Full wwPDB X-ray Structure Validation Report (i)

Oct 4, 2023 – 05:33 PM EDT

PDB ID	:	6OHS
Title	:	Structure of compound 3 (ML299) bound human Phospholipase D2 catalytic domain
Authors	:	Metrick, C.M.; Chodaparambil, J.V.
Deposited on	:	2019-04-06
Resolution	:	3.20 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 (i)) were used in the production of this report:

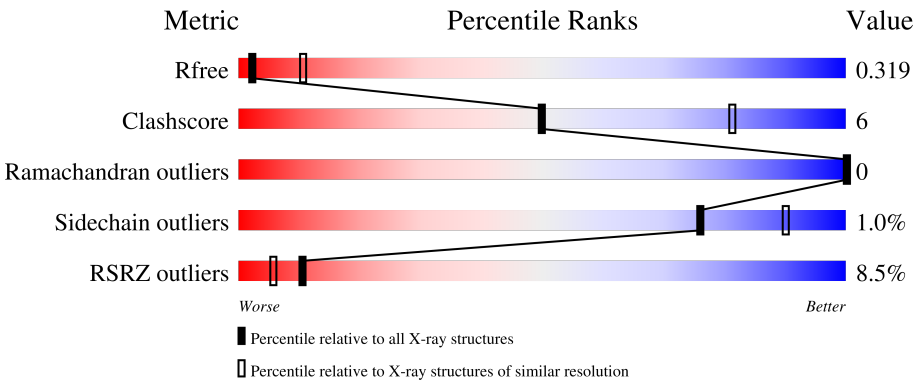
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & 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 3.20 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	1133 (3.20-3.20)
Clashscore	141614	1253 (3.20-3.20)
Ramachandran outliers	138981	1234 (3.20-3.20)
Sidechain outliers	138945	1233 (3.20-3.20)
RSRZ outliers	127900	1095 (3.20-3.20)

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	640	5% 78% 13% 9%
1	B	640	4% 78% 13% 9%
1	C	640	11% 76% 15% 9%
1	D	640	11% 73% 18% 9%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	MJY	A	1001	-	-	-	X
2	MJY	C	1001	-	-	-	X
2	MJY	D	1001	-	-	-	X

2 Entry composition (i)

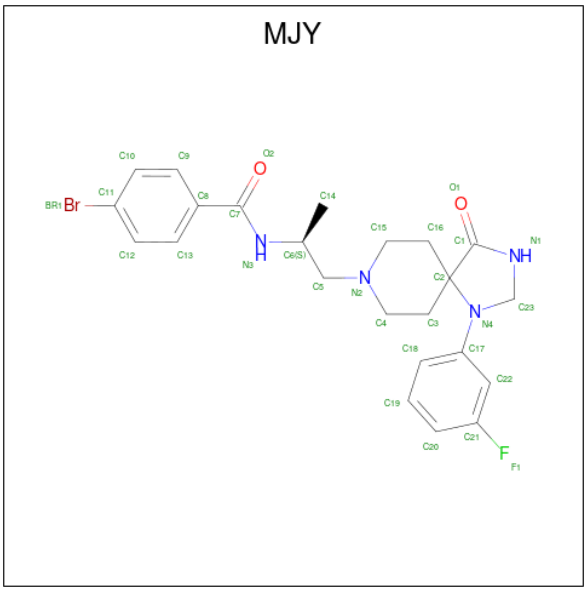
There are 2 unique types of molecules in this entry. The entry contains 18932 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Phospholipase D2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	584	4702	3015	825	846	16	0	0	0
1	B	584	4702	3015	825	846	16	0	0	0
1	C	584	4702	3015	825	846	16	0	0	0
1	D	584	4702	3015	825	846	16	0	0	0

- Molecule 2 is 4-bromo-N-{(2S)-1-[1-(3-fluorophenyl)-4-oxo-1,3,8-triazaspiro[4.5]decan-8-yl]propan-2-yl}benzamide (three-letter code: MJY) (formula: $C_{23}H_{26}BrFN_4O_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
			Total	Br	C	F	N	O		
2	A	1	31	1	23	1	4	2	0	0

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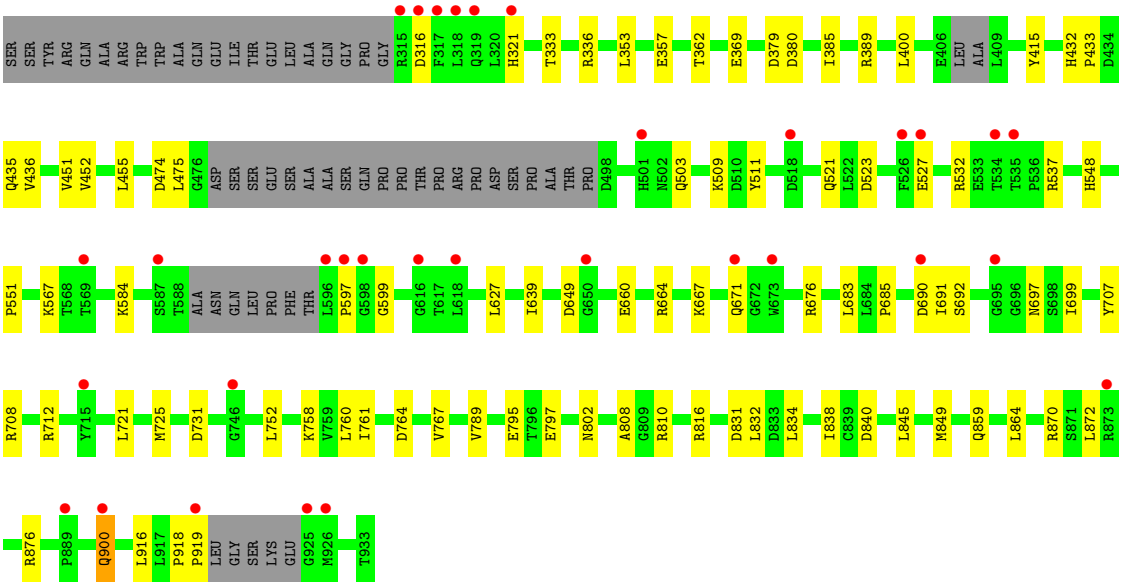
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
			Total	Br	C	F	N	O		
2	B	1	31	1	23	1	4	2	0	0
			Total	Br	C	F	N	O		
2	C	1	31	1	23	1	4	2	0	0
			Total	Br	C	F	N	O		
2	D	1	31	1	23	1	4	2	0	0

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.

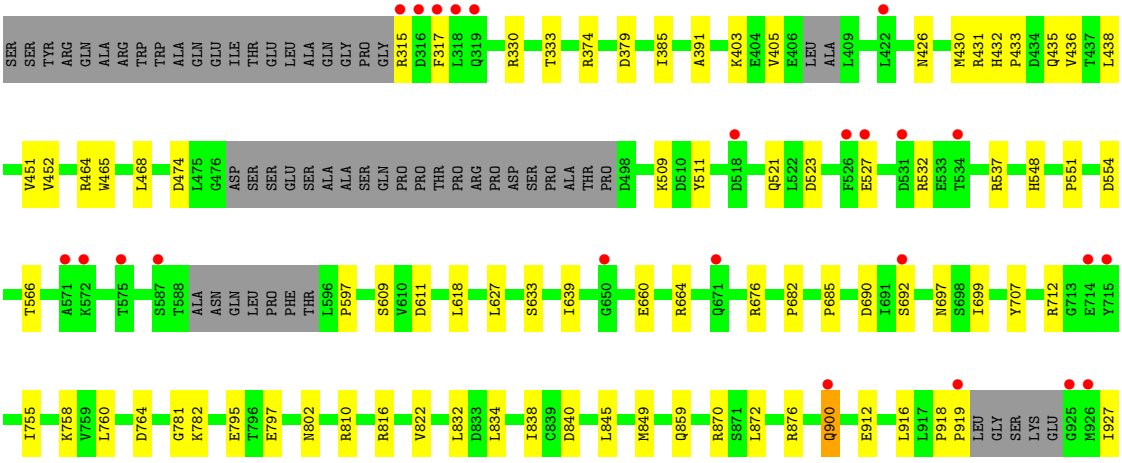
• Molecule 1: Phospholipase D2

Chain A:



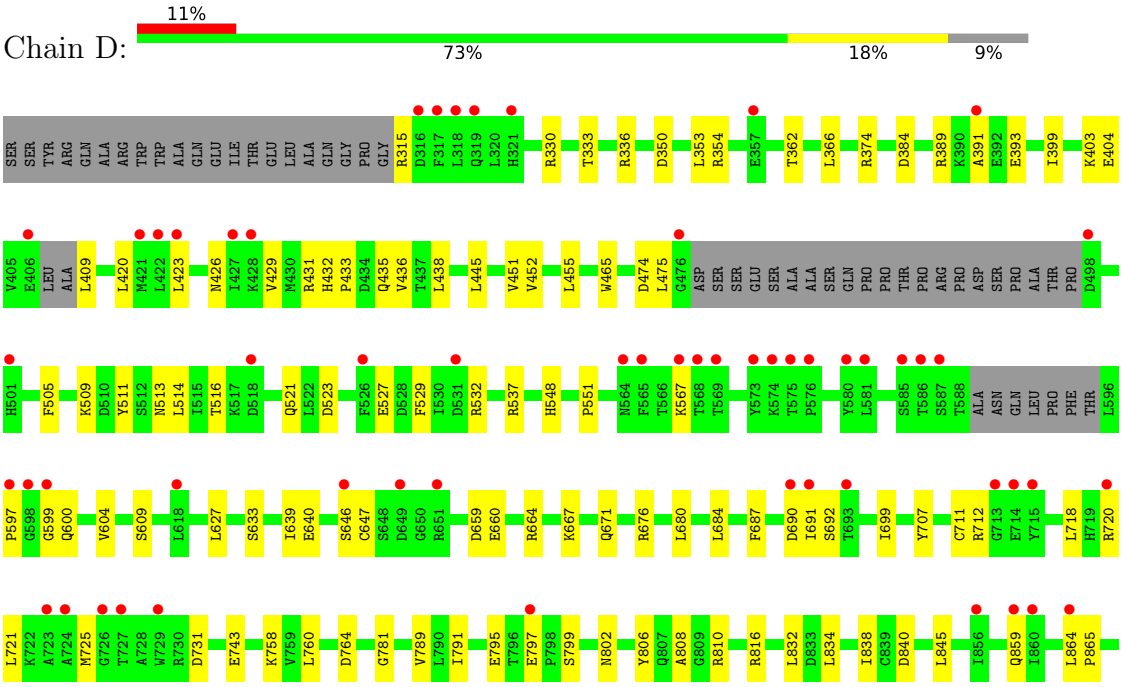
• Molecule 1: Phospholipase D2

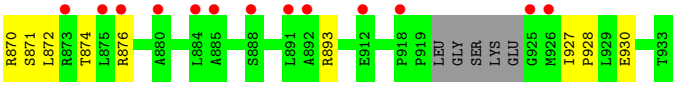
Chain B:



• Molecule 1: Phospholipase D2

Chain D:




R870
S871
L872
R873
T874
L875
R876
A880
L884
A885
S888
L891
A892
R893
E912
P918
P919
LEU
GLY
SER
LYS
GLU
G925
M926
I927
P928
L929
E930
T933

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	89.06Å 132.32Å 114.61Å 90.00° 100.01° 90.00°	Depositor
Resolution (Å)	48.17 – 3.20 48.17 – 3.20	Depositor EDS
% Data completeness (in resolution range)	99.5 (48.17-3.20) 99.5 (48.17-3.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.18 (at 3.19Å)	Xtriage
Refinement program	PHENIX (1.14_3260: ???)	Depositor
R, R_{free}	0.278 , 0.319 0.278 , 0.319	Depositor DCC
R_{free} test set	2146 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å^2)	56.9	Xtriage
Anisotropy	0.503	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 52.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.39$, $< L^2 > = 0.22$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.89	EDS
Total number of atoms	18932	wwPDB-VP
Average B, all atoms (Å^2)	65.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 52.44 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 4.8634e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[1] Intensities estimated from amplitudes.

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

5 Model quality (i)

5.1 Standard geometry (i)

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

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	0.25	0/4823	0.50	1/6553 (0.0%)
1	B	0.26	0/4823	0.50	1/6553 (0.0%)
1	C	0.25	0/4823	0.50	0/6553
1	D	0.25	0/4823	0.50	0/6553
All	All	0.25	0/19292	0.50	2/26212 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	916	LEU	C-N-CA	-5.77	107.27	121.70
1	A	916	LEU	C-N-CA	-5.03	109.12	121.70

There are no chirality outliers.

There are no planarity outliers.

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	4702	0	4634	53	0
1	B	4702	0	4634	49	0
1	C	4702	0	4634	61	1
1	D	4702	0	4634	67	1
2	A	31	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	31	0	0	1	0
2	C	31	0	0	1	0
2	D	31	0	0	1	0
All	All	18932	0	18536	217	1

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 (217) 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:503:GLN:HG2	1:C:831:ASP:HB3	1.65	0.79
1:C:712:ARG:NH2	1:C:910:PHE:O	2.18	0.77
1:D:797:GLU:HG2	1:D:810:ARG:HG2	1.67	0.77
1:B:509:LYS:NZ	1:B:521:GLN:O	2.17	0.76
1:A:797:GLU:HG2	1:A:810:ARG:HG2	1.68	0.73
1:D:816:ARG:NH2	1:D:834:LEU:O	2.19	0.73
1:B:438:LEU:HD21	1:D:438:LEU:HD21	1.72	0.72
1:A:831:ASP:HB3	1:C:503:GLN:HG2	1.71	0.71
1:B:927:ILE:HD13	1:D:927:ILE:HD13	1.73	0.71
1:A:509:LYS:NZ	1:A:521:GLN:O	2.24	0.70
1:B:464:ARG:NH2	2:B:1001:MJY:O2	2.24	0.70
1:C:816:ARG:NH2	1:C:834:LEU:O	2.21	0.69
1:B:816:ARG:NH2	1:B:834:LEU:O	2.23	0.68
1:C:627:LEU:HD22	1:C:660:GLU:HG3	1.76	0.67
1:C:795:GLU:OE1	1:C:810:ARG:NH1	2.28	0.66
1:B:797:GLU:HG2	1:B:810:ARG:HG2	1.75	0.66
1:C:797:GLU:HG2	1:C:810:ARG:HG2	1.77	0.66
1:B:618:LEU:HD13	1:B:782:LYS:HE3	1.77	0.65
1:D:509:LYS:NZ	1:D:521:GLN:O	2.30	0.65
1:B:795:GLU:OE1	1:B:810:ARG:NH1	2.31	0.63
1:A:872:LEU:O	1:A:876:ARG:HD3	1.98	0.63
1:D:627:LEU:HD22	1:D:660:GLU:HG3	1.80	0.63
1:B:832:LEU:HD23	1:B:834:LEU:HD21	1.79	0.63
1:C:872:LEU:O	1:C:876:ARG:HD3	1.98	0.62
1:A:816:ARG:NH2	1:A:834:LEU:O	2.31	0.62
1:B:872:LEU:O	1:B:876:ARG:HD3	2.00	0.61
1:C:676:ARG:NH1	1:C:731:ASP:O	2.30	0.61
1:C:773:ASN:ND2	2:C:1001:MJY:O1	2.34	0.61
1:D:350:ASP:HB3	1:D:354:ARG:HH21	1.64	0.60
1:B:697:ASN:HB2	1:B:918:PRO:HB3	1.81	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:707:TYR:HB3	1:D:712:ARG:HD2	1.82	0.60
1:C:604:VAL:HG22	1:C:791:ILE:HG12	1.84	0.60
1:C:684:LEU:HG	1:C:865:PRO:HD3	1.82	0.60
1:B:405:VAL:HG11	1:D:928:PRO:HB3	1.84	0.60
1:D:676:ARG:NH2	1:D:840:ASP:OD1	2.35	0.60
1:B:627:LEU:HD22	1:B:660:GLU:HG3	1.84	0.59
1:A:795:GLU:OE1	1:A:810:ARG:NH1	2.35	0.59
1:A:503:GLN:CG	1:C:831:ASP:HB3	2.32	0.59
1:B:685:PRO:HD2	1:B:699:ILE:HG23	1.84	0.59
1:D:832:LEU:HD23	1:D:834:LEU:HD21	1.84	0.58
1:C:374:ARG:NH1	1:C:505:PHE:O	2.36	0.58
1:C:676:ARG:NH2	1:C:840:ASP:OD1	2.37	0.58
1:C:832:LEU:HD23	1:C:834:LEU:HD21	1.86	0.57
1:A:548:HIS:NE2	1:A:597:PRO:HD2	2.19	0.57
1:A:676:ARG:NH2	1:A:840:ASP:OD1	2.37	0.57
1:C:797:GLU:N	1:C:808:ALA:O	2.33	0.57
1:D:474:ASP:O	1:D:532:ARG:HD3	2.05	0.56
1:A:802:ASN:HB2	1:A:838:ILE:HD11	1.88	0.56
1:C:455:LEU:HD11	1:C:789:VAL:HG13	1.87	0.56
1:D:455:LEU:HD11	1:D:789:VAL:HG13	1.88	0.56
1:D:509:LYS:HE2	1:D:529:PHE:HB3	1.87	0.55
1:B:391:ALA:HB1	1:B:426:ASN:HB2	1.89	0.55
1:B:403:LYS:HB2	1:B:431:ARG:HB3	1.89	0.55
1:C:509:LYS:NZ	1:C:521:GLN:O	2.40	0.54
1:B:315:ARG:N	1:B:330:ARG:HH12	2.04	0.54
1:B:676:ARG:NH2	1:B:840:ASP:OD1	2.37	0.54
1:A:627:LEU:HD22	1:A:660:GLU:HG3	1.89	0.53
1:A:832:LEU:HD23	1:A:834:LEU:HD21	1.90	0.53
1:B:436:VAL:HG21	1:D:930:GLU:HG3	1.90	0.53
1:A:333:THR:HG21	1:A:551:PRO:HG2	1.91	0.53
1:A:831:ASP:HB3	1:C:503:GLN:CG	2.38	0.53
1:D:333:THR:HG21	1:D:551:PRO:HG2	1.91	0.52
1:D:676:ARG:NH1	1:D:731:ASP:O	2.42	0.52
1:A:380:ASP:OD1	1:A:389:ARG:NH2	2.40	0.52
1:C:474:ASP:O	1:C:532:ARG:HD3	2.10	0.52
1:C:391:ALA:HB1	1:C:426:ASN:HB2	1.91	0.52
1:D:511:TYR:CE2	1:D:537:ARG:HG3	2.45	0.52
1:B:930:GLU:HG3	1:D:436:VAL:HG21	1.92	0.52
1:D:451:VAL:HG23	1:D:452:VAL:HG23	1.92	0.52
1:D:667:LYS:O	1:D:671:GLN:HG2	2.11	0.51
1:C:336:ARG:HB2	1:C:599:GLY:HA2	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:451:VAL:HG23	1:B:452:VAL:HG23	1.93	0.51
1:C:403:LYS:HB2	1:C:431:ARG:HB3	1.92	0.51
1:A:509:LYS:HE3	1:A:527:GLU:O	2.11	0.51
1:D:548:HIS:NE2	1:D:597:PRO:HD2	2.25	0.51
1:C:475:LEU:HD23	1:C:532:ARG:HG2	1.93	0.51
1:D:639:ILE:HG12	1:D:760:LEU:HD12	1.92	0.51
1:D:795:GLU:OE1	1:D:810:ARG:NH1	2.44	0.51
1:A:685:PRO:HD2	1:A:699:ILE:HG23	1.93	0.50
1:C:639:ILE:HG12	1:C:760:LEU:HD12	1.92	0.50
1:D:797:GLU:N	1:D:808:ALA:O	2.38	0.50
1:B:432:HIS:CG	1:B:433:PRO:HA	2.47	0.50
1:D:403:LYS:HB2	1:D:431:ARG:HB3	1.93	0.50
1:A:831:ASP:HB3	1:C:503:GLN:HE21	1.77	0.49
1:B:317:PHE:HZ	1:B:554:ASP:OD1	1.95	0.49
1:D:432:HIS:CG	1:D:433:PRO:HA	2.47	0.49
1:D:475:LEU:HD23	1:D:532:ARG:HG2	1.93	0.49
1:A:451:VAL:HG23	1:A:452:VAL:HG23	1.94	0.49
1:B:435:GLN:HG3	1:B:436:VAL:N	2.28	0.49
1:B:802:ASN:HB2	1:B:838:ILE:HD11	1.93	0.49
1:C:432:HIS:CG	1:C:433:PRO:HA	2.47	0.49
1:B:849:MET:SD	1:B:900:GLN:HG3	2.53	0.49
1:B:764:ASP:OD1	1:B:816:ARG:HD3	2.12	0.49
1:D:690:ASP:OD1	1:D:692:SER:OG	2.30	0.49
1:B:379:ASP:HB3	1:B:385:ILE:HG13	1.95	0.48
1:C:451:VAL:HG23	1:C:452:VAL:HG23	1.94	0.48
1:A:639:ILE:HG12	1:A:760:LEU:HD12	1.95	0.48
1:C:690:ASP:OD1	1:C:692:SER:OG	2.30	0.48
1:C:509:LYS:HE2	1:C:529:PHE:HB3	1.95	0.48
1:A:690:ASP:OD1	1:A:692:SER:OG	2.31	0.48
1:A:676:ARG:NH1	1:A:731:ASP:O	2.43	0.48
1:A:567:LYS:HB3	1:A:567:LYS:HE3	1.71	0.47
1:B:690:ASP:OD1	1:B:692:SER:OG	2.32	0.47
1:D:567:LYS:HB3	1:D:567:LYS:HE3	1.61	0.47
1:D:633:SER:O	1:D:664:ARG:NH2	2.43	0.47
1:C:802:ASN:HB2	1:C:838:ILE:HD11	1.97	0.47
1:D:399:ILE:HB	1:D:429:VAL:HG22	1.97	0.47
1:A:764:ASP:HB3	1:A:808:ALA:HB1	1.97	0.47
1:A:707:TYR:HB3	1:A:712:ARG:HD2	1.97	0.47
1:B:333:THR:HG21	1:B:551:PRO:HG2	1.96	0.47
1:C:509:LYS:HE3	1:C:527:GLU:O	2.15	0.47
1:D:384:ASP:HB2	1:D:423:LEU:HD11	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:687:PHE:HB2	1:D:699:ILE:HD11	1.96	0.46
1:D:659:ASP:HA	1:D:720:ARG:HH22	1.80	0.46
1:A:369:GLU:OE2	1:A:415:TYR:OH	2.22	0.46
1:A:432:HIS:CG	1:A:433:PRO:HA	2.51	0.46
1:B:430:MET:HE3	1:B:566:THR:HB	1.97	0.46
1:B:870:ARG:NE	1:B:912:GLU:OE2	2.49	0.46
1:C:640:GLU:HG3	1:C:680:LEU:HB3	1.97	0.46
1:A:435:GLN:HG3	1:A:436:VAL:N	2.31	0.46
1:B:633:SER:O	1:B:664:ARG:NH2	2.49	0.45
1:D:315:ARG:N	1:D:330:ARG:HH12	2.14	0.45
1:B:374:ARG:HG3	1:B:465:TRP:CE2	2.52	0.45
1:D:684:LEU:HG	1:D:865:PRO:HD3	1.98	0.45
1:A:683:LEU:HB2	1:A:752:LEU:HD22	1.99	0.45
1:A:379:ASP:HB3	1:A:385:ILE:HG13	1.99	0.45
1:A:761:ILE:HG12	1:A:767:VAL:HG22	1.99	0.45
1:B:511:TYR:CE2	1:B:537:ARG:HG3	2.52	0.45
1:B:609:SER:HB3	1:B:781:GLY:HA2	1.98	0.45
1:C:430:MET:HE3	1:C:566:THR:HB	1.99	0.45
1:B:474:ASP:O	1:B:532:ARG:HD3	2.17	0.45
1:C:764:ASP:OD1	1:C:816:ARG:HD3	2.18	0.44
1:D:513:ASN:HB3	1:D:516:THR:HB	2.00	0.44
1:D:799:SER:N	1:D:806:TYR:O	2.47	0.44
1:D:391:ALA:HB1	1:D:426:ASN:HB2	1.99	0.44
1:D:366:LEU:HD22	1:D:420:LEU:HD11	1.99	0.44
1:A:697:ASN:HB2	1:A:918:PRO:HB3	2.00	0.44
1:B:509:LYS:HE3	1:B:527:GLU:O	2.18	0.44
1:C:567:LYS:HB3	1:C:567:LYS:HE3	1.64	0.44
1:D:336:ARG:HB2	1:D:599:GLY:HA2	1.99	0.44
1:D:802:ASN:HB2	1:D:838:ILE:HD11	1.99	0.44
1:A:362:THR:HG22	1:A:400:LEU:HB2	2.00	0.44
1:C:404:GLU:HB2	1:C:409:LEU:HD12	1.99	0.44
1:B:432:HIS:CD2	1:B:433:PRO:HA	2.53	0.44
1:D:435:GLN:HG3	1:D:436:VAL:N	2.33	0.44
1:A:849:MET:SD	1:A:900:GLN:HG3	2.57	0.43
1:B:468:LEU:HD22	1:B:822:VAL:HG21	2.00	0.43
1:C:362:THR:HG23	1:C:559:PHE:HD2	1.83	0.43
1:D:711:CYS:HB3	1:D:718:LEU:HD12	2.00	0.43
1:C:374:ARG:HG3	1:C:465:TRP:CE2	2.53	0.43
1:D:404:GLU:HB2	1:D:409:LEU:HD12	2.01	0.43
1:A:795:GLU:HB3	1:A:810:ARG:NH1	2.34	0.43
1:A:357:GLU:OE2	1:A:584:LYS:NZ	2.24	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:918:PRO:HA	1:B:919:PRO:HD3	1.89	0.43
1:A:503:GLN:HE21	1:C:831:ASP:HB3	1.84	0.43
1:A:511:TYR:CE2	1:A:537:ARG:HG3	2.54	0.43
1:B:611:ASP:OD1	1:B:782:LYS:HD3	2.19	0.43
1:C:366:LEU:HD22	1:C:420:LEU:HD11	2.00	0.43
1:C:384:ASP:HB2	1:C:423:LEU:HD11	2.01	0.43
1:C:435:GLN:HG3	1:C:436:VAL:N	2.34	0.43
1:A:664:ARG:HD2	1:A:664:ARG:HA	1.82	0.42
1:C:425:PRO:O	1:C:428:LYS:HE3	2.18	0.42
1:D:721:LEU:O	1:D:725:MET:HG2	2.18	0.42
1:C:683:LEU:HD11	1:C:904:VAL:HG21	2.01	0.42
1:D:691:ILE:HG23	1:D:864:LEU:HD12	2.01	0.42
1:D:764:ASP:OD1	1:D:816:ARG:HD3	2.18	0.42
1:D:871:SER:OG	1:D:874:THR:HG22	2.20	0.42
1:A:831:ASP:HB3	1:C:503:GLN:NE2	2.34	0.42
1:A:764:ASP:OD1	1:A:816:ARG:HD3	2.19	0.42
1:C:342:ALA:HA	1:C:465:TRP:NE1	2.34	0.42
1:D:609:SER:HB3	1:D:781:GLY:HA2	2.00	0.42
1:B:707:TYR:HB3	1:B:712:ARG:HD2	2.01	0.42
1:D:600:GLN:NE2	1:D:795:GLU:OE1	2.50	0.42
1:A:336:ARG:HB2	1:A:599:GLY:HA2	2.02	0.42
1:B:927:ILE:HD13	1:D:927:ILE:CD1	2.45	0.42
1:C:350:ASP:HB3	1:C:354:ARG:HH21	1.85	0.42
1:D:353:LEU:HD12	1:D:353:LEU:HA	1.89	0.42
1:D:374:ARG:NH1	1:D:505:PHE:O	2.50	0.42
1:A:353:LEU:HD12	1:A:353:LEU:HA	1.86	0.42
1:C:315:ARG:N	1:C:330:ARG:HH12	2.18	0.42
1:C:399:ILE:HB	1:C:429:VAL:HG22	2.02	0.42
1:A:455:LEU:HD11	1:A:789:VAL:HG13	2.01	0.41
1:A:721:LEU:O	1:A:725:MET:HG2	2.19	0.41
1:A:918:PRO:HA	1:A:919:PRO:HD3	1.91	0.41
1:D:604:VAL:HG22	1:D:791:ILE:HG12	2.01	0.41
1:D:640:GLU:HG3	1:D:680:LEU:HB3	2.02	0.41
1:A:691:ILE:HG23	1:A:864:LEU:HD12	2.02	0.41
1:B:682:PRO:HD3	1:B:755:ILE:HB	2.02	0.41
1:A:667:LYS:O	1:A:671:GLN:HG2	2.20	0.41
1:B:639:ILE:HG12	1:B:760:LEU:HD12	2.02	0.41
1:C:683:LEU:HB2	1:C:752:LEU:HD22	2.00	0.41
1:C:707:TYR:HB3	1:C:712:ARG:HD2	2.03	0.41
1:B:548:HIS:NE2	1:B:597:PRO:HD2	2.35	0.41
1:D:389:ARG:O	1:D:393:GLU:HG3	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:743:GLU:CD	1:D:893:ARG:HE	2.23	0.41
1:C:541:ARG:NE	1:C:640:GLU:OE2	2.50	0.41
1:C:774:ILE:HA	1:C:779:LEU:HD11	2.03	0.41
1:D:646:SER:OG	1:D:647:CYS:N	2.52	0.41
1:D:795:GLU:HB3	1:D:810:ARG:NH1	2.35	0.41
1:A:649:ASP:HB3	1:A:708:ARG:HH21	1.86	0.41
1:D:374:ARG:HG3	1:D:465:TRP:CE2	2.56	0.41
1:D:509:LYS:HE3	1:D:527:GLU:O	2.21	0.41
1:D:362:THR:OG1	1:D:445:LEU:HB3	2.20	0.41
1:A:475:LEU:HD23	1:A:532:ARG:HG2	2.03	0.40
1:B:929:LEU:HD23	1:B:929:LEU:HA	1.90	0.40
1:C:389:ARG:O	1:C:393:GLU:HG3	2.20	0.40
1:C:721:LEU:O	1:C:725:MET:HG2	2.20	0.40
1:D:872:LEU:O	1:D:876:ARG:HD3	2.21	0.40
1:A:474:ASP:O	1:A:532:ARG:HD3	2.20	0.40
1:B:685:PRO:HB2	1:B:699:ILE:HD13	2.03	0.40
1:C:664:ARG:HD2	1:C:664:ARG:HA	1.79	0.40
1:D:514:LEU:HD21	2:D:1001:MJY:C14	2.50	0.40
1:A:316:ASP:O	1:A:321:HIS:NE2	2.54	0.40
1:C:527:GLU:HG2	1:C:528:ASP:O	2.21	0.40
1:C:439:TRP:CE2	1:C:783:ARG:HG2	2.57	0.40
1:C:683:LEU:O	1:C:865:PRO:HG3	2.22	0.40
1:D:664:ARG:HD2	1:D:664:ARG:HA	1.83	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:855:ASN:ND2	1:D:671:GLN:O[1_554]	2.02	0.18

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	574/640 (90%)	551 (96%)	23 (4%)	0	100	100
1	B	574/640 (90%)	553 (96%)	21 (4%)	0	100	100
1	C	574/640 (90%)	553 (96%)	21 (4%)	0	100	100
1	D	574/640 (90%)	552 (96%)	22 (4%)	0	100	100
All	All	2296/2560 (90%)	2209 (96%)	87 (4%)	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	504/554 (91%)	498 (99%)	6 (1%)	71	88
1	B	504/554 (91%)	499 (99%)	5 (1%)	76	90
1	C	504/554 (91%)	500 (99%)	4 (1%)	81	93
1	D	504/554 (91%)	499 (99%)	5 (1%)	76	90
All	All	2016/2216 (91%)	1996 (99%)	20 (1%)	76	90

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	523	ASP
1	A	758	LYS
1	A	845	LEU
1	A	859	GLN
1	A	870	ARG
1	A	900	GLN
1	B	523	ASP
1	B	758	LYS
1	B	845	LEU
1	B	859	GLN
1	B	900	GLN
1	C	523	ASP
1	C	758	LYS

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Mol	Chain	Res	Type
1	C	845	LEU
1	C	859	GLN
1	D	523	ASP
1	D	758	LYS
1	D	845	LEU
1	D	859	GLN
1	D	870	ARG

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	642	GLN
1	A	844	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	MJY	C	1001	-	32,34,34	0.31	0	40,49,49	1.48	4 (10%)
2	MJY	B	1001	-	32,34,34	0.42	0	40,49,49	0.76	1 (2%)
2	MJY	A	1001	-	32,34,34	0.35	0	40,49,49	1.44	6 (15%)
2	MJY	D	1001	-	32,34,34	0.42	0	40,49,49	0.79	1 (2%)

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	MJY	C	1001	-	-	4/16/45/45	0/4/4/4
2	MJY	B	1001	-	-	3/16/45/45	0/4/4/4
2	MJY	A	1001	-	-	4/16/45/45	0/4/4/4
2	MJY	D	1001	-	-	2/16/45/45	0/4/4/4

There are no bond length outliers.

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	1001	MJY	C16-C2-N4	7.09	118.09	112.85
2	A	1001	MJY	C16-C2-N4	4.31	116.03	112.85
2	A	1001	MJY	C3-C2-N4	3.66	115.56	112.85
2	A	1001	MJY	C4-C3-C2	3.58	116.16	113.06
2	D	1001	MJY	C16-C2-N4	-3.19	110.49	112.85
2	A	1001	MJY	C15-C16-C2	3.07	115.71	113.06
2	A	1001	MJY	C3-C2-C1	-2.90	106.05	109.93
2	A	1001	MJY	C16-C2-C1	-2.73	106.27	109.93
2	C	1001	MJY	C3-C2-N4	2.70	114.85	112.85
2	B	1001	MJY	C15-C16-C2	-2.59	110.81	113.06
2	C	1001	MJY	C16-C2-C1	-2.40	106.72	109.93
2	C	1001	MJY	C3-C2-C1	-2.31	106.84	109.93

There are no chirality outliers.

All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1001	MJY	N2-C5-C6-C14
2	A	1001	MJY	C8-C7-N3-C6

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Mol	Chain	Res	Type	Atoms
2	B	1001	MJY	C6-C5-N2-C15
2	C	1001	MJY	C18-C17-N4-C23
2	C	1001	MJY	C22-C17-N4-C23
2	C	1001	MJY	C8-C7-N3-C6
2	D	1001	MJY	C6-C5-N2-C15
2	C	1001	MJY	O2-C7-N3-C6
2	A	1001	MJY	O2-C7-N3-C6
2	D	1001	MJY	C5-C6-N3-C7
2	A	1001	MJY	N2-C5-C6-N3
2	B	1001	MJY	N2-C5-C6-C14
2	B	1001	MJY	C5-C6-N3-C7

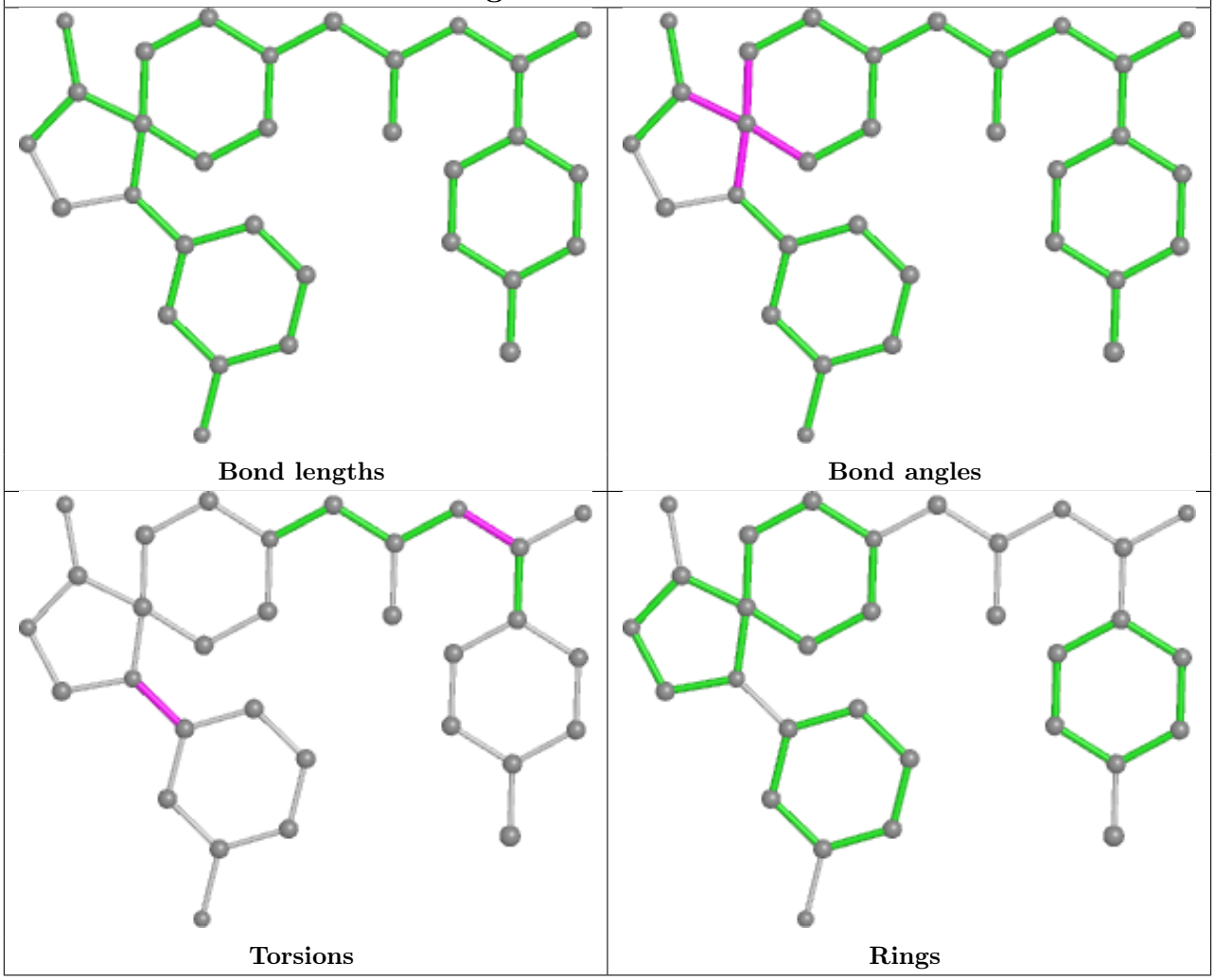
There are no ring outliers.

3 monomers are involved in 3 short contacts:

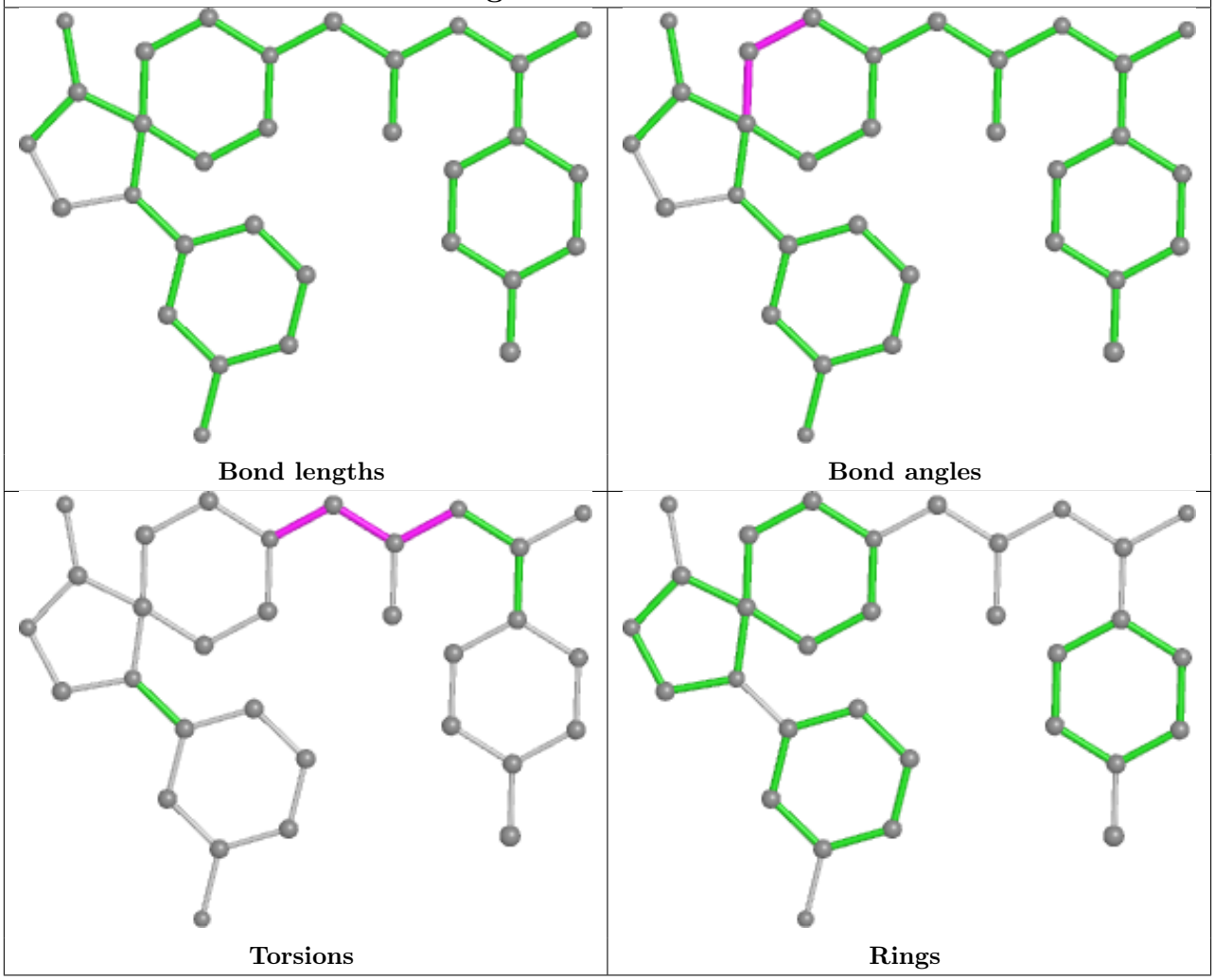
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	1001	MJY	1	0
2	B	1001	MJY	1	0
2	D	1001	MJY	1	0

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.

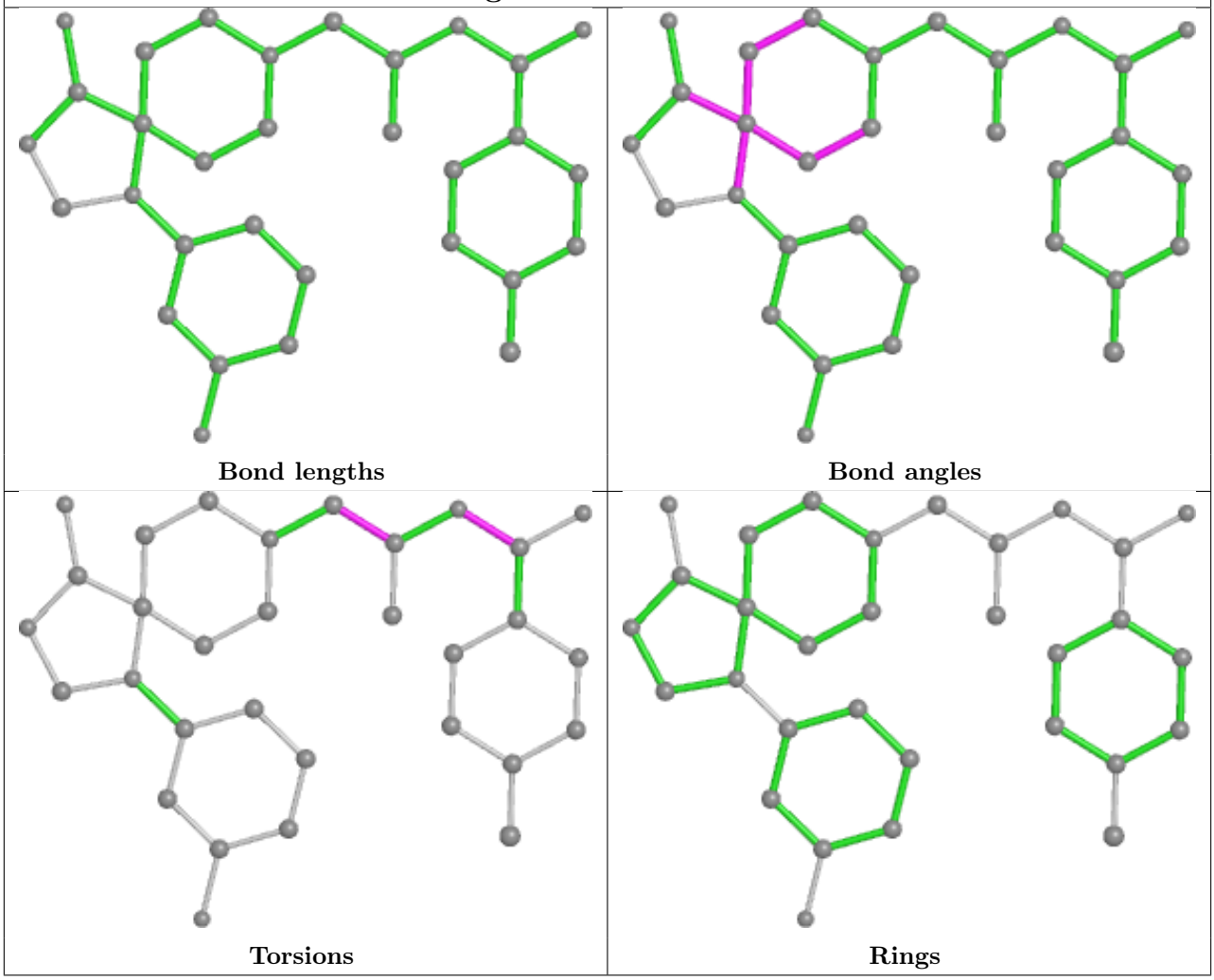
Ligand MJY C 1001



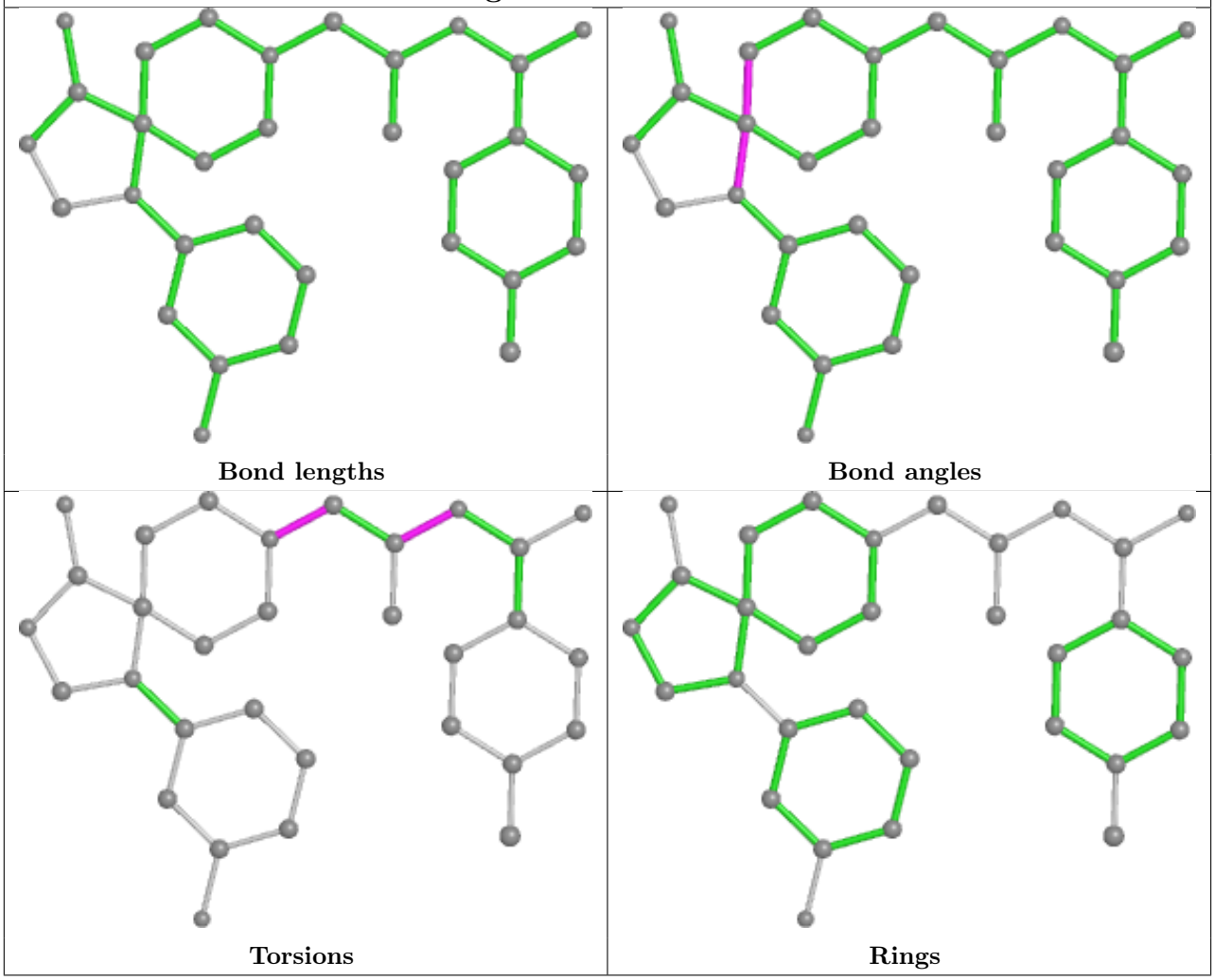
Ligand MJY B 1001



Ligand MJY A 1001



Ligand MJY D 1001



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	584/640 (91%)	0.44	32 (5%)	25	14	28, 54, 105, 178	0
1	B	584/640 (91%)	0.33	24 (4%)	37	24	15, 43, 93, 172	0
1	C	584/640 (91%)	0.86	72 (12%)	4	2	37, 77, 123, 197	0
1	D	584/640 (91%)	0.78	70 (11%)	4	2	34, 69, 115, 180	0
All	All	2336/2560 (91%)	0.60	198 (8%)	10	6	15, 62, 114, 197	0

All (198) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	316	ASP	12.1
1	A	316	ASP	10.0
1	D	501	HIS	8.6
1	D	316	ASP	7.2
1	B	925	GLY	7.1
1	B	926	MET	6.7
1	C	317	PHE	6.6
1	A	319	GLN	6.5
1	A	925	GLY	6.4
1	C	316	ASP	6.2
1	C	925	GLY	6.2
1	D	319	GLN	6.0
1	B	319	GLN	5.8
1	D	318	LEU	5.8
1	C	926	MET	5.5
1	B	315	ARG	5.4
1	D	598	GLY	5.2
1	A	315	ARG	5.2
1	B	318	LEU	5.1
1	C	598	GLY	5.1
1	D	317	PHE	5.0

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Mol	Chain	Res	Type	RSRZ
1	A	671	GLN	4.9
1	D	585	SER	4.9
1	A	926	MET	4.8
1	A	318	LEU	4.8
1	D	880	ALA	4.8
1	C	318	LEU	4.7
1	C	880	ALA	4.7
1	D	726	GLY	4.2
1	A	587	SER	4.1
1	C	327	ALA	4.1
1	C	501	HIS	4.0
1	C	588	THR	4.0
1	B	575	THR	3.9
1	A	919	PRO	3.7
1	C	673	TRP	3.7
1	A	518	ASP	3.7
1	C	531	ASP	3.7
1	C	568	THR	3.7
1	C	587	SER	3.7
1	D	574	LYS	3.6
1	C	581	LEU	3.6
1	B	317	PHE	3.6
1	D	723	ALA	3.5
1	C	574	LYS	3.5
1	C	876	ARG	3.5
1	D	873	ARG	3.5
1	D	691	ILE	3.4
1	C	724	ALA	3.4
1	D	586	THR	3.4
1	D	567	LYS	3.4
1	C	616	GLY	3.4
1	D	568	THR	3.4
1	A	501	HIS	3.4
1	D	422	LEU	3.3
1	B	671	GLN	3.3
1	D	888	SER	3.3
1	C	597	PRO	3.3
1	C	671	GLN	3.2
1	C	726	GLY	3.2
1	D	925	GLY	3.2
1	C	585	SER	3.2
1	A	695	GLY	3.2

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Mol	Chain	Res	Type	RSRZ
1	D	713	GLY	3.2
1	D	526	PHE	3.2
1	B	527	GLU	3.2
1	C	918	PRO	3.1
1	D	892	ALA	3.1
1	C	873	ARG	3.1
1	D	856	ILE	3.1
1	A	900	GLN	3.1
1	C	648	SER	3.0
1	C	745	GLY	3.0
1	C	668	ALA	3.0
1	D	599	GLY	3.0
1	C	634	GLN	2.9
1	A	746	GLY	2.9
1	A	873	ARG	2.9
1	B	714	GLU	2.9
1	D	587	SER	2.9
1	B	919	PRO	2.9
1	A	535	THR	2.9
1	D	597	PRO	2.9
1	C	647	CYS	2.9
1	C	573	TYR	2.9
1	D	321	HIS	2.9
1	C	693	THR	2.8
1	C	691	ILE	2.8
1	D	576	PRO	2.8
1	D	926	MET	2.8
1	D	575	THR	2.8
1	A	598	GLY	2.8
1	C	518	ASP	2.8
1	D	421	MET	2.7
1	C	319	GLN	2.7
1	C	599	GLY	2.7
1	A	527	GLU	2.7
1	C	580	TYR	2.6
1	A	534	THR	2.6
1	C	329	PRO	2.6
1	A	597	PRO	2.6
1	D	531	ASP	2.6
1	D	581	LEU	2.6
1	C	575	THR	2.6
1	D	859	GLN	2.6

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Mol	Chain	Res	Type	RSRZ
1	D	391	ALA	2.5
1	C	321	HIS	2.5
1	A	618	LEU	2.5
1	D	580	TYR	2.5
1	C	886	THR	2.5
1	B	531	ASP	2.5
1	C	692	SER	2.5
1	C	723	ALA	2.5
1	C	729	TRP	2.5
1	B	692	SER	2.5
1	B	900	GLN	2.5
1	D	569	THR	2.5
1	A	317	PHE	2.4
1	D	573	TYR	2.4
1	D	498	ASP	2.4
1	D	476	GLY	2.4
1	D	428	LYS	2.4
1	C	569	THR	2.4
1	C	746	GLY	2.4
1	A	673	TRP	2.4
1	C	649	ASP	2.4
1	C	888	SER	2.4
1	D	918	PRO	2.4
1	B	518	ASP	2.4
1	C	586	THR	2.4
1	D	720	ARG	2.3
1	D	518	ASP	2.3
1	D	423	LEU	2.3
1	D	690	ASP	2.3
1	C	391	ALA	2.3
1	B	650	GLY	2.3
1	C	919	PRO	2.3
1	D	885	ALA	2.3
1	A	321	HIS	2.3
1	D	797	GLU	2.3
1	D	564	ASN	2.3
1	C	879	VAL	2.3
1	C	875	LEU	2.2
1	D	618	LEU	2.2
1	D	884	LEU	2.2
1	D	727	THR	2.2
1	B	571	ALA	2.2

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Mol	Chain	Res	Type	RSRZ
1	D	357	GLU	2.2
1	D	891	LEU	2.2
1	C	863	CYS	2.2
1	C	423	LEU	2.2
1	D	693	THR	2.2
1	A	596	LEU	2.2
1	B	422	LEU	2.2
1	D	864	LEU	2.2
1	B	587	SER	2.2
1	D	714	GLU	2.2
1	D	649	ASP	2.2
1	C	567	LYS	2.2
1	A	690	ASP	2.2
1	C	524	ARG	2.2
1	C	667	LYS	2.2
1	C	877	GLU	2.2
1	C	629	THR	2.2
1	C	414	GLY	2.2
1	C	744	LEU	2.2
1	C	378	SER	2.2
1	A	650	GLY	2.2
1	D	912	GLU	2.1
1	C	435	GLN	2.1
1	D	860	ILE	2.1
1	A	526	PHE	2.1
1	B	572	LYS	2.1
1	D	406	GLU	2.1
1	D	875	LEU	2.1
1	D	729	TRP	2.1
1	D	715	TYR	2.1
1	C	431	ARG	2.1
1	A	715	TYR	2.1
1	B	526	PHE	2.1
1	C	881	VAL	2.1
1	B	534	THR	2.1
1	A	889	PRO	2.1
1	D	427	ILE	2.1
1	B	715	TYR	2.1
1	C	315	ARG	2.1
1	D	646	SER	2.1
1	C	869	THR	2.1
1	C	690	ASP	2.1

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Mol	Chain	Res	Type	RSRZ
1	D	876	ARG	2.0
1	D	565	PHE	2.0
1	C	675	TYR	2.0
1	D	651	ARG	2.0
1	C	844	GLN	2.0
1	A	616	GLY	2.0
1	A	569	THR	2.0
1	C	782	LYS	2.0
1	D	724	ALA	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)

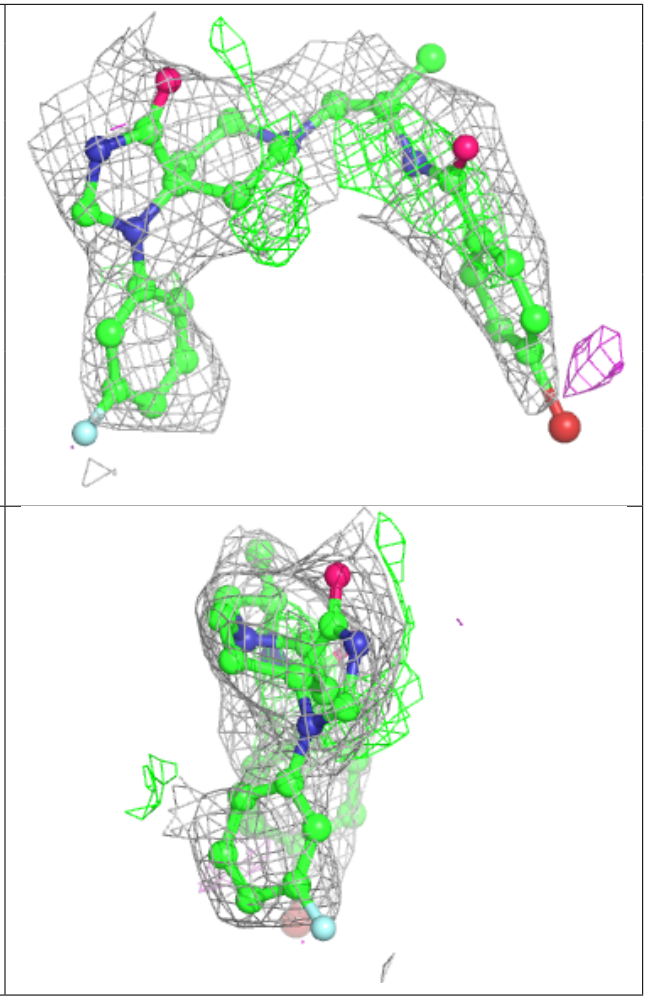
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	MJY	D	1001	31/31	0.69	0.51	71,77,244,300	0
2	MJY	C	1001	31/31	0.72	0.49	85,93,236,291	0
2	MJY	A	1001	31/31	0.79	0.46	59,79,195,242	0
2	MJY	B	1001	31/31	0.84	0.47	64,99,213,269	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.

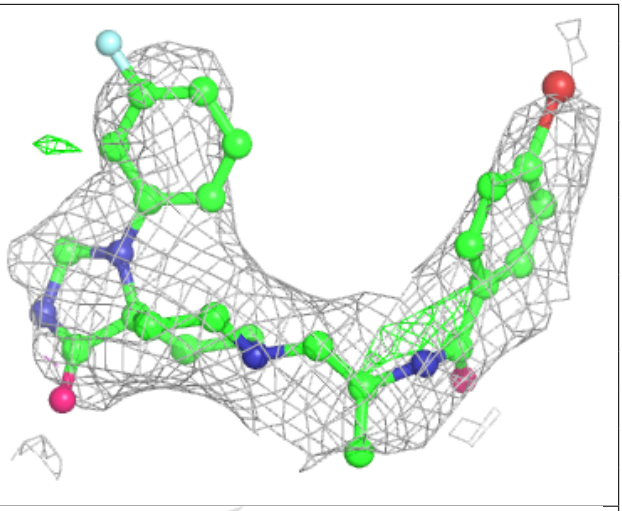
Electron density around MJY D 1001:

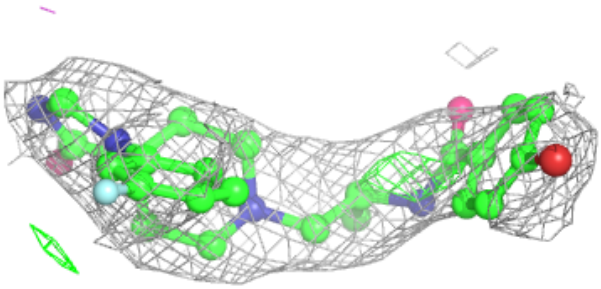
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

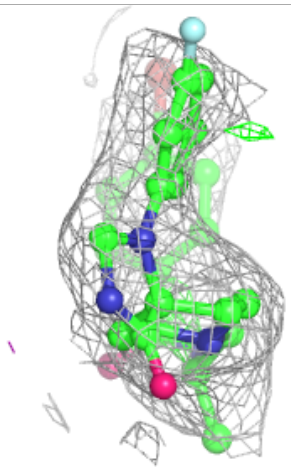


Electron density around MJY C 1001:

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

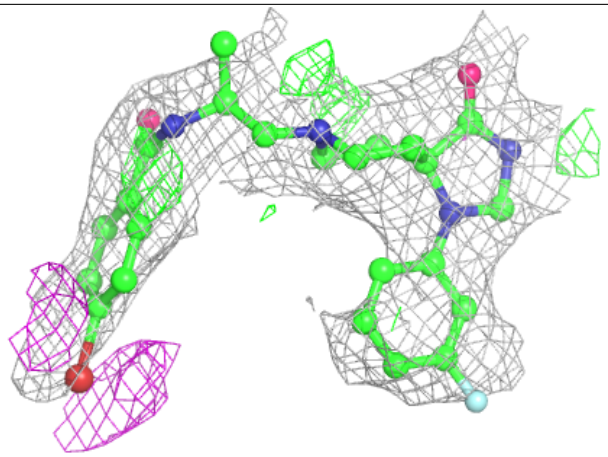


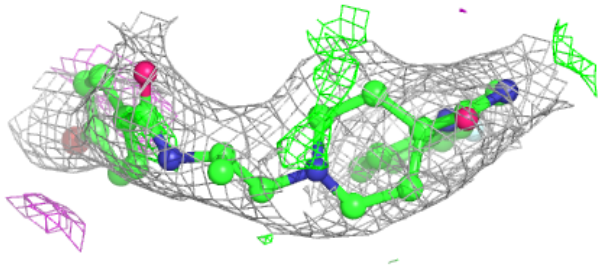




Electron density around MJY A 1001:

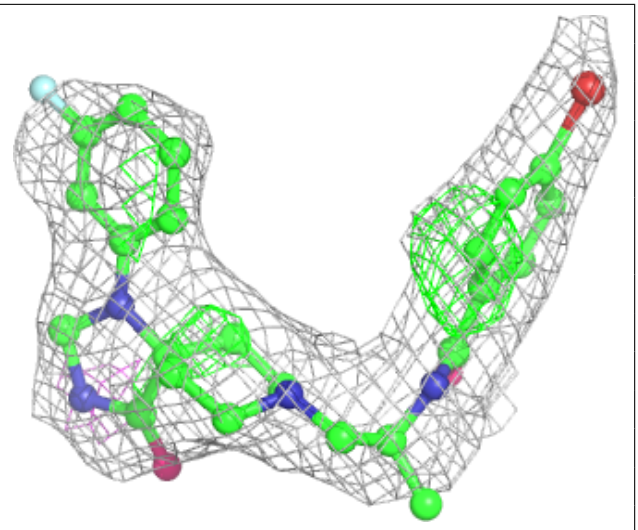
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

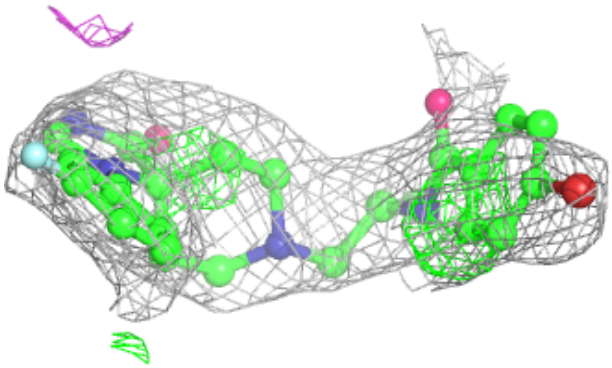


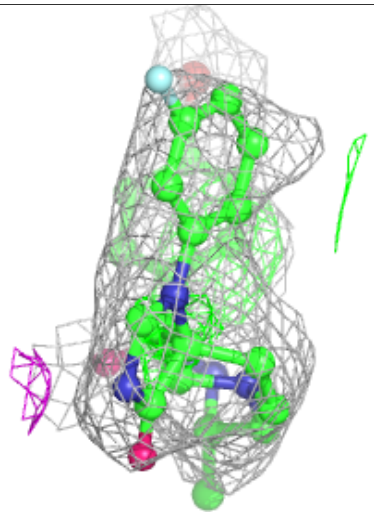


Electron density around MJY B 1001:

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.