Full wwPDB X-ray Structure Validation Report (i)

Dec 8, 2023 – 01:41 am GMT

PDB ID	:	2BM2
Title	:	human beta-II tryptase in complex with 4-(3-Aminomethyl-phenyl)- piperidin-1-yl-(5-phenethyl- pyridin-3-yl)-methanone
Authors	:	Maignan, S.; Guilloteau, J.-P.; Dupuy, A.; Levell, J.; Astles, P.; Eastwood, P.; Cairns, J.; Houille, O.; Aldous, S.; Merriman, G.; Whiteley, B.; Pribish, J.; Czekaj, M.; Liang, G.; Davidson, J.; Harrison, T.; Morley, A.; Watson, S.; Fenton, G.; Mccarthy, C.; Romano, J.; Mathew, R.; Engers, D.; Gardyan, M.; Sides, K.; Kwong, J.; Tsay, J.; Rebello, S.; Shen, L.; Wang, J.; Luo, Y.; Giardino, O.; Lim, H.-K.; Smith, K.; Pauls, H.
Deposited on	:	2005-03-09
Resolution	:	2.20 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 (1)) were used in the production of this report:

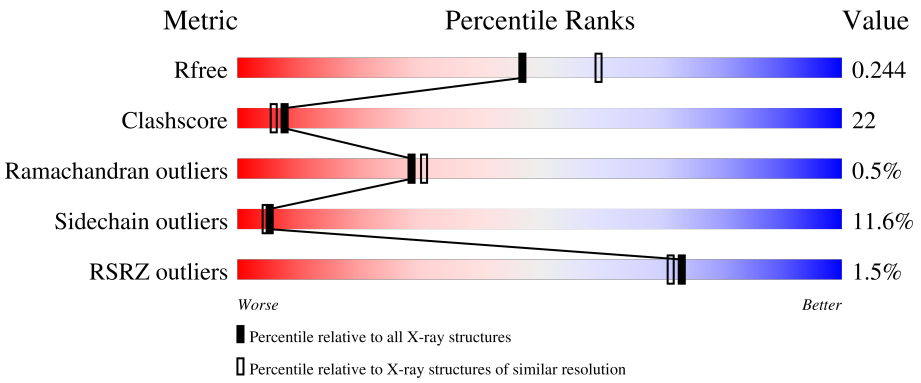
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158

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 2.20 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	4898 (2.20-2.20)
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (2.20-2.20)

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	3% 62% 31% 6% •
1	B	245	2% 58% 36% 6% •

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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

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Mol	Chain	Length	Quality of chain
1	C	245	% 64% 31%
1	D	245	60% 34% 6%

2 Entry composition (i)

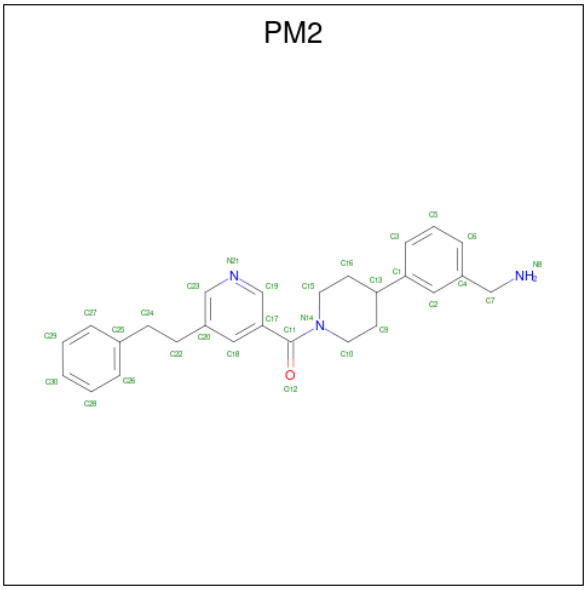
There are 3 unique types of molecules in this entry. The entry contains 8145 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 HUMAN BETA2 TRYPTASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	243	1912	1224	337	339	12	25	0	1
1	B	243	1912	1224	337	339	12	16	0	1
1	C	243	1912	1224	337	339	12	16	0	1
1	D	243	1912	1224	337	339	12	9	0	1

- Molecule 2 is 1-[3-(1-{[5-(2-PHENYLETHYL)PYRIDIN-3-YL]CARBONYL}PIPERIDIN-4-YL)PHENYL]METHANAMINE (three-letter code: PM2) (formula: $C_{26}H_{29}N_3O$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
2	A	1	30	26	3	1	0	0
2	B	1	30	26	3	1	0	0

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
2	C	1	30	26	3	1	0	0
			Total	C	N	O		
2	D	1	30	26	3	1	0	0

- Molecule 3 is water.

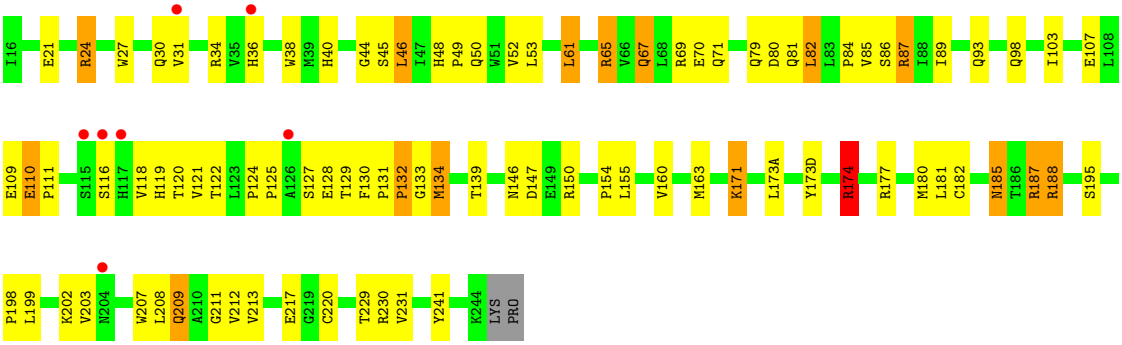
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
3	A	62	62	62	0	0
			Total	O		
3	B	104	104	104	0	0
			Total	O		
3	C	107	107	107	0	0
			Total	O		
3	D	104	104	104	0	0

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.

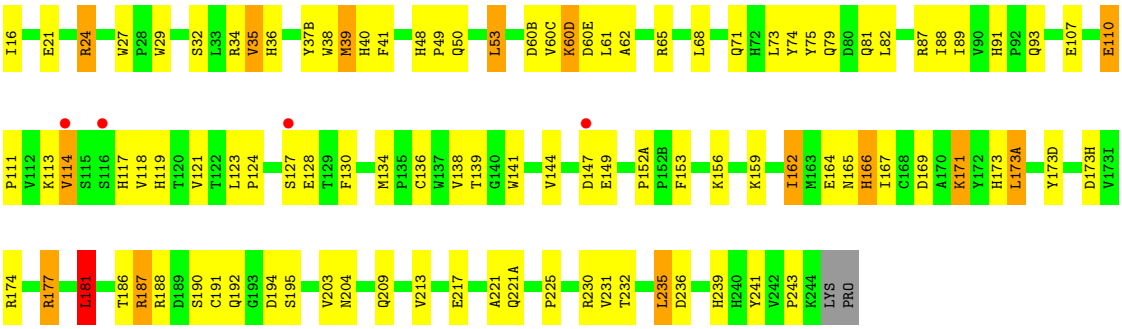
• Molecule 1: HUMAN BETA2 TRYPTASE

Chain A:



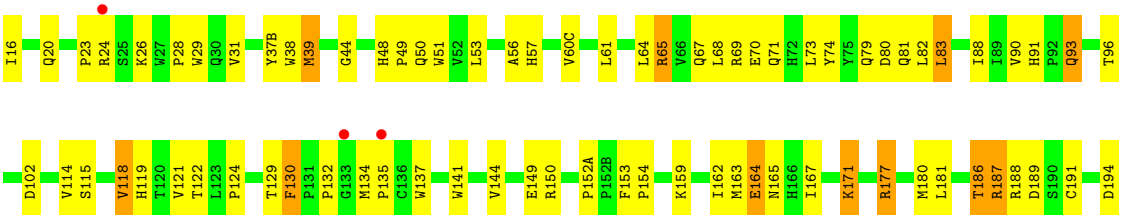
• Molecule 1: HUMAN BETA2 TRYPTASE

Chain B:



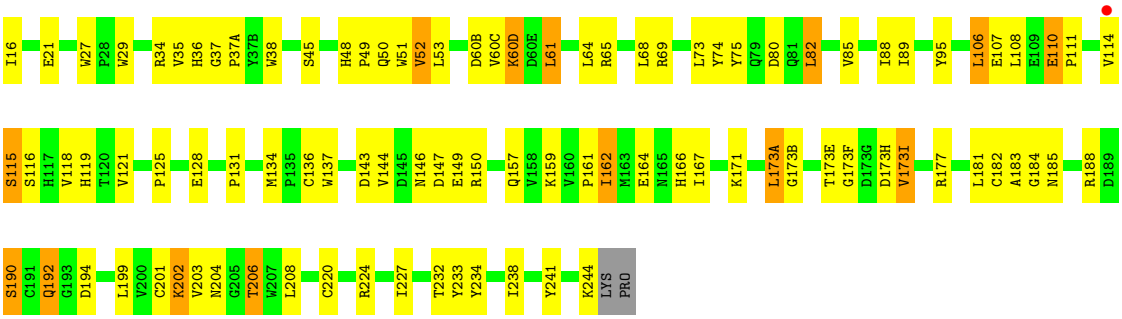
• Molecule 1: HUMAN BETA2 TRYPTASE

Chain C:



• Molecule 1: HUMAN BETA2 TRYPTASE

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 41	Depositor
Cell constants a, b, c, α, β, γ	82.00Å 82.00Å 171.19Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.20 19.94 – 2.20	Depositor EDS
% Data completeness (in resolution range)	91.0 (20.00-2.20) 90.8 (19.94-2.20)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.37 (at 2.19Å)	Xtriage
Refinement program	X-PLOR 981	Depositor
R, R_{free}	0.203 , 0.259 0.194 , 0.244	Depositor DCC
R_{free} test set	3661 reflections (7.06%)	wwPDB-VP
Wilson B-factor (Å^2)	33.9	Xtriage
Anisotropy	0.489	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 53.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.45$, $< L^2 > = 0.28$	Xtriage
Estimated twinning fraction	0.068 for h,-k,-l	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	8145	wwPDB-VP
Average B, all atoms (Å^2)	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.24% 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: PM2

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	0.52	0/1977	1.11	6/2711 (0.2%)
1	B	0.57	0/1977	0.75	2/2711 (0.1%)
1	C	0.54	0/1977	0.74	0/2711
1	D	0.56	0/1977	0.76	1/2711 (0.0%)
All	All	0.55	0/7908	0.85	9/10844 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	D	0	1
All	All	0	2

There are no bond length outliers.

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	174	ARG	NE-CZ-NH2	-31.15	104.72	120.30
1	A	174	ARG	NE-CZ-NH1	29.51	135.06	120.30
1	B	181	LEU	CA-CB-CG	7.33	132.16	115.30
1	A	174	ARG	CG-CD-NE	6.51	125.46	111.80
1	A	174	ARG	CA-CB-CG	6.10	126.83	113.40
1	B	53	LEU	CA-CB-CG	5.67	128.35	115.30
1	A	174	ARG	CD-NE-CZ	5.57	131.40	123.60
1	A	199	LEU	N-CA-C	-5.34	96.57	111.00
1	D	199	LEU	N-CA-C	-5.28	96.74	111.00

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	174	ARG	Sidechain
1	D	95	TYR	Sidechain

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	1912	0	1842	85	0
1	B	1912	0	1842	90	0
1	C	1912	0	1842	83	0
1	D	1912	0	1842	75	0
2	A	30	0	29	0	0
2	B	30	0	29	2	0
2	C	30	0	29	0	0
2	D	30	0	29	1	0
3	A	62	0	0	3	0
3	B	104	0	0	16	0
3	C	107	0	0	8	0
3	D	104	0	0	9	0
All	All	8145	0	7484	328	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 22.

All (328) 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:D:52:VAL:HG23	1:D:106:LEU:HB2	1.25	1.14
1:A:53:LEU:HD11	1:A:103:ILE:HD11	1.32	1.09
1:B:123:LEU:HD12	3:B:2099:HOH:O	1.52	1.09
1:A:24:ARG:HH11	1:A:71:GLN:HG2	1.18	1.05
1:C:65:ARG:HG3	1:C:82:LEU:HB3	1.46	0.96
1:A:69:ARG:HH12	1:A:71:GLN:NE2	1.72	0.87
1:A:185:ASN:HD21	1:A:188:ARG:HG2	1.42	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:146:ASN:HD21	1:A:220:CYS:H	1.22	0.83
1:A:48:HIS:HD2	1:A:50:GLN:H	1.24	0.82
1:B:60(B):ASP:HB2	3:B:2023:HOH:O	1.79	0.82
1:D:27:TRP:HE1	1:D:157:GLN:NE2	1.77	0.81
1:B:166:HIS:HB2	3:B:2066:HOH:O	1.81	0.80
1:C:186:THR:HB	3:C:2083:HOH:O	1.82	0.79
1:D:27:TRP:HE1	1:D:157:GLN:HE21	1.27	0.79
1:B:239:HIS:HE1	3:B:2099:HOH:O	1.64	0.79
1:A:24:ARG:NH1	1:A:71:GLN:HG2	1.99	0.78
1:D:244:LYS:N	3:D:2100:HOH:O	2.17	0.77
1:C:91:HIS:HD2	1:C:93:GLN:H	1.32	0.77
1:D:171:LYS:HA	1:D:173(A):LEU:HD22	1.68	0.76
1:D:52:VAL:CG2	1:D:106:LEU:HB2	2.13	0.75
1:C:217:GLU:HB3	3:C:2094:HOH:O	1.86	0.75
1:A:69:ARG:HH12	1:A:71:GLN:HE21	1.31	0.75
1:B:187:ARG:HG2	1:B:188:ARG:HG3	1.67	0.74
1:C:23:PRO:HD2	1:C:26:LYS:HD2	1.68	0.73
1:A:212:VAL:CG1	1:A:229:THR:HB	2.21	0.70
1:A:48:HIS:CD2	1:A:50:GLN:H	2.07	0.70
1:C:67:GLN:NE2	1:C:70:GLU:HG3	2.07	0.69
1:A:65:ARG:CD	1:A:82:LEU:HB3	2.23	0.69
1:B:187:ARG:HE	1:B:188:ARG:HH11	1.39	0.68
1:A:185:ASN:ND2	1:A:188:ARG:H	1.92	0.68
1:D:164:GLU:HB2	1:D:167:ILE:HD12	1.76	0.68
1:B:91:HIS:HE1	1:B:93:GLN:HE21	1.42	0.67
1:A:146:ASN:HD21	1:A:220:CYS:N	1.90	0.66
1:B:124:PRO:O	1:B:235:LEU:HD21	1.95	0.66
1:B:195:SER:HA	1:B:213:VAL:HG12	1.77	0.66
1:B:60(C):VAL:HG13	1:D:173(B):GLY:O	1.96	0.65
1:D:110:GLU:HG3	1:D:111:PRO:HD2	1.78	0.65
1:C:124:PRO:O	1:C:235:LEU:HD11	1.97	0.65
1:C:48:HIS:HD2	1:C:50:GLN:H	1.44	0.65
1:C:83:LEU:N	1:C:83:LEU:HD12	2.11	0.65
1:A:53:LEU:HD11	1:A:103:ILE:CD1	2.19	0.65
1:D:171:LYS:HA	1:D:173(A):LEU:CD2	2.27	0.65
1:C:91:HIS:CD2	1:C:93:GLN:H	2.12	0.64
1:C:167:ILE:O	1:C:171:LYS:HG2	1.97	0.64
1:A:185:ASN:C	1:A:185:ASN:HD22	2.01	0.63
1:A:27:TRP:O	1:A:69:ARG:HD3	1.99	0.63
1:B:48:HIS:HD2	1:B:50:GLN:H	1.45	0.63
1:C:114:VAL:HG22	1:C:119:HIS:HA	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:211:GLY:HA2	1:A:231:VAL:HG23	1.80	0.62
1:A:181:LEU:HD23	1:A:182:CYS:N	2.14	0.62
1:D:119:HIS:HB2	3:D:2047:HOH:O	2.00	0.61
1:C:134:MET:HG2	1:C:135:PRO:HD2	1.82	0.61
1:A:125:PRO:HD2	1:A:128:GLU:HB2	1.83	0.61
1:D:173(F):GLY:O	1:D:173(I):VAL:HG13	2.00	0.61
1:C:23:PRO:HG2	1:C:26:LYS:HE2	1.83	0.60
1:B:35:VAL:HG13	1:B:41:PHE:CE1	2.37	0.60
1:D:190:SER:HB3	2:D:3211:PM2:H6	1.84	0.60
1:B:60(E):ASP:OD1	1:B:62:ALA:HB3	2.02	0.60
1:B:60(D):LYS:HE2	1:B:60(E):ASP:H	1.67	0.60
1:A:36:HIS:HB2	1:A:38:TRP:CH2	2.37	0.60
1:B:60(D):LYS:CE	1:B:60(E):ASP:H	2.13	0.60
1:C:134:MET:HG2	1:C:135:PRO:CD	2.32	0.60
1:D:146:ASN:HD21	1:D:220:CYS:H	1.49	0.59
1:A:67:GLN:NE2	1:A:70:GLU:HB2	2.17	0.59
1:B:48:HIS:CD2	1:B:50:GLN:H	2.19	0.59
1:B:21:GLU:OE2	3:B:2003:HOH:O	2.17	0.59
1:B:73:LEU:HD23	1:B:74:TYR:CE2	2.38	0.59
1:A:185:ASN:ND2	1:A:187:ARG:H	2.01	0.58
1:C:130:PHE:HA	1:C:134:MET:HE1	1.84	0.58
1:C:171:LYS:HD3	3:C:2074:HOH:O	2.02	0.58
1:C:73:LEU:HB2	1:C:153:PHE:HB2	1.84	0.58
1:C:65:ARG:HG3	1:C:82:LEU:CB	2.26	0.58
1:B:91:HIS:CE1	1:B:93:GLN:HE21	2.21	0.58
1:B:37(B):TYR:OH	1:B:39:MET:HG3	2.03	0.57
1:B:169:ASP:O	1:B:173:HIS:HD2	1.87	0.57
1:C:67:GLN:HE21	1:C:70:GLU:HG3	1.70	0.57
1:D:36:HIS:HB2	1:D:38:TRP:CH2	2.40	0.57
1:A:203:VAL:HG21	1:A:208:LEU:HD12	1.87	0.57
1:C:152(A):PRO:HA	1:C:153:PHE:H	1.69	0.57
1:A:69:ARG:HH22	1:A:71:GLN:HE22	1.51	0.57
1:A:212:VAL:HG12	1:A:229:THR:HB	1.87	0.57
1:A:65:ARG:HG2	1:A:82:LEU:CB	2.34	0.56
1:C:83:LEU:HD11	3:C:2027:HOH:O	2.05	0.56
1:B:134:MET:CE	1:B:203:VAL:HG22	2.35	0.56
1:D:34:ARG:HD2	1:D:38:TRP:O	2.05	0.56
1:A:65:ARG:HG2	1:A:82:LEU:HB3	1.86	0.56
1:A:173(D):TYR:CE2	1:C:60(C):VAL:HA	2.40	0.56
1:D:125:PRO:HG2	1:D:128:GLU:HG2	1.86	0.56
1:A:65:ARG:HG2	1:A:82:LEU:HG	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:48:HIS:CE1	1:B:243:PRO:HG2	2.41	0.56
1:A:65:ARG:HD2	1:A:82:LEU:HB3	1.86	0.56
1:B:50:GLN:NE2	3:B:2017:HOH:O	2.39	0.56
1:B:110:GLU:HG3	1:B:111:PRO:HD2	1.87	0.56
1:B:181:LEU:HD22	3:B:2094:HOH:O	2.05	0.56
1:A:130:PHE:HA	1:A:134:MET:HE3	1.87	0.56
1:B:128:GLU:HG3	1:B:130:PHE:CE2	2.40	0.55
1:B:209:GLN:HG2	1:B:231:VAL:HG21	1.88	0.55
1:D:73:LEU:O	1:D:75:TYR:HD2	1.89	0.55
1:B:24:ARG:HE	1:B:117:HIS:CE1	2.24	0.55
1:C:124:PRO:HA	1:C:208:LEU:HD12	1.88	0.55
1:C:91:HIS:CD2	1:C:93:GLN:HB2	2.41	0.55
1:B:87:ARG:HB2	1:B:107:GLU:HB3	1.89	0.55
1:B:152(A):PRO:HA	1:B:153:PHE:H	1.71	0.54
1:B:29:TRP:CG	1:B:121:VAL:HB	2.42	0.54
1:C:61:LEU:CD1	1:C:88:ILE:HD12	2.37	0.54
1:B:152(A):PRO:HA	1:B:153:PHE:N	2.22	0.54
1:A:125:PRO:HG2	1:A:128:GLU:HB2	1.90	0.54
1:C:57:HIS:HD2	1:C:102:ASP:OD2	1.91	0.54
1:A:34:ARG:HD3	1:A:40:HIS:HA	1.89	0.54
1:B:217:GLU:OE2	3:B:2087:HOH:O	2.18	0.54
1:A:131:PRO:O	1:A:132:PRO:O	2.25	0.54
1:C:152(A):PRO:HA	1:C:153:PHE:N	2.23	0.54
1:C:29:TRP:CG	1:C:121:VAL:HB	2.43	0.53
1:B:195:SER:HA	1:B:213:VAL:CG1	2.38	0.53
1:B:136:CYS:SG	1:B:162:ILE:CD1	2.97	0.53
1:B:177:ARG:NH1	3:B:2068:HOH:O	2.41	0.53
1:A:67:GLN:HE22	1:A:70:GLU:HB2	1.72	0.53
1:C:31:VAL:HG22	1:C:44:GLY:C	2.29	0.53
1:A:163:MET:O	3:A:2030:HOH:O	2.19	0.53
1:C:164:GLU:HG2	1:C:167:ILE:HG12	1.91	0.53
1:D:21:GLU:OE1	3:D:2004:HOH:O	2.18	0.53
1:D:164:GLU:OE2	1:D:166:HIS:HE1	1.92	0.53
1:C:130:PHE:HA	1:C:134:MET:CE	2.39	0.53
1:C:186:THR:HG23	1:C:186:THR:O	2.09	0.53
1:B:110:GLU:O	3:B:2047:HOH:O	2.18	0.53
1:D:114:VAL:CG1	1:D:115:SER:N	2.72	0.52
1:A:119:HIS:HD2	1:A:120:THR:O	1.91	0.52
1:D:114:VAL:HG13	1:D:115:SER:N	2.25	0.52
1:D:144:VAL:HG23	1:D:149:GLU:HB3	1.91	0.52
1:D:173(B):GLY:O	3:D:2068:HOH:O	2.19	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:185:ASN:HD22	1:A:188:ARG:H	1.57	0.52
1:B:232:THR:HA	1:B:235:LEU:HD22	1.92	0.52
1:C:48:HIS:CD2	1:C:50:GLN:H	2.27	0.52
1:B:187:ARG:HH21	1:B:188:ARG:NH1	2.07	0.52
1:D:131:PRO:O	1:D:162:ILE:HG13	2.10	0.51
1:B:65:ARG:HB3	1:B:82:LEU:HB3	1.92	0.51
1:A:173(D):TYR:CD2	1:C:90:VAL:HG21	2.44	0.51
1:A:65:ARG:CG	1:A:82:LEU:HB3	2.40	0.51
1:A:71:GLN:NE2	1:A:71:GLN:HA	2.26	0.51
1:C:16:ILE:N	1:C:194:ASP:OD2	2.44	0.51
1:B:173(D):TYR:CE2	1:D:60(C):VAL:HA	2.45	0.51
1:D:60(B):ASP:OD1	3:D:2018:HOH:O	2.20	0.51
1:B:192:GLN:OE1	3:B:2075:HOH:O	2.19	0.50
1:B:37(B):TYR:CZ	1:B:39:MET:HG3	2.47	0.50
1:C:164:GLU:O	1:C:164:GLU:HG3	2.11	0.50
1:C:217:GLU:OE2	3:C:2094:HOH:O	2.20	0.50
1:A:71:GLN:HE21	1:A:71:GLN:HA	1.77	0.50
1:B:164:GLU:CD	1:B:166:HIS:H	2.15	0.50
1:C:65:ARG:CG	1:C:82:LEU:HB3	2.29	0.50
1:B:89:ILE:HD13	1:B:241:TYR:CD1	2.47	0.50
1:C:187:ARG:HB2	1:C:187:ARG:CZ	2.40	0.50
1:A:203:VAL:CG2	1:A:208:LEU:HD12	2.41	0.50
1:B:134:MET:HE3	1:B:203:VAL:HG22	1.93	0.50
1:A:185:ASN:ND2	1:A:188:ARG:N	2.60	0.50
1:D:162:ILE:HG12	3:D:2048:HOH:O	2.10	0.50
1:A:84:PRO:HG2	1:A:109:GLU:HB2	1.94	0.50
1:C:73:LEU:HG	1:C:141:TRP:CD1	2.47	0.50
1:C:177:ARG:HG3	1:C:180:MET:CE	2.42	0.50
1:D:233:TYR:O	1:D:233:TYR:CD1	2.64	0.49
1:D:137:TRP:NE1	1:D:159:LYS:HB2	2.27	0.49
1:A:131:PRO:HD2	1:A:134:MET:HG3	1.95	0.49
1:D:143:ASP:OD2	1:D:192:GLN:CG	2.60	0.49
1:C:61:LEU:HD11	1:C:88:ILE:HD12	1.93	0.49
1:B:164:GLU:OE1	1:B:166:HIS:N	2.45	0.49
1:A:86:SER:OG	1:A:107:GLU:HG2	2.13	0.49
1:A:61:LEU:HD13	1:A:85:VAL:O	2.12	0.49
1:C:164:GLU:HG3	1:C:167:ILE:H	1.77	0.49
1:B:29:TRP:CD2	1:B:121:VAL:HB	2.47	0.48
1:C:48:HIS:CD2	1:C:49:PRO:HD2	2.48	0.48
1:C:189:ASP:HA	3:C:2087:HOH:O	2.12	0.48
1:A:124:PRO:HB2	1:A:125:PRO:HD2	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:61:LEU:HD12	1:D:88:ILE:CD1	2.43	0.48
1:A:30:GLN:NE2	1:A:139:THR:OG1	2.47	0.48
1:B:34:ARG:HG3	1:B:34:ARG:HH11	1.78	0.48
1:A:212:VAL:HG13	1:A:229:THR:HB	1.95	0.48
1:C:37(B):TYR:CZ	1:C:39:MET:HG3	2.48	0.48
1:C:48:HIS:HB3	1:C:51:TRP:HB2	1.95	0.48
1:B:204:ASN:HB3	3:B:2082:HOH:O	2.13	0.48
1:D:232:THR:HG23	3:D:2084:HOH:O	2.13	0.48
1:D:89:ILE:HD13	1:D:241:TYR:CD1	2.49	0.48
1:D:173(F):GLY:O	1:D:173(I):VAL:CG1	2.62	0.48
1:A:195:SER:HA	1:A:213:VAL:CG1	2.44	0.48
1:B:16:ILE:N	1:B:194:ASP:OD1	2.47	0.48
1:B:36:HIS:HB2	1:B:38:TRP:CH2	2.49	0.47
1:B:73:LEU:HD13	1:B:141:TRP:CD2	2.49	0.47
1:C:186:THR:O	1:C:186:THR:CG2	2.61	0.47
1:B:24:ARG:O	1:B:24:ARG:HG3	2.14	0.47
1:B:35:VAL:HG13	1:B:41:PHE:CD1	2.49	0.47
1:B:48:HIS:O	1:B:50:GLN:N	2.47	0.47
1:C:191:CYS:O	1:C:194:ASP:HB2	2.13	0.47
1:B:32:SER:HB2	1:B:141:TRP:CZ3	2.49	0.47
1:B:60(D):LYS:HD2	1:B:60(D):LYS:HA	1.47	0.47
1:D:51:TRP:CH2	1:D:107:GLU:HB2	2.50	0.47
1:C:38:TRP:CE3	1:C:65:ARG:HB2	2.50	0.47
1:D:51:TRP:CZ3	1:D:107:GLU:HB2	2.50	0.47
1:D:48:HIS:CG	1:D:49:PRO:HD2	2.50	0.47
1:A:185:ASN:HD22	1:A:187:ARG:H	1.61	0.47
1:C:80:ASP:O	1:C:81:GLN:HG2	2.15	0.46
1:A:31:VAL:HG22	1:A:44:GLY:C	2.36	0.46
1:A:160:VAL:HG12	1:A:188:ARG:HB2	1.96	0.46
1:B:171:LYS:HA	1:B:173(A):LEU:HD22	1.98	0.46
1:C:124:PRO:CA	1:C:208:LEU:HD12	2.45	0.46
1:C:164:GLU:HG2	1:C:167:ILE:CG1	2.45	0.46
1:B:87:ARG:HE	1:B:89:ILE:HD11	1.81	0.46
1:D:134:MET:HB2	1:D:162:ILE:HD11	1.98	0.46
1:B:177:ARG:NH1	3:B:2067:HOH:O	2.48	0.46
1:D:136:CYS:SG	1:D:162:ILE:CD1	3.04	0.46
1:D:29:TRP:CG	1:D:121:VAL:HB	2.51	0.46
1:A:110:GLU:HB2	1:A:111:PRO:HD2	1.97	0.45
1:D:173(H):ASP:HB2	3:D:2063:HOH:O	2.17	0.45
1:A:171:LYS:HE3	1:A:173(A):LEU:HD11	1.98	0.45
1:B:68:LEU:HD22	1:B:118:VAL:HG21	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:65:ARG:HG3	1:D:82:LEU:HB3	1.98	0.45
1:C:28:PRO:HB2	1:C:119:HIS:H	1.81	0.45
1:D:27:TRP:NE1	1:D:157:GLN:NE2	2.56	0.45
1:A:171:LYS:HE3	1:A:171:LYS:HA	1.99	0.45
1:C:118:VAL:HG22	1:C:118:VAL:O	2.16	0.45
1:B:204:ASN:CB	3:B:2082:HOH:O	2.64	0.45
1:A:30:GLN:HE22	1:A:198:PRO:HD2	1.81	0.45
1:C:61:LEU:HG	1:C:88:ILE:HD12	1.98	0.45
1:C:149:GLU:HG3	3:C:2066:HOH:O	2.16	0.45
1:C:16:ILE:O	1:C:144:VAL:HA	2.17	0.44
1:C:57:HIS:HE1	3:C:2089:HOH:O	1.99	0.44
1:A:202:LYS:HE3	1:A:207:TRP:CE2	2.52	0.44
1:D:73:LEU:O	1:D:75:TYR:CD2	2.70	0.44
1:A:125:PRO:CG	1:A:128:GLU:HB2	2.47	0.44
1:A:209:GLN:OE1	1:A:211:GLY:O	2.35	0.44
1:B:61:LEU:CD2	1:B:88:ILE:HG13	2.47	0.44
1:B:188:ARG:NH2	3:B:2072:HOH:O	2.50	0.44
1:B:144:VAL:HG12	1:B:156:LYS:HE2	1.99	0.44
1:C:137:TRP:CH2	1:C:159:LYS:HB2	2.53	0.44
1:D:203:VAL:HB	1:D:208:LEU:HD12	2.00	0.44
1:A:125:PRO:CD	1:A:128:GLU:HB2	2.46	0.44
1:B:134:MET:HE2	1:B:203:VAL:HG22	2.00	0.44
1:C:64:LEU:O	1:C:65:ARG:HD3	2.17	0.44
1:C:74:TYR:HA	1:C:80:ASP:OD1	2.18	0.44
1:D:115:SER:HB2	1:D:118:VAL:H	1.83	0.44
1:D:143:ASP:OD2	1:D:192:GLN:HG2	2.17	0.43
1:D:161:PRO:O	1:D:183:ALA:HA	2.18	0.43
1:A:131:PRO:O	1:A:134:MET:HB2	2.19	0.43
1:B:171:LYS:O	1:B:173(A):LEU:HB2	2.18	0.43
1:C:81:GLN:O	1:C:83:LEU:HD12	2.18	0.43
1:A:21:GLU:HG3	1:A:154:PRO:HB2	1.98	0.43
1:A:65:ARG:HG2	1:A:82:LEU:CG	2.47	0.43
1:D:65:ARG:CG	1:D:82:LEU:HB3	2.48	0.43
1:A:70:GLU:OE1	1:A:80:ASP:OD1	2.37	0.43
1:D:137:TRP:CE2	1:D:159:LYS:HB2	2.54	0.43
1:B:164:GLU:OE1	1:B:166:HIS:HB3	2.19	0.43
1:D:45:SER:O	1:D:52:VAL:HA	2.18	0.43
1:B:73:LEU:HD13	1:B:141:TRP:CG	2.53	0.43
1:C:73:LEU:HB2	1:C:153:PHE:CB	2.49	0.43
1:D:134:MET:HB3	1:D:134:MET:HE2	1.29	0.43
1:D:161:PRO:HD2	1:D:184:GLY:HA2	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:181:LEU:HD23	1:D:182:CYS:N	2.34	0.43
1:A:121:VAL:HG22	1:A:122:THR:N	2.33	0.43
1:A:217:GLU:HB3	3:A:2051:HOH:O	2.17	0.43
1:B:114:VAL:HG12	1:B:119:HIS:HA	2.01	0.43
1:C:206:THR:O	1:C:208:LEU:HD23	2.18	0.43
1:D:185:ASN:HD21	1:D:188:ARG:HD2	1.83	0.43
1:D:234:TYR:O	1:D:238:ILE:HG13	2.19	0.43
1:C:203:VAL:HG13	1:C:203:VAL:O	2.19	0.43
1:D:16:ILE:N	1:D:194:ASP:OD2	2.52	0.43
1:B:225:PRO:HA	3:B:2074:HOH:O	2.19	0.42
1:A:89:ILE:HD13	1:A:241:TYR:CE1	2.55	0.42
1:B:27:TRP:CG	1:B:139:THR:HG21	2.54	0.42
1:B:187:ARG:C	1:B:188:ARG:HG3	2.38	0.42
1:D:35:VAL:HG22	1:D:36:HIS:N	2.33	0.42
1:C:83:LEU:N	1:C:83:LEU:CD1	2.81	0.42
1:B:165:ASN:HD21	1:B:230:ARG:HH21	1.68	0.42
1:D:52:VAL:HG23	1:D:106:LEU:CB	2.19	0.42
1:A:46:LEU:HD23	1:A:46:LEU:HA	1.83	0.42
1:A:132:PRO:O	1:A:134:MET:N	2.53	0.42
1:B:40:HIS:CB	1:B:73:LEU:HD21	2.50	0.42
1:C:56:ALA:HB1	1:C:90:VAL:HG13	2.01	0.42
1:C:207:TRP:C	1:C:208:LEU:HD22	2.40	0.42
1:D:60(B):ASP:O	1:D:60(D):LYS:HD2	2.20	0.42
1:D:61:LEU:HD12	1:D:88:ILE:HD12	2.01	0.42
1:A:93:GLN:NE2	3:A:2016:HOH:O	2.52	0.42
1:B:34:ARG:HD2	1:B:38:TRP:O	2.18	0.42
1:D:173(E):THR:HG22	1:D:173(I):VAL:HG13	2.01	0.42
1:B:190:SER:OG	2:B:3211:PM2:H7C1	2.20	0.41
1:D:182:CYS:SG	1:D:227:ILE:HD12	2.60	0.41
1:A:131:PRO:HD2	1:A:134:MET:HE3	2.01	0.41
1:C:61:LEU:CG	1:C:88:ILE:HD12	2.51	0.41
1:C:165:ASN:HD21	1:C:181:LEU:HA	1.86	0.41
1:D:37:GLY:HA3	1:D:37(A):PRO:HD2	1.87	0.41
1:D:171:LYS:O	1:D:173(A):LEU:HB2	2.20	0.41
1:A:87:ARG:NE	1:A:89:ILE:HD11	2.35	0.41
1:C:71:GLN:O	1:C:154:PRO:HA	2.20	0.41
1:C:73:LEU:HG	1:C:141:TRP:CG	2.56	0.41
1:D:68:LEU:O	1:D:69:ARG:C	2.59	0.41
1:A:48:HIS:O	1:A:49:PRO:C	2.59	0.41
1:A:132:PRO:C	1:A:134:MET:H	2.24	0.41
1:D:203:VAL:O	1:D:206:THR:HG23	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:98:GLN:HG2	1:C:96:THR:HG21	2.02	0.41
1:A:185:ASN:ND2	1:A:185:ASN:C	2.72	0.41
1:C:203:VAL:O	1:C:204:ASN:HB2	2.20	0.41
1:D:64:LEU:O	1:D:65:ARG:HD2	2.21	0.41
1:A:31:VAL:HG21	1:A:52:VAL:HG11	2.02	0.41
1:B:34:ARG:HD3	1:B:40:HIS:HA	2.03	0.41
1:B:61:LEU:HD21	1:B:88:ILE:HG13	2.01	0.41
1:D:202:LYS:CB	1:D:202:LYS:NZ	2.83	0.41
1:A:180:MET:C	1:A:230:ARG:HG3	2.41	0.41
1:B:186:THR:O	1:B:221:ALA:HB1	2.21	0.41
1:A:45:SER:OG	1:A:209:GLN:NE2	2.54	0.41
1:A:69:ARG:NH1	1:A:71:GLN:NE2	2.55	0.41
1:B:60(D):LYS:NZ	1:B:60(E):ASP:H	2.18	0.41
1:B:166:HIS:ND1	1:B:167:ILE:N	2.69	0.41
1:B:167:ILE:HD13	1:B:167:ILE:HA	1.78	0.41
1:B:181:LEU:CD1	1:B:181:LEU:C	2.90	0.41
1:B:191:CYS:O	1:B:194:ASP:HB2	2.21	0.41
1:B:192:GLN:HE21	2:B:3211:PM2:H152	1.86	0.41
1:B:235:LEU:HD12	1:B:235:LEU:HA	1.76	0.41
1:D:134:MET:HE1	1:D:201:CYS:HB3	2.03	0.41
1:A:195:SER:HA	1:A:213:VAL:HG12	2.02	0.41
1:B:34:ARG:HG3	1:B:34:ARG:NH1	2.36	0.40
1:C:23:PRO:CD	1:C:26:LYS:HD2	2.45	0.40
1:C:70:GLU:O	1:C:141:TRP:HZ2	2.03	0.40
1:D:74:TYR:HA	1:D:80:ASP:OD1	2.22	0.40
1:D:136:CYS:SG	1:D:162:ILE:HD12	2.61	0.40
1:D:224:ARG:HG3	3:D:2087:HOH:O	2.21	0.40
1:C:129:THR:O	1:C:130:PHE:HB2	2.21	0.40
1:C:228:TYR:CD1	1:C:228:TYR:N	2.89	0.40
1:A:185:ASN:HD21	1:A:188:ARG:N	2.20	0.40
1:C:171:LYS:HE2	1:C:223:ASN:HD22	1.86	0.40
1:D:61:LEU:CD1	1:D:88:ILE:HD12	2.51	0.40
1:C:115:SER:O	1:C:119:HIS:HD2	2.04	0.40
1:C:162:ILE:HG22	1:C:163:MET:N	2.35	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	241/245 (98%)	221 (92%)	18 (8%)	2 (1%)	19	19
1	B	241/245 (98%)	223 (92%)	17 (7%)	1 (0%)	34	37
1	C	241/245 (98%)	219 (91%)	20 (8%)	2 (1%)	19	19
1	D	241/245 (98%)	226 (94%)	15 (6%)	0	100	100
All	All	964/980 (98%)	889 (92%)	70 (7%)	5 (0%)	29	31

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	132	PRO
1	B	49	PRO
1	C	132	PRO
1	A	133	GLY
1	C	130	PHE

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	207/210 (99%)	182 (88%)	25 (12%)	5	4
1	B	207/210 (99%)	178 (86%)	29 (14%)	3	3
1	C	207/210 (99%)	188 (91%)	19 (9%)	9	9
1	D	207/210 (99%)	184 (89%)	23 (11%)	6	5
All	All	828/840 (99%)	732 (88%)	96 (12%)	5	5

All (96) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	24	ARG
1	A	46	LEU
1	A	61	LEU
1	A	65	ARG
1	A	67	GLN
1	A	79	GLN
1	A	81	GLN
1	A	82	LEU
1	A	87	ARG
1	A	110	GLU
1	A	116	SER
1	A	118	VAL
1	A	127	SER
1	A	129	THR
1	A	134	MET
1	A	147	ASP
1	A	150	ARG
1	A	155	LEU
1	A	171	LYS
1	A	174	ARG
1	A	177	ARG
1	A	185	ASN
1	A	187	ARG
1	A	188	ARG
1	A	209	GLN
1	B	24	ARG
1	B	35	VAL
1	B	39	MET
1	B	53	LEU
1	B	60(D)	LYS
1	B	71	GLN
1	B	75	TYR
1	B	79	GLN
1	B	81	GLN
1	B	110	GLU
1	B	113	LYS
1	B	114	VAL
1	B	127	SER
1	B	138	VAL
1	B	147	ASP
1	B	149	GLU
1	B	159	LYS

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Mol	Chain	Res	Type
1	B	162	ILE
1	B	166	HIS
1	B	171	LYS
1	B	173(A)	LEU
1	B	173(H)	ASP
1	B	174	ARG
1	B	177	ARG
1	B	181	LEU
1	B	187	ARG
1	B	221(A)	GLN
1	B	235	LEU
1	B	236	ASP
1	C	20	GLN
1	C	24	ARG
1	C	39	MET
1	C	53	LEU
1	C	65	ARG
1	C	68	LEU
1	C	69	ARG
1	C	79	GLN
1	C	83	LEU
1	C	93	GLN
1	C	118	VAL
1	C	122	THR
1	C	150	ARG
1	C	164	GLU
1	C	171	LYS
1	C	177	ARG
1	C	186	THR
1	C	187	ARG
1	C	188	ARG
1	D	50	GLN
1	D	52	VAL
1	D	53	LEU
1	D	60(D)	LYS
1	D	61	LEU
1	D	82	LEU
1	D	85	VAL
1	D	106	LEU
1	D	108	LEU
1	D	110	GLU
1	D	115	SER

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Mol	Chain	Res	Type
1	D	116	SER
1	D	147	ASP
1	D	150	ARG
1	D	162	ILE
1	D	173(A)	LEU
1	D	173(I)	VAL
1	D	177	ARG
1	D	190	SER
1	D	192	GLN
1	D	202	LYS
1	D	204	ASN
1	D	206	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (42) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	30	GLN
1	A	48	HIS
1	A	50	GLN
1	A	71	GLN
1	A	72	HIS
1	A	93	GLN
1	A	117	HIS
1	A	119	HIS
1	A	146	ASN
1	A	185	ASN
1	A	192	GLN
1	A	209	GLN
1	B	48	HIS
1	B	50	GLN
1	B	71	GLN
1	B	81	GLN
1	B	93	GLN
1	B	117	HIS
1	B	165	ASN
1	B	173	HIS
1	B	192	GLN
1	B	223	ASN
1	B	239	HIS
1	C	30	GLN
1	C	36	HIS
1	C	48	HIS

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Mol	Chain	Res	Type
1	C	57	HIS
1	C	79	GLN
1	C	91	HIS
1	C	165	ASN
1	C	204	ASN
1	C	209	GLN
1	C	223	ASN
1	C	239	HIS
1	D	30	GLN
1	D	50	GLN
1	D	93	GLN
1	D	119	HIS
1	D	146	ASN
1	D	157	GLN
1	D	166	HIS
1	D	240	HIS

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	PM2	D	3211	-	33,33,33	2.31	16 (48%)	44,44,44	1.04	3 (6%)
2	PM2	B	3211	-	33,33,33	2.36	17 (51%)	44,44,44	1.11	2 (4%)
2	PM2	A	3211	-	33,33,33	2.48	15 (45%)	44,44,44	1.15	2 (4%)
2	PM2	C	3211	-	33,33,33	2.53	15 (45%)	44,44,44	0.98	2 (4%)

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	PM2	D	3211	-	-	0/19/29/29	0/4/4/4
2	PM2	B	3211	-	-	0/19/29/29	0/4/4/4
2	PM2	A	3211	-	-	0/19/29/29	0/4/4/4
2	PM2	C	3211	-	-	0/19/29/29	0/4/4/4

All (63) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	3211	PM2	C3-C1	5.31	1.47	1.39
2	A	3211	PM2	C18-C20	4.96	1.47	1.39
2	A	3211	PM2	C28-C26	4.57	1.48	1.38
2	B	3211	PM2	C3-C1	4.44	1.46	1.39
2	C	3211	PM2	C18-C20	4.42	1.46	1.39
2	A	3211	PM2	C18-C17	4.38	1.45	1.39
2	A	3211	PM2	C3-C1	4.25	1.45	1.39
2	C	3211	PM2	C2-C1	4.18	1.45	1.39
2	B	3211	PM2	C2-C4	4.07	1.46	1.39
2	C	3211	PM2	C18-C17	4.04	1.45	1.39
2	D	3211	PM2	C3-C1	4.04	1.45	1.39
2	B	3211	PM2	C2-C1	4.00	1.45	1.39
2	D	3211	PM2	C18-C20	3.82	1.45	1.39
2	C	3211	PM2	C27-C25	3.80	1.47	1.38
2	B	3211	PM2	C18-C20	3.80	1.45	1.39
2	A	3211	PM2	C6-C4	3.80	1.47	1.38
2	B	3211	PM2	C28-C26	3.80	1.46	1.38
2	C	3211	PM2	C28-C26	3.79	1.46	1.38
2	D	3211	PM2	C27-C25	3.76	1.47	1.38
2	C	3211	PM2	C6-C4	3.72	1.46	1.38
2	B	3211	PM2	C27-C25	3.59	1.46	1.38
2	A	3211	PM2	C11-N14	3.56	1.42	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	3211	PM2	C5-C6	3.55	1.46	1.38
2	D	3211	PM2	C2-C1	3.54	1.44	1.39
2	A	3211	PM2	C27-C25	3.51	1.46	1.38
2	D	3211	PM2	C28-C26	3.48	1.46	1.38
2	D	3211	PM2	C6-C4	3.45	1.46	1.38
2	D	3211	PM2	C18-C17	3.44	1.44	1.39
2	D	3211	PM2	C11-N14	3.37	1.42	1.34
2	C	3211	PM2	C5-C3	3.24	1.45	1.38
2	B	3211	PM2	C18-C17	3.18	1.44	1.39
2	A	3211	PM2	C15-N14	2.95	1.52	1.47
2	B	3211	PM2	C6-C4	2.94	1.45	1.38
2	A	3211	PM2	C5-C3	2.88	1.45	1.38
2	B	3211	PM2	C30-C29	2.87	1.45	1.38
2	A	3211	PM2	C2-C1	2.87	1.43	1.39
2	C	3211	PM2	C30-C29	2.87	1.45	1.38
2	D	3211	PM2	C30-C29	2.87	1.45	1.38
2	B	3211	PM2	C11-N14	2.81	1.40	1.34
2	C	3211	PM2	C2-C4	2.80	1.44	1.39
2	D	3211	PM2	C5-C6	2.75	1.44	1.38
2	C	3211	PM2	C30-C28	2.71	1.45	1.38
2	D	3211	PM2	C19-C17	2.69	1.43	1.39
2	C	3211	PM2	C11-N14	2.68	1.40	1.34
2	D	3211	PM2	C29-C27	2.54	1.44	1.38
2	A	3211	PM2	C30-C29	2.53	1.44	1.38
2	B	3211	PM2	C26-C25	2.46	1.44	1.38
2	A	3211	PM2	C5-C6	2.45	1.44	1.38
2	B	3211	PM2	C30-C28	2.42	1.44	1.38
2	A	3211	PM2	C30-C28	2.42	1.44	1.38
2	C	3211	PM2	C29-C27	2.39	1.44	1.38
2	B	3211	PM2	C5-C3	2.38	1.43	1.38
2	A	3211	PM2	C29-C27	2.36	1.43	1.38
2	D	3211	PM2	C5-C3	2.36	1.43	1.38
2	D	3211	PM2	C30-C28	2.33	1.44	1.38
2	B	3211	PM2	C19-C17	2.32	1.42	1.39
2	B	3211	PM2	C29-C27	2.25	1.43	1.38
2	C	3211	PM2	C26-C25	2.20	1.43	1.38
2	A	3211	PM2	C9-C13	2.20	1.59	1.53
2	B	3211	PM2	C9-C13	2.15	1.59	1.53
2	B	3211	PM2	C9-C10	2.10	1.58	1.52
2	D	3211	PM2	C2-C4	2.05	1.42	1.39
2	D	3211	PM2	C16-C13	2.01	1.58	1.53

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	3211	PM2	C17-C11-N14	4.72	124.72	118.72
2	B	3211	PM2	C17-C11-N14	4.17	124.01	118.72
2	C	3211	PM2	C17-C11-N14	3.97	123.76	118.72
2	D	3211	PM2	C17-C11-N14	3.87	123.62	118.72
2	B	3211	PM2	O12-C11-C17	-3.53	113.37	120.23
2	A	3211	PM2	O12-C11-C17	-3.28	113.84	120.23
2	D	3211	PM2	O12-C11-C17	-2.98	114.44	120.23
2	C	3211	PM2	O12-C11-C17	-2.59	115.18	120.23
2	D	3211	PM2	C10-N14-C11	2.01	129.15	122.78

There are no chirality outliers.

There are no torsion outliers.

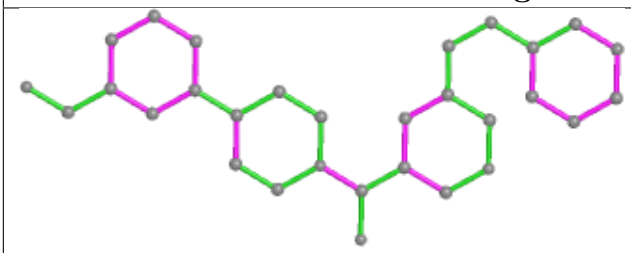
There are no ring outliers.

2 monomers are involved in 3 short contacts:

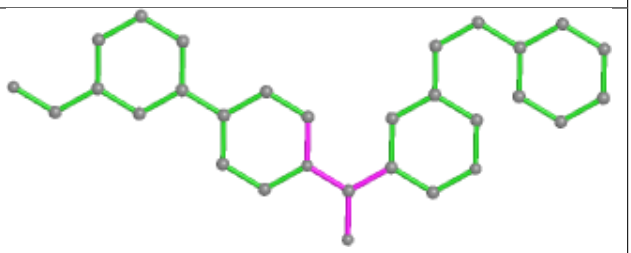
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	3211	PM2	1	0
2	B	3211	PM2	2	0

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.

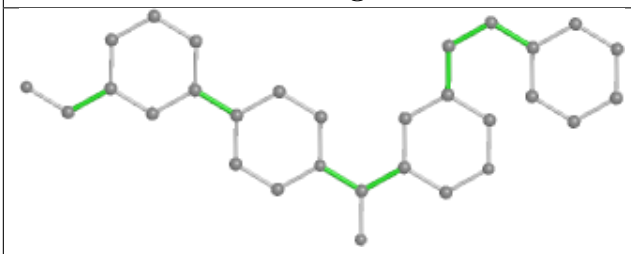
Ligand PM2 D 3211



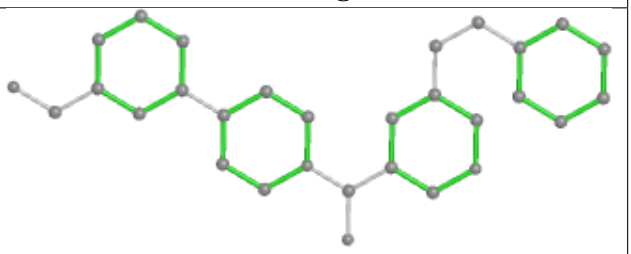
Bond lengths



Bond angles

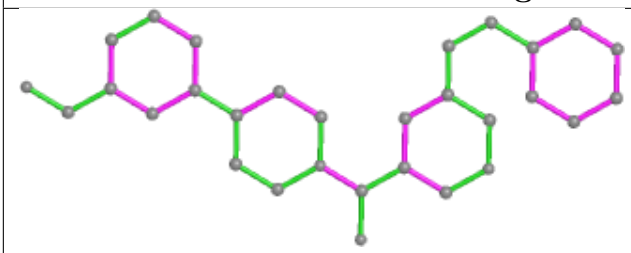


Torsions

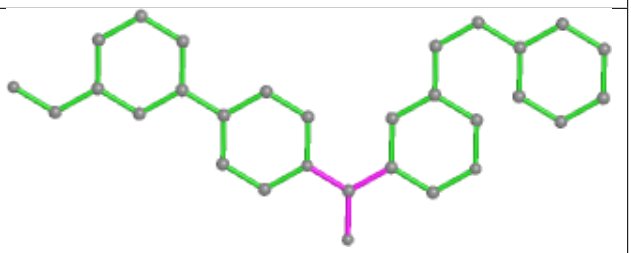


Rings

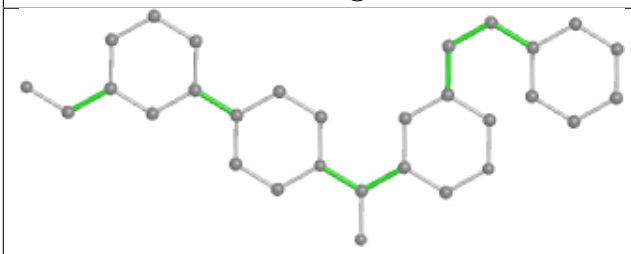
Ligand PM2 B 3211



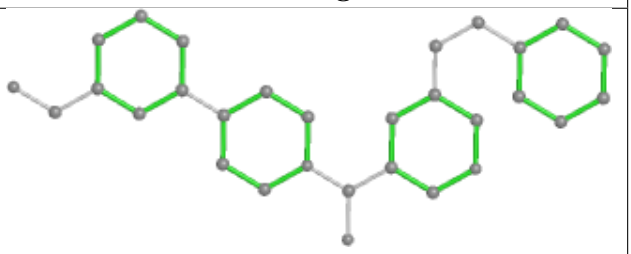
Bond lengths



Bond angles

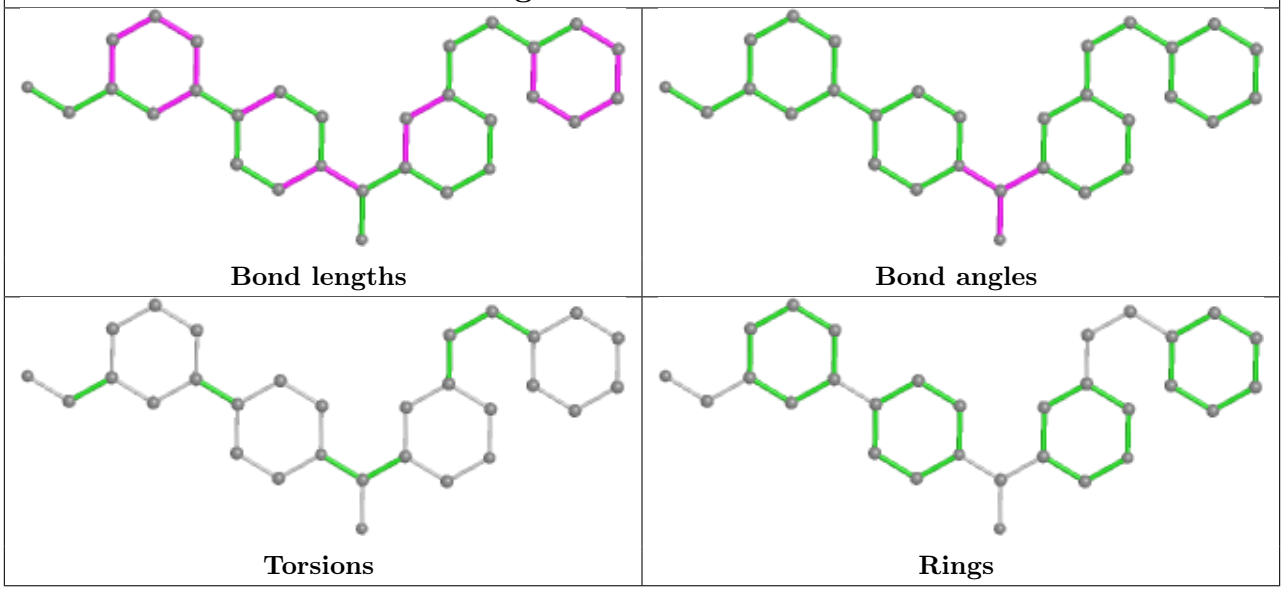


Torsions

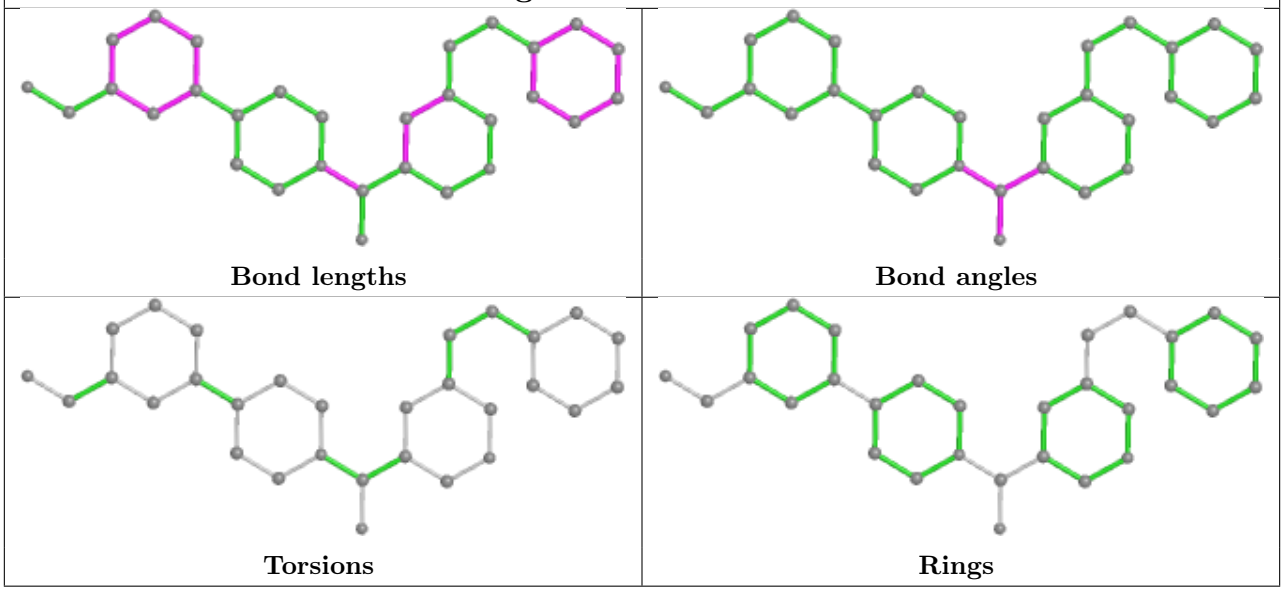


Rings

Ligand PM2 A 3211



Ligand PM2 C 3211



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%)	-0.06	7 (2%)	51	49	21, 38, 63, 75	6 (2%)
1	B	243/245 (99%)	-0.21	4 (1%)	72	70	18, 34, 59, 68	3 (1%)
1	C	243/245 (99%)	-0.19	3 (1%)	79	77	17, 33, 56, 70	3 (1%)
1	D	243/245 (99%)	-0.21	1 (0%)	92	91	20, 33, 57, 67	2 (0%)
All	All	972/980 (99%)	-0.17	15 (1%)	73	72	17, 34, 60, 75	14 (1%)

All (15) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	114	VAL	3.5
1	B	147	ASP	3.1
1	A	117	HIS	3.0
1	B	114	VAL	2.8
1	A	115	SER	2.5
1	C	135	PRO	2.5
1	B	116	SER	2.4
1	B	127	SER	2.4
1	A	204	ASN	2.4
1	A	116	SER	2.4
1	A	36	HIS	2.2
1	A	31	VAL	2.2
1	C	24	ARG	2.2
1	A	126	ALA	2.1
1	C	133	GLY	2.1

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)

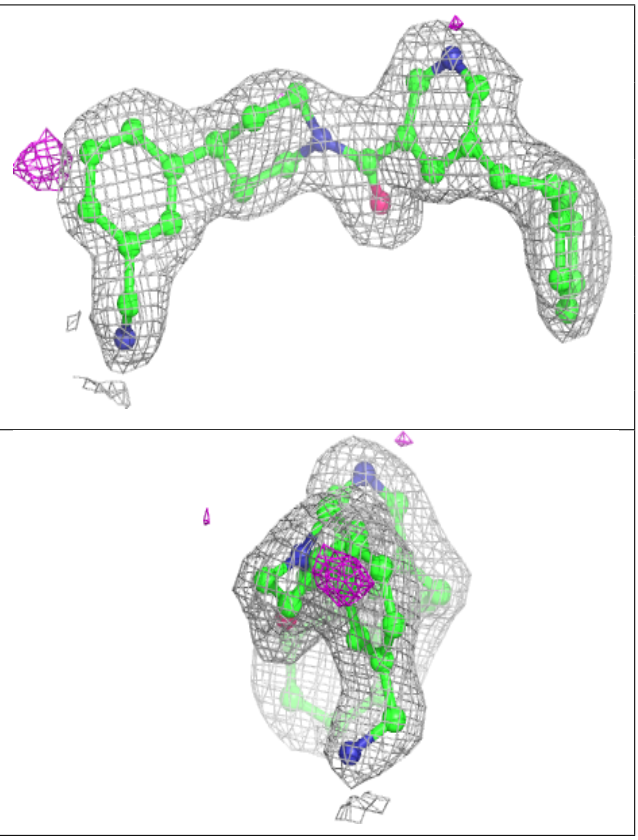
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	PM2	A	3211	30/30	0.92	0.13	22,33,36,37	0
2	PM2	B	3211	30/30	0.94	0.11	18,28,36,36	0
2	PM2	C	3211	30/30	0.94	0.11	24,31,35,38	0
2	PM2	D	3211	30/30	0.94	0.12	22,30,41,45	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.

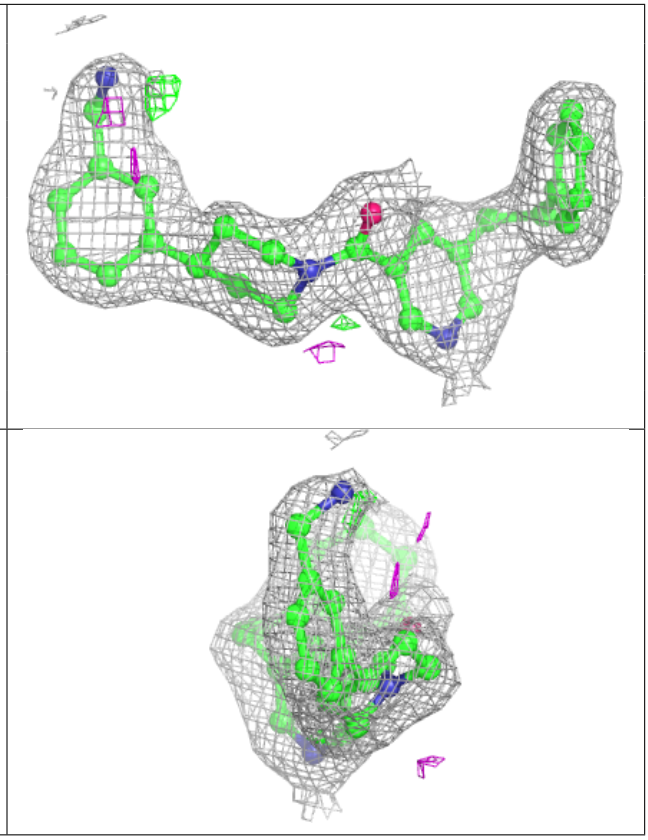
Electron density around PM2 A 3211:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative) and green (positive)



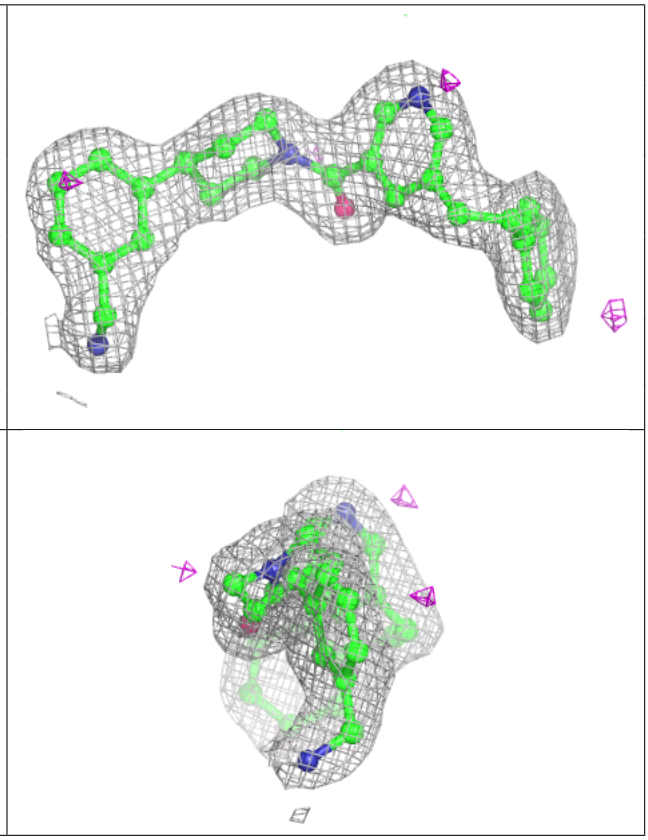
Electron density around PM2 B 3211:

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



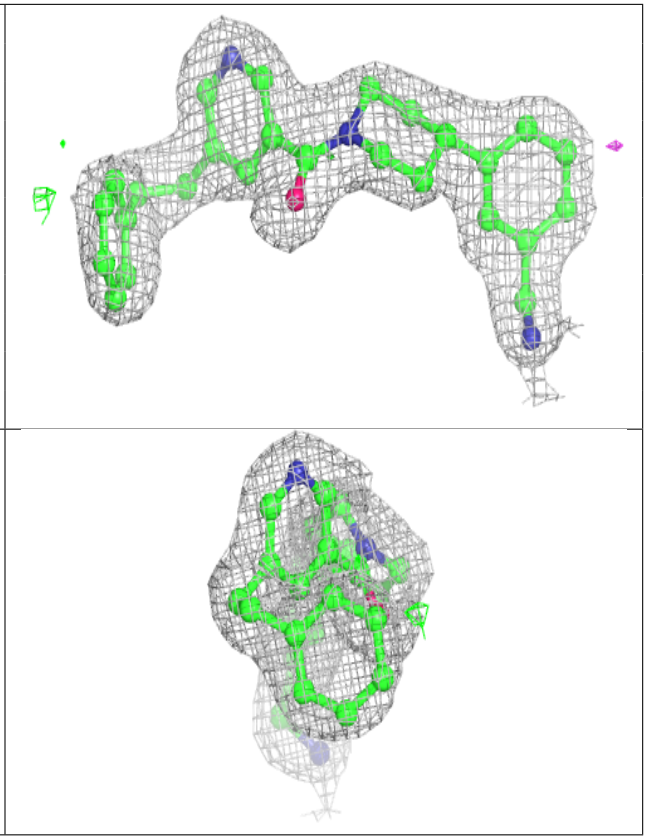
Electron density around PM2 C 3211:

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



Electron density around PM2 D 3211:

$2mF_o$-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.