Full wwPDB X-ray Structure Validation Report ⓘ

Sep 26, 2023 – 01:20 PM EDT

PDB ID	:	6CXS
Title	:	Crystal Structure of Clostridium perfringens beta-glucuronidase bound with a novel, potent inhibitor 4-(8-(piperazin-1-yl)-1,2,3,4-tetrahydro-[1,2,3]triazino[4',5':4,5]thieno[2,3-c]isoquinolin-5-yl)morpholine
Authors	:	Wallace, B.D.; Redinbo, M.R.
Deposited on	:	2018-04-04
Resolution	:	2.80 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references ⓘ) were used in the production of this report:

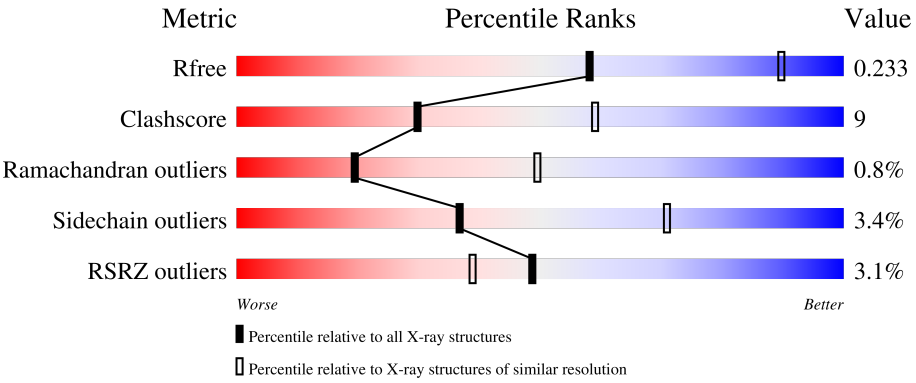
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh &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

1 Overall quality at a glance (i)

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

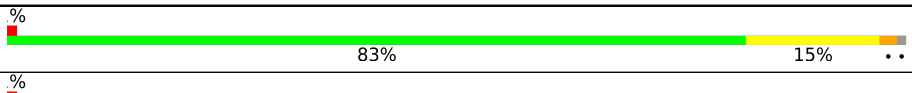
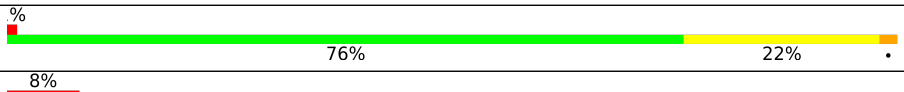
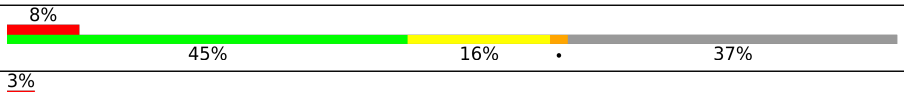
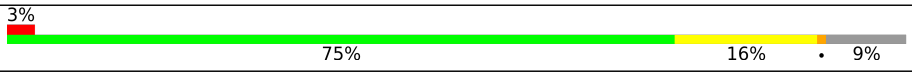
The reported resolution of this entry is 2.80 Å.

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	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)

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	602	
1	B	602	
2	C	398	
2	D	398	

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 14610 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 Beta-glucuronidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	598	Total	C	N	O	S	0	2	0
			4852	3102	807	923	20			
1	B	599	Total	C	N	O	S	0	1	0
			4844	3095	806	924	19			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	SER	-	expression tag	UNP Q8XP19
A	-1	ASN	-	expression tag	UNP Q8XP19
A	0	ALA	-	expression tag	UNP Q8XP19
B	-2	SER	-	expression tag	UNP Q8XP19
B	-1	ASN	-	expression tag	UNP Q8XP19
B	0	ALA	-	expression tag	UNP Q8XP19

- Molecule 2 is a protein called Maltose/maltodextrin-binding periplasmic protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	252	Total	C	N	O	S	0	0	0
			1858	1180	304	368	6			
2	D	362	Total	C	N	O	S	0	0	0
			2653	1693	433	521	6			

There are 64 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	-4	HIS	-	expression tag	UNP P0AEX9
C	-3	HIS	-	expression tag	UNP P0AEX9
C	-2	HIS	-	expression tag	UNP P0AEX9
C	-1	HIS	-	expression tag	UNP P0AEX9
C	0	HIS	-	expression tag	UNP P0AEX9
C	1	HIS	-	expression tag	UNP P0AEX9

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Chain	Residue	Modelled	Actual	Comment	Reference
C	2	GLY	-	expression tag	UNP P0AEX9
C	369	ASN	-	expression tag	UNP P0AEX9
C	370	SER	-	expression tag	UNP P0AEX9
C	371	SER	-	expression tag	UNP P0AEX9
C	372	SER	-	expression tag	UNP P0AEX9
C	373	ASN	-	expression tag	UNP P0AEX9
C	374	ASN	-	expression tag	UNP P0AEX9
C	375	ASN	-	expression tag	UNP P0AEX9
C	376	ASN	-	expression tag	UNP P0AEX9
C	377	ASN	-	expression tag	UNP P0AEX9
C	378	ASN	-	expression tag	UNP P0AEX9
C	379	ASN	-	expression tag	UNP P0AEX9
C	380	ASN	-	expression tag	UNP P0AEX9
C	381	ASN	-	expression tag	UNP P0AEX9
C	382	ASN	-	expression tag	UNP P0AEX9
C	383	ARG	-	expression tag	UNP P0AEX9
C	384	ASP	-	expression tag	UNP P0AEX9
C	385	LEU	-	expression tag	UNP P0AEX9
C	386	GLY	-	expression tag	UNP P0AEX9
C	387	THR	-	expression tag	UNP P0AEX9
C	388	GLU	-	expression tag	UNP P0AEX9
C	389	ASN	-	expression tag	UNP P0AEX9
C	390	LEU	-	expression tag	UNP P0AEX9
C	391	TYR	-	expression tag	UNP P0AEX9
C	392	PHE	-	expression tag	UNP P0AEX9
C	393	GLN	-	expression tag	UNP P0AEX9
D	3	HIS	-	expression tag	UNP P0AEX9
D	4	HIS	-	expression tag	UNP P0AEX9
D	5	HIS	-	expression tag	UNP P0AEX9
D	6	HIS	-	expression tag	UNP P0AEX9
D	7	HIS	-	expression tag	UNP P0AEX9
D	8	HIS	-	expression tag	UNP P0AEX9
D	9	GLY	-	expression tag	UNP P0AEX9
D	376	ASN	-	expression tag	UNP P0AEX9
D	377	SER	-	expression tag	UNP P0AEX9
D	378	SER	-	expression tag	UNP P0AEX9
D	379	SER	-	expression tag	UNP P0AEX9
D	380	ASN	-	expression tag	UNP P0AEX9
D	381	ASN	-	expression tag	UNP P0AEX9
D	382	ASN	-	expression tag	UNP P0AEX9
D	383	ASN	-	expression tag	UNP P0AEX9
D	384	ASN	-	expression tag	UNP P0AEX9

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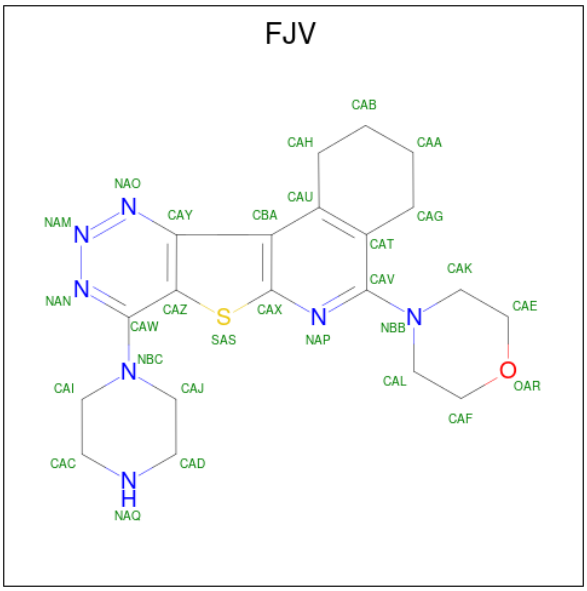
Chain	Residue	Modelled	Actual	Comment	Reference
D	385	ASN	-	expression tag	UNP P0AEX9
D	386	ASN	-	expression tag	UNP P0AEX9
D	387	ASN	-	expression tag	UNP P0AEX9
D	388	ASN	-	expression tag	UNP P0AEX9
D	389	ASN	-	expression tag	UNP P0AEX9
D	390	ARG	-	expression tag	UNP P0AEX9
D	391	ASP	-	expression tag	UNP P0AEX9
D	392	LEU	-	expression tag	UNP P0AEX9
D	393	GLY	-	expression tag	UNP P0AEX9
D	394	THR	-	expression tag	UNP P0AEX9
D	395	GLU	-	expression tag	UNP P0AEX9
D	396	ASN	-	expression tag	UNP P0AEX9
D	397	LEU	-	expression tag	UNP P0AEX9
D	398	TYR	-	expression tag	UNP P0AEX9
D	399	PHE	-	expression tag	UNP P0AEX9
D	400	GLN	-	expression tag	UNP P0AEX9

- Molecule 3 is 4-(8-(piperazin-1-yl)-1,2,3,4-tetrahydro-[1,2,3]triazino[4',5':4,5]thieno[2,3-c]isoquinolin-5-yl)morpholine (three-letter code: FJV) (formula: $C_{20}H_{25}N_7OS$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	S	0	0
			29	20	7	1	1		
3	B	1	Total	C	N	O	S	0	0
			29	20	7	1	1		

- Molecule 4 is water.

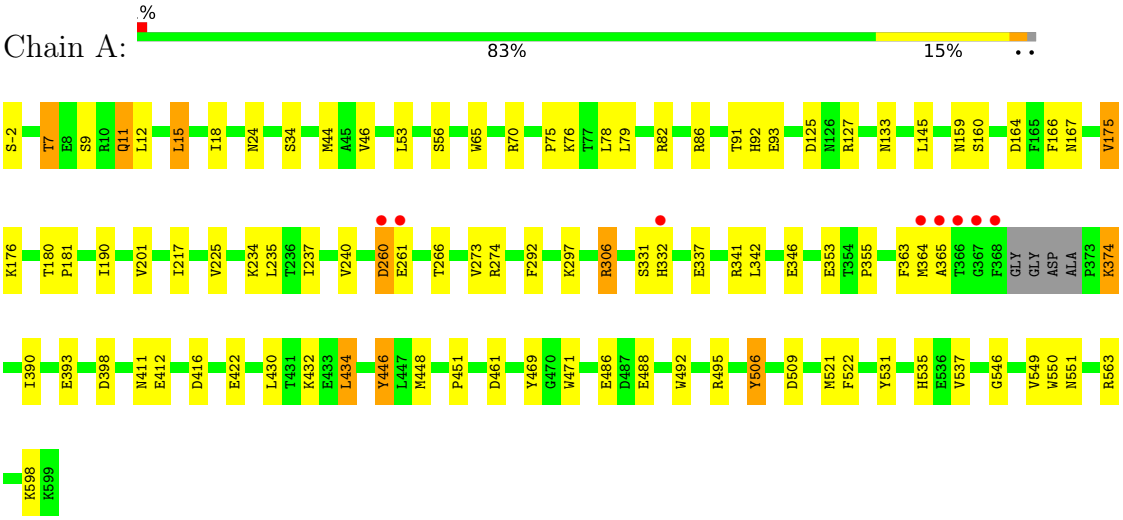
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	193	Total O 193 193	0	0
4	B	94	Total O 94 94	0	0
4	C	35	Total O 35 35	0	0
4	D	23	Total O 23 23	0	0

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.

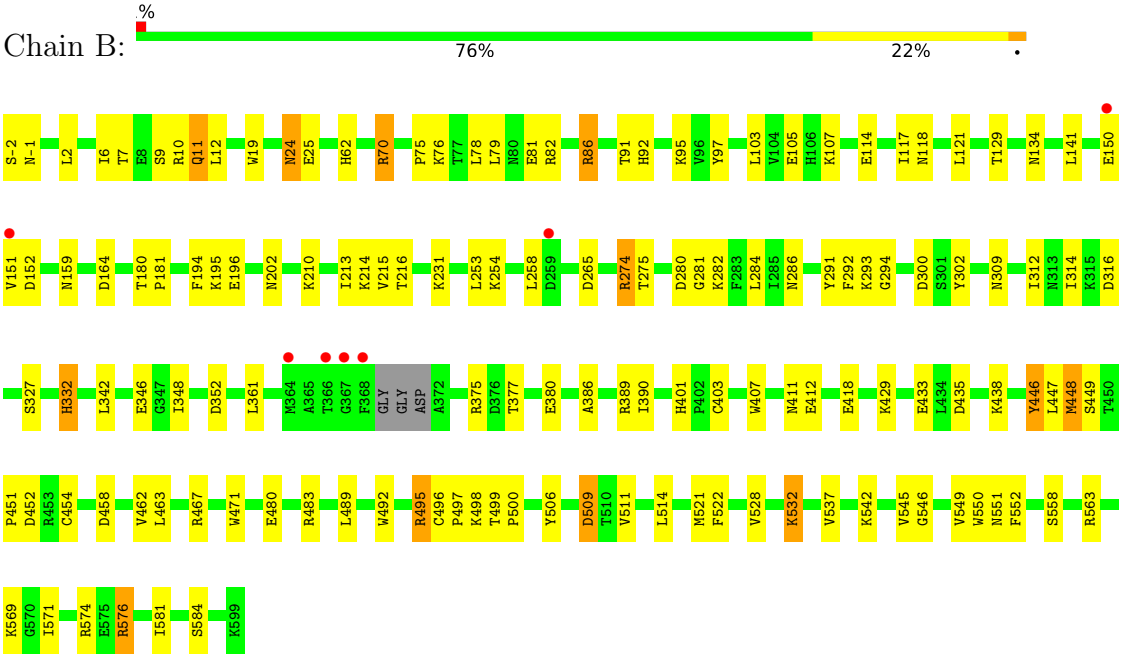
• Molecule 1: Beta-glucuronidase

Chain A:

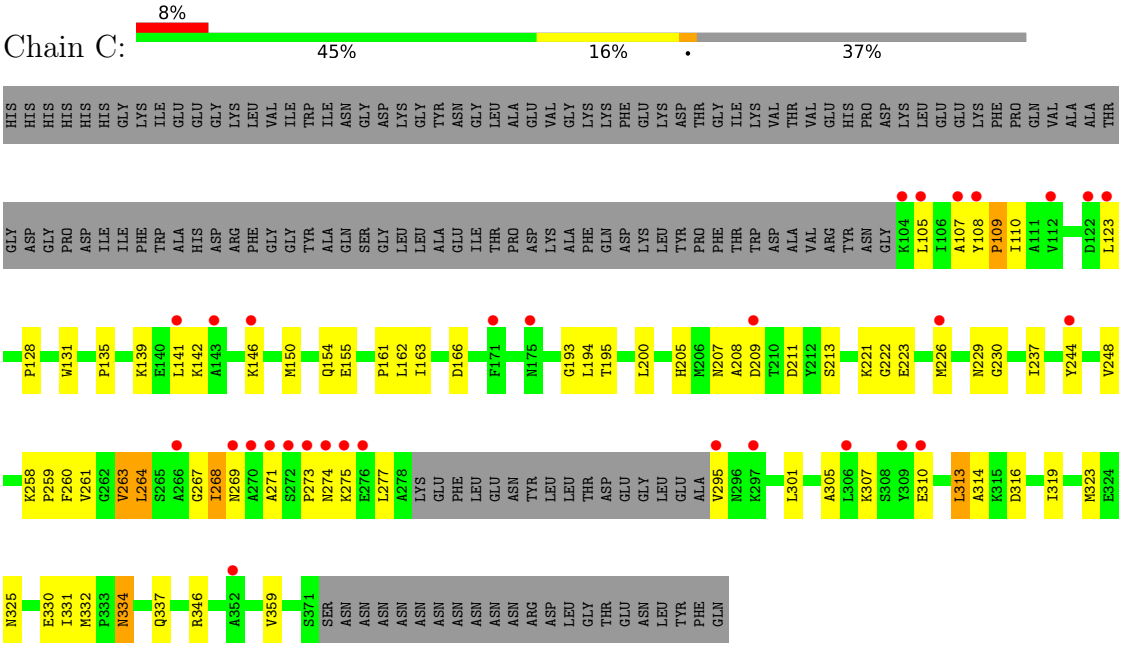


• Molecule 1: Beta-glucuronidase

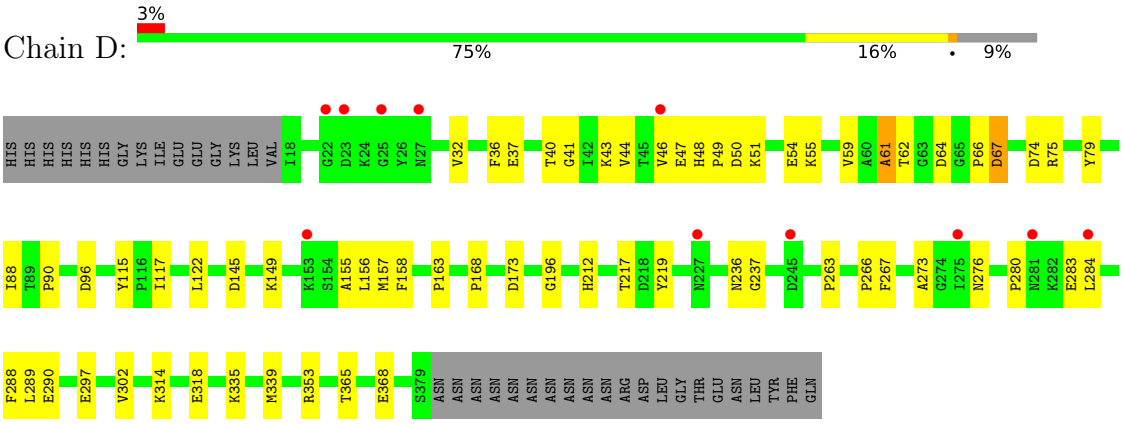
Chain B:



• Molecule 2: Maltose/maltodextrin-binding periplasmic protein



• Molecule 2: Maltose/maltodextrin-binding periplasmic protein



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	71.29Å 292.09Å 240.47Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.68 – 2.80 48.68 – 2.69	Depositor EDS
% Data completeness (in resolution range)	98.7 (48.68-2.80) 98.8 (48.68-2.69)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.10	Depositor
$< I/\sigma(I) >$ [1]	1.94 (at 2.69Å)	Xtriage
Refinement program	PHENIX 1.13_2998	Depositor
R, R_{free}	0.200 , 0.236 0.198 , 0.233	Depositor DCC
R_{free} test set	3512 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å^2)	62.0	Xtriage
Anisotropy	0.204	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 52.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	14610	wwPDB-VP
Average B, all atoms (Å^2)	61.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.53% 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: FJV

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	0.27	0/4968	0.50	0/6725
1	B	0.27	0/4957	0.51	1/6715 (0.0%)
2	C	0.31	0/1899	0.57	0/2594
2	D	0.27	0/2717	0.48	0/3718
All	All	0.27	0/14541	0.51	1/19752 (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
2	C	0	2
2	D	0	1
All	All	0	3

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	532	LYS	CD-CE-NZ	-6.06	97.76	111.70

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	C	105	LEU	Peptide
2	C	263	VAL	Peptide
2	D	61	ALA	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	4852	0	4767	70	0
1	B	4844	0	4740	100	0
2	C	1858	0	1759	56	0
2	D	2653	0	2443	44	0
3	A	29	0	0	1	0
3	B	29	0	0	3	0
4	A	193	0	0	8	0
4	B	94	0	0	4	0
4	C	35	0	0	2	0
4	D	23	0	0	1	0
All	All	14610	0	13709	262	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 (262) 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)
2:D:48:HIS:NE2	2:D:289:LEU:HD23	1.48	1.24
2:C:123:LEU:O	2:C:123:LEU:HD23	1.58	1.01
1:A:332:HIS:CE1	1:A:411:ASN:ND2	2.30	0.99
2:C:263:VAL:H	2:C:264:LEU:HB2	1.31	0.94
1:A:332:HIS:CE1	1:A:411:ASN:CG	2.43	0.92
1:A:160:SER:OG	4:A:701:HOH:O	1.94	0.86
2:D:297:GLU:OE2	2:D:297:GLU:N	2.13	0.81
2:D:48:HIS:CD2	2:D:289:LEU:HD23	2.14	0.80
2:C:268:ILE:HG23	2:C:269:ASN:H	1.47	0.79
1:A:332:HIS:HE1	1:A:411:ASN:CG	1.82	0.79
1:B:7:THR:HG23	1:B:9:SER:H	1.48	0.78
2:C:123:LEU:HD11	2:C:141:LEU:CD1	2.13	0.78
1:B:2:LEU:O	1:B:86:ARG:NH2	2.18	0.76
1:B:82:ARG:HH11	1:B:180:THR:HG21	1.50	0.76
2:C:123:LEU:HD11	2:C:141:LEU:HD11	1.65	0.76
2:D:48:HIS:NE2	2:D:289:LEU:CD2	2.40	0.74
2:C:268:ILE:HD11	2:C:271:ALA:HB3	1.69	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:284:LEU:HD22	2:D:288:PHE:CZ	2.24	0.73
1:B:216:THR:HG23	1:B:254:LYS:HB3	1.70	0.72
1:A:346:GLU:OE1	4:A:702:HOH:O	2.08	0.71
2:C:141:LEU:HD11	2:C:146:LYS:HB2	1.73	0.71
2:D:61:ALA:O	2:D:62:THR:HG23	1.91	0.71
2:C:248:VAL:HA	2:C:325:ASN:HD21	1.56	0.70
1:A:145:LEU:HD12	4:A:701:HOH:O	1.91	0.70
1:A:486:GLU:HG3	1:A:537:VAL:HG13	1.73	0.69
2:D:280:PRO:HD2	2:D:283:GLU:HB3	1.73	0.69
1:B:509:ASP:OD1	1:B:569:LYS:NZ	2.26	0.69
1:B:449:SER:OG	1:B:454:CYS:SG	2.50	0.68
1:B:213:ILE:HD12	1:B:231:LYS:HG3	1.75	0.67
1:B:151:VAL:HG12	1:B:152:ASP:HA	1.76	0.67
2:D:284:LEU:HD23	2:D:284:LEU:O	1.95	0.67
1:B:86:ARG:NH1	1:B:114:GLU:OE1	2.27	0.67
1:A:260:ASP:HB3	1:A:261:GLU:OE1	1.94	0.66
2:C:221:LYS:HD3	2:C:223:GLU:OE2	1.94	0.66
1:B:292:PHE:HB2	1:B:546:GLY:HA3	1.78	0.66
1:B:-2:SER:OG	1:B:-1:ASN:N	2.29	0.66
2:C:135:PRO:O	2:C:139:LYS:HG3	1.95	0.66
1:B:346:GLU:OE2	4:B:701:HOH:O	2.14	0.66
2:C:313:LEU:HD11	2:C:323:MET:HG3	1.78	0.66
2:C:154:GLN:NE2	2:C:208:ALA:O	2.29	0.65
2:C:135:PRO:HG3	2:C:200:LEU:HD21	1.78	0.65
1:B:151:VAL:CG1	1:B:152:ASP:HA	2.28	0.63
2:C:155:GLU:OE1	2:C:346:ARG:NH2	2.31	0.63
1:B:309:ASN:O	1:B:312:ILE:HG22	1.98	0.62
1:B:361:LEU:HD12	1:B:377:THR:HA	1.82	0.62
1:B:214:LYS:NZ	1:B:258:LEU:HD12	2.15	0.62
1:B:532:LYS:N	1:B:532:LYS:HD2	2.14	0.62
1:A:7:THR:HG23	1:A:9:SER:H	1.64	0.61
1:A:292:PHE:HB2	1:A:546:GLY:HA3	1.81	0.61
2:C:109:PRO:HD3	2:C:263:VAL:HG13	1.81	0.61
2:C:260:PHE:HB3	2:C:332:MET:HG3	1.83	0.61
2:C:307:LYS:HA	2:C:319:ILE:HD11	1.81	0.61
1:B:275:THR:H	1:B:286:ASN:ND2	1.99	0.60
1:A:412:GLU:OE1	3:A:601:FJV:NAQ	2.35	0.60
2:D:59:VAL:HG21	2:D:302:VAL:O	2.02	0.60
1:A:75:PRO:HG2	1:B:11[A]:GLN:HG2	1.84	0.60
2:C:267:GLY:HA3	2:C:268:ILE:HB	1.83	0.59
2:C:128:PRO:HD2	2:C:226:MET:HE1	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:139:LYS:HG2	2:C:205:HIS:HE1	1.67	0.59
2:C:229:ASN:OD1	2:C:230:GLY:N	2.34	0.58
1:A:82:ARG:HH11	1:A:180:THR:HG21	1.69	0.58
2:C:194:LEU:HD23	2:C:359:VAL:HG13	1.85	0.58
1:B:107:LYS:HB2	1:B:389:ARG:HH12	1.69	0.58
1:B:386:ALA:O	1:B:390:ILE:HG12	2.04	0.58
1:B:551:ASN:OD1	1:B:552:PHE:N	2.36	0.57
2:D:314:LYS:O	2:D:318:GLU:HG3	2.03	0.57
1:B:361:LEU:H	1:B:377:THR:HG22	1.69	0.57
1:A:86:ARG:NH1	4:A:710:HOH:O	2.28	0.57
1:A:355:PRO:HD2	1:A:390:ILE:HG12	1.86	0.56
1:A:261:GLU:OE1	1:A:261:GLU:N	2.32	0.56
1:B:471:TRP:CZ2	1:B:509:ASP:HB2	2.40	0.56
1:B:497:PRO:O	1:B:498:LYS:HE2	2.06	0.56
1:B:6:ILE:HG12	1:B:12:LEU:HB2	1.88	0.56
1:B:447:LEU:HD11	3:B:601:FJV:SAS	2.45	0.56
1:A:412:GLU:HG2	1:A:446:TYR:HB3	1.86	0.56
1:B:202:ASN:ND2	4:B:715:HOH:O	2.39	0.56
1:A:93:GLU:HB3	1:A:133:ASN:HB3	1.88	0.55
1:A:190:ILE:HG23	1:A:201:VAL:HG23	1.89	0.55
1:B:82:ARG:HB3	1:B:180:THR:HG22	1.87	0.55
1:A:332:HIS:HE1	1:A:411:ASN:ND2	1.93	0.55
1:B:151:VAL:HG12	1:B:152:ASP:CA	2.36	0.55
1:A:521:MET:O	1:A:522:PHE:HB2	2.07	0.54
2:D:46:VAL:O	2:D:50:ASP:HB2	2.07	0.54
2:D:47:GLU:HA	2:D:50:ASP:CB	2.37	0.54
1:A:471:TRP:CZ2	1:A:509:ASP:HB2	2.42	0.54
2:D:156:LEU:HD21	2:D:158:PHE:CD1	2.43	0.54
2:D:276:ASN:HB3	2:D:280:PRO:HG3	1.90	0.54
1:B:231:LYS:HD2	1:B:231:LYS:N	2.23	0.53
2:D:284:LEU:CD2	2:D:288:PHE:CZ	2.90	0.53
1:B:480:GLU:OE2	1:B:483:ARG:NH1	2.41	0.53
2:C:109:PRO:HD3	2:C:263:VAL:O	2.07	0.53
2:C:263:VAL:N	2:C:264:LEU:HB2	2.12	0.53
1:B:446:TYR:O	1:B:467:ARG:NH1	2.41	0.53
1:A:506:TYR:OH	1:A:535:HIS:NE2	2.35	0.53
2:D:284:LEU:CD2	2:D:288:PHE:CE2	2.92	0.52
1:A:432:LYS:NZ	1:A:461:ASP:OD2	2.42	0.52
1:B:451:PRO:HB3	1:B:492:TRP:CD2	2.45	0.52
1:A:11[B]:GLN:HG2	1:B:11[B]:GLN:NE2	2.25	0.52
1:B:95:LYS:HG2	1:B:105:GLU:HG2	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:195:THR:HG23	2:C:359:VAL:HG11	1.91	0.52
2:C:274:ASN:HB3	2:C:275:LYS:HG2	1.91	0.52
1:B:81:GLU:O	1:B:118:ASN:ND2	2.38	0.52
1:B:316:ASP:OD1	1:B:576:ARG:NH1	2.39	0.52
1:A:11[A]:GLN:HG2	1:B:75:PRO:HG2	1.91	0.52
1:A:217:ILE:HG13	1:A:235:LEU:HD23	1.92	0.52
2:D:236:ASN:OD1	2:D:237:GLY:N	2.38	0.52
1:B:215:VAL:HG13	1:B:253:LEU:HD11	1.90	0.52
1:A:337:GLU:O	1:A:341:ARG:HG3	2.10	0.51
1:B:332:HIS:CE1	1:B:411:ASN:CG	2.84	0.51
1:B:361:LEU:HD13	1:B:375:ARG:NH1	2.24	0.51
1:B:281:GLY:H	1:B:282:LYS:NZ	2.09	0.51
1:B:117:ILE:O	1:B:121:LEU:HG	2.11	0.51
1:B:274:ARG:HB2	1:B:286:ASN:HD21	1.75	0.51
1:B:24:ASN:ND2	1:B:25:GLU:O	2.43	0.51
2:D:365:THR:HG23	2:D:368:GLU:H	1.75	0.51
2:C:161:PRO:HG3	2:C:259:PRO:HB3	1.92	0.51
2:D:163:PRO:HD3	2:D:353:ARG:HB2	1.92	0.51
1:A:240:VAL:CG2	1:A:273:VAL:HG11	2.40	0.51
1:A:598:LYS:O	4:A:703:HOH:O	2.19	0.51
2:C:301:LEU:HA	2:C:305:ALA:HA	1.92	0.51
2:C:211:ASP:OD1	2:C:213:SER:N	2.42	0.51
1:B:528:VAL:HG13	1:B:532:LYS:HZ3	1.76	0.50
1:B:446:TYR:CZ	1:B:448:MET:HB2	2.46	0.50
1:A:167:ASN:ND2	4:A:715:HOH:O	2.32	0.50
1:A:234:LYS:NZ	4:A:724:HOH:O	2.45	0.50
1:B:418:GLU:OE2	1:B:418:GLU:N	2.27	0.50
1:B:462:VAL:HG22	1:B:500:PRO:HG2	1.92	0.50
1:A:11[A]:GLN:NE2	1:B:11[A]:GLN:OE1	2.44	0.49
2:C:267:GLY:CA	2:C:268:ILE:HB	2.41	0.49
2:D:32:VAL:HG22	2:D:75:ARG:NH1	2.27	0.49
1:A:76:LYS:HA	1:A:79:LEU:HD13	1.94	0.49
1:A:240:VAL:HG21	1:A:273:VAL:HG11	1.93	0.49
1:B:438:LYS:HB3	2:C:166:ASP:OD1	2.11	0.49
2:C:295:VAL:N	4:C:408:HOH:O	2.45	0.49
2:D:48:HIS:H	2:D:49:PRO:HD2	1.78	0.49
1:A:190:ILE:HG23	1:A:201:VAL:CG2	2.42	0.49
1:B:302:TYR:CE2	1:B:574:ARG:HB3	2.48	0.49
1:B:275:THR:H	1:B:286:ASN:HD22	1.60	0.49
2:C:142:LYS:HA	2:C:146:LYS:O	2.13	0.49
2:D:157:MET:HG2	2:D:217:THR:HG21	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:214:LYS:HZ2	1:B:258:LEU:HD12	1.77	0.49
1:A:91:THR:HA	1:A:92:HIS:HA	1.64	0.48
1:B:401:HIS:NE2	4:B:711:HOH:O	2.35	0.48
2:C:207:ASN:OD1	2:C:209:ASP:HB2	2.12	0.48
1:B:91:THR:HA	1:B:92:HIS:HA	1.58	0.48
1:A:164:ASP:CG	1:A:563:ARG:HH21	2.17	0.48
1:B:348:ILE:O	1:B:403:CYS:HB2	2.13	0.48
1:A:332:HIS:HE1	1:A:411:ASN:OD1	1.94	0.48
2:D:88:ILE:HG13	2:D:90:PRO:HD3	1.96	0.48
1:A:180:THR:HG23	1:A:181:PRO:O	2.13	0.48
2:D:32:VAL:HG21	2:D:79:TYR:OH	2.14	0.48
2:C:123:LEU:O	2:C:123:LEU:CD2	2.48	0.47
2:C:274:ASN:CB	2:C:275:LYS:HA	2.43	0.47
1:A:18:ILE:HD12	1:B:314:ILE:HD11	1.96	0.47
2:D:115:TYR:CD1	2:D:290:GLU:HG2	2.49	0.47
1:A:201:VAL:HG11	1:A:217:ILE:CD1	2.44	0.47
1:B:294:GLY:HA3	1:B:327:SER:O	2.15	0.47
1:B:429:LYS:O	1:B:433:GLU:HG3	2.14	0.47
2:D:64:ASP:OD2	4:D:501:HOH:O	2.21	0.47
2:D:122:LEU:HD22	2:D:236:ASN:HA	1.96	0.47
1:A:7:THR:HG21	1:A:266:THR:O	2.16	0.46
1:A:82:ARG:HB3	1:A:180:THR:HG22	1.98	0.46
1:B:451:PRO:HB3	1:B:492:TRP:CE3	2.50	0.46
2:D:145:ASP:HA	2:D:155:ALA:HB2	1.96	0.46
2:D:219:TYR:OH	2:D:236:ASN:ND2	2.46	0.46
1:A:201:VAL:HG11	1:A:217:ILE:HD11	1.98	0.46
1:B:164:ASP:OD2	1:B:563:ARG:NH1	2.49	0.46
1:B:194:PHE:O	1:B:195:LYS:HG3	2.16	0.46
1:B:412:GLU:OE1	3:B:601:FJV:NAQ	2.49	0.46
1:B:532:LYS:HD2	1:B:532:LYS:H	1.80	0.46
2:C:277:LEU:H	2:C:277:LEU:HD22	1.81	0.46
1:B:549:VAL:HG11	1:B:571:ILE:HD11	1.98	0.46
1:B:293:LYS:HE3	1:B:293:LYS:HB2	1.80	0.45
1:B:210:LYS:HD2	1:B:210:LYS:HA	1.82	0.45
1:A:78:LEU:HD11	1:B:11[B]:GLN:HE22	1.80	0.45
2:C:310:GLU:HA	2:C:310:GLU:OE1	2.17	0.45
2:D:59:VAL:HG22	2:D:302:VAL:HG13	1.97	0.45
1:A:34:SER:O	1:A:127:ARG:NH2	2.48	0.45
1:B:407:TRP:NE1	1:B:435:ASP:OD1	2.49	0.45
2:C:163:ILE:HA	2:C:193:GLY:HA3	1.98	0.45
2:D:51:LYS:HA	2:D:54:GLU:HG3	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:281:GLY:H	1:B:282:LYS:HZ3	1.64	0.45
1:B:489:LEU:HD12	1:B:537:VAL:HG12	1.99	0.45
1:A:15:LEU:HB2	1:A:175:VAL:HG22	1.98	0.45
1:B:458:ASP:OD2	1:B:495:ARG:NH1	2.34	0.45
1:A:225:VAL:HG11	1:A:237:ILE:HG23	1.97	0.45
1:B:141:LEU:HD12	1:B:390:ILE:HG13	1.99	0.45
1:A:166:PHE:O	1:A:306:ARG:NH2	2.50	0.45
1:B:550:TRP:HA	1:B:551:ASN:HA	1.71	0.45
1:A:-2:SER:N	1:A:393:GLU:HG2	2.32	0.44
1:B:7:THR:HG22	1:B:10:ARG:HB2	1.99	0.44
2:C:141:LEU:CD1	2:C:146:LYS:HB2	2.46	0.44
2:D:66:PRO:O	2:D:67:ASP:HB2	2.17	0.44
1:B:9:SER:OG	1:B:265:ASP:OD1	2.30	0.44
2:D:157:MET:HB2	2:D:157:MET:HE3	1.85	0.44
1:B:300:ASP:O	1:B:576:ARG:NH2	2.50	0.44
2:C:237:ILE:HG13	2:C:244:TYR:CE2	2.52	0.44
2:C:334:ASN:OD1	2:C:334:ASN:N	2.50	0.44
2:D:48:HIS:N	2:D:49:PRO:HD2	2.32	0.44
2:D:55:LYS:HE3	2:D:55:LYS:HB2	1.83	0.44
1:A:374:LYS:HB2	1:A:374:LYS:HE2	1.75	0.44
2:C:108:TYR:HB3	2:C:109:PRO:HA	2.00	0.44
2:C:123:LEU:HD23	2:C:123:LEU:C	2.35	0.44
1:B:231:LYS:HD2	1:B:231:LYS:H	1.80	0.44
2:D:267:PHE:HB3	2:D:339:MET:HE2	1.99	0.44
1:A:44:MET:SD	1:A:53:LEU:HD12	2.57	0.44
1:A:550:TRP:HA	1:A:551:ASN:HA	1.72	0.44
1:B:97:TYR:HB2	1:B:129:THR:HB	1.99	0.43
1:B:280:ASP:HA	1:B:498:LYS:HD3	1.99	0.43
2:C:261:VAL:HB	2:C:331:ILE:HA	2.00	0.43
2:C:337:GLN:H	2:C:337:GLN:CD	2.21	0.43
1:B:150:GLU:HB3	1:B:151:VAL:HA	2.01	0.43
1:B:496:CYS:HB3	1:B:499:THR:HG23	2.00	0.43
1:B:521:MET:O	1:B:522:PHE:HB2	2.19	0.43
2:C:146:LYS:HE3	2:C:222:GLY:O	2.18	0.43
2:D:173:ASP:O	2:D:196:GLY:HA3	2.18	0.43
1:A:164:ASP:OD2	1:A:563:ARG:NH2	2.44	0.43
2:C:123:LEU:HD11	2:C:141:LEU:HD13	1.95	0.43
1:A:297:LYS:O	1:A:331:SER:HB2	2.19	0.43
1:B:151:VAL:HG12	1:B:152:ASP:CB	2.49	0.43
1:A:331:SER:O	1:A:332:HIS:HB2	2.19	0.42
1:A:451:PRO:HG3	1:A:492:TRP:CD2	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:6:ILE:CG1	1:B:12:LEU:HB2	2.48	0.42
2:D:96:ASP:O	2:D:314:LYS:NZ	2.51	0.42
1:A:7:THR:CG2	1:A:9:SER:H	2.29	0.42
2:D:40:THR:OG1	2:D:41:GLY:N	2.53	0.42
2:C:313:LEU:CD1	2:C:323:MET:HG3	2.48	0.42
1:A:486:GLU:HG3	1:A:537:VAL:CG1	2.47	0.42
2:D:263:PRO:HB3	2:D:335:LYS:HD3	2.02	0.42
1:B:454:CYS:O	1:B:495:ARG:NH2	2.53	0.42
1:B:447:LEU:CD1	3:B:601:FJV:SAS	3.08	0.42
1:B:511:VAL:HB	1:B:514:LEU:HD12	2.01	0.42
2:D:168:PRO:HG3	2:D:266:PRO:HA	2.01	0.42
2:C:267:GLY:HA3	2:C:268:ILE:CB	2.50	0.41
1:B:10:ARG:NH1	4:B:721:HOH:O	2.44	0.41
1:B:214:LYS:HZ3	1:B:258:LEU:HD12	1.83	0.41
2:D:117:ILE:HD11	2:D:273:ALA:HB2	2.02	0.41
1:A:65:TRP:CZ2	1:A:133:ASN:HB2	2.56	0.41
1:B:375:ARG:NH1	1:B:380:GLU:OE1	2.42	0.41
1:A:332:HIS:N	1:A:353:GLU:OE1	2.53	0.41
1:B:19:TRP:CE2	1:B:70:ARG:HG2	2.56	0.41
2:D:145:ASP:OD2	2:D:212:HIS:ND1	2.41	0.41
2:C:131:TRP:CE2	2:C:162:LEU:HD13	2.55	0.41
1:A:297:LYS:HZ2	1:A:297:LYS:HB3	1.84	0.41
1:A:531:TYR:OH	1:A:549:VAL:HG13	2.21	0.41
1:B:571:ILE:HG23	1:B:581:ILE:HG23	2.03	0.41
1:A:469:TYR:OH	1:A:488:GLU:OE1	2.32	0.40
1:B:62:HIS:O	1:B:134:ASN:ND2	2.50	0.40
1:B:180:THR:HG23	1:B:181:PRO:O	2.21	0.40
1:B:429:LYS:HZ3	2:C:258:LYS:HE2	1.86	0.40
1:A:398:ASP:OD1	4:A:704:HOH:O	2.22	0.40
1:A:430:LEU:HG	1:A:434:LEU:HD22	2.03	0.40
2:C:248:VAL:HA	2:C:325:ASN:ND2	2.30	0.40
2:C:260:PHE:HA	2:C:330:GLU:O	2.22	0.40
2:C:264:LEU:HD22	2:C:264:LEU:HA	1.80	0.40
2:C:314:ALA:HB3	4:C:407:HOH:O	2.21	0.40
2:D:284:LEU:HD22	2:D:288:PHE:HZ	1.83	0.40
1:A:416:ASP:OD1	1:A:416:ASP:N	2.52	0.40
1:B:11[B]:GLN:OE1	1:B:78:LEU:HD21	2.21	0.40
1:B:291:TYR:HA	1:B:545:VAL:O	2.20	0.40
1:A:12:LEU:HD22	1:A:176:LYS:HD2	2.04	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	596/602 (99%)	570 (96%)	24 (4%)	2 (0%)	41	72
1	B	596/602 (99%)	561 (94%)	33 (6%)	2 (0%)	41	72
2	C	248/398 (62%)	221 (89%)	20 (8%)	7 (3%)	5	17
2	D	360/398 (90%)	331 (92%)	25 (7%)	4 (1%)	14	41
All	All	1800/2000 (90%)	1683 (94%)	102 (6%)	15 (1%)	19	49

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	452	ASP
2	C	107	ALA
2	C	268	ILE
1	A	365	ALA
2	C	110	ILE
2	C	273	PRO
2	C	313	LEU
1	A	260	ASP
1	B	196	GLU
2	C	264	LEU
2	D	43	LYS
2	C	109	PRO
2	D	44	VAL
2	D	67	ASP
2	D	37	GLU

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	531/531 (100%)	508 (96%)	23 (4%)	29	62
1	B	528/531 (99%)	504 (96%)	24 (4%)	27	60
2	C	184/323 (57%)	181 (98%)	3 (2%)	62	88
2	D	251/323 (78%)	248 (99%)	3 (1%)	71	92
All	All	1494/1708 (88%)	1441 (96%)	53 (4%)	37	70

All (53) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	THR
1	A	11[A]	GLN
1	A	11[B]	GLN
1	A	15	LEU
1	A	24	ASN
1	A	46	VAL
1	A	56	SER
1	A	70	ARG
1	A	125	ASP
1	A	159	ASN
1	A	175	VAL
1	A	274	ARG
1	A	306	ARG
1	A	342	LEU
1	A	364[A]	MET
1	A	364[B]	MET
1	A	374	LYS
1	A	422	GLU
1	A	434	LEU
1	A	446	TYR
1	A	448	MET
1	A	495	ARG
1	A	506	TYR
1	B	11[A]	GLN
1	B	11[B]	GLN
1	B	24	ASN
1	B	70	ARG
1	B	76	LYS
1	B	79	LEU
1	B	86	ARG
1	B	103	LEU

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Mol	Chain	Res	Type
1	B	159	ASN
1	B	274	ARG
1	B	284	LEU
1	B	332	HIS
1	B	342	LEU
1	B	352	ASP
1	B	446	TYR
1	B	448	MET
1	B	463	LEU
1	B	495	ARG
1	B	506	TYR
1	B	509	ASP
1	B	542	LYS
1	B	558	SER
1	B	576	ARG
1	B	584	SER
2	C	150	MET
2	C	316	ASP
2	C	334	ASN
2	D	36	PHE
2	D	74	ASP
2	D	149	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	332	HIS
1	A	411	ASN
1	B	286	ASN
1	B	332	HIS
2	C	154	GLN
2	C	187	ASN
2	D	58	GLN

5.3.3 RNA

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)

2 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	FJV	B	601	-	29,34,34	2.48	3 (10%)	28,49,49	2.89	10 (35%)
3	FJV	A	601	-	29,34,34	2.50	4 (13%)	28,49,49	2.86	10 (35%)

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
3	FJV	B	601	-	-	3/8/31/31	0/6/6/6
3	FJV	A	601	-	-	2/8/31/31	0/6/6/6

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	601	FJV	NAN-NAM	-9.01	1.23	1.32
3	B	601	FJV	NAN-NAM	-8.64	1.23	1.32
3	A	601	FJV	NAO-NAM	-8.40	1.23	1.32
3	B	601	FJV	NAO-NAM	-8.34	1.24	1.32
3	B	601	FJV	CAV-NAP	2.70	1.34	1.31
3	A	601	FJV	CAV-NAP	2.46	1.34	1.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	601	FJV	CAV-NBB	2.04	1.42	1.37

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	601	FJV	CAB-CAH-CAU	7.49	123.86	112.49
3	B	601	FJV	CAB-CAH-CAU	7.41	123.74	112.49
3	B	601	FJV	CAG-CAT-CAU	-7.26	112.32	121.11
3	A	601	FJV	CAG-CAT-CAU	-6.62	113.09	121.11
3	A	601	FJV	NAP-CAV-NBB	-5.94	113.39	117.62
3	B	601	FJV	CAA-CAG-CAT	5.89	124.92	112.84
3	A	601	FJV	CAA-CAG-CAT	5.45	124.03	112.84
3	B	601	FJV	NAP-CAV-NBB	-5.29	113.86	117.62
3	A	601	FJV	CAV-NAP-CAX	3.33	122.75	116.74
3	B	601	FJV	CAT-CAV-NAP	-3.33	117.87	122.78
3	B	601	FJV	CAV-NAP-CAX	3.19	122.50	116.74
3	A	601	FJV	CAT-CAV-NAP	-2.94	118.44	122.78
3	B	601	FJV	CAK-NBB-CAV	2.81	128.82	119.05
3	A	601	FJV	CAL-NBB-CAV	2.56	127.97	119.05
3	B	601	FJV	CAB-CAA-CAG	-2.56	101.19	112.55
3	B	601	FJV	CAA-CAB-CAH	-2.54	101.27	112.55
3	A	601	FJV	CAB-CAA-CAG	-2.54	101.28	112.55
3	A	601	FJV	CAA-CAB-CAH	-2.54	101.30	112.55
3	A	601	FJV	CAT-CAU-CBA	2.25	120.88	118.99
3	B	601	FJV	CAI-NBC-CAW	2.06	124.60	118.73

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	601	FJV	CAZ-CAW-NBC-CAJ
3	B	601	FJV	CAZ-CAW-NBC-CAJ
3	B	601	FJV	CAT-CAV-NBB-CAK
3	B	601	FJV	NAP-CAV-NBB-CAK
3	A	601	FJV	NAN-CAW-NBC-CAJ

There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	601	FJV	3	0

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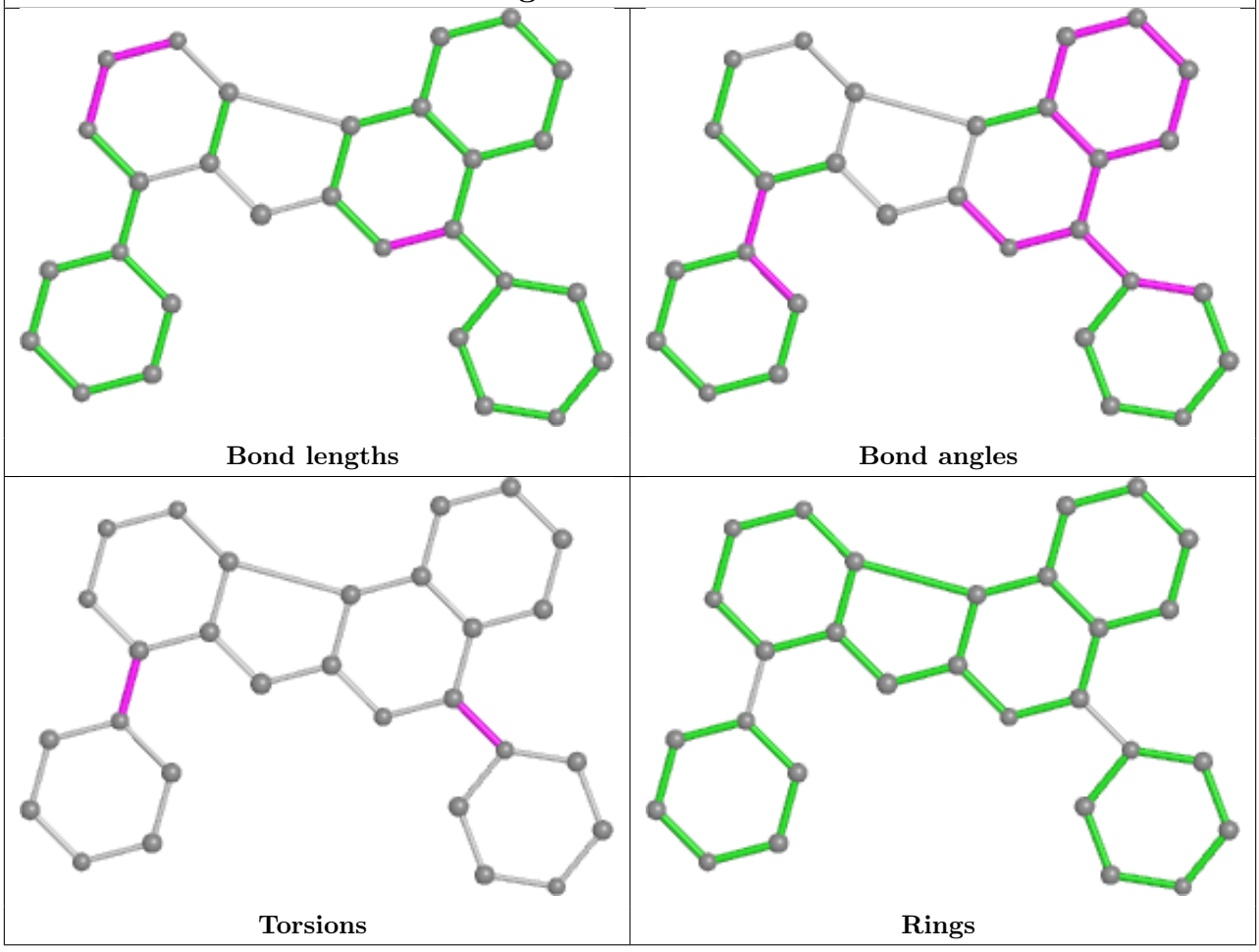
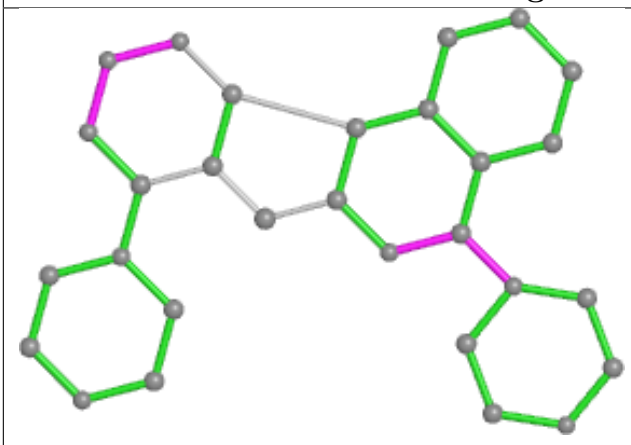
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	601	FJV	1	0

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.

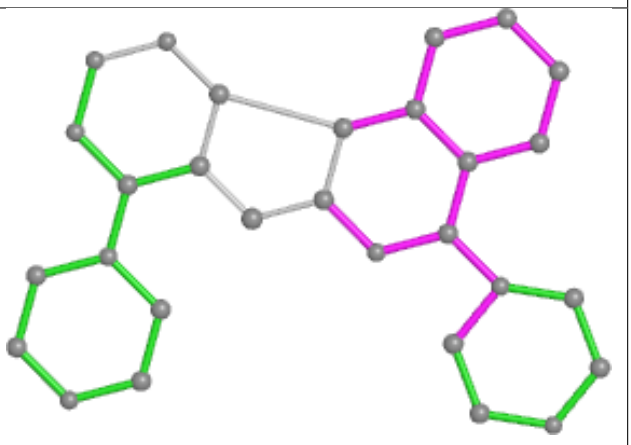
Ligand FJV B 601



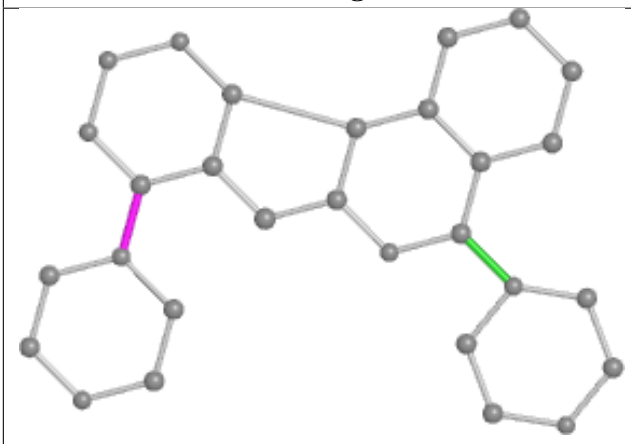
Ligand FJV A 601



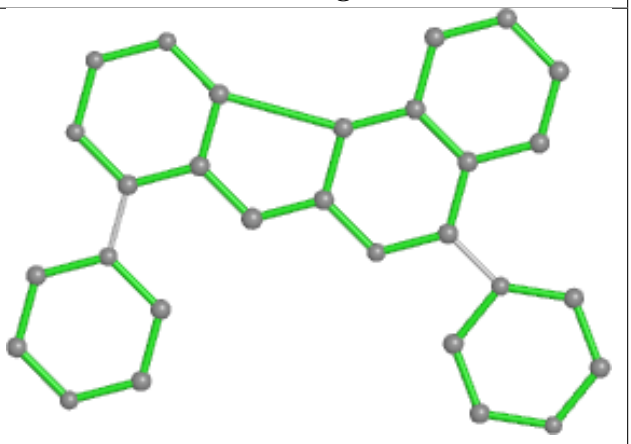
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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	598/602 (99%)	-0.35	8 (1%) 77 72	25, 41, 69, 143	0
1	B	599/602 (99%)	-0.27	7 (1%) 79 73	34, 53, 85, 149	0
2	C	252/398 (63%)	0.57	30 (11%) 4 2	62, 93, 120, 136	0
2	D	362/398 (90%)	-0.09	11 (3%) 50 40	41, 75, 116, 134	0
All	All	1811/2000 (90%)	-0.14	56 (3%) 49 39	25, 56, 109, 149	0

All (56) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	C	105	LEU	7.5
1	B	368	PHE	7.4
2	C	272	SER	7.0
1	A	367	GLY	6.4
2	C	273	PRO	5.7
2	C	276	GLU	4.9
1	A	260	ASP	4.6
1	B	151	VAL	4.5
1	A	366	THR	4.5
2	D	22	GLY	4.5
1	A	368	PHE	4.4
1	B	367	GLY	4.3
2	C	310	GLU	4.2
2	C	108	TYR	4.2
2	C	275	LYS	3.9
2	D	46	VAL	3.8
1	B	364	MET	3.7
1	B	366	THR	3.6
2	D	284	LEU	3.6
2	D	281	ASN	3.5
2	C	123	LEU	3.4

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Mol	Chain	Res	Type	RSRZ
2	C	271	ALA	3.3
2	D	23	ASP	3.2
2	C	104	LYS	3.2
2	C	122	ASP	3.2
2	C	270	ALA	3.2
2	C	141	LEU	3.1
2	C	297	LYS	3.1
1	A	364[A]	MET	2.7
2	D	245	ASP	2.7
1	B	150	GLU	2.6
2	D	27	ASN	2.6
2	C	175	ASN	2.6
2	C	274	ASN	2.5
2	D	153	LYS	2.5
2	C	146	LYS	2.4
2	C	266	ALA	2.4
2	C	306	LEU	2.4
2	C	269	ASN	2.3
2	D	227	ASN	2.3
2	C	309	TYR	2.3
2	C	112	VAL	2.3
2	C	107	ALA	2.3
2	C	244	TYR	2.2
1	A	365	ALA	2.2
2	C	171	PHE	2.2
1	B	259	ASP	2.2
2	C	209	ASP	2.2
2	C	295	VAL	2.2
2	C	352	ALA	2.2
2	D	25	GLY	2.1
1	A	261	GLU	2.1
1	A	332	HIS	2.1
2	D	275	ILE	2.1
2	C	226	MET	2.1
2	C	143	ALA	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)

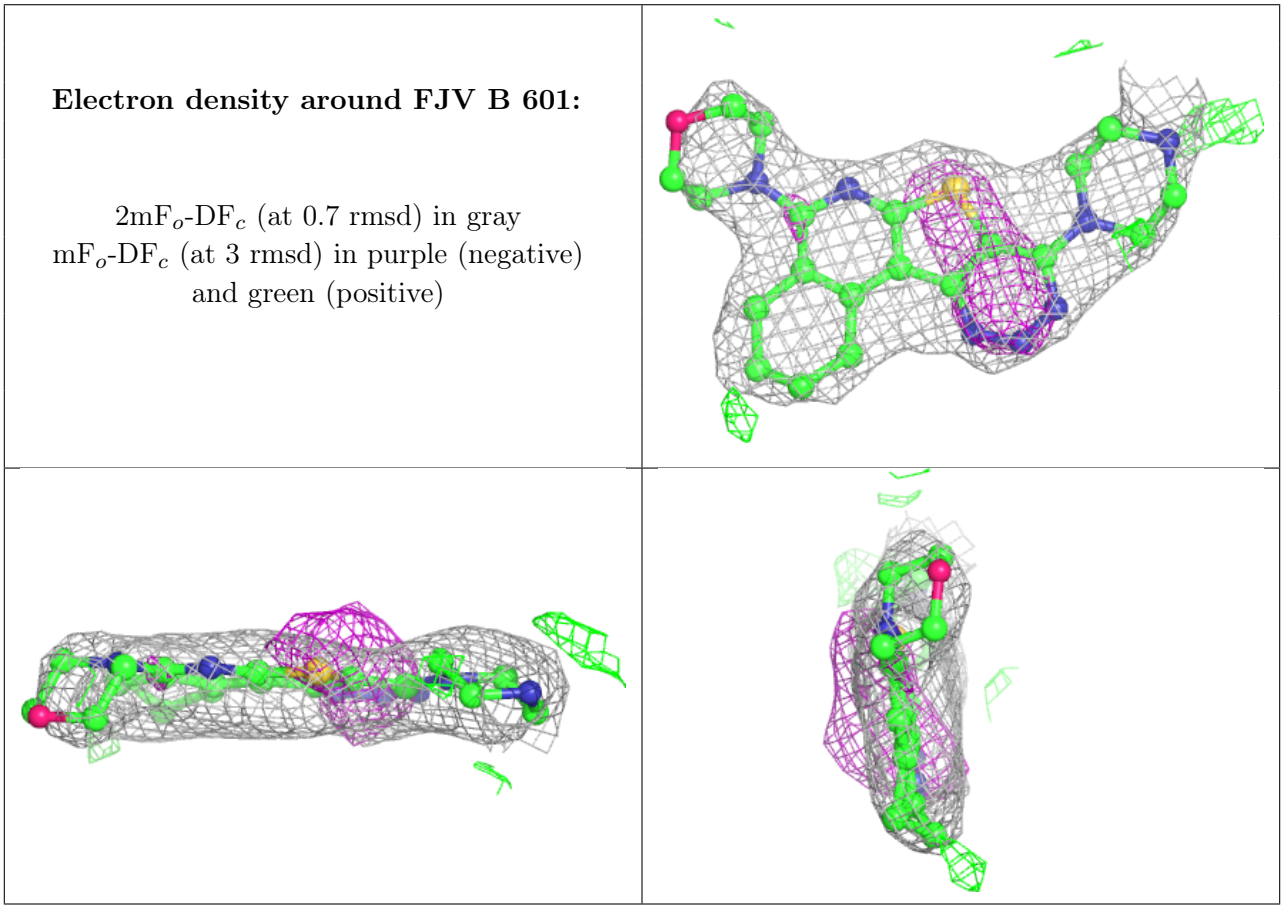
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' 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
3	FJV	B	601	29/29	0.89	0.22	59,71,89,103	0
3	FJV	A	601	29/29	0.92	0.23	44,57,71,85	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.

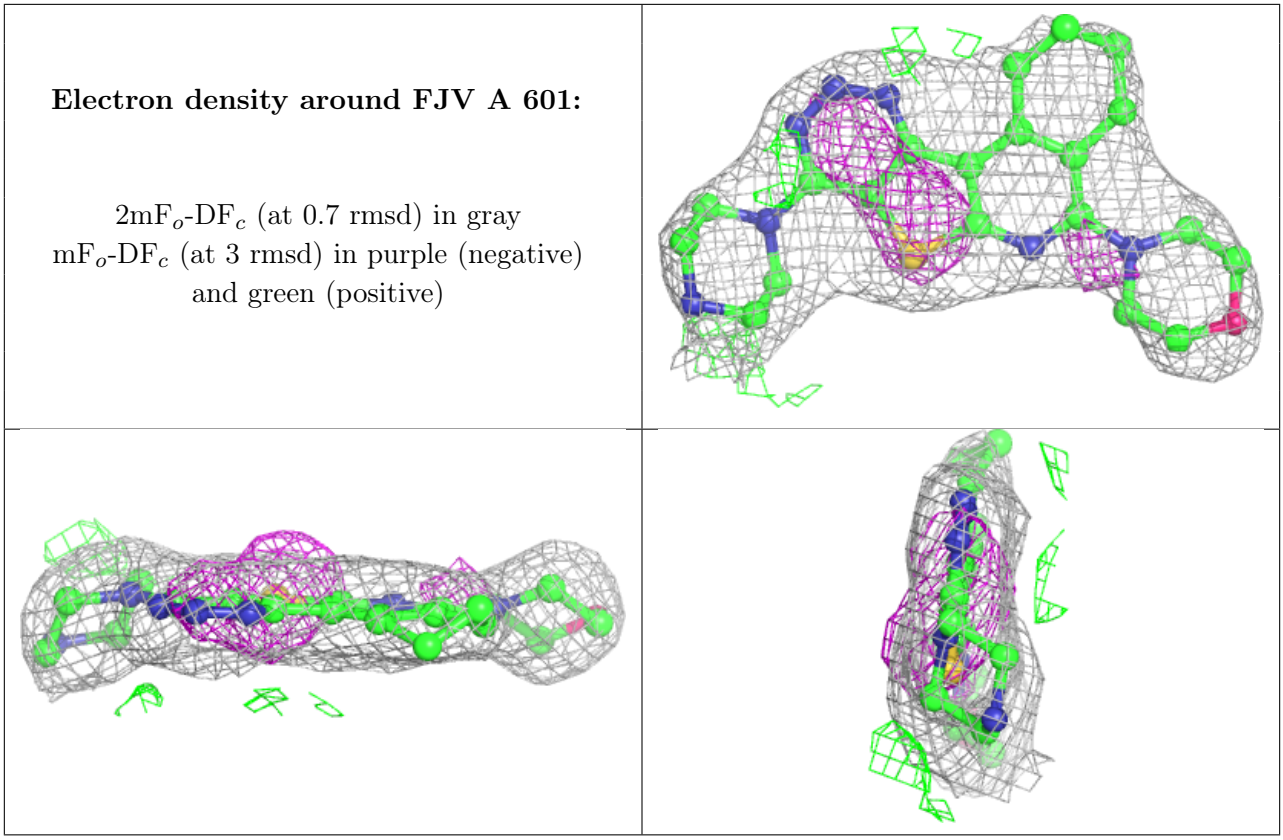
Electron density around FJV B 601:

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



Electron density around FJV A 601:

$2mF_o$-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.