Full wwPDB X-ray Structure Validation Report (i)

Sep 9, 2023 – 08:08 PM EDT

PDB ID	:	4HHY
Title	:	Crystal structure of PARP catalytic domain in complex with novel inhibitors
Authors	:	Liu, Q.F.; Chen, T.T.; Xu, Y.C.
Deposited on	:	2012-10-10
Resolution	:	2.36 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:

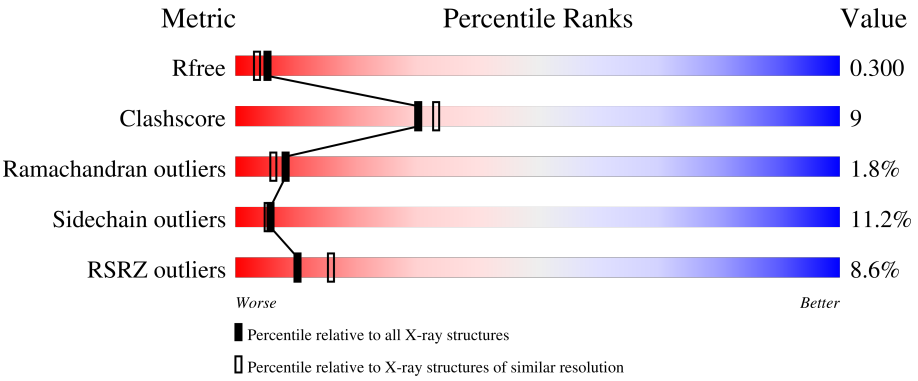
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & 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 2.36 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	1164 (2.36-2.36)
Clashscore	141614	1232 (2.36-2.36)
Ramachandran outliers	138981	1211 (2.36-2.36)
Sidechain outliers	138945	1212 (2.36-2.36)
RSRZ outliers	127900	1150 (2.36-2.36)

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	355	4% 71% 24%
1	B	355	76% 16%
1	C	355	6% 71% 22%
1	D	355	23% 55% 28% 13%

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
4	PEG	A	403	-	-	X	-

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 10721 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.

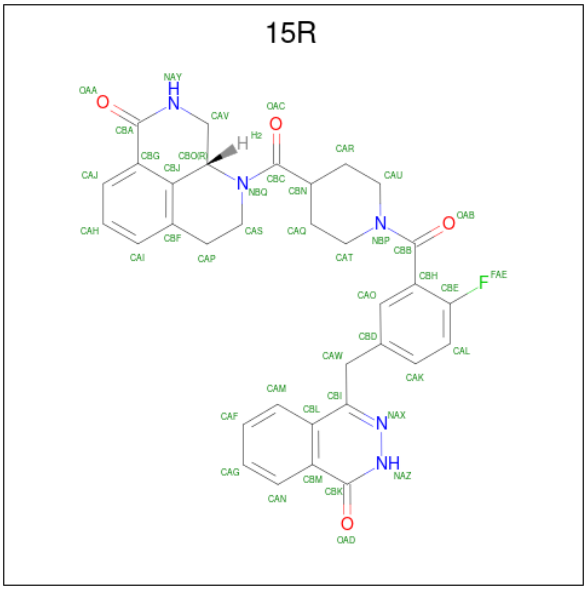
- Molecule 1 is a protein called Poly [ADP-ribose] polymerase 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	349	Total	C	N	O	S	0	0	0
			2733	1739	462	521	11			
1	B	340	Total	C	N	O	S	0	0	0
			2653	1694	443	505	11			
1	C	345	Total	C	N	O	S	0	0	0
			2661	1689	448	513	11			
1	D	309	Total	C	N	O	S	0	0	0
			2401	1521	408	464	8			

There are 20 discrepancies between the modelled and reference sequences:

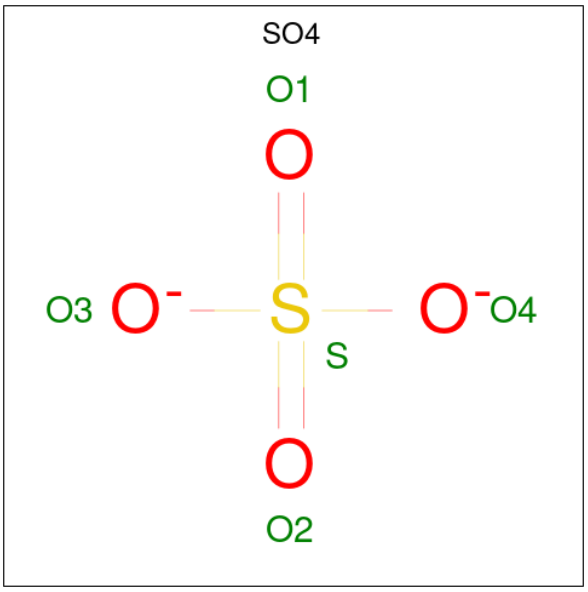
Chain	Residue	Modelled	Actual	Comment	Reference
A	-4	GLY	-	expression tag	UNP P09874
A	-3	PRO	-	expression tag	UNP P09874
A	-2	LEU	-	expression tag	UNP P09874
A	0	SER	THR	conflict	UNP P09874
A	101	ALA	VAL	conflict	UNP P09874
B	-4	GLY	-	expression tag	UNP P09874
B	-3	PRO	-	expression tag	UNP P09874
B	-2	LEU	-	expression tag	UNP P09874
B	0	SER	THR	conflict	UNP P09874
B	101	ALA	VAL	conflict	UNP P09874
C	-4	GLY	-	expression tag	UNP P09874
C	-3	PRO	-	expression tag	UNP P09874
C	-2	LEU	-	expression tag	UNP P09874
C	0	SER	THR	conflict	UNP P09874
C	101	ALA	VAL	conflict	UNP P09874
D	-4	GLY	-	expression tag	UNP P09874
D	-3	PRO	-	expression tag	UNP P09874
D	-2	LEU	-	expression tag	UNP P09874
D	0	SER	THR	conflict	UNP P09874
D	101	ALA	VAL	conflict	UNP P09874

- Molecule 2 is (9aR)-1-[(1-{2-fluoro-5-[(4-oxo-3,4-dihydrophthalazin-1-yl)methyl]benzoyl}piperidin-4-yl)carbonyl]-1,2,3,8,9,9a-hexahydro-7H-benzo[de][1,7]naphthyridin-7-one (three-letter code: 15R) (formula: $C_{33}H_{30}FN_5O_4$).



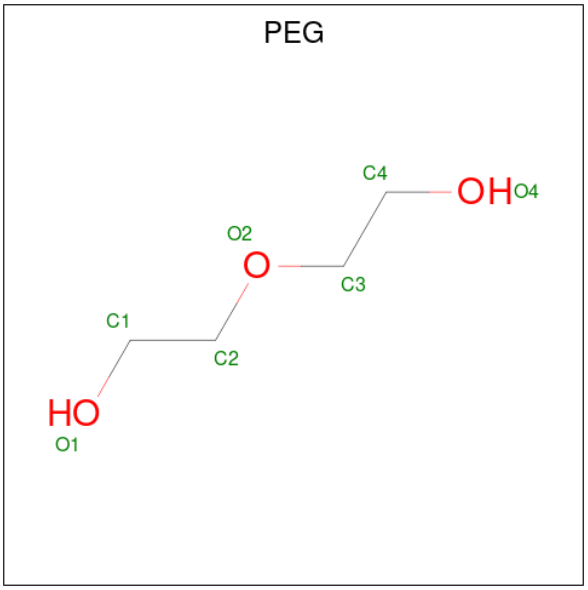
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	F	N	O	0	0
			43	33	1	5	4		
2	B	1	Total	C	F	N	O	0	0
			43	33	1	5	4		
2	C	1	Total	C	F	N	O	0	0
			43	33	1	5	4		
2	D	1	Total	C	F	N	O	0	0
			43	33	1	5	4		

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



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

- Molecule 4 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: $C_4H_{10}O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 7 4 3	0	0

- Molecule 5 is water.

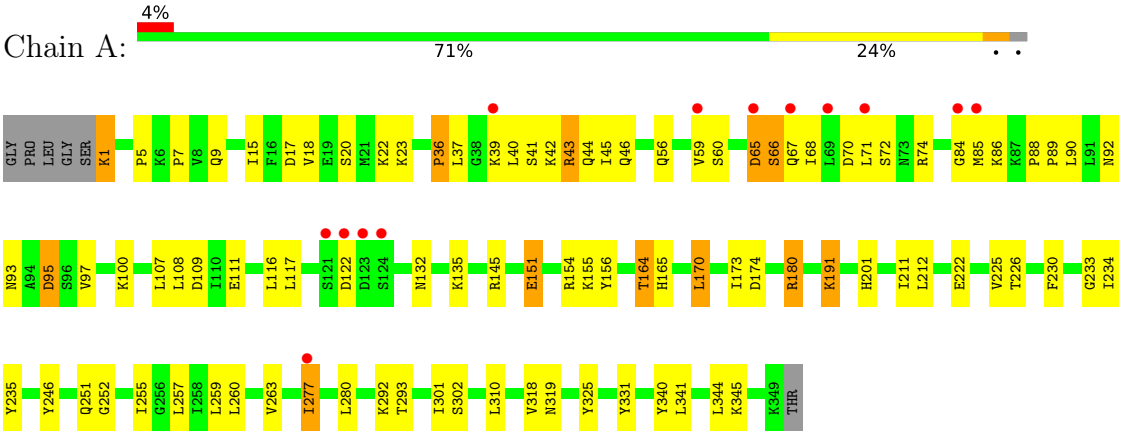
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	32	Total O 32 32	0	0
5	B	27	Total O 27 27	0	0
5	C	18	Total O 18 18	0	0
5	D	7	Total O 7 7	0	0

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.

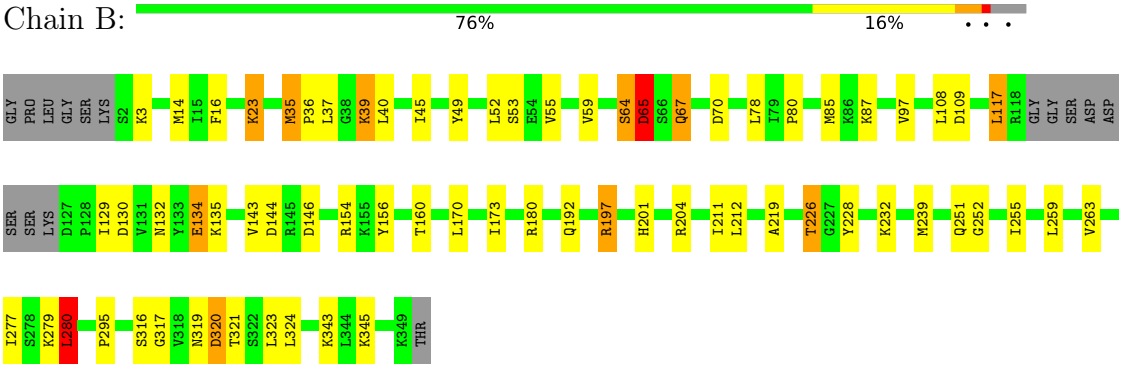
• Molecule 1: Poly [ADP-ribose] polymerase 1

Chain A:



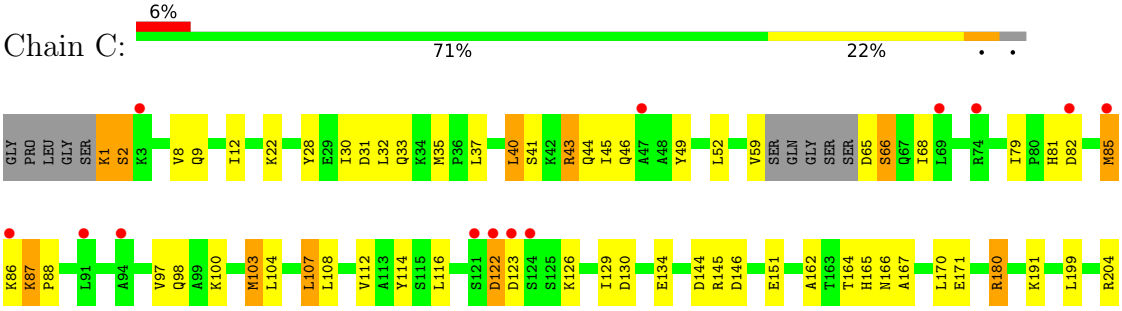
• Molecule 1: Poly [ADP-ribose] polymerase 1

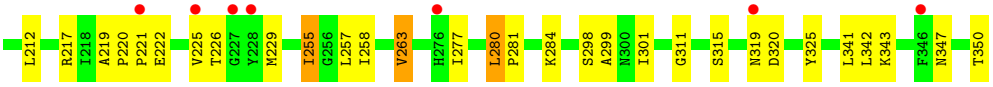
Chain B:



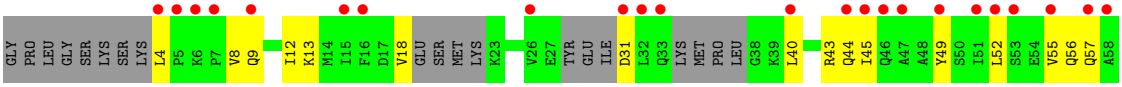
• Molecule 1: Poly [ADP-ribose] polymerase 1

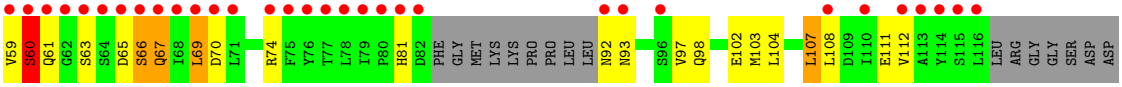
Chain C:

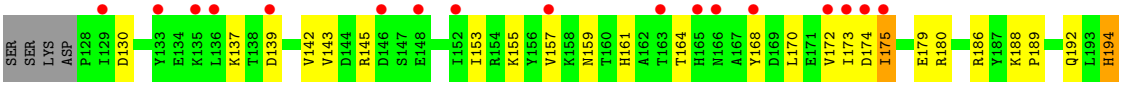


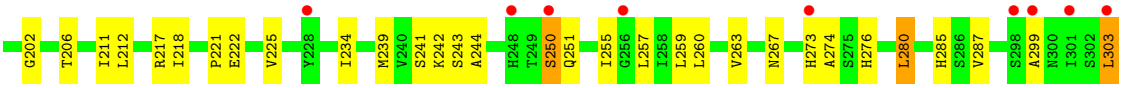


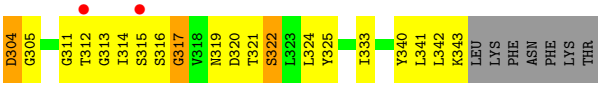
• Molecule 1: Poly [ADP-ribose] polymerase 1











4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	103.80Å 107.55Å 143.11Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	43.61 – 2.36 43.61 – 2.36	Depositor EDS
% Data completeness (in resolution range)	97.9 (43.61-2.36) 97.9 (43.61-2.36)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.34 (at 2.37Å)	Xtriage
Refinement program	PHENIX 1.8_1069	Depositor
R, R_{free}	0.237 , 0.299 0.238 , 0.300	Depositor DCC
R_{free} test set	3288 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å^2)	45.1	Xtriage
Anisotropy	0.154	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 34.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.015 for k,h,-l	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	10721	wwPDB-VP
Average B, all atoms (Å^2)	22.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.45% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PEG, 15R, SO4

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	0.51	0/2785	0.66	2/3761 (0.1%)
1	B	0.50	0/2704	0.67	0/3658
1	C	0.43	0/2711	0.62	2/3673 (0.1%)
1	D	0.38	0/2440	0.58	0/3298
All	All	0.46	0/10640	0.64	4/14390 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	C	0	1

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	180	ARG	NE-CZ-NH2	-6.47	117.06	120.30
1	C	180	ARG	NE-CZ-NH2	-5.68	117.46	120.30
1	C	66	SER	N-CA-C	-5.58	95.92	111.00
1	A	180	ARG	NE-CZ-NH1	5.01	122.81	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	65	ASP	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	2733	0	2763	53	0
1	B	2653	0	2660	40	0
1	C	2661	0	2624	46	0
1	D	2401	0	2394	58	0
2	A	43	0	30	10	0
2	B	43	0	30	2	0
2	C	43	0	30	2	0
2	D	43	0	30	6	0
3	A	5	0	0	0	0
3	B	5	0	0	0	0
4	A	7	0	10	4	0
5	A	32	0	0	2	0
5	B	27	0	0	1	0
5	C	18	0	0	1	0
5	D	7	0	0	0	0
All	All	10721	0	10571	197	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 9.

All (197) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:14:MET:HE1	1:B:343:LYS:HE2	1.63	0.80
2:A:401:15R:FAE	2:A:401:15R:H18	1.76	0.74
1:D:260:LEU:HB2	1:D:340:TYR:HB2	1.69	0.73
1:C:171:GLU:OE2	1:C:347:ASN:ND2	2.23	0.72
1:C:180:ARG:HD2	1:C:212:LEU:O	1.90	0.71
1:C:9:GLN:HG2	1:C:129:ILE:HG21	1.72	0.71
1:C:165:HIS:O	1:C:167:ALA:N	2.21	0.70
1:A:84:GLY:HA2	1:A:86:LYS:H	1.57	0.69
1:B:226:THR:HB	1:B:228:TYR:H	1.56	0.69
1:A:117:LEU:HD11	1:B:85:MET:HG2	1.74	0.69
1:D:45:ILE:HG23	1:D:104:LEU:HD22	1.75	0.69
1:D:66:SER:HA	1:D:69:LEU:HD23	1.75	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:299:ALA:HB3	1:D:311:GLY:HA2	1.75	0.69
1:C:66:SER:O	1:C:68:ILE:N	2.23	0.68
1:C:41:SER:HB3	1:C:44:GLN:HB2	1.75	0.67
1:A:180:ARG:HD2	1:A:212:LEU:O	1.94	0.67
1:B:279:LYS:O	1:B:280:LEU:HB2	1.93	0.66
1:B:35:MET:HE1	1:B:40:LEU:HD23	1.77	0.66
1:B:201:HIS:CE1	2:B:401:15R:H30	2.32	0.65
1:C:257:LEU:HD22	1:C:341:LEU:HD21	1.80	0.64
1:C:299:ALA:HB3	1:C:311:GLY:HA2	1.80	0.64
1:D:65:ASP:O	1:D:67:GLN:N	2.31	0.63
1:A:65:ASP:O	1:A:67:GLN:N	2.31	0.63
1:C:31:ASP:HB2	1:C:82:ASP:HB2	1.81	0.63
1:D:218:ILE:O	2:D:401:15R:H26	1.97	0.62
1:D:316:SER:OG	1:D:317:GLY:N	2.26	0.62
1:A:319:ASN:HB2	1:D:273:HIS:HD2	1.64	0.62
1:D:241:SER:HA	1:D:244:ALA:HB3	1.81	0.62
1:B:173:ILE:HD11	1:B:345:LYS:HB2	1.80	0.62
1:C:255:ILE:HD11	1:C:343:LYS:HE2	1.80	0.61
1:A:132:ASN:HD21	1:B:85:MET:HG3	1.66	0.61
1:C:30:ILE:HD11	1:C:103:MET:HE3	1.83	0.61
1:A:319:ASN:HB2	1:D:273:HIS:CD2	2.37	0.60
1:C:45:ILE:HG23	1:C:104:LEU:HD22	1.82	0.60
1:B:180:ARG:HD2	1:B:212:LEU:O	2.01	0.60
2:D:401:15R:FAE	2:D:401:15R:H18	1.92	0.60
1:A:151:GLU:HG2	1:A:154:ARG:NH1	2.16	0.60
2:A:401:15R:H19	4:A:403:PEG:H42	1.83	0.59
2:D:401:15R:CAK	2:D:401:15R:H25	2.33	0.59
1:C:281:PRO:HG2	1:C:284:LYS:HG3	1.84	0.59
1:C:85:MET:N	1:C:85:MET:SD	2.77	0.58
1:C:162:ALA:HB3	1:C:165:HIS:CD2	2.38	0.58
1:A:211:ILE:HG12	4:A:403:PEG:H32	1.85	0.58
1:C:162:ALA:HB3	1:C:165:HIS:HD2	1.68	0.58
1:D:143:VAL:HB	1:D:175:ILE:HG12	1.85	0.58
1:A:235:TYR:HB2	2:A:401:15R:H12	1.85	0.58
1:A:17:ASP:OD1	1:A:20:SER:OG	2.19	0.57
1:D:9:GLN:O	1:D:13:LYS:N	2.37	0.57
1:C:52:LEU:HD22	1:C:97:VAL:HG23	1.87	0.57
1:D:234:ILE:HD11	1:D:333:ILE:HG22	1.87	0.57
1:D:98:GLN:NE2	1:D:102:GLU:OE1	2.38	0.56
1:D:312:THR:O	1:D:314:ILE:N	2.38	0.56
1:C:85:MET:O	1:C:87:LYS:N	2.31	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:84:GLY:HA2	1:A:86:LYS:N	2.20	0.56
2:A:401:15R:H1	5:A:520:HOH:O	2.05	0.55
1:B:64:SER:HB2	1:B:67:GLN:H	1.71	0.55
1:D:139:ASP:HB3	1:D:179:GLU:HB3	1.87	0.55
1:B:109:ASP:OD1	2:B:401:15R:H26	2.07	0.55
1:C:8:VAL:O	1:C:12:ILE:HG12	2.06	0.55
1:A:257:LEU:HD22	1:A:341:LEU:HD21	1.89	0.54
1:A:132:ASN:ND2	1:B:85:MET:HG3	2.23	0.54
1:D:59:VAL:HG12	1:D:60:SER:H	1.73	0.54
1:D:239:MET:HG3	1:D:325:TYR:CD1	2.43	0.54
1:D:155:LYS:O	1:D:159:ASN:N	2.38	0.53
1:D:70:ASP:O	1:D:74:ARG:HG3	2.09	0.53
1:B:154:ARG:HG3	5:B:504:HOH:O	2.09	0.52
1:A:260:LEU:HB2	1:A:340:TYR:HB2	1.92	0.52
1:A:201:HIS:HE1	2:A:401:15R:H11	1.75	0.51
1:A:164:THR:HB	1:A:325:TYR:OH	2.09	0.51
1:A:39:LYS:HG3	1:C:33:GLN:HG2	1.92	0.51
1:A:277:ILE:HG12	1:A:331:TYR:CZ	2.45	0.51
1:C:258:ILE:HG22	1:C:342:LEU:HB2	1.91	0.51
1:C:45:ILE:HD13	1:C:107:LEU:HB3	1.92	0.51
1:C:162:ALA:HB1	1:C:325:TYR:CZ	2.46	0.51
1:D:55:VAL:O	1:D:59:VAL:HG23	2.10	0.51
1:D:273:HIS:CG	1:D:274:ALA:N	2.79	0.51
1:B:132:ASN:HA	1:B:135:LYS:HD2	1.93	0.50
1:D:45:ILE:HG21	1:D:108:LEU:HG	1.92	0.50
1:D:59:VAL:O	1:D:61:GLN:N	2.44	0.50
1:B:35:MET:O	1:B:35:MET:HG3	2.12	0.50
1:A:93:ASN:HD22	1:A:95:ASP:H	1.59	0.50
1:D:242:LYS:HD2	1:D:325:TYR:HB2	1.93	0.50
2:D:401:15R:H18	2:D:401:15R:CBE	2.42	0.50
1:A:173:ILE:HD11	1:A:345:LYS:HE2	1.93	0.50
1:A:234:ILE:HA	2:A:401:15R:H14	1.92	0.50
1:B:39:LYS:O	1:B:39:LYS:HG3	2.11	0.49
2:C:401:15R:H17	2:C:401:15R:CBE	2.41	0.49
1:D:280:LEU:HD11	1:D:287:VAL:HG23	1.93	0.49
1:B:239:MET:HE3	1:B:295:PRO:HG3	1.94	0.49
1:A:301:ILE:HD12	1:A:310:LEU:HD21	1.93	0.49
1:C:37:LEU:O	1:C:40:LEU:HB2	2.13	0.49
2:D:401:15R:H25	2:D:401:15R:CBD	2.42	0.49
1:C:108:LEU:HB3	2:C:401:15R:CAF	2.43	0.49
1:B:36:PRO:HD2	1:B:39:LYS:HG2	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:252:GLY:HA3	1:B:252:GLY:HA3	1.95	0.49
1:B:64:SER:O	1:B:65:ASP:HB2	2.13	0.49
1:D:273:HIS:CG	1:D:274:ALA:H	2.30	0.49
1:B:160:THR:HB	1:B:239:MET:HA	1.95	0.48
1:D:303:LEU:O	1:D:305:GLY:N	2.41	0.48
1:B:160:THR:HA	1:B:239:MET:HE1	1.95	0.48
1:B:45:ILE:HG21	1:B:108:LEU:HG	1.95	0.48
1:D:234:ILE:HA	2:D:401:15R:H14	1.94	0.48
1:D:267:ASN:H	1:D:285:HIS:CE1	2.31	0.48
1:C:28:TYR:CG	1:C:103:MET:HG3	2.49	0.48
1:A:66:SER:OG	1:A:67:GLN:N	2.47	0.48
1:D:319:ASN:N	1:D:319:ASN:OD1	2.46	0.48
1:D:194:HIS:ND1	1:D:194:HIS:N	2.61	0.48
1:C:122:ASP:N	1:C:122:ASP:OD1	2.47	0.47
1:D:4:LEU:HD13	1:D:130:ASP:OD2	2.13	0.47
1:D:202:GLY:HA3	1:D:243:SER:O	2.14	0.47
1:D:225:VAL:HG13	1:D:276:HIS:CD2	2.49	0.47
1:C:37:LEU:HD13	1:C:114:TYR:CD1	2.50	0.47
1:A:164:THR:HG22	1:A:165:HIS:CD2	2.49	0.47
1:C:108:LEU:O	1:C:112:VAL:HG23	2.14	0.47
1:B:16:PHE:HD1	1:B:117:LEU:HD22	1.79	0.47
1:B:320:ASP:N	1:B:320:ASP:OD1	2.48	0.47
1:C:1:LYS:HD2	1:C:1:LYS:HA	1.68	0.47
1:A:109:ASP:OD1	4:A:403:PEG:H11	2.15	0.47
1:B:35:MET:HG2	1:B:80:PRO:HD2	1.97	0.47
1:C:79:ILE:O	1:C:81:HIS:ND1	2.46	0.47
1:C:319:ASN:HA	1:C:320:ASP:HA	1.58	0.47
1:C:2:SER:OG	1:C:130:ASP:OD2	2.32	0.47
1:D:59:VAL:HG21	1:D:92:ASN:O	2.15	0.47
1:A:1:LYS:HB3	1:A:1:LYS:HE3	1.70	0.46
1:C:219:ALA:HA	1:C:220:PRO:HD3	1.76	0.46
1:D:8:VAL:HG13	1:D:12:ILE:HD13	1.96	0.46
1:C:41:SER:O	1:C:45:ILE:HG13	2.15	0.46
1:A:41:SER:HA	1:A:43:ARG:HH21	1.80	0.46
1:B:316:SER:N	1:B:317:GLY:HA2	2.31	0.46
1:A:59:VAL:HG21	1:A:92:ASN:HA	1.98	0.45
1:A:292:LYS:HE2	1:D:273:HIS:CE1	2.50	0.45
1:B:211:ILE:HG21	1:B:259:LEU:HD11	1.98	0.45
1:B:280:LEU:HD12	1:B:280:LEU:HA	1.80	0.45
1:C:41:SER:OG	1:C:43:ARG:HG2	2.17	0.45
1:D:137:LYS:HE2	1:D:137:LYS:HB3	1.70	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:23:LYS:HE3	1:B:23:LYS:HD3	1.97	0.45
1:A:90:LEU:HD23	1:A:92:ASN:ND2	2.31	0.45
1:B:134:GLU:H	1:B:134:GLU:HG2	1.41	0.45
1:B:239:MET:CE	1:B:295:PRO:HG3	2.47	0.45
1:D:180:ARG:HD2	1:D:212:LEU:O	2.16	0.45
1:A:18:VAL:HG12	1:A:22:LYS:HD2	1.99	0.45
1:A:70:ASP:OD1	1:A:74:ARG:NH2	2.50	0.44
1:A:225:VAL:HG13	5:A:518:HOH:O	2.17	0.44
1:B:219:ALA:HB3	1:B:232:LYS:HD3	1.99	0.44
1:A:211:ILE:HG21	1:A:259:LEU:HD11	1.99	0.44
1:C:126:LYS:NZ	1:C:134:GLU:OE2	2.51	0.44
1:A:170:LEU:HG	1:A:344:LEU:HD13	2.00	0.44
1:A:7:PRO:HB3	1:A:174:ASP:OD1	2.18	0.44
1:C:32:LEU:HA	1:C:35:MET:O	2.18	0.44
1:C:87:LYS:HA	1:C:88:PRO:HD3	1.85	0.44
1:D:57:GLN:O	1:D:61:GLN:HB3	2.17	0.44
1:C:199:LEU:HD12	1:C:263:VAL:CG1	2.48	0.43
1:C:199:LEU:HD12	1:C:263:VAL:HG13	2.00	0.43
1:A:36:PRO:HG2	1:A:39:LYS:HE2	2.00	0.43
1:B:35:MET:HE3	1:B:35:MET:HB2	1.81	0.43
1:D:107:LEU:HD22	1:D:107:LEU:HA	1.76	0.43
1:D:108:LEU:O	1:D:112:VAL:HG23	2.18	0.43
1:A:39:LYS:O	1:A:40:LEU:HD23	2.19	0.43
1:A:191:LYS:HE2	1:A:191:LYS:O	2.19	0.43
1:D:186:ARG:O	1:D:189:PRO:HD2	2.19	0.42
2:A:401:15R:CAO	4:A:403:PEG:H42	2.48	0.42
1:A:90:LEU:HD23	1:A:92:ASN:HD22	1.85	0.42
1:A:108:LEU:HB3	2:A:401:15R:CAF	2.50	0.42
1:B:52:LEU:HD23	1:B:52:LEU:HA	1.91	0.42
1:D:92:ASN:OD1	1:D:93:ASN:N	2.51	0.42
1:A:88:PRO:HA	1:A:89:PRO:HD2	1.86	0.42
1:B:197:ARG:HE	1:B:197:ARG:HB2	1.58	0.42
1:A:230:PHE:O	1:A:277:ILE:HG23	2.20	0.42
1:D:40:LEU:HA	1:D:44:GLN:NE2	2.35	0.42
1:D:211:ILE:HG21	1:D:259:LEU:HD11	2.02	0.42
1:A:46:GLN:NE2	1:A:222:GLU:OE2	2.29	0.41
1:D:104:LEU:HD23	1:D:104:LEU:HA	1.95	0.41
1:D:153:ILE:CG2	1:D:342:LEU:HD21	2.50	0.41
1:B:130:ASP:O	1:B:134:GLU:HG2	2.20	0.41
1:D:31:ASP:HB2	1:D:81:HIS:C	2.40	0.41
1:B:55:VAL:O	1:B:59:VAL:HG23	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:273:HIS:CG	1:D:322:SER:HG	2.38	0.41
1:A:116:LEU:O	1:A:135:LYS:HD3	2.20	0.41
1:C:229:MET:HE2	1:C:229:MET:HB3	1.72	0.41
1:C:299:ALA:HB3	1:C:311:GLY:CA	2.48	0.41
1:D:188:LYS:HB3	1:D:189:PRO:HD3	2.03	0.41
1:C:204:ARG:HG3	5:C:509:HOH:O	2.21	0.41
1:D:257:LEU:HD23	1:D:343:LYS:HA	2.03	0.41
1:A:45:ILE:HG21	1:A:108:LEU:HG	2.03	0.40
1:B:319:ASN:OD1	1:B:319:ASN:N	2.54	0.40
1:A:246:TYR:CZ	2:A:401:15R:H9	2.56	0.40
1:A:5:PRO:O	1:A:9:GLN:HG3	2.21	0.40
1:A:233:GLY:O	2:A:401:15R:H17	2.21	0.40
1:A:277:ILE:O	1:A:277:ILE:HG13	2.20	0.40
1:C:116:LEU:HD23	1:C:116:LEU:HA	1.81	0.40
1:D:52:LEU:HD12	1:D:104:LEU:HD12	2.04	0.40
1:D:173:ILE:HG22	1:D:174:ASP:OD1	2.22	0.40
1:D:250:SER:HB2	1:D:251:GLN:H	1.58	0.40
1:B:39:LYS:HE2	1:B:39:LYS:HB2	1.78	0.40
1:C:280:LEU:HA	1:C:280:LEU:HD12	1.86	0.40
1:D:49:TYR:HE2	1:D:108:LEU:HD11	1.87	0.40
1:D:221:PRO:HD2	1:D:222:GLU:OE2	2.22	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	347/355 (98%)	327 (94%)	14 (4%)	6 (2%)	9 7
1	B	336/355 (95%)	318 (95%)	13 (4%)	5 (2%)	10 8
1	C	341/355 (96%)	321 (94%)	15 (4%)	5 (2%)	10 8
1	D	297/355 (84%)	263 (89%)	26 (9%)	8 (3%)	5 2

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	1321/1420 (93%)	1229 (93%)	68 (5%)	24 (2%)	8 6

All (24) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	66	SER
1	C	166	ASN
1	D	66	SER
1	D	317	GLY
1	A	36	PRO
1	A	37	LEU
1	A	60	SER
1	B	64	SER
1	B	65	ASP
1	B	280	LEU
1	C	277	ILE
1	D	304	ASP
1	D	313	GLY
1	D	315	SER
1	C	87	LYS
1	A	65	ASP
1	D	60	SER
1	D	250	SER
1	D	320	ASP
1	A	122	ASP
1	B	226	THR
1	C	86	LYS
1	C	221	PRO
1	B	87	LYS

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	303/310 (98%)	272 (90%)	31 (10%)	7 6

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	B	292/310 (94%)	260 (89%)	32 (11%)	6 5
1	C	288/310 (93%)	255 (88%)	33 (12%)	5 5
1	D	264/310 (85%)	231 (88%)	33 (12%)	4 4
All	All	1147/1240 (92%)	1018 (89%)	129 (11%)	6 5

All (129) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	LYS
1	A	15	ILE
1	A	42	LYS
1	A	43	ARG
1	A	44	GLN
1	A	56	GLN
1	A	68	ILE
1	A	71	LEU
1	A	72	SER
1	A	85	MET
1	A	95	ASP
1	A	97	VAL
1	A	100	LYS
1	A	107	LEU
1	A	111	GLU
1	A	145	ARG
1	A	151	GLU
1	A	155	LYS
1	A	156	TYR
1	A	164	THR
1	A	170	LEU
1	A	191	LYS
1	A	226	THR
1	A	251	GLN
1	A	255	ILE
1	A	263	VAL
1	A	277	ILE
1	A	280	LEU
1	A	293	THR
1	A	302	SER
1	A	318	VAL
1	B	3	LYS
1	B	23	LYS

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Mol	Chain	Res	Type
1	B	35	MET
1	B	37	LEU
1	B	39	LYS
1	B	49	TYR
1	B	53	SER
1	B	65	ASP
1	B	67	GLN
1	B	70	ASP
1	B	78	LEU
1	B	97	VAL
1	B	117	LEU
1	B	129	ILE
1	B	134	GLU
1	B	143	VAL
1	B	144	ASP
1	B	146	ASP
1	B	156	TYR
1	B	170	LEU
1	B	192	GLN
1	B	197	ARG
1	B	204	ARG
1	B	251	GLN
1	B	255	ILE
1	B	263	VAL
1	B	277	ILE
1	B	280	LEU
1	B	320	ASP
1	B	321	THR
1	B	323	LEU
1	B	324	LEU
1	C	1	LYS
1	C	2	SER
1	C	22	LYS
1	C	40	LEU
1	C	43	ARG
1	C	46	GLN
1	C	49	TYR
1	C	59	VAL
1	C	85	MET
1	C	98	GLN
1	C	100	LYS
1	C	103	MET

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Mol	Chain	Res	Type
1	C	107	LEU
1	C	122	ASP
1	C	123	ASP
1	C	144	ASP
1	C	145	ARG
1	C	146	ASP
1	C	151	GLU
1	C	164	THR
1	C	170	LEU
1	C	191	LYS
1	C	217	ARG
1	C	222	GLU
1	C	225	VAL
1	C	226	THR
1	C	255	ILE
1	C	263	VAL
1	C	280	LEU
1	C	298	SER
1	C	301	ILE
1	C	315	SER
1	C	350	THR
1	D	18	VAL
1	D	43	ARG
1	D	56	GLN
1	D	60	SER
1	D	63	SER
1	D	67	GLN
1	D	69	LEU
1	D	97	VAL
1	D	103	MET
1	D	107	LEU
1	D	111	GLU
1	D	142	VAL
1	D	145	ARG
1	D	157	VAL
1	D	161	HIS
1	D	164	THR
1	D	168	TYR
1	D	170	LEU
1	D	172	VAL
1	D	175	ILE
1	D	192	GLN

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Mol	Chain	Res	Type
1	D	194	HIS
1	D	206	THR
1	D	217	ARG
1	D	255	ILE
1	D	263	VAL
1	D	280	LEU
1	D	303	LEU
1	D	304	ASP
1	D	321	THR
1	D	322	SER
1	D	324	LEU
1	D	341	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	D	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)

7 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	$\#\|Z\| > 2$
3	SO4	A	402	-	4,4,4	0.18	0	6,6,6	0.43	0
2	15R	A	401	-	48,49,49	2.59	16 (33%)	59,72,72	3.14	28 (47%)
2	15R	B	401	-	48,49,49	2.71	18 (37%)	59,72,72	3.06	22 (37%)
3	SO4	B	402	-	4,4,4	0.09	0	6,6,6	0.23	0
4	PEG	A	403	-	6,6,6	0.48	0	5,5,5	1.74	2 (40%)
2	15R	C	401	-	48,49,49	2.71	16 (33%)	59,72,72	3.04	24 (40%)
2	15R	D	401	-	48,49,49	2.71	17 (35%)	59,72,72	3.01	28 (47%)

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	15R	A	401	-	-	9/20/52/52	1/7/7/7
2	15R	B	401	-	-	2/20/52/52	0/7/7/7
4	PEG	A	403	-	-	2/4/4/4	-
2	15R	C	401	-	-	0/20/52/52	0/7/7/7
2	15R	D	401	-	-	5/20/52/52	0/7/7/7

All (67) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	401	15R	OAA-CBA	9.25	1.42	1.23
2	D	401	15R	OAA-CBA	8.40	1.40	1.23
2	A	401	15R	OAA-CBA	8.13	1.39	1.23
2	B	401	15R	OAA-CBA	7.87	1.39	1.23
2	A	401	15R	OAD-CBK	7.60	1.38	1.23
2	C	401	15R	OAD-CBK	7.57	1.38	1.23
2	D	401	15R	OAD-CBK	7.36	1.38	1.23
2	B	401	15R	OAD-CBK	7.03	1.37	1.23
2	A	401	15R	CAJ-CBG	5.52	1.48	1.39
2	B	401	15R	CAJ-CBG	5.15	1.48	1.39
2	C	401	15R	CAV-CBO	5.08	1.58	1.52
2	D	401	15R	CAJ-CBG	4.87	1.47	1.39
2	D	401	15R	CAV-CBO	4.84	1.58	1.52
2	C	401	15R	CBI-NAX	4.74	1.32	1.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	401	15R	CAI-CBF	4.67	1.47	1.39
2	B	401	15R	CBH-CBB	-4.61	1.43	1.50
2	A	401	15R	CAI-CBF	4.54	1.47	1.39
2	C	401	15R	CAJ-CBG	4.52	1.47	1.39
2	B	401	15R	CAI-CBF	4.36	1.47	1.39
2	B	401	15R	CBI-NAX	4.30	1.31	1.29
2	A	401	15R	CAW-CBD	-4.29	1.44	1.51
2	B	401	15R	CAV-CBO	4.07	1.57	1.52
2	C	401	15R	CAI-CBF	4.04	1.46	1.39
2	B	401	15R	CBC-NBQ	3.92	1.43	1.34
2	D	401	15R	CBI-NAX	3.89	1.31	1.29
2	D	401	15R	CAW-CBD	-3.85	1.45	1.51
2	A	401	15R	CBI-NAX	3.77	1.31	1.29
2	A	401	15R	CAH-CAJ	3.69	1.46	1.38
2	D	401	15R	CBH-CBB	-3.65	1.45	1.50
2	B	401	15R	CBG-CBJ	-3.57	1.36	1.40
2	C	401	15R	CAH-CAJ	3.52	1.46	1.38
2	C	401	15R	CAN-CBM	3.46	1.45	1.39
2	C	401	15R	CBC-NBQ	3.45	1.42	1.34
2	D	401	15R	CBC-NBQ	3.41	1.42	1.34
2	B	401	15R	CAH-CAJ	3.37	1.46	1.38
2	D	401	15R	CAH-CAJ	3.30	1.45	1.38
2	B	401	15R	CAW-CBD	-3.30	1.46	1.51
2	D	401	15R	CBG-CBJ	-3.29	1.36	1.40
2	A	401	15R	CBC-NBQ	3.24	1.42	1.34
2	D	401	15R	CAN-CBM	3.22	1.45	1.39
2	B	401	15R	CAN-CBM	3.20	1.45	1.39
2	D	401	15R	OAB-CBB	-3.14	1.16	1.22
2	C	401	15R	CAW-CBD	-3.13	1.46	1.51
2	B	401	15R	CBN-CBC	3.08	1.56	1.51
2	B	401	15R	OAB-CBB	-2.94	1.16	1.22
2	C	401	15R	CBO-NBQ	2.93	1.50	1.47
2	A	401	15R	CAN-CBM	2.92	1.44	1.39
2	C	401	15R	CAM-CBL	2.90	1.44	1.39
2	C	401	15R	OAB-CBB	-2.82	1.17	1.22
2	B	401	15R	FAE-CBE	-2.67	1.28	1.35
2	C	401	15R	CBH-CBB	-2.65	1.46	1.50
2	D	401	15R	CAM-CBL	2.62	1.44	1.39
2	A	401	15R	FAE-CBE	-2.61	1.28	1.35
2	D	401	15R	CBO-NBQ	2.52	1.50	1.47
2	A	401	15R	CAV-CBO	2.51	1.55	1.52
2	A	401	15R	OAB-CBB	-2.49	1.17	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	401	15R	FAE-CBE	-2.38	1.29	1.35
2	A	401	15R	CAQ-CAT	-2.36	1.45	1.52
2	D	401	15R	CAQ-CAT	-2.35	1.45	1.52
2	C	401	15R	FAE-CBE	-2.33	1.29	1.35
2	A	401	15R	CAW-CBI	-2.21	1.48	1.52
2	B	401	15R	CAG-CAF	2.10	1.43	1.38
2	B	401	15R	CAS-NBQ	2.09	1.50	1.47
2	A	401	15R	CAH-CAI	2.08	1.43	1.38
2	C	401	15R	CAQ-CAT	-2.05	1.46	1.52
2	A	401	15R	CAM-CBL	2.03	1.43	1.39
2	B	401	15R	CBO-NBQ	2.01	1.49	1.47

All (104) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	401	15R	CAJ-CBG-CBA	-10.14	105.10	120.19
2	B	401	15R	CAJ-CBG-CBA	-8.79	107.11	120.19
2	D	401	15R	CAJ-CBG-CBA	-8.68	107.26	120.19
2	A	401	15R	CBH-CBB-NBP	7.96	131.00	118.28
2	B	401	15R	CBG-CBJ-CBF	-7.73	112.81	119.81
2	B	401	15R	CBK-NAZ-NAX	-7.09	119.93	127.98
2	B	401	15R	OAA-CBA-CBG	-6.88	111.37	123.30
2	A	401	15R	CBK-NAZ-NAX	-6.80	120.27	127.98
2	C	401	15R	CBK-NAZ-NAX	-6.74	120.33	127.98
2	D	401	15R	CBK-NAZ-NAX	-6.67	120.41	127.98
2	D	401	15R	OAA-CBA-CBG	-6.63	111.81	123.30
2	A	401	15R	OAC-CBC-NBQ	-6.55	109.70	121.38
2	C	401	15R	OAA-CBA-CBG	-6.27	112.44	123.30
2	B	401	15R	CBM-CBK-NAZ	6.26	122.37	115.03
2	A	401	15R	CAQ-CBN-CBC	-6.15	98.70	109.83
2	A	401	15R	OAC-CBC-CBN	-6.14	111.45	120.81
2	D	401	15R	CBJ-CBG-CBA	-5.96	115.37	120.61
2	A	401	15R	CBG-CBA-NAY	-5.91	107.97	116.03
2	B	401	15R	OAC-CBC-CBN	-5.89	111.83	120.81
2	A	401	15R	CBM-CBK-NAZ	5.87	121.92	115.03
2	C	401	15R	CBM-CBK-NAZ	5.87	121.92	115.03
2	D	401	15R	CBM-CBK-NAZ	5.77	121.80	115.03
2	B	401	15R	CAR-CBN-CBC	5.57	119.89	109.83
2	A	401	15R	CAJ-CBG-CBA	-5.47	112.05	120.19
2	D	401	15R	OAC-CBC-CBN	-5.39	112.60	120.81
2	D	401	15R	CBG-CBJ-CBF	-5.30	115.01	119.81
2	C	401	15R	OAC-CBC-CBN	-5.28	112.77	120.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	401	15R	CAJ-CBG-CBJ	-4.99	111.85	119.78
2	D	401	15R	CAQ-CBN-CBC	-4.98	100.82	109.83
2	C	401	15R	CAP-CBF-CAI	-4.97	110.54	120.98
2	B	401	15R	CBF-CBJ-CBO	-4.97	112.29	120.83
2	A	401	15R	CBJ-CBG-CBA	-4.96	116.25	120.61
2	C	401	15R	CBG-CBJ-CBF	-4.87	115.40	119.81
2	A	401	15R	OAA-CBA-CBG	-4.78	115.02	123.30
2	B	401	15R	CAP-CBF-CAI	-4.58	111.37	120.98
2	A	401	15R	OAB-CBB-NBP	-4.36	115.12	122.34
2	D	401	15R	CAP-CBF-CAI	-4.36	111.82	120.98
2	C	401	15R	CAR-CAU-NBP	4.34	117.42	110.82
2	C	401	15R	CAP-CAS-NBQ	4.34	115.69	109.48
2	D	401	15R	CBH-CBB-NBP	4.31	125.17	118.28
2	D	401	15R	CAH-CAI-CBF	-4.30	114.47	120.89
2	A	401	15R	CAR-CBN-CBC	4.19	117.41	109.83
2	C	401	15R	OAB-CBB-NBP	-4.11	115.55	122.34
2	A	401	15R	CBO-NBQ-CBC	4.08	136.41	121.53
2	C	401	15R	CBG-CBA-NAY	-3.98	110.61	116.03
2	B	401	15R	CAP-CAS-NBQ	3.79	114.90	109.48
2	A	401	15R	FAE-CBE-CBH	3.76	126.04	119.67
2	C	401	15R	CAT-CAQ-CBN	-3.76	104.16	110.41
2	D	401	15R	CAM-CBL-CBI	3.72	126.40	121.14
2	C	401	15R	CBH-CBB-NBP	3.71	124.21	118.28
2	D	401	15R	CAJ-CBG-CBJ	-3.62	114.03	119.78
2	C	401	15R	CBJ-CBG-CBA	-3.59	117.45	120.61
2	B	401	15R	CAQ-CBN-CBC	-3.55	103.42	109.83
2	B	401	15R	CAL-CBE-CBH	-3.52	119.28	123.11
2	B	401	15R	CAR-CAU-NBP	3.50	116.14	110.82
2	C	401	15R	OAC-CBC-NBQ	-3.45	115.23	121.38
2	B	401	15R	CBD-CAW-CBI	-3.32	106.26	114.34
2	C	401	15R	CAH-CAI-CBF	-3.26	116.03	120.89
2	A	401	15R	CAP-CBF-CAI	-3.19	114.27	120.98
2	B	401	15R	CBJ-CBG-CBA	-3.19	117.80	120.61
2	D	401	15R	CAL-CBE-CBH	-3.12	119.71	123.11
2	D	401	15R	OAC-CBC-NBQ	-3.10	115.85	121.38
2	D	401	15R	CAQ-CAT-NBP	-3.09	106.12	110.82
2	A	401	15R	OAB-CBB-CBH	-3.08	113.84	120.06
2	B	401	15R	CAO-CBH-CBE	3.08	120.41	116.66
2	A	401	15R	OAD-CBK-CBM	-3.02	118.06	123.30
2	B	401	15R	CAJ-CBG-CBJ	-3.01	114.99	119.78
2	C	401	15R	OAD-CBK-CBM	-2.99	118.12	123.30
2	A	401	15R	CAP-CAS-NBQ	-2.95	105.24	109.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	401	15R	CAN-CBM-CBL	2.92	122.51	119.26
2	D	401	15R	CAP-CAS-NBQ	2.82	113.51	109.48
2	A	401	15R	CAS-NBQ-CBO	-2.81	109.22	115.35
2	C	401	15R	CAL-CBE-CBH	-2.79	120.07	123.11
2	C	401	15R	CAR-CBN-CBC	2.79	114.87	109.83
2	A	401	15R	CAH-CAI-CBF	-2.76	116.78	120.89
2	D	401	15R	CAU-CAR-CBN	2.73	114.95	110.41
2	A	401	15R	CBL-CBM-CBK	-2.72	116.87	119.52
2	C	401	15R	CBL-CBM-CBK	-2.71	116.88	119.52
2	A	401	15R	CBF-CBJ-CBO	-2.69	116.20	120.83
2	D	401	15R	OAB-CBB-NBP	-2.66	117.94	122.34
2	A	401	15R	CBG-CBJ-CBF	-2.62	117.44	119.81
2	B	401	15R	CBG-CBA-NAY	-2.60	112.49	116.03
2	C	401	15R	CBO-NBQ-CBC	2.55	130.82	121.53
2	B	401	15R	CBL-CBM-CBK	-2.50	117.08	119.52
2	A	401	15R	FAE-CBE-CAL	-2.48	113.06	118.59
2	D	401	15R	CBD-CAW-CBI	2.48	120.37	114.34
2	D	401	15R	CAQ-CBN-CAR	2.43	115.11	109.97
4	A	403	PEG	O2-C3-C4	2.41	120.66	110.07
2	C	401	15R	CAT-NBP-CAU	2.40	117.24	112.62
2	A	401	15R	CAS-NBQ-CBC	-2.39	113.90	122.59
2	D	401	15R	CBO-NBQ-CBC	2.35	130.09	121.53
2	D	401	15R	FAE-CBE-CBH	2.28	123.54	119.67
2	B	401	15R	OAD-CBK-CBM	-2.28	119.35	123.30
2	B	401	15R	CAG-CAF-CAM	2.26	123.63	120.19
2	D	401	15R	CAI-CAH-CAJ	-2.17	117.17	120.25
2	A	401	15R	CAH-CAJ-CBG	-2.14	115.76	119.81
2	C	401	15R	CAK-CAL-CBE	2.13	121.63	119.05
2	A	401	15R	CAJ-CBG-CBJ	-2.13	116.39	119.78
2	D	401	15R	OAD-CBK-NAZ	-2.10	118.14	120.90
2	D	401	15R	CAK-CAL-CBE	2.07	121.55	119.05
2	A	401	15R	CAL-CBE-CBH	-2.04	120.89	123.11
4	A	403	PEG	O2-C2-C1	2.04	119.01	110.07
2	D	401	15R	CAN-CBM-CBL	2.04	121.52	119.26
2	D	401	15R	CBG-CBA-NAY	-2.02	113.28	116.03

There are no chirality outliers.

All (18) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	401	15R	NBP-CBB-CBH-CBE
2	A	401	15R	OAB-CBB-CBH-CBE

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Mol	Chain	Res	Type	Atoms
2	D	401	15R	CBD-CAW-CBI-NAX
2	D	401	15R	CBD-CAW-CBI-CBL
2	A	401	15R	NBP-CBB-CBH-CAO
2	A	401	15R	OAB-CBB-CBH-CAO
2	A	401	15R	OAC-CBC-CBN-CAR
4	A	403	PEG	O1-C1-C2-O2
2	A	401	15R	NBQ-CBC-CBN-CAR
4	A	403	PEG	C1-C2-O2-C3
2	A	401	15R	CBD-CAW-CBI-CBL
2	B	401	15R	CBD-CAW-CBI-CBL
2	A	401	15R	CBD-CAW-CBI-NAX
2	B	401	15R	CBD-CAW-CBI-NAX
2	D	401	15R	OAB-CBB-CBH-CBE
2	D	401	15R	NBP-CBB-CBH-CAO
2	D	401	15R	OAB-CBB-CBH-CAO
2	A	401	15R	NBQ-CBC-CBN-CAQ

All (1) ring outliers are listed below:

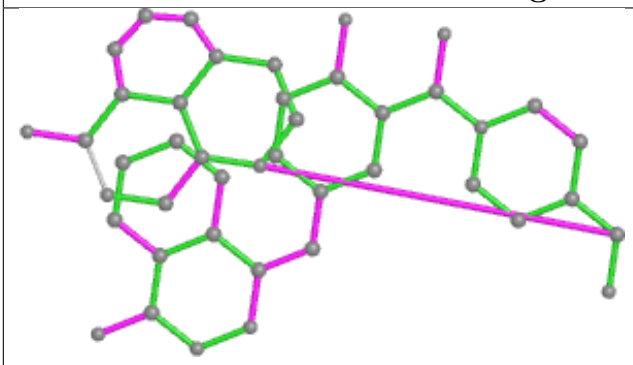
Mol	Chain	Res	Type	Atoms
2	A	401	15R	CAQ-CAR-CAT-CAU-CBN-NBP

5 monomers are involved in 22 short contacts:

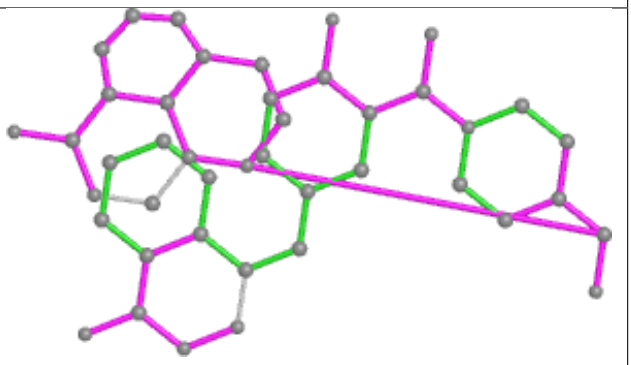
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	401	15R	10	0
2	B	401	15R	2	0
4	A	403	PEG	4	0
2	C	401	15R	2	0
2	D	401	15R	6	0

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.

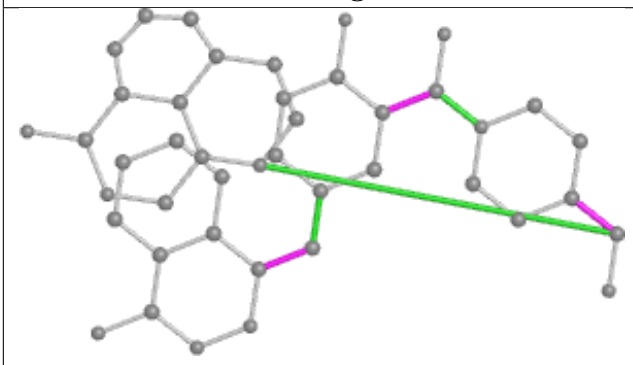
Ligand 15R A 401



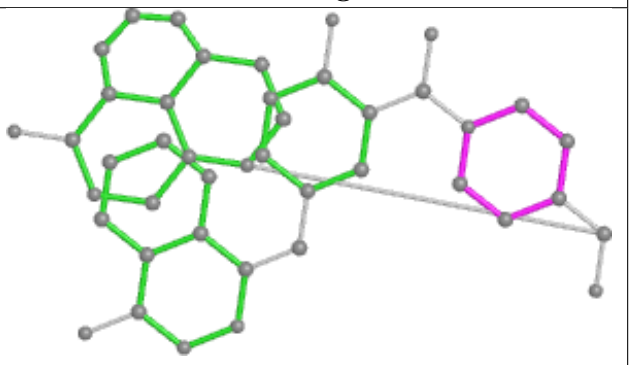
Bond lengths



Bond angles

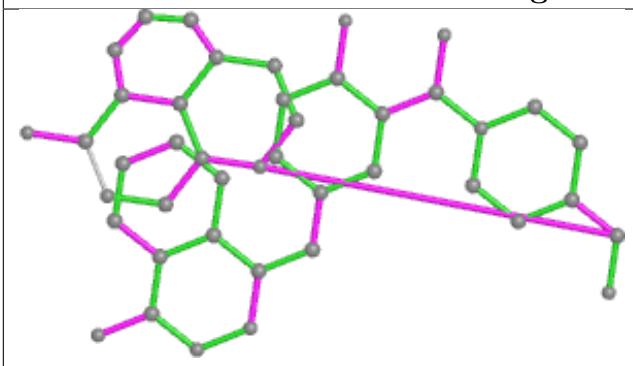


Torsions

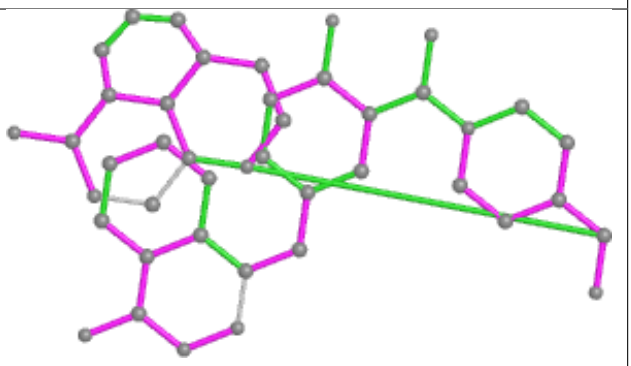


Rings

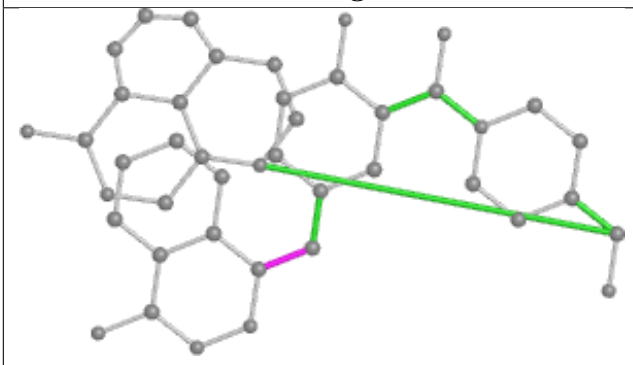
Ligand 15R B 401



Bond lengths



Bond angles



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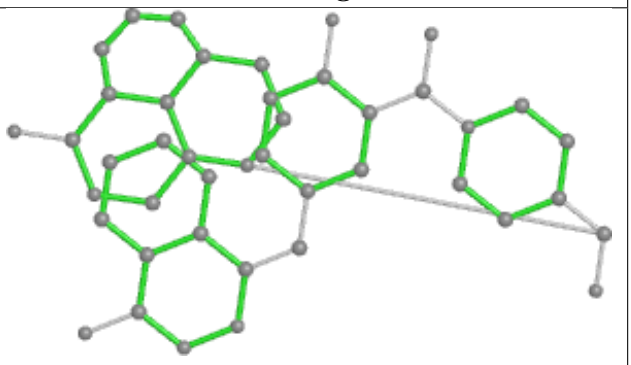
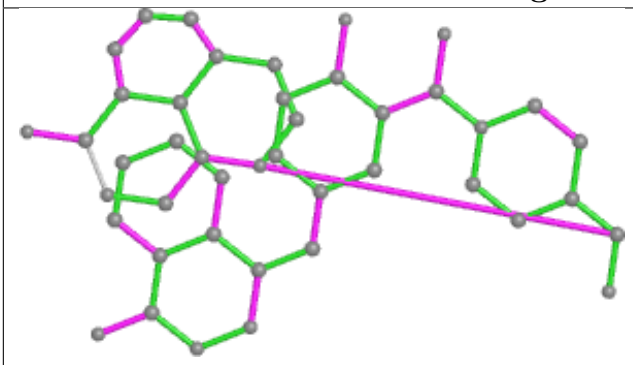
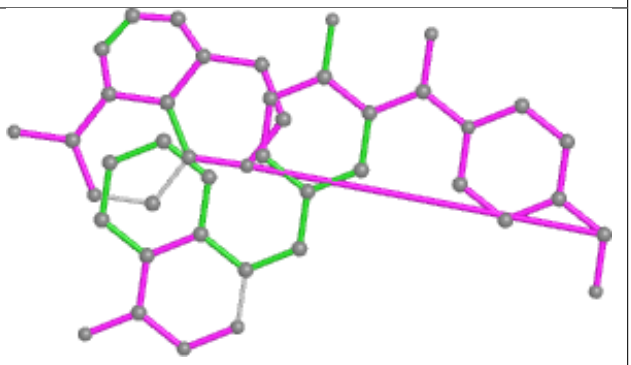


Rings

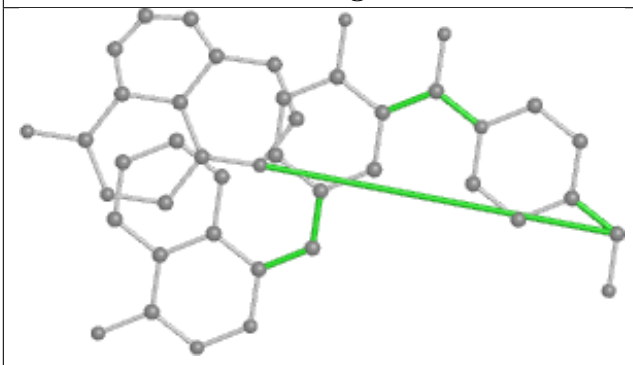
Ligand 15R C 401



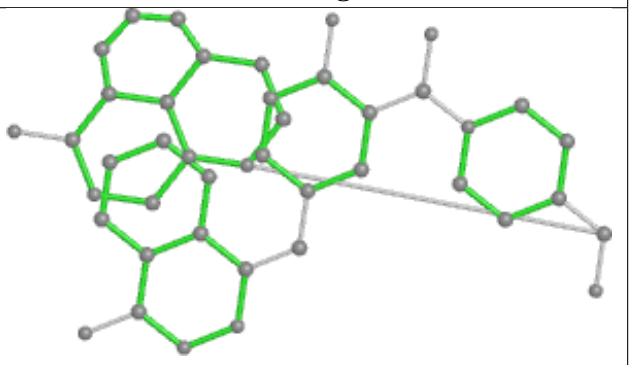
Bond lengths



Bond angles

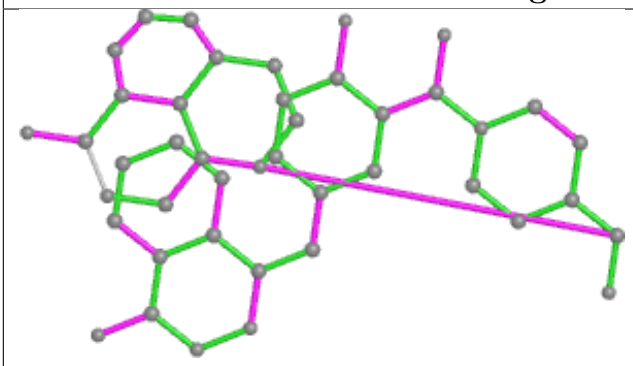


Torsions

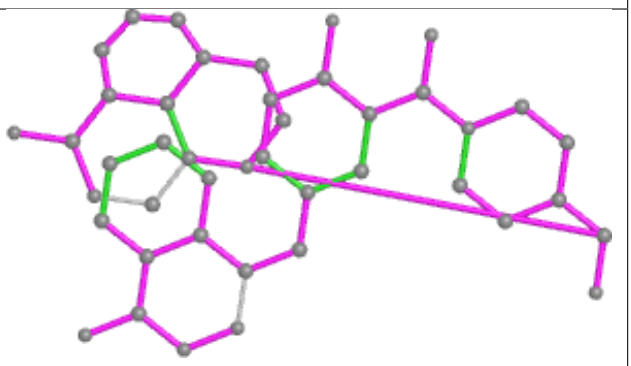


Rings

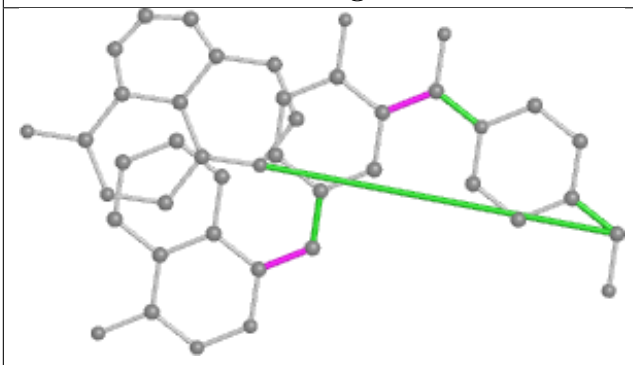
Ligand 15R D 401



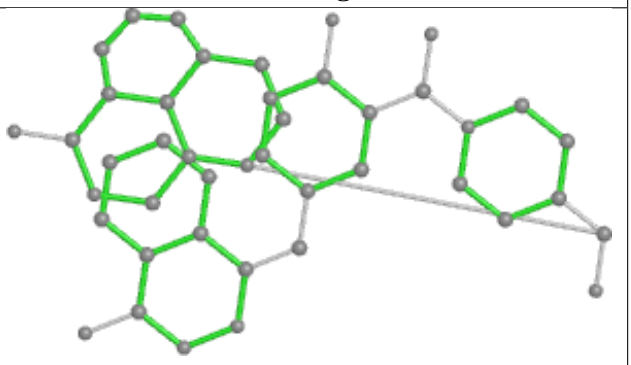
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	349/355 (98%)	0.24	13 (3%) 41 54	0, 10, 39, 78	0
1	B	340/355 (95%)	0.13	0 100 100	0, 10, 32, 44	0
1	C	345/355 (97%)	0.37	20 (5%) 23 33	2, 22, 51, 76	0
1	D	309/355 (87%)	1.23	83 (26%) 0 0	5, 42, 72, 92	0
All	All	1343/1420 (94%)	0.48	116 (8%) 10 16	0, 17, 61, 92	0

All (116) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	69	LEU	7.8
1	A	122	ASP	6.2
1	D	68	ILE	6.2
1	D	32	LEU	5.7
1	D	52	LEU	5.7
1	D	114	TYR	5.6
1	C	122	ASP	5.2
1	D	62	GLY	5.2
1	D	79	ILE	5.1
1	D	96	SER	5.0
1	D	45	ILE	4.7
1	D	60	SER	4.7
1	D	63	SER	4.6
1	C	276	HIS	4.6
1	D	66	SER	4.5
1	A	85	MET	4.4
1	A	124	SER	4.3
1	D	75	PHE	4.2
1	D	80	PRO	4.1
1	D	53	SER	3.9
1	C	85	MET	3.7

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Mol	Chain	Res	Type	RSRZ
1	D	78	LEU	3.7
1	D	47	ALA	3.7
1	D	7	PRO	3.7
1	D	315	SER	3.7
1	D	82	ASP	3.7
1	A	69	LEU	3.6
1	D	71	LEU	3.6
1	C	225	VAL	3.5
1	D	15	ILE	3.5
1	C	91	LEU	3.5
1	D	46	GLN	3.5
1	D	136	LEU	3.5
1	D	135	LYS	3.5
1	D	172	VAL	3.4
1	D	93	ASN	3.4
1	D	61	GLN	3.4
1	A	121	SER	3.4
1	D	113	ALA	3.3
1	D	77	THR	3.2
1	D	81	HIS	3.1
1	D	312	THR	3.1
1	D	115	SER	3.1
1	D	112	VAL	3.1
1	D	165	HIS	3.1
1	D	139	ASP	3.1
1	D	129	ILE	3.1
1	C	123	ASP	3.1
1	D	76	TYR	3.0
1	D	40	LEU	3.0
1	D	175	ILE	3.0
1	D	163	THR	2.9
1	C	3	LYS	2.9
1	D	26	VAL	2.9
1	A	84	GLY	2.9
1	C	227	GLY	2.8
1	D	58	ALA	2.8
1	C	94	ALA	2.8
1	D	250	SER	2.8
1	D	44	GLN	2.8
1	A	67	GLN	2.8
1	A	123	ASP	2.7
1	D	9	GLN	2.7

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Mol	Chain	Res	Type	RSRZ
1	D	273	HIS	2.7
1	D	31	ASP	2.7
1	D	157	VAL	2.7
1	D	166	ASN	2.7
1	D	6	LYS	2.6
1	D	133	TYR	2.6
1	C	74	ARG	2.6
1	D	174	ASP	2.6
1	D	168	TYR	2.6
1	D	70	ASP	2.6
1	C	228	TYR	2.6
1	D	5	PRO	2.6
1	D	64	SER	2.5
1	D	248	HIS	2.5
1	D	67	GLN	2.5
1	D	299	ALA	2.5
1	D	51	ILE	2.5
1	D	16	PHE	2.5
1	C	221	PRO	2.5
1	A	59	VAL	2.4
1	D	298	SER	2.4
1	C	86	LYS	2.4
1	C	82	ASP	2.4
1	D	110	ILE	2.4
1	D	57	GLN	2.4
1	D	59	VAL	2.4
1	A	39	LYS	2.4
1	D	228	TYR	2.4
1	D	65	ASP	2.4
1	D	108	LEU	2.4
1	A	71	LEU	2.3
1	C	69	LEU	2.3
1	C	124	SER	2.3
1	D	146	ASP	2.3
1	D	152	ILE	2.3
1	C	121	SER	2.3
1	D	55	VAL	2.3
1	D	33	GLN	2.3
1	D	301	ILE	2.2
1	D	49	TYR	2.2
1	A	65	ASP	2.2
1	D	256	GLY	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	277	ILE	2.2
1	D	173	ILE	2.2
1	D	4	LEU	2.2
1	D	92	ASN	2.1
1	D	74	ARG	2.1
1	C	319	ASN	2.1
1	D	303	LEU	2.1
1	C	346	PHE	2.1
1	D	116	LEU	2.1
1	C	47	ALA	2.0
1	D	148	GLU	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

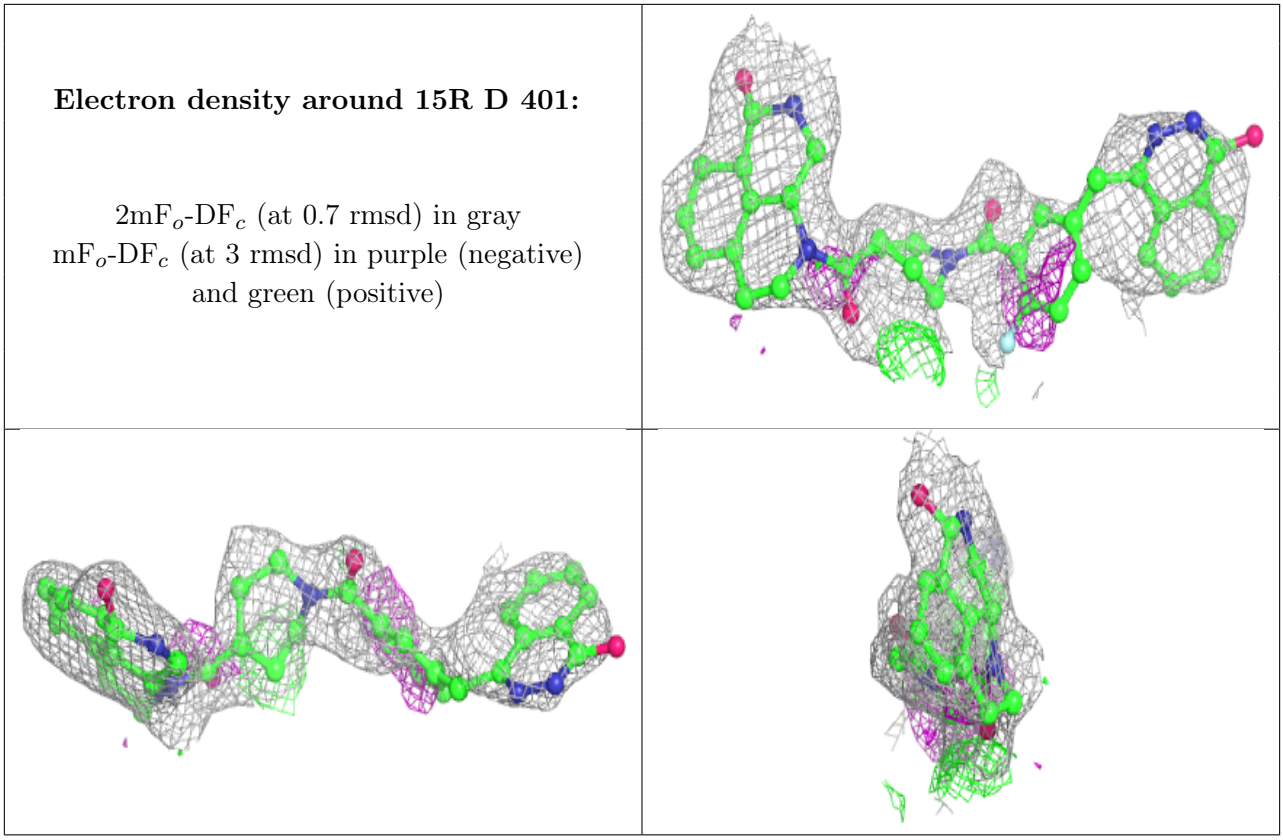
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	15R	D	401	43/43	0.78	0.28	11,37,56,58	0
2	15R	A	401	43/43	0.84	0.24	0,13,27,37	0
2	15R	C	401	43/43	0.85	0.23	3,26,42,51	0
4	PEG	A	403	7/7	0.89	0.13	7,9,15,16	0
2	15R	B	401	43/43	0.91	0.18	1,12,19,22	0
3	SO4	B	402	5/5	0.94	0.15	11,14,20,26	0
3	SO4	A	402	5/5	0.98	0.11	7,9,17,17	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.

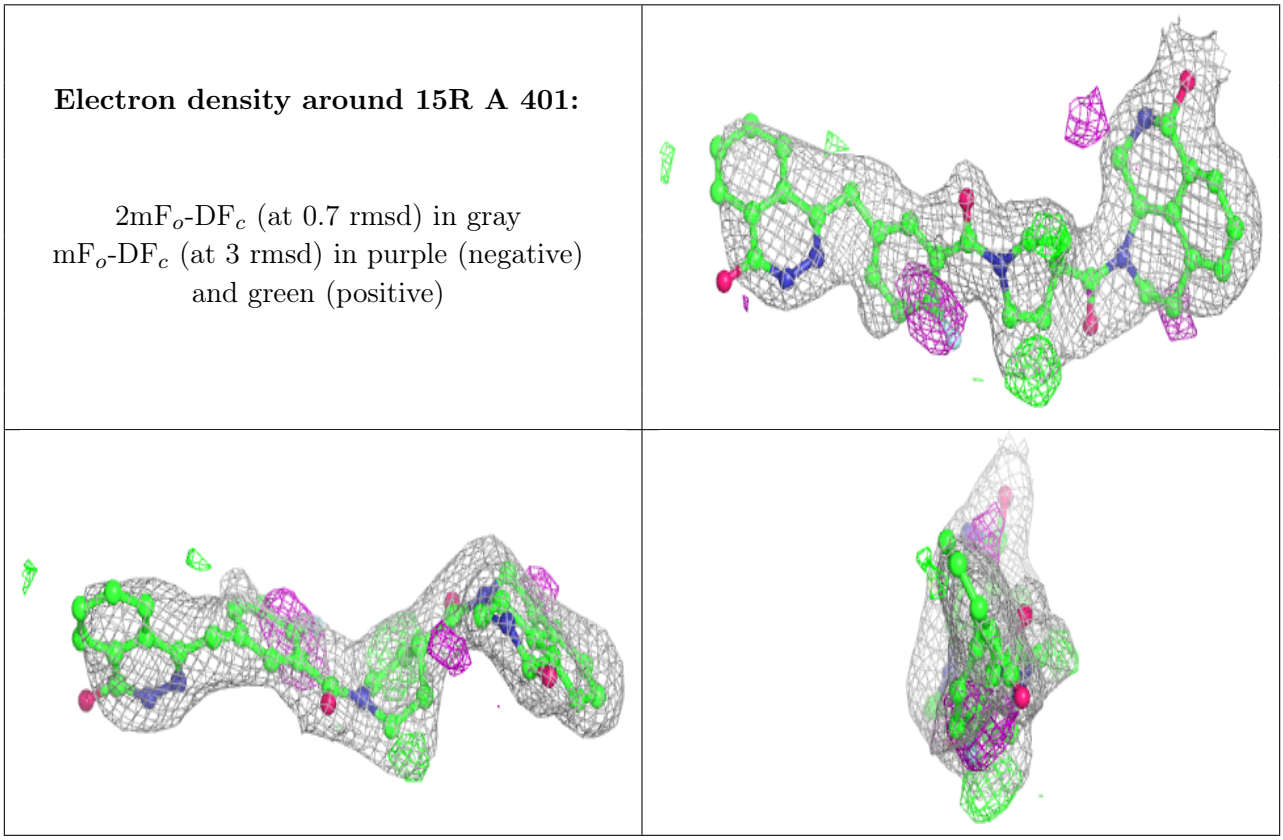
Electron density around 15R D 401:

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



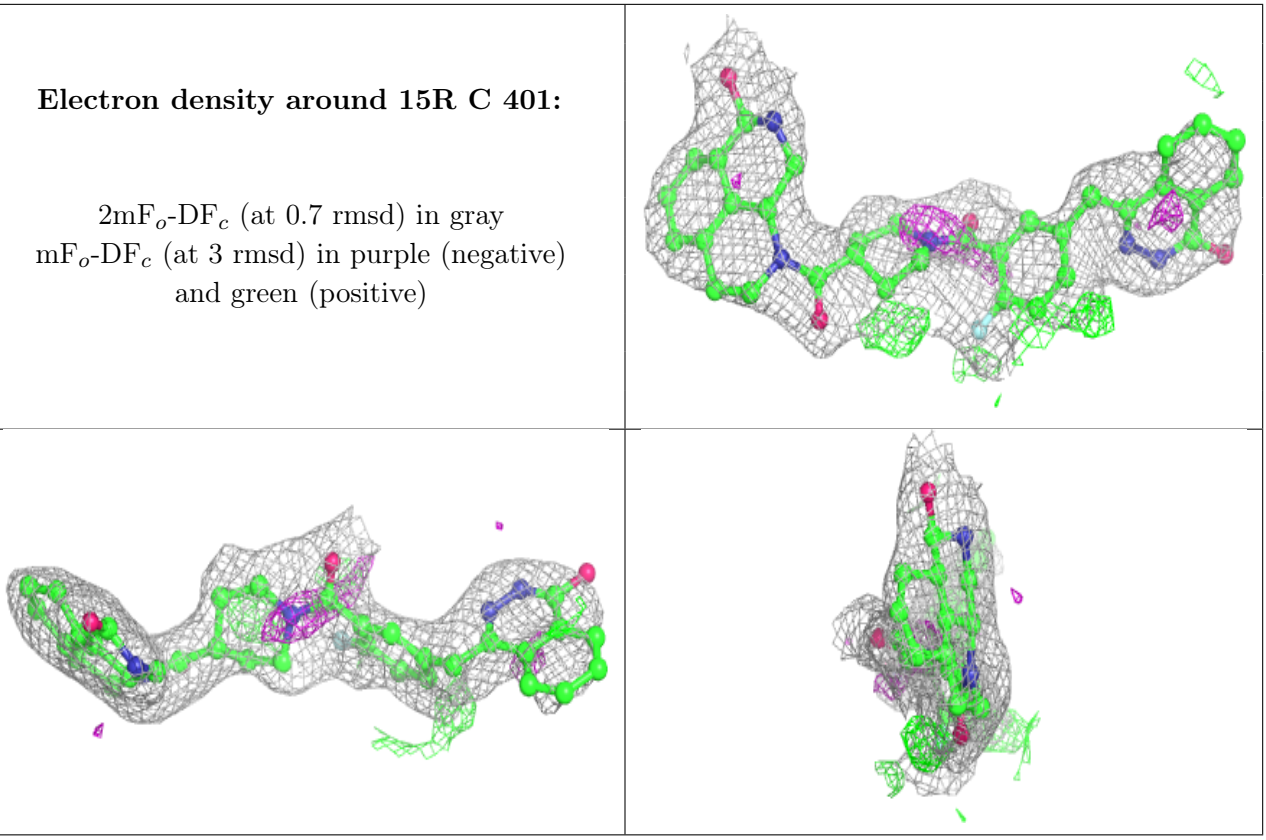
Electron density around 15R A 401:

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



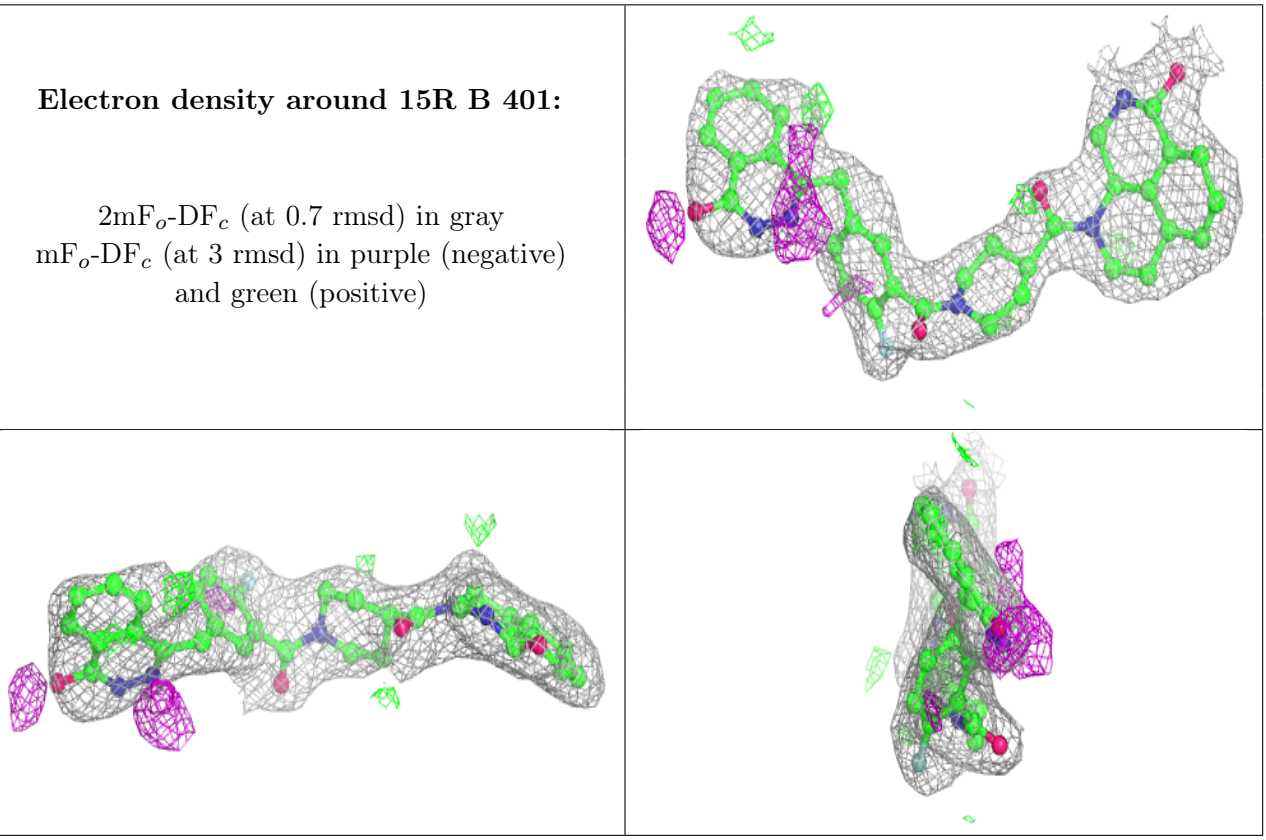
Electron density around 15R C 401:

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



Electron density around 15R B 401:

$2mF_o$-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.