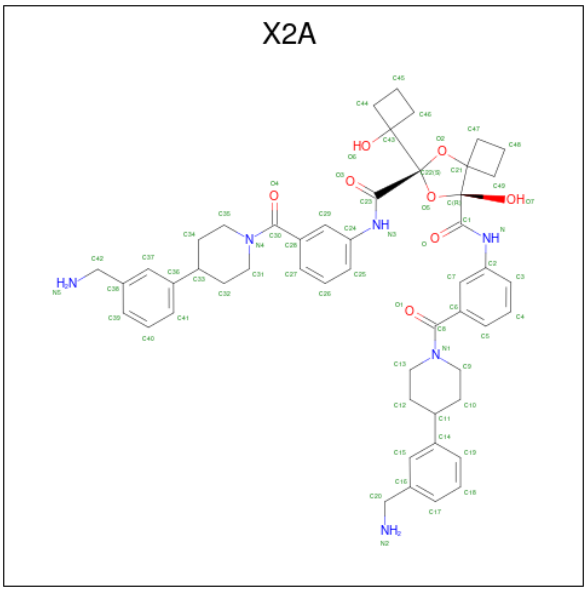
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	O	S		
3	A	1	5	4	1	0	0
3	B	1	5	4	1	0	0
3	B	1	5	4	1	0	0
3	B	1	5	4	1	0	0

- Molecule 4 is TETRAETHYLENE GLYCOL (three-letter code: PG4) (formula: $C_8H_{18}O_5$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
4	A	1	13	8	5	0	0
			Total	C	O		
4	B	1	13	8	5	0	0

- Molecule 5 is (6S,8R)-N,N'-bis[3-({4-[3-(aminomethyl)phenyl]piperidin-1-yl}carbonyl)phenyl]-8-hydroxy-6-(1-hydroxycyclobutyl)-5,7-dioxaspiro[3.4]octane-6,8-dicarboxamide (three-letter code: X2A) (formula: $C_{50}H_{58}N_6O_8$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
5	B	1	256	200	24	32	0	1

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
6	A	274	274	274	0	0
			Total	O		
6	B	241	241	241	0	0

3 Residue-property plots (i)

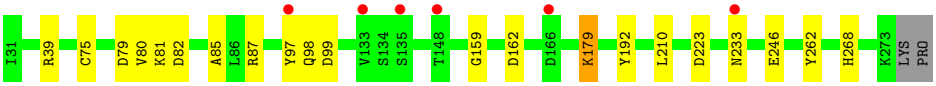
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Tryptase alpha/beta-1

Chain A:

• Molecule 1: Tryptase alpha/beta-1

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α, β, γ	78.16Å 78.16Å 165.04Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	19.80 – 1.65 19.73 – 1.65	Depositor EDS
% Data completeness (in resolution range)	99.3 (19.80-1.65) 99.4 (19.73-1.65)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.02 (at 1.65Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, R_{free}	0.178 , 0.216 0.188 , 0.222	Depositor DCC
R_{free} test set	3575 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å^2)	20.7	Xtriage
Anisotropy	0.033	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.38 , 40.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	0.024 for -h,-k,l	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	4793	wwPDB-VP
Average B, all atoms (Å^2)	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.65% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: SO4, PG4, X2A, MES

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	1.19	1/2074 (0.0%)	1.18	13/2837 (0.5%)
1	B	1.17	3/2024 (0.1%)	1.16	6/2773 (0.2%)
All	All	1.18	4/4098 (0.1%)	1.17	19/5610 (0.3%)

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

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	87	ARG	CZ-NH1	5.97	1.40	1.33
1	B	268	HIS	N-CA	5.05	1.56	1.46
1	B	159	GLY	N-CA	-5.04	1.38	1.46
1	B	75	CYS	CB-SG	-5.00	1.73	1.81

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	87	ARG	NE-CZ-NH1	11.54	126.07	120.30
1	A	87	ARG	NE-CZ-NH2	-7.75	116.42	120.30
1	A	253	ARG	NE-CZ-NH2	-7.48	116.56	120.30
1	B	82	ASP	CB-CG-OD2	-6.92	112.07	118.30
1	A	162	ASP	CB-CG-OD1	6.79	124.41	118.30
1	B	162	ASP	CB-CG-OD1	6.41	124.07	118.30
1	A	58	PHE	CB-CG-CD1	6.13	125.09	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	99	ASP	CB-CG-OD1	5.95	123.66	118.30
1	A	189	ASP	CB-CG-OD1	5.90	123.61	118.30
1	A	259	ARG	NE-CZ-NH2	5.76	123.18	120.30
1	A	99	ASP	CB-CG-OD1	5.50	123.25	118.30
1	A	176	LYS	CD-CE-NZ	5.42	124.17	111.70
1	A	164	ASP	CB-CG-OD1	5.33	123.10	118.30
1	A	99	ASP	CB-CG-OD2	-5.32	113.52	118.30
1	B	87	ARG	NE-CZ-NH2	-5.30	117.65	120.30
1	B	262	TYR	CB-CG-CD1	5.26	124.16	121.00
1	B	223	ASP	CB-CG-OD1	-5.25	113.58	118.30
1	A	207	ASP	CB-CG-OD2	-5.13	113.69	118.30
1	A	206	ARG	NE-CZ-NH2	-5.08	117.76	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	272	PRO	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	1999	0	1932	18	0
1	B	1953	0	1884	13	0
2	A	12	0	13	0	0
2	B	12	0	13	1	0
3	A	5	0	0	0	0
3	B	15	0	0	1	0
4	A	13	0	18	4	0
4	B	13	0	18	2	0
5	B	256	0	231	31	0
6	A	274	0	0	7	0
6	B	241	0	0	9	0
All	All	4793	0	4109	62	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 7.

All (62) 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)
5:B:301[B]:X2A:H39	5:B:301[B]:X2A:H36	1.41	1.01
6:A:532:HOH:O	5:B:301[A]:X2A:H33	1.72	0.90
1:B:81:LYS:NZ	6:B:516:HOH:O	2.02	0.80
5:B:301[B]:X2A:H36	5:B:301[B]:X2A:C7	2.13	0.76
1:B:179[A]:LYS:HB3	1:B:179[A]:LYS:HZ2	1.52	0.75
5:B:301[C]:X2A:H36	6:B:513:HOH:O	1.90	0.71
5:B:301[C]:X2A:H31	5:B:301[C]:X2A:N	2.07	0.69
5:B:301[A]:X2A:C49	5:B:301[A]:X2A:H23	2.07	0.67
5:B:301[D]:X2A:H26	5:B:301[D]:X2A:H22	1.76	0.66
1:A:81:LYS:HG3	6:A:517:HOH:O	1.96	0.64
5:B:301[C]:X2A:C47	6:B:513:HOH:O	2.42	0.63
2:B:302:MES:H22	3:B:305:SO4:O1	2.00	0.62
1:B:179[A]:LYS:HB3	1:B:179[A]:LYS:NZ	2.13	0.62
5:B:301[D]:X2A:H35	5:B:301[D]:X2A:H39	1.83	0.61
1:B:210:LEU:C	1:B:210:LEU:HD23	2.22	0.60
1:A:246[B]:GLU:HA	5:B:301[B]:X2A:H40	1.84	0.58
1:A:136[B]:HIS:NE2	6:A:535:HOH:O	2.26	0.58
5:B:301[C]:X2A:C48	6:B:513:HOH:O	2.53	0.56
4:A:303:PG4:H41	6:A:525:HOH:O	2.05	0.55
4:A:303:PG4:H71	6:A:525:HOH:O	2.06	0.55
1:A:153:MET:HG3	1:A:154:PRO:HD2	1.89	0.55
1:B:97:TYR:CD2	1:B:98:GLN:HG2	2.43	0.54
1:B:85:ALA:HB3	4:B:306:PG4:H41	1.90	0.54
5:B:301[C]:X2A:H33	6:B:513:HOH:O	2.08	0.53
5:B:301[A]:X2A:C29	5:B:301[A]:X2A:H32	2.39	0.52
1:A:197:TYR:CE1	1:B:80[B]:VAL:HG12	2.45	0.52
5:B:301[A]:X2A:O6	5:B:301[A]:X2A:N	2.44	0.51
5:B:301[C]:X2A:N	5:B:301[C]:X2A:C49	2.73	0.50
1:B:39[A]:ARG:HG3	6:B:575:HOH:O	2.11	0.49
5:B:301[A]:X2A:C49	5:B:301[A]:X2A:N3	2.73	0.49
5:B:301[C]:X2A:C29	5:B:301[C]:X2A:H2	2.40	0.49
5:B:301[A]:X2A:H23	5:B:301[A]:X2A:C21	2.24	0.49
5:B:301[A]:X2A:N3	5:B:301[A]:X2A:C21	2.76	0.48
5:B:301[C]:X2A:O6	5:B:301[C]:X2A:H32	2.13	0.48
1:A:186:HIS:HD2	6:A:647:HOH:O	1.96	0.48
1:A:246[A]:GLU:HA	5:B:301[A]:X2A:H19	1.96	0.47
1:A:41[A]:LYS:NZ	6:A:558:HOH:O	2.25	0.46
5:B:301[A]:X2A:H32	5:B:301[A]:X2A:C24	2.46	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:197:TYR:CE2	1:B:80[B]:VAL:HA	2.51	0.45
1:A:191[B]:LYS:HD3	1:A:191[B]:LYS:HA	1.80	0.45
5:B:301[C]:X2A:H31	5:B:301[C]:X2A:H39	1.99	0.45
1:B:192:TYR:HE2	1:B:246[B]:GLU:HG3	1.82	0.45
1:A:149:PHE:O	1:A:182:ILE:HG21	2.18	0.44
1:A:81:LYS:HA	4:A:303:PG4:H21	1.99	0.43
1:B:233:ASN:ND2	6:B:617:HOH:O	2.29	0.43
5:B:301[D]:X2A:H39	5:B:301[D]:X2A:C47	2.48	0.42
1:A:90:LEU:O	1:A:91[A]:ARG:C	2.57	0.42
5:B:301[A]:X2A:H32	5:B:301[A]:X2A:N3	2.35	0.42
1:A:224:SER:HA	1:A:242:VAL:CG1	2.50	0.41
5:B:301[B]:X2A:N3	5:B:301[B]:X2A:H29	2.35	0.41
1:A:224:SER:HA	1:A:242:VAL:HG12	2.02	0.41
5:B:301[C]:X2A:N3	5:B:301[C]:X2A:O7	2.53	0.41
1:A:81:LYS:HB3	4:A:303:PG4:H52	2.03	0.41
5:B:301[D]:X2A:H25	6:B:513:HOH:O	2.19	0.41
4:B:306:PG4:C3	6:B:484:HOH:O	2.69	0.41
1:B:79:ASP:O	1:B:81:LYS:HE3	2.20	0.41
1:A:34:GLY:H	1:A:176:LYS:HZ1	1.69	0.41
1:B:98:GLN:HE21	1:B:98:GLN:HA	1.86	0.41
1:A:95:LEU:HG	1:A:160:TRP:CD1	2.57	0.40
5:B:301[C]:X2A:O7	5:B:301[C]:X2A:C23	2.70	0.40
5:B:301[C]:X2A:O3	5:B:301[C]:X2A:H26	2.20	0.40
5:B:301[D]:X2A:O	5:B:301[D]:X2A:C44	2.69	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	251/245 (102%)	241 (96%)	10 (4%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	246/245 (100%)	241 (98%)	5 (2%)	0	100	100
All	All	497/490 (101%)	482 (97%)	15 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	218/210 (104%)	214 (98%)	4 (2%)	59	34
1	B	211/210 (100%)	209 (99%)	2 (1%)	78	63
All	All	429/420 (102%)	423 (99%)	6 (1%)	76	45

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	66	PRO
1	A	98	GLN
1	A	136[A]	HIS
1	A	136[B]	HIS
1	B	179[A]	LYS
1	B	179[B]	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	112	GLN
1	B	98	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)

12 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	$\#\|Z\| > 2$
5	X2A	B	301[A]	-	68,72,72	1.70	15 (22%)	81,108,108	1.87	15 (18%)
5	X2A	B	301[D]	-	68,72,72	1.89	15 (22%)	81,108,108	2.35	20 (24%)
3	SO4	B	304	-	4,4,4	0.55	0	6,6,6	0.59	0
3	SO4	B	305	-	4,4,4	0.67	0	6,6,6	1.02	1 (16%)
5	X2A	B	301[B]	-	68,72,72	2.36	19 (27%)	81,108,108	2.25	25 (30%)
5	X2A	B	301[C]	-	68,72,72	2.02	14 (20%)	81,108,108	2.10	21 (25%)
2	MES	B	302	-	12,12,12	1.32	2 (16%)	15,16,16	1.46	2 (13%)
3	SO4	A	302	-	4,4,4	0.57	0	6,6,6	0.66	0
4	PG4	A	303	-	12,12,12	0.74	0	11,11,11	0.73	0
3	SO4	B	303	-	4,4,4	0.73	0	6,6,6	0.40	0
2	MES	A	301	-	12,12,12	1.44	2 (16%)	15,16,16	1.29	2 (13%)
4	PG4	B	306	-	12,12,12	0.72	0	11,11,11	0.44	0

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
5	X2A	B	301[A]	-	-	10/42/114/114	0/9/9/9

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	X2A	B	301[D]	-	2/2/12/14	7/42/114/114	0/9/9/9
5	X2A	B	301[B]	-	-	8/42/114/114	0/9/9/9
5	X2A	B	301[C]	-	2/2/12/14	7/42/114/114	0/9/9/9
2	MES	B	302	-	-	1/6/14/14	0/1/1/1
2	MES	A	301	-	-	4/6/14/14	0/1/1/1
4	PG4	A	303	-	-	8/10/10/10	-
4	PG4	B	306	-	-	5/10/10/10	-

All (67) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	301[B]	X2A	C-C1	-9.23	1.42	1.54
5	B	301[D]	X2A	C22-C23	-7.17	1.45	1.54
5	B	301[C]	X2A	C-C1	-6.82	1.45	1.54
5	B	301[B]	X2A	C2-N	-6.27	1.29	1.41
5	B	301[A]	X2A	C22-C23	-6.13	1.46	1.54
5	B	301[B]	X2A	C24-N3	-6.05	1.29	1.41
5	B	301[B]	X2A	C22-C23	-5.98	1.46	1.54
5	B	301[C]	X2A	C2-N	-5.97	1.29	1.41
5	B	301[C]	X2A	C22-C23	-5.74	1.47	1.54
5	B	301[D]	X2A	C-C1	-5.49	1.47	1.54
5	B	301[B]	X2A	O2-C21	-5.18	1.40	1.45
5	B	301[A]	X2A	C24-N3	-4.69	1.32	1.41
5	B	301[D]	X2A	O2-C21	-4.28	1.41	1.45
5	B	301[D]	X2A	C2-N	-4.28	1.33	1.41
5	B	301[A]	X2A	C2-N	-4.12	1.33	1.41
5	B	301[C]	X2A	C29-C28	-3.92	1.33	1.39
5	B	301[C]	X2A	C1-N	-3.83	1.26	1.35
5	B	301[B]	X2A	C29-C28	-3.78	1.33	1.39
5	B	301[C]	X2A	C24-N3	-3.76	1.34	1.41
2	A	301	MES	C8-S	-3.65	1.72	1.77
5	B	301[C]	X2A	O2-C21	-3.64	1.42	1.45
5	B	301[D]	X2A	C24-N3	-3.34	1.34	1.41
5	B	301[B]	X2A	C7-C6	-3.33	1.34	1.39
5	B	301[B]	X2A	C23-N3	-3.24	1.28	1.35
5	B	301[C]	X2A	C7-C6	-3.12	1.34	1.39
5	B	301[A]	X2A	C-C1	-3.06	1.50	1.54
5	B	301[B]	X2A	C4-C3	-3.04	1.33	1.38
5	B	301[D]	X2A	C1-N	-3.02	1.28	1.35
5	B	301[B]	X2A	C1-N	-2.83	1.29	1.35
2	B	302	MES	C8-S	-2.79	1.73	1.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	301[B]	X2A	C18-C17	-2.77	1.34	1.38
5	B	301[B]	X2A	C37-C36	-2.75	1.35	1.39
5	B	301[A]	X2A	C40-C39	-2.73	1.34	1.38
5	B	301[D]	X2A	C18-C17	-2.73	1.34	1.38
5	B	301[C]	X2A	C40-C39	-2.71	1.34	1.38
5	B	301[C]	X2A	C15-C14	-2.70	1.35	1.39
5	B	301[A]	X2A	C15-C14	-2.69	1.35	1.39
5	B	301[D]	X2A	C37-C36	-2.69	1.35	1.39
5	B	301[D]	X2A	C29-C28	-2.69	1.35	1.39
2	B	302	MES	C5-N4	2.64	1.54	1.46
5	B	301[B]	X2A	O4-C30	-2.61	1.17	1.22
5	B	301[B]	X2A	O7-C	2.61	1.44	1.39
5	B	301[A]	X2A	O2-C21	-2.60	1.43	1.45
5	B	301[C]	X2A	O1-C8	-2.45	1.17	1.22
5	B	301[A]	X2A	O7-C	2.43	1.44	1.39
5	B	301[B]	X2A	C31-N4	-2.42	1.42	1.47
5	B	301[C]	X2A	C9-N1	-2.36	1.42	1.47
5	B	301[D]	X2A	O7-C	2.32	1.43	1.39
5	B	301[A]	X2A	O5-C	-2.30	1.38	1.42
5	B	301[D]	X2A	C31-N4	-2.23	1.43	1.47
5	B	301[A]	X2A	C23-N3	-2.22	1.30	1.35
5	B	301[D]	X2A	O4-C30	-2.21	1.18	1.22
5	B	301[A]	X2A	C13-N1	-2.16	1.43	1.47
5	B	301[B]	X2A	C19-C14	-2.15	1.35	1.39
5	B	301[D]	X2A	C19-C14	-2.15	1.35	1.39
5	B	301[C]	X2A	C41-C36	-2.14	1.35	1.39
5	B	301[B]	X2A	C26-C25	-2.14	1.35	1.38
5	B	301[A]	X2A	C41-C36	-2.11	1.35	1.39
5	B	301[D]	X2A	C4-C3	-2.10	1.35	1.38
5	B	301[A]	X2A	C1-N	-2.08	1.30	1.35
5	B	301[B]	X2A	C4-C5	-2.08	1.35	1.38
5	B	301[C]	X2A	O7-C	2.06	1.43	1.39
5	B	301[B]	X2A	C14-C11	-2.02	1.48	1.52
2	A	301	MES	O1S-S	2.02	1.50	1.45
5	B	301[A]	X2A	C36-C33	-2.01	1.48	1.52
5	B	301[A]	X2A	O1-C8	-2.01	1.18	1.22
5	B	301[D]	X2A	C46-C43	-2.01	1.52	1.53

All (86) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	B	301[D]	X2A	O5-C22-C23	-13.58	88.24	109.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	B	301[B]	X2A	O5-C22-C23	-9.76	94.30	109.81
5	B	301[C]	X2A	O5-C22-C23	-9.13	95.31	109.81
5	B	301[A]	X2A	O5-C22-C23	-9.03	95.47	109.81
5	B	301[C]	X2A	O5-C-C1	-7.47	93.50	109.35
5	B	301[D]	X2A	O5-C-C1	-6.74	95.05	109.35
5	B	301[B]	X2A	C3-C2-C7	5.91	126.80	119.66
5	B	301[A]	X2A	O5-C-C1	-5.43	97.83	109.35
5	B	301[B]	X2A	C4-C5-C6	5.19	125.46	120.36
5	B	301[A]	X2A	C28-C30-N4	4.52	124.31	118.66
5	B	301[D]	X2A	C6-C8-N1	4.51	124.30	118.66
5	B	301[B]	X2A	C6-C8-N1	4.43	124.19	118.66
5	B	301[C]	X2A	O7-C-C1	4.35	120.72	108.96
5	B	301[B]	X2A	C25-C24-C29	4.21	124.74	119.66
5	B	301[C]	X2A	C3-C2-C7	4.14	124.66	119.66
5	B	301[B]	X2A	C4-C3-C2	-4.00	115.11	119.73
5	B	301[B]	X2A	O-C1-N	3.98	133.14	123.34
5	B	301[D]	X2A	C24-N3-C23	-3.97	119.79	126.86
5	B	301[A]	X2A	O7-C-C1	3.97	119.67	108.96
5	B	301[D]	X2A	C4-C5-C6	3.78	124.08	120.36
5	B	301[B]	X2A	C26-C27-C28	3.74	124.04	120.36
5	B	301[D]	X2A	O3-C23-N3	3.67	132.39	123.34
5	B	301[B]	X2A	C2-N-C1	-3.67	120.33	126.86
5	B	301[C]	X2A	C28-C30-N4	3.58	123.13	118.66
5	B	301[A]	X2A	C26-C27-C28	3.54	123.85	120.36
5	B	301[D]	X2A	C45-C44-C43	3.38	92.07	88.55
5	B	301[C]	X2A	C24-N3-C23	-3.38	120.86	126.86
5	B	301[B]	X2A	C6-C7-C2	-3.31	116.17	120.44
5	B	301[D]	X2A	C45-C46-C43	3.28	91.97	88.55
2	B	302	MES	O2S-S-C8	3.27	111.67	106.73
5	B	301[D]	X2A	C28-C30-N4	3.14	122.59	118.66
5	B	301[A]	X2A	C25-C24-C29	3.08	123.37	119.66
5	B	301[C]	X2A	C7-C2-N	-3.01	110.34	120.13
5	B	301[C]	X2A	C4-C3-C2	-3.01	116.26	119.73
5	B	301[C]	X2A	C26-C27-C28	3.01	123.32	120.36
5	B	301[B]	X2A	C28-C30-N4	2.95	122.34	118.66
5	B	301[B]	X2A	O1-C8-C6	-2.94	114.45	120.29
5	B	301[C]	X2A	O2-C22-C23	2.92	114.44	109.81
5	B	301[B]	X2A	C25-C24-N3	-2.88	110.76	120.41
5	B	301[C]	X2A	O3-C23-N3	2.83	130.32	123.34
5	B	301[B]	X2A	O3-C23-N3	2.81	130.27	123.34
5	B	301[B]	X2A	C35-C34-C33	2.79	114.26	111.00
5	B	301[C]	X2A	C6-C8-N1	2.77	122.13	118.66

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	B	301[B]	X2A	C10-C9-N1	-2.77	105.23	110.66
5	B	301[B]	X2A	C32-C31-N4	-2.77	105.24	110.66
5	B	301[D]	X2A	C12-C13-N1	-2.77	105.25	110.66
2	A	301	MES	O2S-S-O1S	-2.76	104.84	113.82
5	B	301[C]	X2A	C13-C12-C11	2.73	114.19	111.00
5	B	301[A]	X2A	C34-C35-N4	-2.73	105.32	110.66
5	B	301[C]	X2A	C10-C9-N1	-2.72	105.33	110.66
2	B	302	MES	O2S-S-O1S	-2.72	104.97	113.82
5	B	301[B]	X2A	C26-C25-C24	-2.70	116.61	119.73
5	B	301[A]	X2A	C6-C8-N1	2.69	122.02	118.66
5	B	301[D]	X2A	C3-C2-C7	2.69	122.90	119.66
5	B	301[D]	X2A	C35-C34-C33	2.68	114.13	111.00
5	B	301[D]	X2A	C32-C31-N4	-2.65	105.47	110.66
5	B	301[C]	X2A	C34-C35-N4	-2.62	105.53	110.66
5	B	301[A]	X2A	C9-C10-C11	2.61	114.06	111.00
5	B	301[B]	X2A	C3-C2-N	-2.56	111.81	120.41
5	B	301[C]	X2A	O7-C-O5	2.55	114.30	110.54
5	B	301[C]	X2A	C4-C5-C6	2.50	122.83	120.36
5	B	301[C]	X2A	C12-C13-N1	-2.47	105.82	110.66
5	B	301[D]	X2A	C34-C35-N4	-2.45	105.86	110.66
5	B	301[C]	X2A	C41-C36-C37	-2.42	115.93	118.74
5	B	301[B]	X2A	C34-C35-N4	-2.42	105.93	110.66
5	B	301[A]	X2A	C41-C36-C37	-2.41	115.94	118.74
5	B	301[B]	X2A	O5-C-C1	-2.38	104.30	109.35
5	B	301[A]	X2A	O3-C23-N3	2.38	129.20	123.34
5	B	301[D]	X2A	O1-C8-C6	-2.37	115.59	120.29
5	B	301[D]	X2A	C19-C14-C15	-2.36	116.00	118.74
5	B	301[D]	X2A	C2-N-C1	-2.35	122.67	126.86
5	B	301[A]	X2A	O4-C30-C28	-2.34	115.64	120.29
5	B	301[A]	X2A	C12-C13-N1	-2.33	106.10	110.66
5	B	301[B]	X2A	C19-C14-C15	-2.29	116.08	118.74
5	B	301[A]	X2A	C10-C9-N1	-2.28	106.19	110.66
2	A	301	MES	C5-N4-C3	-2.25	104.00	108.84
5	B	301[B]	X2A	O4-C30-C28	-2.22	115.89	120.29
5	B	301[C]	X2A	O4-C30-C28	-2.17	115.98	120.29
5	B	301[D]	X2A	C28-C29-C24	2.13	123.17	120.44
5	B	301[B]	X2A	C24-N3-C23	-2.11	123.11	126.86
5	B	301[D]	X2A	C7-C6-C8	2.10	124.80	120.13
5	B	301[B]	X2A	C28-C29-C24	-2.08	117.76	120.44
3	B	305	SO4	O4-S-O2	-2.04	98.88	109.56
5	B	301[C]	X2A	C27-C28-C29	-2.03	116.90	119.25
5	B	301[A]	X2A	C37-C36-C33	2.02	125.87	120.88

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	B	301[D]	X2A	C15-C14-C11	2.00	125.83	120.88

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
5	B	301[C]	X2A	C22
5	B	301[C]	X2A	C
5	B	301[D]	X2A	C22
5	B	301[D]	X2A	C

All (50) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	301	MES	C7-C8-S-O2S
5	B	301[A]	X2A	C22-C23-N3-C24
5	B	301[A]	X2A	O5-C22-C23-N3
5	B	301[B]	X2A	O3-C23-N3-C24
5	B	301[B]	X2A	C22-C23-N3-C24
5	B	301[B]	X2A	O5-C22-C23-N3
5	B	301[B]	X2A	O5-C22-C23-O3
5	B	301[C]	X2A	O3-C23-N3-C24
5	B	301[C]	X2A	C22-C23-N3-C24
5	B	301[C]	X2A	O5-C-C1-O
5	B	301[C]	X2A	O5-C-C1-N
5	B	301[C]	X2A	C-C1-N-C2
5	B	301[D]	X2A	C22-C23-N3-C24
5	B	301[D]	X2A	C-C1-N-C2
5	B	301[D]	X2A	O-C1-N-C2
5	B	301[A]	X2A	O3-C23-N3-C24
5	B	301[C]	X2A	O-C1-N-C2
5	B	301[D]	X2A	O3-C23-N3-C24
5	B	301[A]	X2A	C29-C24-N3-C23
5	B	301[A]	X2A	C25-C24-N3-C23
4	B	306	PG4	O1-C1-C2-O2
4	A	303	PG4	O3-C5-C6-O4
4	B	306	PG4	O2-C3-C4-O3
2	A	301	MES	N4-C7-C8-S
2	B	302	MES	N4-C7-C8-S
4	A	303	PG4	O1-C1-C2-O2
2	A	301	MES	C8-C7-N4-C3
5	B	301[A]	X2A	O5-C22-C23-O3
5	B	301[A]	X2A	C7-C2-N-C1

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Mol	Chain	Res	Type	Atoms
5	B	301[B]	X2A	C-C1-N-C2
4	A	303	PG4	O2-C3-C4-O3
4	A	303	PG4	C6-C5-O3-C4
4	B	306	PG4	C8-C7-O4-C6
5	B	301[A]	X2A	O-C1-N-C2
4	A	303	PG4	C1-C2-O2-C3
5	B	301[A]	X2A	C3-C2-N-C1
2	A	301	MES	C8-C7-N4-C5
4	B	306	PG4	C3-C4-O3-C5
5	B	301[B]	X2A	C3-C2-N-C1
5	B	301[A]	X2A	O5-C-C1-N
5	B	301[C]	X2A	O5-C22-C23-N3
5	B	301[D]	X2A	O5-C22-C23-N3
5	B	301[D]	X2A	O5-C-C1-N
4	B	306	PG4	C1-C2-O2-C3
4	A	303	PG4	C4-C3-O2-C2
5	B	301[B]	X2A	C7-C2-N-C1
5	B	301[B]	X2A	O5-C-C1-O
5	B	301[D]	X2A	O5-C-C1-O
4	A	303	PG4	C3-C4-O3-C5
4	A	303	PG4	C5-C6-O4-C7

There are no ring outliers.

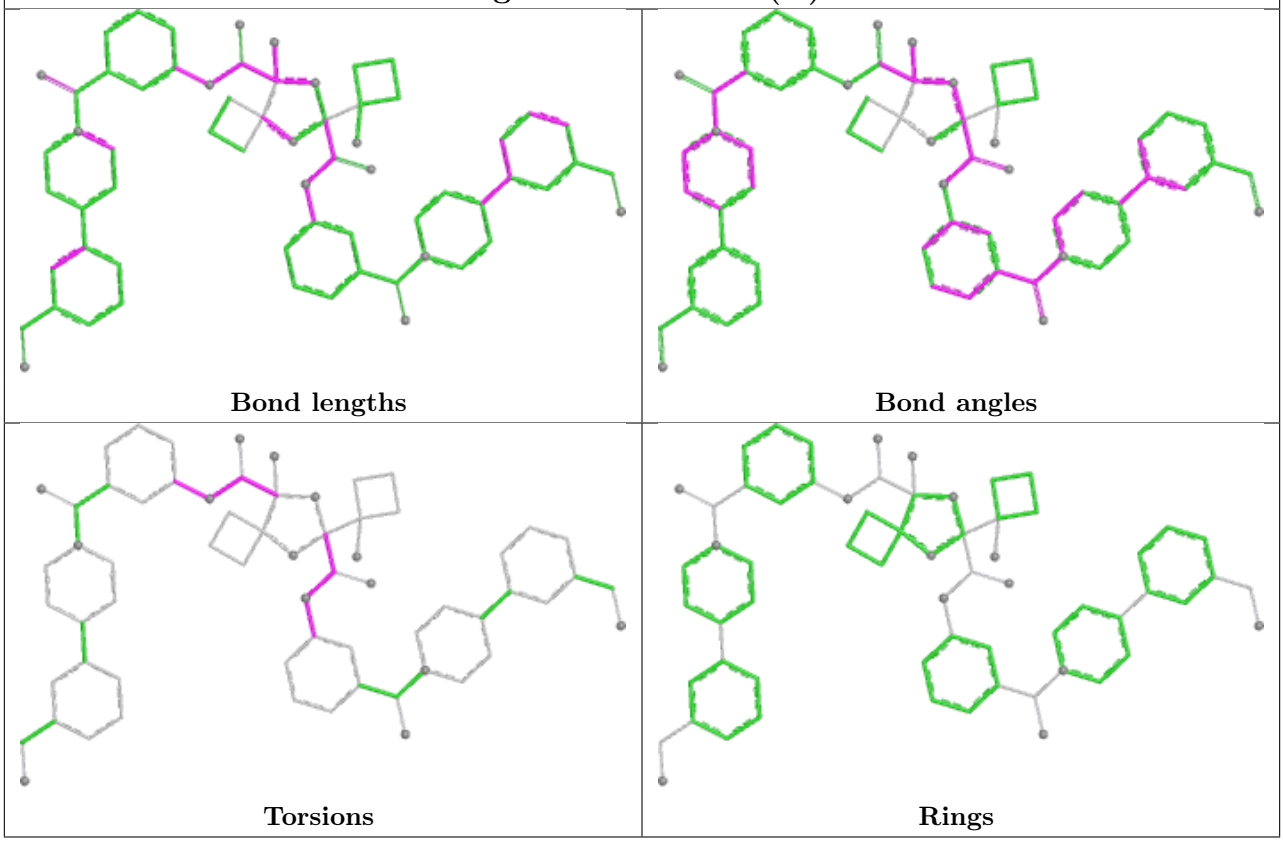
8 monomers are involved in 38 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	301[A]	X2A	10	0
5	B	301[D]	X2A	5	0
3	B	305	SO4	1	0
5	B	301[B]	X2A	4	0
5	B	301[C]	X2A	12	0
2	B	302	MES	1	0
4	A	303	PG4	4	0
4	B	306	PG4	2	0

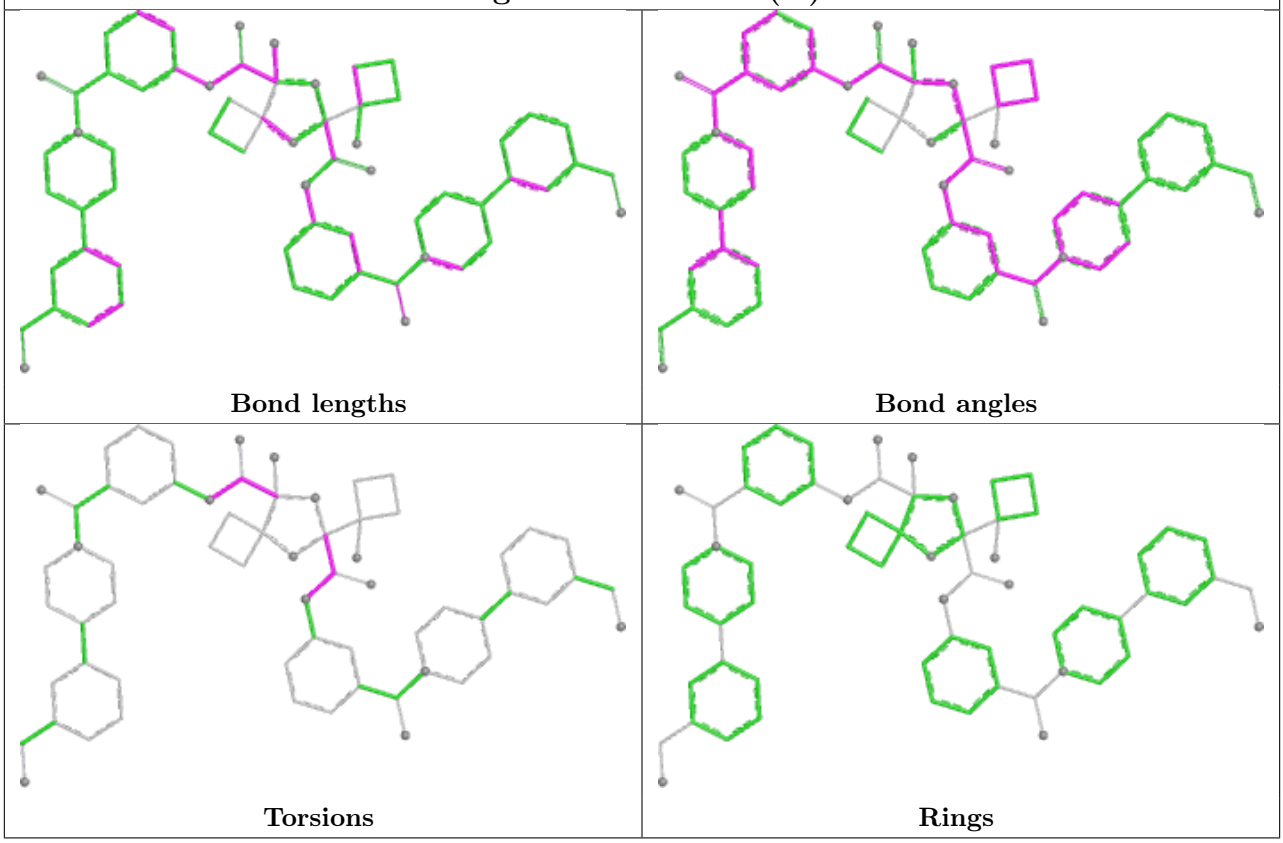
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

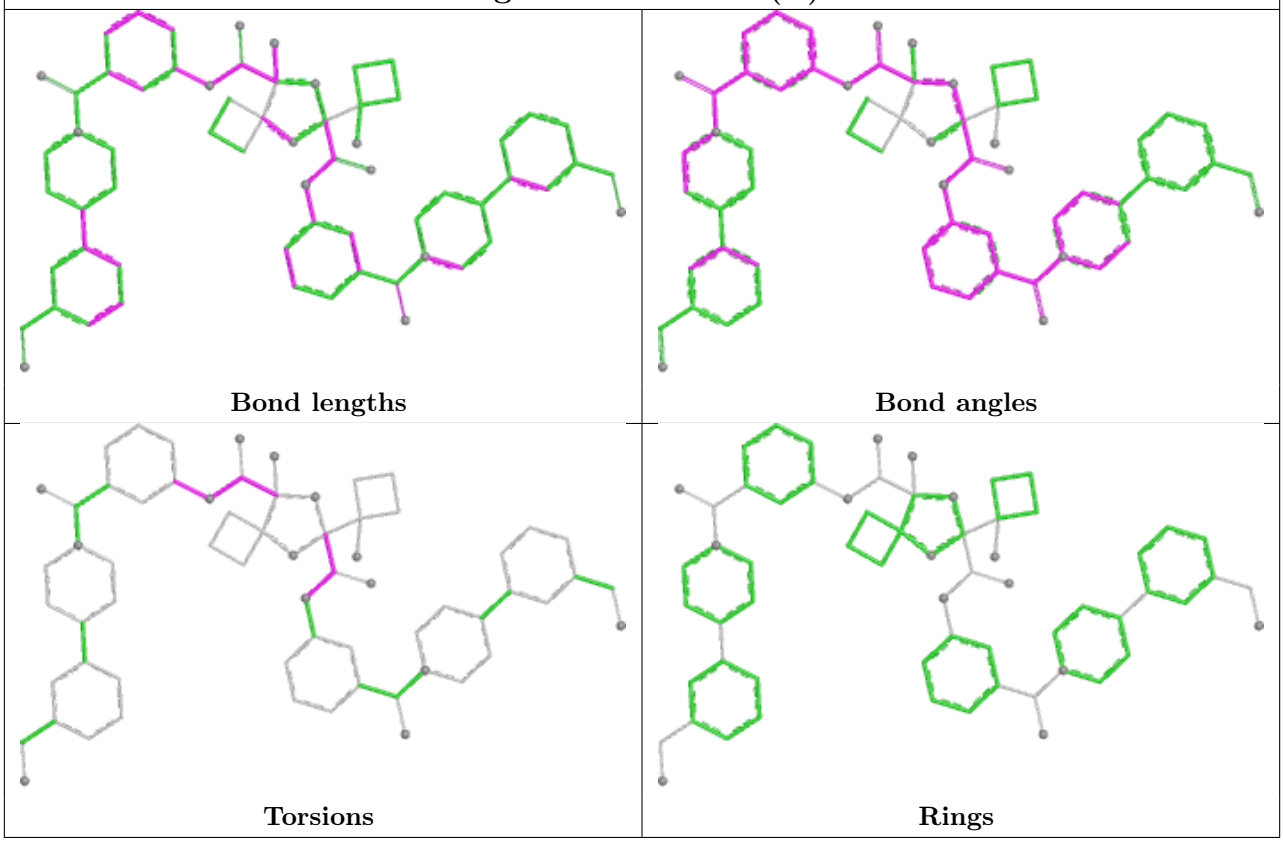
Ligand X2A B 301 (A)



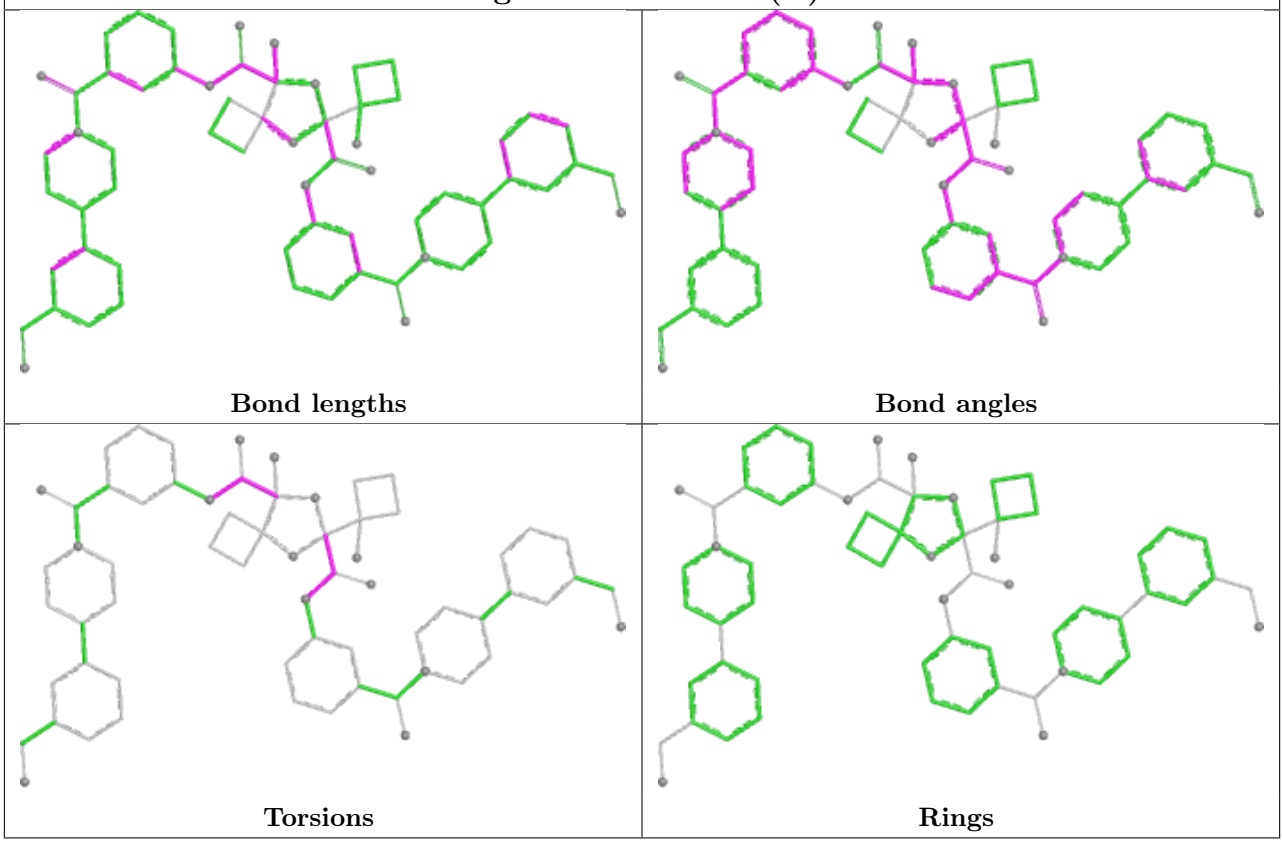
Ligand X2A B 301 (D)



Ligand X2A B 301 (B)



Ligand X2A B 301 (C)



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	243/245 (99%)	-0.32	3 (1%)	79	79	14, 20, 34, 52	0
1	B	243/245 (99%)	-0.26	6 (2%)	57	56	15, 22, 38, 51	0
All	All	486/490 (99%)	-0.29	9 (1%)	66	67	14, 21, 37, 52	0

All (9) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	97	TYR	3.0
1	B	133	VAL	2.8
1	B	148	THR	2.6
1	B	233	ASN	2.5
1	A	97	TYR	2.3
1	A	233	ASN	2.1
1	B	166	ASP	2.1
1	A	166	ASP	2.0
1	B	135	SER	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

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

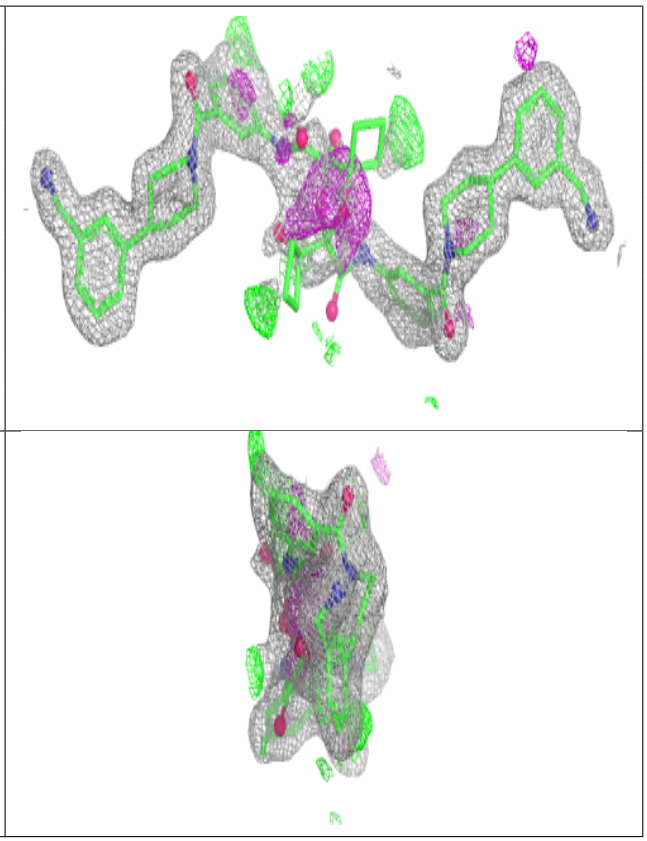
median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	PG4	A	303	13/13	0.80	0.16	24,44,54,62	0
5	X2A	B	301[A]	64/64	0.81	0.23	18,37,56,58	64
5	X2A	B	301[B]	64/64	0.81	0.23	23,40,56,64	64
5	X2A	B	301[C]	64/64	0.81	0.23	18,36,55,60	64
5	X2A	B	301[D]	64/64	0.81	0.23	14,28,54,56	64
4	PG4	B	306	13/13	0.85	0.17	32,45,55,57	0
2	MES	A	301	12/12	0.93	0.17	28,32,42,45	0
3	SO4	B	305	5/5	0.94	0.16	37,39,45,47	0
3	SO4	B	303	5/5	0.96	0.18	44,44,47,53	0
2	MES	B	302	12/12	0.98	0.06	21,27,29,30	0
3	SO4	A	302	5/5	0.98	0.12	28,30,35,40	0
3	SO4	B	304	5/5	0.99	0.07	25,30,37,38	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.

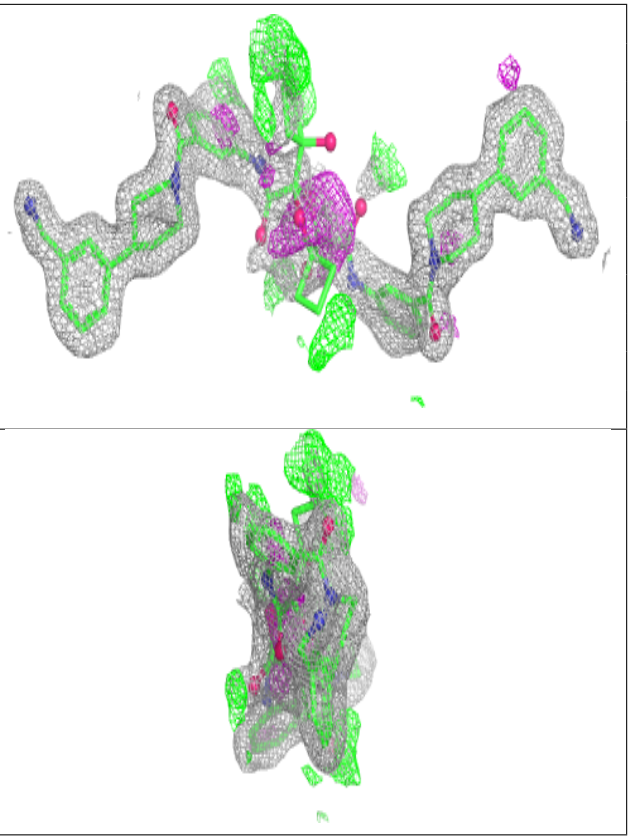
Electron density around X2A B 301 (A):

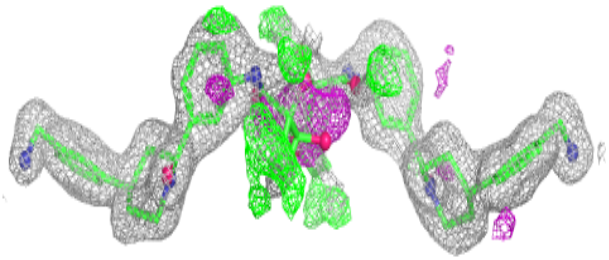
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



Electron density around X2A B 301 (B):

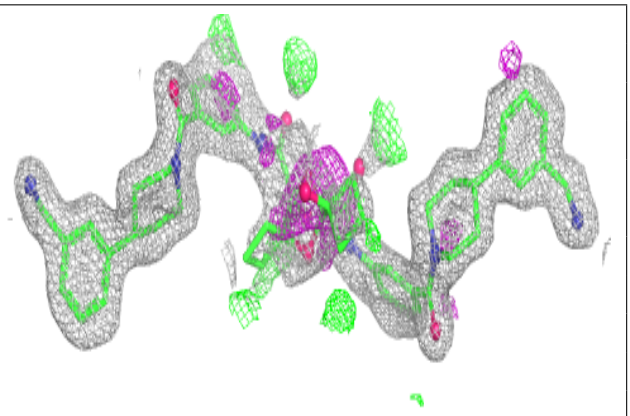
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

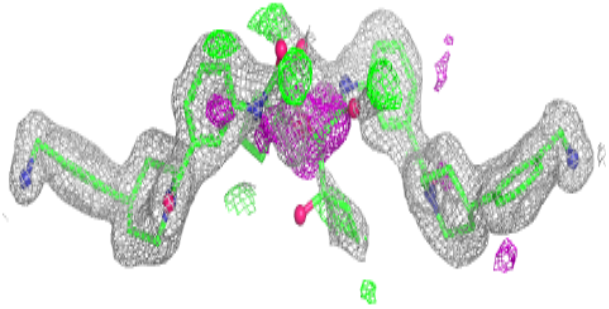


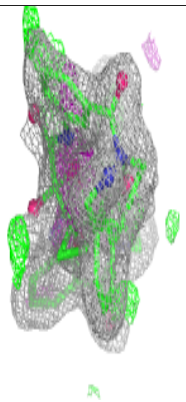


Electron density around X2A B 301 (C):

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

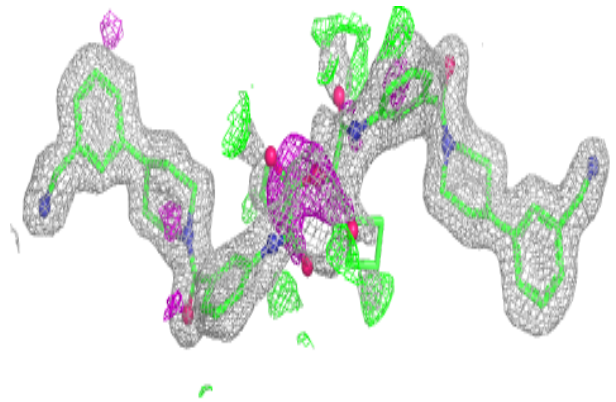


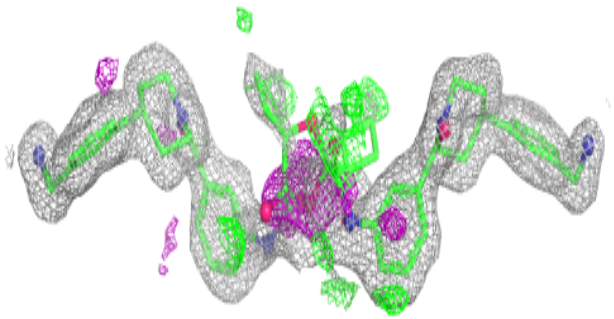


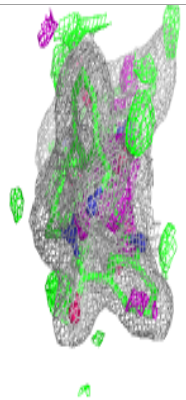


Electron density around X2A B 301 (D):

$2mF_o$-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.