



Full wwPDB X-ray Structure Validation Report ⓘ

May 23, 2020 – 08:03 pm BST

PDB ID : 6MRG
Title : FAAH bound to non covalent inhibitor
Authors : Saha, A.; Shih, A.; Mirzadegan, T.; Seierstad, M.
Deposited on : 2018-10-12
Resolution : 2.77 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 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	:	2.11
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)	:	2.11

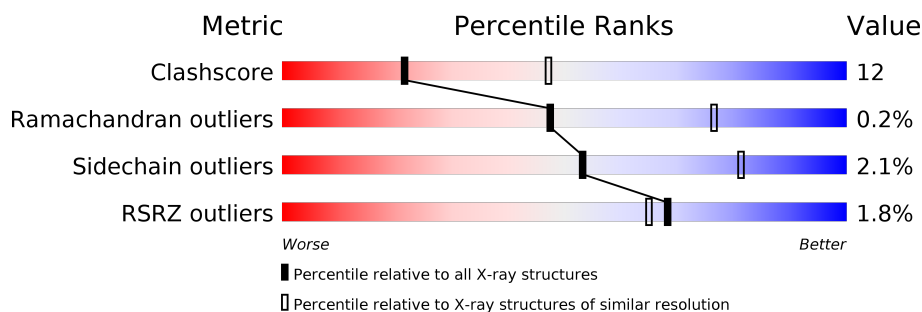
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.77 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))
Clashscore	141614	4575 (2.80-2.76)
Ramachandran outliers	138981	4487 (2.80-2.76)
Sidechain outliers	138945	4489 (2.80-2.76)
RSRZ outliers	127900	4027 (2.80-2.76)

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 on 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 $\leq 5\%$. 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	580	<div> <div>2%</div> <div>79%</div> <div>14%</div> <div>6%</div> </div>
1	B	580	<div> <div>%</div> <div>77%</div> <div>16%</div> <div>7%</div> </div>
1	C	580	<div> <div>2%</div> <div>79%</div> <div>14%</div> <div>7%</div> </div>
1	D	580	<div> <div>2%</div> <div>78%</div> <div>15%</div> <div>7%</div> </div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 16863 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 Fatty-acid amide hydrolase 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	543	Total	C	N	O	S	63	1	0
			4196	2677	716	773	30			
1	B	542	Total	C	N	O	S	70	1	0
			4189	2673	715	771	30			
1	C	542	Total	C	N	O	S	89	0	0
			4180	2668	713	769	30			
1	D	542	Total	C	N	O	S	72	0	0
			4180	2668	713	769	30			

There are 152 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	GLY	-	expression tag	UNP P97612
A	1	SER	-	expression tag	UNP P97612
A	2	GLY	-	expression tag	UNP P97612
A	3	MET	-	expression tag	UNP P97612
A	4	LYS	-	expression tag	UNP P97612
A	5	GLU	-	expression tag	UNP P97612
A	6	THR	-	expression tag	UNP P97612
A	7	ALA	-	expression tag	UNP P97612
A	8	ALA	-	expression tag	UNP P97612
A	9	ALA	-	expression tag	UNP P97612
A	10	LYS	-	expression tag	UNP P97612
A	11	PHE	-	expression tag	UNP P97612
A	12	GLU	-	expression tag	UNP P97612
A	13	ARG	-	expression tag	UNP P97612
A	14	GLN	-	expression tag	UNP P97612
A	15	HIS	-	expression tag	UNP P97612
A	16	MET	-	expression tag	UNP P97612
A	17	ASP	-	expression tag	UNP P97612
A	18	SER	-	expression tag	UNP P97612
A	19	PRO	-	expression tag	UNP P97612
A	20	ASP	-	expression tag	UNP P97612

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Chain	Residue	Modelled	Actual	Comment	Reference
A	21	LEU	-	expression tag	UNP P97612
A	22	GLY	-	expression tag	UNP P97612
A	23	THR	-	expression tag	UNP P97612
A	24	ASP	-	expression tag	UNP P97612
A	25	ASP	-	expression tag	UNP P97612
A	26	ASP	-	expression tag	UNP P97612
A	27	ASP	-	expression tag	UNP P97612
A	28	LYS	-	expression tag	UNP P97612
A	29	ALA	-	expression tag	UNP P97612
A	30	MET	-	expression tag	UNP P97612
A	31	GLU	-	expression tag	UNP P97612
A	192	PHE	LEU	conflict	UNP P97612
A	194	TYR	PHE	conflict	UNP P97612
A	377	THR	ALA	conflict	UNP P97612
A	435	ASN	SER	conflict	UNP P97612
A	491	VAL	ILE	conflict	UNP P97612
A	495	MET	VAL	conflict	UNP P97612
B	0	GLY	-	expression tag	UNP P97612
B	1	SER	-	expression tag	UNP P97612
B	2	GLY	-	expression tag	UNP P97612
B	3	MET	-	expression tag	UNP P97612
B	4	LYS	-	expression tag	UNP P97612
B	5	GLU	-	expression tag	UNP P97612
B	6	THR	-	expression tag	UNP P97612
B	7	ALA	-	expression tag	UNP P97612
B	8	ALA	-	expression tag	UNP P97612
B	9	ALA	-	expression tag	UNP P97612
B	10	LYS	-	expression tag	UNP P97612
B	11	PHE	-	expression tag	UNP P97612
B	12	GLU	-	expression tag	UNP P97612
B	13	ARG	-	expression tag	UNP P97612
B	14	GLN	-	expression tag	UNP P97612
B	15	HIS	-	expression tag	UNP P97612
B	16	MET	-	expression tag	UNP P97612
B	17	ASP	-	expression tag	UNP P97612
B	18	SER	-	expression tag	UNP P97612
B	19	PRO	-	expression tag	UNP P97612
B	20	ASP	-	expression tag	UNP P97612
B	21	LEU	-	expression tag	UNP P97612
B	22	GLY	-	expression tag	UNP P97612
B	23	THR	-	expression tag	UNP P97612
B	24	ASP	-	expression tag	UNP P97612

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Chain	Residue	Modelled	Actual	Comment	Reference
B	25	ASP	-	expression tag	UNP P97612
B	26	ASP	-	expression tag	UNP P97612
B	27	ASP	-	expression tag	UNP P97612
B	28	LYS	-	expression tag	UNP P97612
B	29	ALA	-	expression tag	UNP P97612
B	30	MET	-	expression tag	UNP P97612
B	31	GLU	-	expression tag	UNP P97612
B	192	PHE	LEU	conflict	UNP P97612
B	194	TYR	PHE	conflict	UNP P97612
B	377	THR	ALA	conflict	UNP P97612
B	435	ASN	SER	conflict	UNP P97612
B	491	VAL	ILE	conflict	UNP P97612
B	495	MET	VAL	conflict	UNP P97612
C	0	GLY	-	expression tag	UNP P97612
C	1	SER	-	expression tag	UNP P97612
C	2	GLY	-	expression tag	UNP P97612
C	3	MET	-	expression tag	UNP P97612
C	4	LYS	-	expression tag	UNP P97612
C	5	GLU	-	expression tag	UNP P97612
C	6	THR	-	expression tag	UNP P97612
C	7	ALA	-	expression tag	UNP P97612
C	8	ALA	-	expression tag	UNP P97612
C	9	ALA	-	expression tag	UNP P97612
C	10	LYS	-	expression tag	UNP P97612
C	11	PHE	-	expression tag	UNP P97612
C	12	GLU	-	expression tag	UNP P97612
C	13	ARG	-	expression tag	UNP P97612
C	14	GLN	-	expression tag	UNP P97612
C	15	HIS	-	expression tag	UNP P97612
C	16	MET	-	expression tag	UNP P97612
C	17	ASP	-	expression tag	UNP P97612
C	18	SER	-	expression tag	UNP P97612
C	19	PRO	-	expression tag	UNP P97612
C	20	ASP	-	expression tag	UNP P97612
C	21	LEU	-	expression tag	UNP P97612
C	22	GLY	-	expression tag	UNP P97612
C	23	THR	-	expression tag	UNP P97612
C	24	ASP	-	expression tag	UNP P97612
C	25	ASP	-	expression tag	UNP P97612
C	26	ASP	-	expression tag	UNP P97612
C	27	ASP	-	expression tag	UNP P97612
C	28	LYS	-	expression tag	UNP P97612

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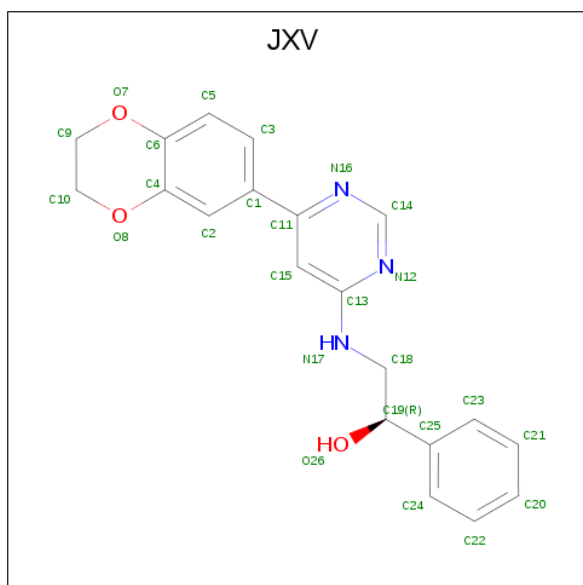
Chain	Residue	Modelled	Actual	Comment	Reference
C	29	ALA	-	expression tag	UNP P97612
C	30	MET	-	expression tag	UNP P97612
C	31	GLU	-	expression tag	UNP P97612
C	192	PHE	LEU	conflict	UNP P97612
C	194	TYR	PHE	conflict	UNP P97612
C	377	THR	ALA	conflict	UNP P97612
C	435	ASN	SER	conflict	UNP P97612
C	491	VAL	ILE	conflict	UNP P97612
C	495	MET	VAL	conflict	UNP P97612
D	0	GLY	-	expression tag	UNP P97612
D	1	SER	-	expression tag	UNP P97612
D	2	GLY	-	expression tag	UNP P97612
D	3	MET	-	expression tag	UNP P97612
D	4	LYS	-	expression tag	UNP P97612
D	5	GLU	-	expression tag	UNP P97612
D	6	THR	-	expression tag	UNP P97612
D	7	ALA	-	expression tag	UNP P97612
D	8	ALA	-	expression tag	UNP P97612
D	9	ALA	-	expression tag	UNP P97612
D	10	LYS	-	expression tag	UNP P97612
D	11	PHE	-	expression tag	UNP P97612
D	12	GLU	-	expression tag	UNP P97612
D	13	ARG	-	expression tag	UNP P97612
D	14	GLN	-	expression tag	UNP P97612
D	15	HIS	-	expression tag	UNP P97612
D	16	MET	-	expression tag	UNP P97612
D	17	ASP	-	expression tag	UNP P97612
D	18	SER	-	expression tag	UNP P97612
D	19	PRO	-	expression tag	UNP P97612
D	20	ASP	-	expression tag	UNP P97612
D	21	LEU	-	expression tag	UNP P97612
D	22	GLY	-	expression tag	UNP P97612
D	23	THR	-	expression tag	UNP P97612
D	24	ASP	-	expression tag	UNP P97612
D	25	ASP	-	expression tag	UNP P97612
D	26	ASP	-	expression tag	UNP P97612
D	27	ASP	-	expression tag	UNP P97612
D	28	LYS	-	expression tag	UNP P97612
D	29	ALA	-	expression tag	UNP P97612
D	30	MET	-	expression tag	UNP P97612
D	31	GLU	-	expression tag	UNP P97612
D	192	PHE	LEU	conflict	UNP P97612

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Chain	Residue	Modelled	Actual	Comment	Reference
D	194	TYR	PHE	conflict	UNP P97612
D	377	THR	ALA	conflict	UNP P97612
D	435	ASN	SER	conflict	UNP P97612
D	491	VAL	ILE	conflict	UNP P97612
D	495	MET	VAL	conflict	UNP P97612

- Molecule 2 is (1R)-2-{{[6-(2,3-dihydro-1,4-benzodioxin-6-yl)pyrimidin-4-yl]amino}-1-phenylethan-1-ol (three-letter code: JXV) (formula: C₂₀H₁₉N₃O₃).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			26	20	3	3		
2	B	1	Total	C	N	O	0	0
			26	20	3	3		
2	C	1	Total	C	N	O	0	0
			26	20	3	3		
2	D	1	Total	C	N	O	0	0
			26	20	3	3		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	2	Total	O	0	0
			2	2		
3	B	6	Total	O	0	0
			6	6		

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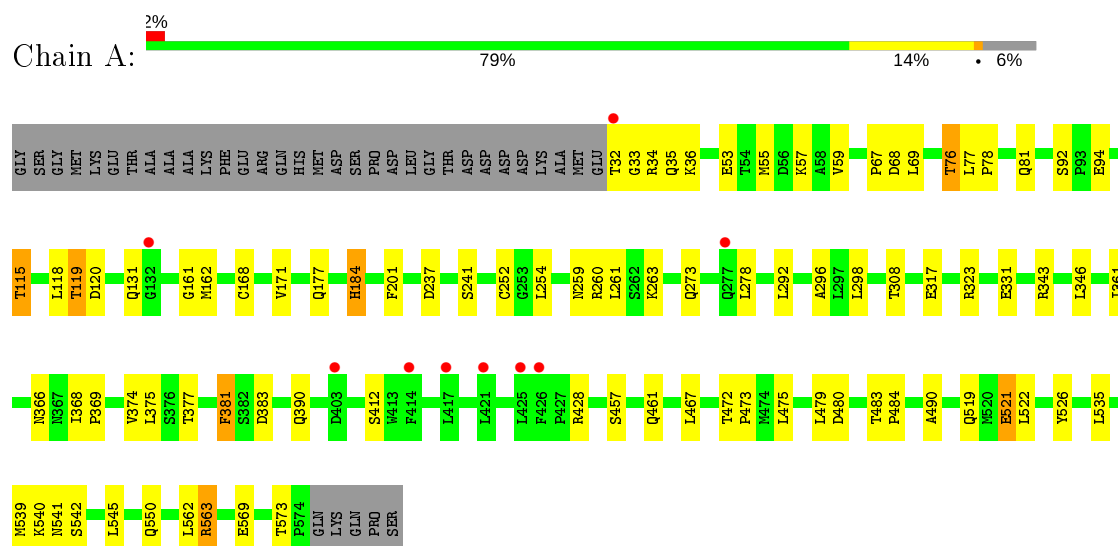
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	C	3	Total	O	0	0
			3	3		
3	D	3	Total	O	0	0
			3	3		

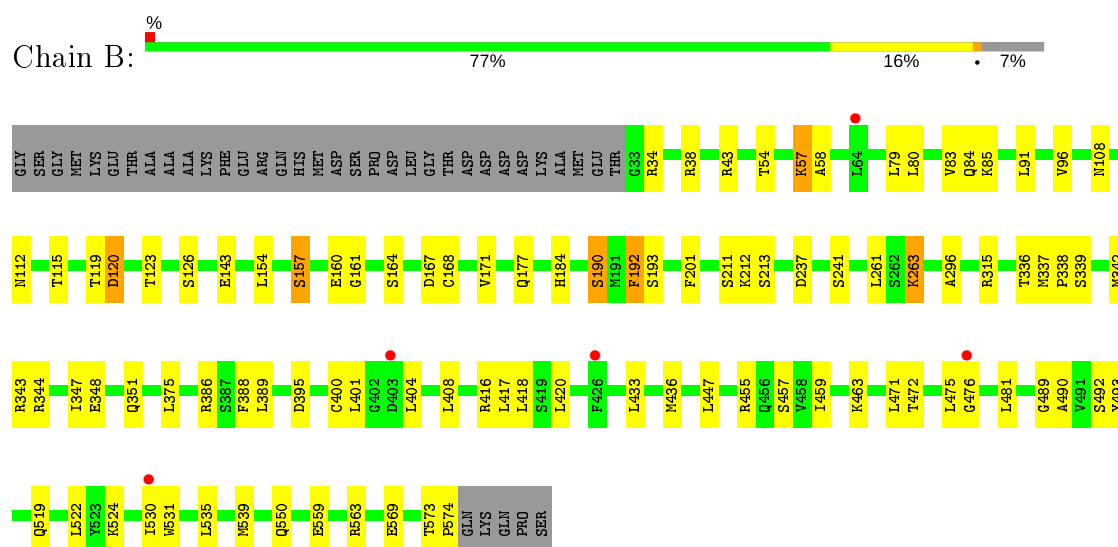
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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.

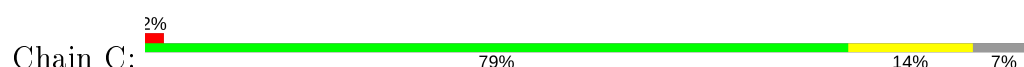
• Molecule 1: Fatty-acid amide hydrolase 1

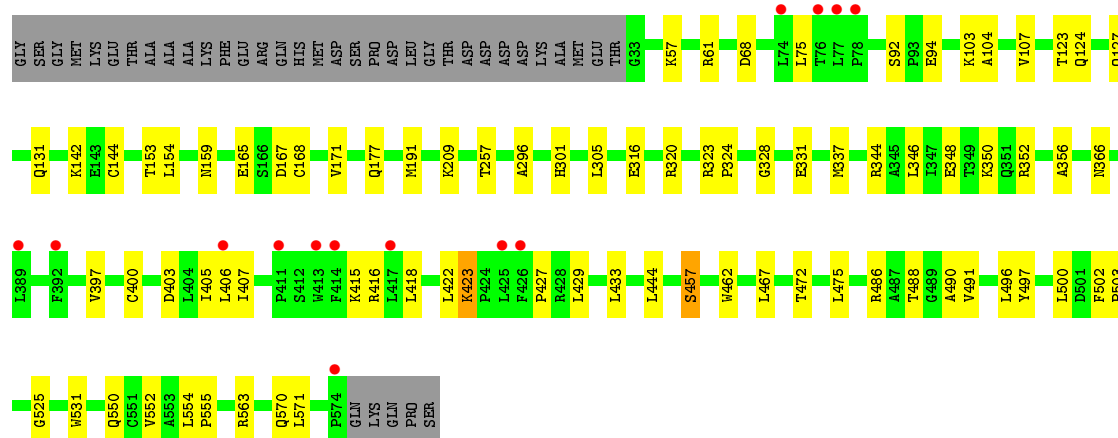


• Molecule 1: Fatty-acid amide hydrolase 1

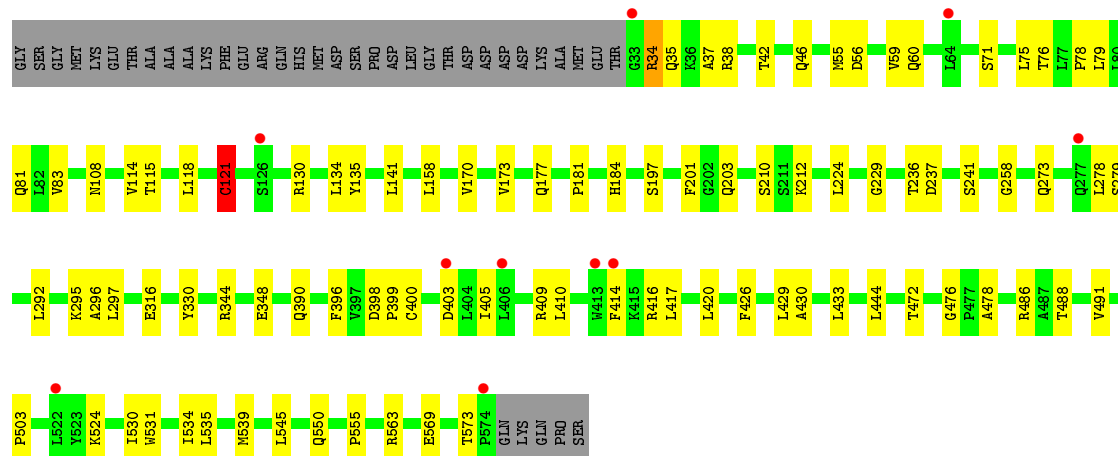
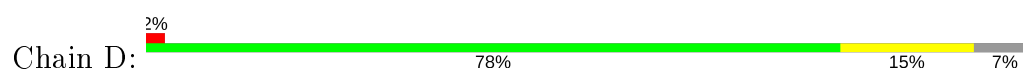


• Molecule 1: Fatty-acid amide hydrolase 1





• Molecule 1: Fatty-acid amide hydrolase 1



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	144.21Å 152.01Å 299.91Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.39 – 2.77 49.39 – 2.77	Depositor EDS
% Data completeness (in resolution range)	92.2 (49.39-2.77) 92.3 (49.39-2.77)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.27 (at 2.77Å)	Xtriage
Refinement program	PHENIX 1.13_2998	Depositor
R, R_{free}	0.195 , 0.240 0.192 , (Not available)	Depositor DCC
R_{free} test set	684 reflections (0.88%)	wwPDB-VP
Wilson B-factor (Å ²)	62.6	Xtriage
Anisotropy	0.723	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 37.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	16863	wwPDB-VP
Average B, all atoms (Å ²)	63.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.04% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ 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: JXV

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	0.58	1/4290 (0.0%)	0.70	1/5821 (0.0%)
1	B	0.57	0/4283	0.69	0/5811
1	C	0.56	0/4274	0.67	0/5799
1	D	0.57	0/4274	0.68	0/5799
All	All	0.57	1/17121 (0.0%)	0.69	1/23230 (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	A	0	5
1	C	0	1
1	D	0	2
All	All	0	8

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	252	CYS	CB-SG	-5.31	1.73	1.81

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	428	ARG	NE-CZ-NH1	5.54	123.07	120.30

There are no chirality outliers.

All (8) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	115	THR	Mainchain
1	A	131	GLN	Mainchain
1	A	390	GLN	Mainchain
1	A	521	GLU	Mainchain
1	A	76	THR	Mainchain
1	C	131	GLN	Mainchain
1	D	121	CYS	Mainchain
1	D	390	GLN	Mainchain

5.2 Too-close contacts

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	4196	0	4247	89	0
1	B	4189	0	4240	99	0
1	C	4180	0	4233	101	0
1	D	4180	0	4233	108	0
2	A	26	0	0	0	0
2	B	26	0	0	0	0
2	C	26	0	0	0	0
2	D	26	0	0	1	0
3	A	2	0	0	0	0
3	B	6	0	0	0	0
3	C	3	0	0	1	0
3	D	3	0	0	0	0
All	All	16863	0	16953	394	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 12.

All (394) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:130:ARG:HD3	1:D:135:TYR:CZ	1.52	1.41
1:D:130:ARG:HD3	1:D:135:TYR:CE2	1.64	1.32
1:D:429:LEU:O	1:D:433:LEU:HD12	1.36	1.24
1:D:130:ARG:HG2	1:D:135:TYR:CE1	1.71	1.24

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:366:ASN:HD22	1:A:461:GLN:NE2	1.42	1.16
1:C:418:LEU:HD11	1:C:433:LEU:CD1	1.78	1.12
1:B:337:MET:CE	1:B:343:ARG:HH11	1.62	1.11
1:C:142:LYS:HE2	1:C:191:MET:HE2	1.29	1.11
1:B:337:MET:HE3	1:B:343:ARG:HH11	1.08	1.10
1:A:519:GLN:OE1	1:A:522:LEU:HD12	1.51	1.09
1:A:535:LEU:HD21	1:A:539:MET:HE2	1.34	1.08
1:D:429:LEU:C	1:D:433:LEU:HD12	1.75	1.07
1:A:259:ASN:O	1:A:259:ASN:OD1	1.73	1.04
1:D:130:ARG:CD	1:D:135:TYR:CZ	2.40	1.04
1:A:535:LEU:HD21	1:A:539:MET:CE	1.87	1.04
1:C:418:LEU:HD11	1:C:433:LEU:HD11	1.40	1.01
1:C:344:ARG:O	1:C:348:GLU:HG3	1.60	1.01
1:D:130:ARG:CG	1:D:135:TYR:CE1	2.46	0.99
1:C:337:MET:CE	1:C:525:GLY:H	1.77	0.97
1:C:123:THR:O	1:C:127:GLN:HG2	1.64	0.96
1:C:301:HIS:O	1:C:305:LEU:HD13	1.67	0.94
1:A:535:LEU:CD2	1:A:539:MET:CE	2.46	0.94
1:B:212:LYS:C	1:B:481:LEU:HD11	1.89	0.93
1:C:418:LEU:CD1	1:C:433:LEU:CD1	2.46	0.93
1:A:535:LEU:CD2	1:A:539:MET:HE2	1.98	0.93
1:D:78:PRO:HD2	1:D:81:GLN:HG3	1.49	0.93
1:B:192:PHE:CD2	1:B:388:PHE:CE1	2.56	0.92
1:A:168:CYS:SG	1:A:171:VAL:HG23	2.10	0.92
1:C:488:THR:O	1:C:491:VAL:HG22	1.72	0.90
1:D:530:ILE:HD12	1:D:530:ILE:H	1.36	0.90
1:C:142:LYS:HE2	1:C:191:MET:CE	2.02	0.90
1:B:337:MET:HE3	1:B:343:ARG:NH1	1.88	0.89
1:D:429:LEU:O	1:D:433:LEU:CD1	2.19	0.89
1:D:278:LEU:HD12	1:D:279:SER:H	1.36	0.88
1:C:429:LEU:HD22	1:C:531:TRP:CZ2	2.09	0.88
1:A:254:LEU:HD22	1:A:562:LEU:HD21	1.55	0.88
1:A:366:ASN:HD22	1:A:461:GLN:HE21	0.92	0.88
1:B:404:LEU:O	1:B:408:LEU:HG	1.74	0.88
1:A:366:ASN:ND2	1:A:461:GLN:HE21	1.71	0.87
1:C:124:GLN:HA	1:C:127:GLN:CG	2.05	0.86
1:B:212:LYS:O	1:B:481:LEU:HD11	1.75	0.86
1:A:35:GLN:CD	1:A:35:GLN:H	1.78	0.86
1:A:366:ASN:H	1:A:461:GLN:HE22	1.19	0.86
1:B:212:LYS:C	1:B:481:LEU:CD1	2.45	0.85
1:D:130:ARG:CD	1:D:135:TYR:CE2	2.55	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:480:ASP:HB2	1:A:483:THR:HG21	1.59	0.84
1:B:337:MET:CE	1:B:343:ARG:NH1	2.40	0.84
1:C:418:LEU:CD1	1:C:433:LEU:HD11	2.06	0.84
1:B:115:THR:OG1	1:B:201:PHE:CE1	2.32	0.83
1:D:344:ARG:O	1:D:348:GLU:HG3	1.77	0.83
1:B:471:LEU:HD12	1:B:472:THR:H	1.40	0.83
1:C:496:LEU:HD23	1:C:497:TYR:CE1	2.14	0.83
1:D:130:ARG:HD3	1:D:135:TYR:CE1	2.15	0.82
1:A:78:PRO:HD2	1:A:81:GLN:HG3	1.60	0.82
1:D:417:LEU:HA	1:D:420:LEU:CD1	2.08	0.82
1:D:410:LEU:HD22	1:D:414:PHE:CD2	2.16	0.81
1:B:315:ARG:N	1:B:559:GLU:OE1	2.14	0.81
1:C:337:MET:HE2	1:C:525:GLY:H	1.45	0.81
1:B:347:ILE:O	1:B:351:GLN:HG3	1.81	0.81
1:D:34:ARG:HG3	1:D:37:ALA:HB3	1.63	0.80
1:D:130:ARG:CD	1:D:135:TYR:CE1	2.66	0.79
1:A:331:GLU:OE1	1:A:343:ARG:NH2	2.17	0.78
1:B:336:THR:OG1	1:B:493:TYR:CE2	2.38	0.77
1:D:224:LEU:HD11	1:D:229:GLY:O	1.84	0.77
1:D:236:THR:HB	1:D:278:LEU:HD11	1.64	0.77
1:D:535:LEU:O	1:D:539:MET:HG3	1.85	0.77
1:C:502:PHE:CE2	1:C:554:LEU:HD23	2.19	0.77
1:B:115:THR:OG1	1:B:201:PHE:CD1	2.37	0.77
1:C:144:CYS:SG	1:C:191:MET:HE1	2.26	0.76
1:C:144:CYS:SG	1:C:191:MET:CE	2.74	0.76
1:D:278:LEU:HD12	1:D:279:SER:N	2.01	0.76
1:C:415:LYS:HA	1:C:433:LEU:HD21	1.68	0.74
1:A:32:THR:O	1:A:35:GLN:NE2	2.19	0.74
1:C:429:LEU:HD22	1:C:531:TRP:CE2	2.23	0.74
1:B:91:LEU:HD23	1:B:96:VAL:CG2	2.18	0.74
1:D:115:THR:HG22	1:D:201:PHE:CG	2.21	0.74
1:C:301:HIS:O	1:C:305:LEU:CD1	2.34	0.74
1:A:366:ASN:ND2	1:A:461:GLN:NE2	2.28	0.74
1:D:398:ASP:OD2	1:D:399:PRO:N	2.21	0.73
1:A:542:SER:HB3	1:A:545:LEU:HD12	1.70	0.73
1:B:192:PHE:HD2	1:B:388:PHE:HE1	1.37	0.73
1:D:417:LEU:HA	1:D:420:LEU:HD12	1.71	0.73
1:D:130:ARG:HG2	1:D:135:TYR:CD1	2.24	0.72
1:C:167:ASP:HB3	1:C:171:VAL:CG2	2.20	0.72
1:C:144:CYS:HB3	1:C:191:MET:HE3	1.72	0.72
1:B:339:SER:OG	1:B:342:MET:HG3	1.89	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:91:LEU:HD23	1:B:96:VAL:HG23	1.73	0.71
1:D:212:LYS:HG3	1:D:545:LEU:HD11	1.73	0.71
1:C:337:MET:CE	1:C:525:GLY:N	2.52	0.71
1:C:418:LEU:HD11	1:C:433:LEU:HD12	1.72	0.70
1:D:71:SER:O	1:D:75:LEU:HD12	1.91	0.70
1:C:168:CYS:SG	1:C:171:VAL:HG13	2.30	0.70
1:D:295:LYS:NZ	1:D:316:GLU:OE2	2.25	0.69
1:C:429:LEU:CD2	1:C:531:TRP:CE2	2.76	0.69
1:D:78:PRO:CD	1:D:81:GLN:HG3	2.20	0.69
1:C:415:LYS:O	1:C:433:LEU:HD22	1.93	0.69
1:B:115:THR:OG1	1:B:201:PHE:CZ	2.45	0.69
1:C:486:ARG:NH1	3:C:701:HOH:O	2.26	0.69
1:D:212:LYS:HE3	1:D:478:ALA:O	1.93	0.68
1:B:192:PHE:CD2	1:B:388:PHE:HE1	2.08	0.68
1:D:292:LEU:HD23	1:D:292:LEU:C	2.13	0.68
1:B:123:THR:O	1:B:126:SER:OG	2.10	0.68
1:C:167:ASP:HB3	1:C:171:VAL:HG23	1.76	0.67
1:D:38:ARG:O	1:D:42:THR:HG23	1.91	0.67
1:A:535:LEU:CD2	1:A:539:MET:HE3	2.23	0.67
1:B:168:CYS:SG	1:B:171:VAL:HG12	2.34	0.67
1:B:211:SER:O	1:B:481:LEU:HD13	1.93	0.67
1:D:130:ARG:HD3	1:D:135:TYR:CD2	2.29	0.67
1:A:519:GLN:OE1	1:A:522:LEU:CD1	2.37	0.66
1:B:79:LEU:HD11	1:B:83:VAL:CG1	2.25	0.66
1:A:521:GLU:OE1	1:A:540:LYS:NZ	2.28	0.66
1:B:79:LEU:CD1	1:B:83:VAL:CG1	2.74	0.66
1:B:471:LEU:HD12	1:B:472:THR:N	2.10	0.66
1:C:429:LEU:CD2	1:C:531:TRP:CZ2	2.79	0.66
1:A:261:LEU:CD2	1:A:298:LEU:HD21	2.26	0.65
1:C:337:MET:HE1	1:C:525:GLY:N	2.12	0.65
1:C:415:LYS:CA	1:C:433:LEU:HD21	2.24	0.65
1:A:119:THR:OG1	1:A:120:ASP:OD1	2.13	0.65
1:D:34:ARG:HD2	1:D:396:PHE:CE1	2.32	0.65
1:B:237:ASP:HA	1:B:241:SER:HB2	1.79	0.65
1:C:142:LYS:HD3	1:C:144:CYS:SG	2.37	0.65
1:C:415:LYS:O	1:C:433:LEU:CD2	2.44	0.65
1:B:190:SER:HG	1:B:388:PHE:HE1	1.44	0.64
1:D:569:GLU:O	1:D:573:THR:HG23	1.98	0.64
1:B:34:ARG:O	1:B:38:ARG:HG3	1.97	0.64
1:D:134:LEU:HD21	1:D:292:LEU:CD2	2.28	0.64
1:B:80:LEU:O	1:B:83:VAL:HG22	1.97	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:34:ARG:HD2	1:D:396:PHE:CD1	2.32	0.64
1:C:433:LEU:O	1:C:433:LEU:HD23	1.97	0.64
1:B:79:LEU:HD12	1:B:83:VAL:HG13	1.79	0.64
1:D:417:LEU:CA	1:D:420:LEU:HD12	2.27	0.64
1:B:535:LEU:HD12	1:B:539:MET:HG3	1.78	0.63
1:A:490:ALA:HB2	1:A:535:LEU:HD12	1.79	0.63
1:A:78:PRO:CD	1:A:81:GLN:HG3	2.27	0.63
1:A:161:GLY:O	1:A:162:MET:HE3	1.97	0.63
1:D:76:THR:CG2	1:D:76:THR:O	2.47	0.63
1:B:213:SER:N	1:B:481:LEU:CD1	2.62	0.63
1:A:483:THR:OG1	1:A:484:PRO:HD3	1.99	0.62
1:A:260:ARG:O	1:A:261:LEU:HD23	1.99	0.62
1:B:192:PHE:HD2	1:B:388:PHE:CE1	2.08	0.62
1:B:336:THR:HG21	1:B:490:ALA:HA	1.79	0.62
1:C:472:THR:HG21	1:C:550:GLN:HE21	1.64	0.62
1:B:337:MET:HE1	1:B:343:ARG:NH1	2.14	0.62
1:D:79:LEU:O	1:D:83:VAL:HG13	2.00	0.62
1:A:33:GLY:HA2	1:A:35:GLN:OE1	1.99	0.62
1:B:342:MET:SD	1:B:475:LEU:HA	2.40	0.62
1:B:418:LEU:HD12	1:B:418:LEU:O	2.00	0.62
1:A:254:LEU:HD22	1:A:562:LEU:CD2	2.28	0.61
1:A:161:GLY:O	1:A:162:MET:CE	2.48	0.61
1:C:144:CYS:SG	1:C:191:MET:HE3	2.39	0.61
1:B:344:ARG:O	1:B:348:GLU:HG3	2.01	0.61
1:D:405:ILE:O	1:D:409:ARG:HG3	2.00	0.61
1:D:416:ARG:O	1:D:420:LEU:HD12	2.00	0.61
1:D:78:PRO:HD2	1:D:81:GLN:CG	2.27	0.60
1:B:315:ARG:HB2	1:B:559:GLU:OE1	2.02	0.60
1:C:554:LEU:HB3	1:C:555:PRO:HD2	1.83	0.60
1:D:170:VAL:O	1:D:173:VAL:HG22	2.00	0.60
1:D:433:LEU:HG	2:D:601:JXV:C20	2.32	0.60
1:B:167:ASP:HB3	1:B:171:VAL:HG13	1.83	0.60
1:C:429:LEU:HD21	1:C:531:TRP:CD2	2.37	0.60
1:B:315:ARG:HD3	1:B:559:GLU:OE1	2.01	0.60
1:C:416:ARG:HG3	1:C:416:ARG:HH11	1.67	0.60
1:C:337:MET:HE1	1:C:525:GLY:H	1.59	0.59
1:D:76:THR:O	1:D:76:THR:HG22	2.01	0.59
1:C:124:GLN:CA	1:C:127:GLN:CG	2.80	0.59
1:A:519:GLN:HE22	1:A:522:LEU:HD11	1.67	0.59
1:B:143:GLU:OE1	1:B:154:LEU:N	2.27	0.58
1:B:416:ARG:O	1:B:420:LEU:HG	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:530:ILE:HG22	1:D:534:ILE:HD12	1.83	0.58
1:A:115:THR:HB	1:A:184:HIS:O	2.03	0.58
1:A:77:LEU:HD22	1:A:81:GLN:CB	2.33	0.58
1:B:459:ILE:O	1:B:463:LYS:HG3	2.02	0.58
1:C:144:CYS:CB	1:C:191:MET:HE3	2.33	0.58
1:D:429:LEU:HD23	1:D:531:TRP:CZ2	2.39	0.58
1:C:497:TYR:CE2	1:C:552:VAL:HG21	2.39	0.57
1:D:472:THR:HB	1:D:550:GLN:HB3	1.85	0.57
1:A:366:ASN:N	1:A:461:GLN:HE22	1.96	0.57
1:A:535:LEU:HD23	1:A:535:LEU:O	2.04	0.57
1:B:338:PRO:HA	1:B:342:MET:HE3	1.86	0.57
1:B:79:LEU:CD1	1:B:83:VAL:HG13	2.34	0.57
1:B:177:GLN:HG2	1:B:296:ALA:HB1	1.87	0.57
1:D:224:LEU:HD11	1:D:229:GLY:C	2.25	0.57
1:D:398:ASP:OD2	1:D:398:ASP:C	2.42	0.57
1:D:410:LEU:HD22	1:D:414:PHE:CE2	2.39	0.57
1:D:59:VAL:HG13	1:D:60:GLN:NE2	2.20	0.57
1:C:337:MET:HE2	1:C:525:GLY:N	2.17	0.56
1:A:55:MET:O	1:A:59:VAL:HG23	2.06	0.56
1:B:213:SER:N	1:B:481:LEU:HD12	2.20	0.56
1:B:342:MET:SD	1:B:476:GLY:N	2.78	0.56
1:C:497:TYR:CD1	1:C:500:LEU:HD12	2.40	0.56
1:C:144:CYS:HB3	1:C:191:MET:CE	2.36	0.56
1:D:130:ARG:CG	1:D:135:TYR:CZ	2.83	0.56
1:C:416:ARG:NH1	1:C:416:ARG:HG3	2.21	0.56
1:A:479:LEU:HB3	1:A:483:THR:OG1	2.05	0.55
1:C:344:ARG:O	1:C:348:GLU:CG	2.45	0.55
1:B:315:ARG:CB	1:B:559:GLU:OE1	2.54	0.55
1:A:535:LEU:HD23	1:A:535:LEU:C	2.28	0.54
1:B:190:SER:OG	1:B:388:PHE:HE1	1.91	0.54
1:B:43:ARG:NH1	1:B:160:GLU:OE1	2.40	0.54
1:D:398:ASP:OD2	1:D:399:PRO:CD	2.56	0.54
1:D:130:ARG:CD	1:D:135:TYR:CD2	2.90	0.54
1:D:530:ILE:HD12	1:D:530:ILE:N	2.17	0.54
1:B:193:SER:HB2	1:B:401:LEU:HD23	1.90	0.54
1:C:475:LEU:HD22	1:C:490:ALA:HB1	1.90	0.54
1:A:366:ASN:H	1:A:461:GLN:NE2	1.96	0.54
1:D:170:VAL:HA	1:D:173:VAL:HG22	1.89	0.53
1:B:337:MET:HE1	1:B:343:ARG:HH11	1.56	0.53
1:C:328:GLY:N	1:C:467:LEU:HD22	2.23	0.53
1:C:328:GLY:CA	1:C:467:LEU:HD22	2.39	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:130:ARG:HA	1:D:135:TYR:CD1	2.44	0.53
1:A:535:LEU:HD23	1:A:539:MET:HG3	1.90	0.52
1:A:308:THR:HG22	1:B:455:ARG:CZ	2.39	0.52
1:A:53:GLU:O	1:A:57:LYS:HG3	2.08	0.52
1:D:34:ARG:HG3	1:D:34:ARG:O	2.09	0.52
1:A:535:LEU:CD2	1:A:539:MET:HG3	2.40	0.52
1:C:323:ARG:HG2	1:C:324:PRO:O	2.10	0.52
1:B:336:THR:CG2	1:B:490:ALA:HA	2.38	0.52
1:A:168:CYS:SG	1:A:171:VAL:CG2	2.92	0.52
1:D:430:ALA:N	1:D:433:LEU:HD12	2.24	0.52
1:C:497:TYR:HD1	1:C:500:LEU:HD12	1.75	0.52
1:B:79:LEU:O	1:B:83:VAL:HG13	2.10	0.52
1:A:472:THR:HG22	1:A:473:PRO:O	2.10	0.52
1:A:472:THR:HG21	1:A:550:GLN:HE21	1.74	0.52
1:B:519:GLN:O	1:B:522:LEU:HB2	2.10	0.52
1:C:433:LEU:HD23	1:C:433:LEU:C	2.30	0.51
1:A:35:GLN:NE2	1:A:35:GLN:H	2.08	0.51
1:B:84:GLN:NE2	1:B:85:LYS:NZ	2.58	0.51
1:C:403:ASP:HB2	1:C:407:ILE:HD11	1.92	0.51
1:D:118:LEU:O	1:D:121:CYS:SG	2.68	0.51
1:B:336:THR:CG2	1:B:492:SER:OG	2.59	0.51
1:C:316:GLU:OE1	1:C:320:ARG:NE	2.44	0.51
1:A:77:LEU:HD22	1:A:81:GLN:HB3	1.92	0.51
1:B:54:THR:O	1:B:57:LYS:HG3	2.11	0.51
1:D:134:LEU:HD21	1:D:292:LEU:HD22	1.92	0.51
1:D:56:ASP:O	1:D:60:GLN:NE2	2.43	0.51
1:A:475:LEU:HD11	1:A:535:LEU:HD11	1.93	0.51
1:C:92:SER:HB2	1:C:94:GLU:OE2	2.11	0.51
1:D:398:ASP:OD2	1:D:399:PRO:HD2	2.11	0.51
1:A:535:LEU:HD21	1:A:539:MET:SD	2.51	0.50
1:B:375:LEU:HA	1:B:447:LEU:HD11	1.93	0.50
1:A:92:SER:HB2	1:A:94:GLU:OE1	2.12	0.50
1:B:573:THR:HB	1:B:574:PRO:HD2	1.91	0.50
1:C:124:GLN:HA	1:C:127:GLN:HG3	1.89	0.50
1:B:535:LEU:HD11	1:B:539:MET:SD	2.52	0.50
1:B:57:LYS:HD2	1:B:58:ALA:N	2.26	0.50
1:D:78:PRO:CG	1:D:81:GLN:HG3	2.41	0.50
1:C:75:LEU:HD13	1:C:103:LYS:HD3	1.94	0.50
1:C:423:LYS:HE2	1:C:427:PRO:HA	1.94	0.50
1:C:462:TRP:CD1	1:C:554:LEU:HD11	2.46	0.50
1:D:212:LYS:HG3	1:D:545:LEU:CD1	2.40	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:344:ARG:HG2	1:D:348:GLU:OE1	2.12	0.50
1:B:389:LEU:HD21	1:B:408:LEU:HB2	1.93	0.50
1:C:403:ASP:O	1:C:407:ILE:HG13	2.12	0.50
1:B:339:SER:OG	1:B:342:MET:CG	2.59	0.49
1:D:330:TYR:CZ	1:D:472:THR:HG23	2.47	0.49
1:A:34:ARG:H	1:A:35:GLN:HE22	1.58	0.49
1:B:115:THR:OG1	1:B:201:PHE:CE2	2.63	0.49
1:C:124:GLN:CA	1:C:127:GLN:HG2	2.43	0.49
1:C:177:GLN:HG2	1:C:296:ALA:HB1	1.94	0.49
1:C:403:ASP:O	1:C:407:ILE:CD1	2.61	0.49
1:B:261:LEU:O	1:B:263:LYS:HE2	2.13	0.49
1:A:34:ARG:H	1:A:35:GLN:NE2	2.11	0.49
1:A:526:TYR:HE1	1:C:165:GLU:HG2	1.78	0.49
1:A:490:ALA:HB2	1:A:535:LEU:CD1	2.43	0.48
1:A:521:GLU:CD	1:A:540:LYS:NZ	2.67	0.48
1:D:237:ASP:HA	1:D:241:SER:HB2	1.94	0.48
1:B:84:GLN:HE22	1:B:85:LYS:HZ2	1.61	0.48
1:D:78:PRO:O	1:D:81:GLN:HB2	2.13	0.48
1:B:336:THR:HG23	1:B:492:SER:OG	2.13	0.48
1:C:570:GLN:OE1	1:C:571:LEU:CD2	2.61	0.48
1:B:57:LYS:HD2	1:B:57:LYS:C	2.34	0.48
1:B:408:LEU:HD21	1:B:436:MET:HE3	1.95	0.48
1:C:429:LEU:CD2	1:C:531:TRP:CH2	2.96	0.48
1:C:496:LEU:HD23	1:C:497:TYR:CZ	2.47	0.48
1:D:55:MET:O	1:D:59:VAL:HG12	2.13	0.48
1:A:34:ARG:N	1:A:35:GLN:NE2	2.62	0.48
1:B:417:LEU:HA	1:B:420:LEU:HD12	1.94	0.48
1:B:79:LEU:HD12	1:B:83:VAL:CG1	2.41	0.48
1:D:530:ILE:H	1:D:530:ILE:CD1	2.12	0.48
1:A:317:GLU:CD	1:A:317:GLU:H	2.16	0.47
1:A:361:ILE:HD12	1:A:467:LEU:CD2	2.44	0.47
1:B:569:GLU:O	1:B:573:THR:HG23	2.14	0.47
1:C:429:LEU:CD2	1:C:531:TRP:CD2	2.96	0.47
1:A:260:ARG:C	1:A:261:LEU:HD23	2.34	0.47
1:C:418:LEU:CG	1:C:433:LEU:HD11	2.44	0.47
1:C:444:LEU:O	1:C:444:LEU:HD12	2.14	0.47
1:D:115:THR:OG1	1:D:184:HIS:O	2.28	0.47
1:C:257:THR:OG1	1:C:503:PRO:HD3	2.14	0.47
1:B:472:THR:HG21	1:B:550:GLN:HE21	1.80	0.47
1:D:398:ASP:OD2	1:D:400:CYS:N	2.42	0.46
1:D:488:THR:O	1:D:491:VAL:HG22	2.14	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:34:ARG:HD2	1:D:396:PHE:CZ	2.49	0.46
1:D:56:ASP:OD1	1:D:60:GLN:NE2	2.48	0.46
1:D:476:GLY:O	1:D:539:MET:CE	2.63	0.46
1:C:168:CYS:O	1:C:171:VAL:HG22	2.15	0.46
1:A:331:GLU:HB3	1:A:346:LEU:HD12	1.97	0.46
1:C:123:THR:C	1:C:127:GLN:HG2	2.32	0.46
1:C:418:LEU:CD1	1:C:433:LEU:HD13	2.38	0.46
1:D:429:LEU:HD23	1:D:531:TRP:CE2	2.50	0.46
1:B:418:LEU:HG	1:B:433:LEU:HD21	1.97	0.46
1:D:34:ARG:CG	1:D:34:ARG:O	2.63	0.46
1:A:263:LYS:HD3	1:A:278:LEU:O	2.16	0.46
1:A:77:LEU:HD22	1:A:81:GLN:HB2	1.98	0.46
1:D:130:ARG:CD	1:D:135:TYR:CD1	2.98	0.46
1:D:444:LEU:HD12	1:D:444:LEU:O	2.16	0.46
1:A:78:PRO:HD2	1:A:81:GLN:CG	2.40	0.46
1:C:104:ALA:O	1:C:107:VAL:HG22	2.15	0.46
1:D:177:GLN:HG2	1:D:296:ALA:HB1	1.96	0.46
1:D:426:PHE:HB3	1:D:429:LEU:HD12	1.98	0.46
1:B:160:GLU:HG2	1:B:161:GLY:H	1.81	0.46
1:C:406:LEU:HD23	1:C:406:LEU:O	2.16	0.46
1:C:418:LEU:HD12	1:C:422:LEU:HD12	1.96	0.46
1:D:292:LEU:CD2	1:D:292:LEU:C	2.82	0.45
1:B:54:THR:HA	1:B:57:LYS:HG3	1.97	0.45
1:D:292:LEU:HD23	1:D:292:LEU:O	2.16	0.45
1:A:34:ARG:N	1:A:35:GLN:HE22	2.14	0.45
1:C:57:LYS:O	1:C:61:ARG:HG3	2.16	0.45
1:C:403:ASP:O	1:C:407:ILE:HD12	2.17	0.45
1:A:33:GLY:CA	1:A:35:GLN:HE22	2.30	0.45
1:B:213:SER:N	1:B:481:LEU:HD11	2.28	0.45
1:C:570:GLN:OE1	1:C:571:LEU:HD21	2.17	0.45
1:D:34:ARG:HD2	1:D:396:PHE:CG	2.52	0.45
1:B:84:GLN:HE22	1:B:85:LYS:NZ	2.14	0.45
1:C:124:GLN:O	1:C:127:GLN:HG3	2.16	0.45
1:D:141:LEU:HD11	1:D:181:PRO:HB3	1.99	0.45
1:D:197:SER:OG	1:D:203:GLN:HB2	2.17	0.45
1:A:115:THR:HG23	1:A:201:PHE:CZ	2.52	0.44
1:C:496:LEU:CD2	1:C:497:TYR:CE1	2.93	0.44
1:D:429:LEU:O	1:D:433:LEU:CG	2.64	0.44
1:C:331:GLU:HG2	1:C:346:LEU:HD12	2.00	0.44
1:D:410:LEU:HD22	1:D:414:PHE:HD2	1.77	0.44
1:A:76:THR:O	1:A:76:THR:HG22	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:79:LEU:HD11	1:B:83:VAL:HG12	1.95	0.44
1:A:81:GLN:HG2	1:A:81:GLN:H	1.60	0.44
1:C:418:LEU:HD12	1:C:433:LEU:HD13	2.00	0.44
1:A:308:THR:HG22	1:B:455:ARG:NH2	2.33	0.44
1:B:530:ILE:HG23	1:B:531:TRP:CD1	2.53	0.44
1:C:423:LYS:HE2	1:C:427:PRO:CA	2.46	0.44
1:D:115:THR:HG22	1:D:201:PHE:CD1	2.52	0.44
1:A:33:GLY:CA	1:A:35:GLN:OE1	2.65	0.43
1:D:429:LEU:C	1:D:433:LEU:CD1	2.65	0.43
1:A:261:LEU:HD21	1:A:298:LEU:HD21	2.00	0.43
1:C:570:GLN:CD	1:C:571:LEU:HD23	2.39	0.43
1:D:59:VAL:HG13	1:D:60:GLN:HE22	1.83	0.43
1:B:389:LEU:HD11	1:B:408:LEU:HB3	2.00	0.43
1:D:158:LEU:N	1:D:158:LEU:HD23	2.33	0.43
1:D:403:ASP:OD1	1:D:486:ARG:NH2	2.51	0.43
1:B:192:PHE:CE2	1:B:388:PHE:CD1	3.06	0.43
1:D:134:LEU:CD2	1:D:292:LEU:HD21	2.48	0.43
1:B:108:ASN:OD1	1:B:112:ASN:HA	2.18	0.43
1:D:38:ARG:HG2	1:D:396:PHE:CZ	2.54	0.43
1:C:153:THR:HA	1:C:159:ASN:HB2	2.00	0.43
1:C:154:LEU:HD22	1:C:191:MET:SD	2.58	0.43
1:B:190:SER:OG	1:B:190:SER:O	2.37	0.43
1:C:366:ASN:ND2	1:C:457:SER:OG	2.49	0.43
1:A:177:GLN:HG2	1:A:296:ALA:HB1	2.00	0.43
1:B:119:THR:O	1:B:120:ASP:CB	2.67	0.42
1:D:173:VAL:HG23	1:D:297:LEU:HD23	2.01	0.42
1:A:368:ILE:N	1:A:369:PRO:CD	2.82	0.42
1:A:472:THR:CG2	1:A:550:GLN:HE21	2.32	0.42
1:C:144:CYS:CB	1:C:191:MET:CE	2.96	0.42
1:C:554:LEU:HB3	1:C:555:PRO:CD	2.48	0.42
1:C:356:ALA:HB2	1:C:571:LEU:CD1	2.49	0.42
1:D:130:ARG:CG	1:D:135:TYR:CD1	2.94	0.42
1:D:503:PRO:HD3	1:D:555:PRO:HA	2.01	0.42
1:C:415:LYS:O	1:C:433:LEU:HD21	2.19	0.42
1:A:261:LEU:HD23	1:A:298:LEU:HD21	2.01	0.42
1:A:323:ARG:O	1:A:563:ARG:NH1	2.52	0.42
1:C:433:LEU:CD2	1:C:433:LEU:C	2.88	0.42
1:A:374:VAL:HG12	1:A:375:LEU:HD23	2.01	0.42
1:D:212:LYS:HD2	1:D:212:LYS:HA	1.81	0.42
1:A:569:GLU:O	1:A:573:THR:HG23	2.20	0.42
1:B:472:THR:CG2	1:B:550:GLN:HE21	2.33	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:254:LEU:CD2	1:A:562:LEU:HD21	2.37	0.42
1:B:336:THR:CG2	1:B:489:GLY:O	2.68	0.42
1:B:54:THR:HA	1:B:57:LYS:CG	2.50	0.42
1:B:43:ARG:HD2	1:B:160:GLU:OE2	2.19	0.41
1:B:157:SER:HB3	1:B:395:ASP:OD1	2.20	0.41
1:D:38:ARG:HG2	1:D:396:PHE:CE2	2.55	0.41
1:A:237:ASP:HA	1:A:241:SER:HB2	2.01	0.41
1:D:134:LEU:CD2	1:D:292:LEU:CD2	2.98	0.41
1:A:535:LEU:HD22	1:A:539:MET:HE2	1.93	0.41
1:C:502:PHE:CE2	1:C:554:LEU:CD2	2.97	0.41
1:B:192:PHE:CD2	1:B:388:PHE:CD1	3.06	0.41
1:C:406:LEU:C	1:C:406:LEU:HD23	2.41	0.41
1:D:416:ARG:O	1:D:420:LEU:CD1	2.67	0.41
1:A:118:LEU:O	1:A:120:ASP:N	2.54	0.41
1:D:108:ASN:ND2	1:D:114:VAL:H	2.19	0.41
1:A:361:ILE:HD12	1:A:467:LEU:HD23	2.02	0.41
1:A:292:LEU:HD12	1:A:292:LEU:O	2.21	0.40
1:A:33:GLY:HA2	1:A:35:GLN:NE2	2.37	0.40
1:A:377:THR:O	1:A:381:PHE:HD1	2.03	0.40
1:B:79:LEU:O	1:B:79:LEU:HD12	2.20	0.40
1:C:397:VAL:HG13	1:C:405:ILE:HG13	2.03	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	542/580 (93%)	518 (96%)	22 (4%)	2 (0%)	34	64
1	B	541/580 (93%)	516 (95%)	24 (4%)	1 (0%)	47	76
1	C	540/580 (93%)	518 (96%)	22 (4%)	0	100	100
1	D	540/580 (93%)	520 (96%)	19 (4%)	1 (0%)	47	76

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	2163/2320 (93%)	2072 (96%)	87 (4%)	4 (0%)	47 76

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	119	THR
1	B	120	ASP
1	D	258	GLY
1	A	67	PRO

5.3.2 Protein sidechains ⓘ

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	462/491 (94%)	451 (98%)	11 (2%)	49 78
1	B	461/491 (94%)	449 (97%)	12 (3%)	46 76
1	C	460/491 (94%)	452 (98%)	8 (2%)	60 85
1	D	460/491 (94%)	452 (98%)	8 (2%)	60 85
All	All	1843/1964 (94%)	1804 (98%)	39 (2%)	53 81

All (39) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	36	LYS
1	A	68	ASP
1	A	69	LEU
1	A	184	HIS
1	A	273	GLN
1	A	381	PHE
1	A	383	ASP
1	A	412	SER
1	A	457	SER
1	A	541	ASN
1	A	563	ARG

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Mol	Chain	Res	Type
1	B	57	LYS
1	B	157	SER
1	B	164	SER
1	B	184	HIS
1	B	190	SER
1	B	192	PHE
1	B	263	LYS
1	B	386	ARG
1	B	400	CYS
1	B	457	SER
1	B	524	LYS
1	B	563	ARG
1	C	68	ASP
1	C	209	LYS
1	C	350	LYS
1	C	352	ARG
1	C	400	CYS
1	C	423	LYS
1	C	457	SER
1	C	563	ARG
1	D	34	ARG
1	D	35	GLN
1	D	46	GLN
1	D	121	CYS
1	D	210	SER
1	D	273	GLN
1	D	524	LYS
1	D	563	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	461	GLN
1	A	541	ASN
1	B	84	GLN
1	B	390	GLN
1	D	46	GLN
1	D	60	GLN
1	D	84	GLN
1	D	87	GLN
1	D	108	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

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	JXV	A	601	-	29,29,29	1.68	5 (17%)	38,39,39	1.96	7 (18%)
2	JXV	C	601	-	29,29,29	1.68	4 (13%)	38,39,39	1.92	7 (18%)
2	JXV	B	601	-	29,29,29	1.81	5 (17%)	38,39,39	2.01	9 (23%)
2	JXV	D	601	-	29,29,29	1.77	5 (17%)	38,39,39	1.87	7 (18%)

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	JXV	A	601	-	-	0/13/20/20	0/4/4/4
2	JXV	C	601	-	-	0/13/20/20	0/4/4/4
2	JXV	B	601	-	-	0/13/20/20	0/4/4/4
2	JXV	D	601	-	-	0/13/20/20	0/4/4/4

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	601	JXV	C13-N17	6.46	1.45	1.36
2	D	601	JXV	C13-N17	6.03	1.45	1.36
2	A	601	JXV	C13-N17	6.02	1.45	1.36
2	C	601	JXV	C13-N17	5.58	1.44	1.36
2	D	601	JXV	O26-C19	-3.87	1.34	1.42
2	B	601	JXV	O26-C19	-3.80	1.34	1.42
2	C	601	JXV	O26-C19	-3.80	1.34	1.42
2	A	601	JXV	O26-C19	-3.76	1.34	1.42
2	D	601	JXV	O7-C6	2.95	1.40	1.37
2	C	601	JXV	O7-C6	2.72	1.40	1.37
2	B	601	JXV	O7-C6	2.39	1.40	1.37
2	A	601	JXV	C6-C4	-2.31	1.35	1.40
2	A	601	JXV	O7-C6	2.24	1.40	1.37
2	A	601	JXV	C14-N12	2.23	1.38	1.33
2	D	601	JXV	C14-N12	2.20	1.38	1.33
2	D	601	JXV	C6-C4	-2.19	1.36	1.40
2	B	601	JXV	C6-C4	-2.15	1.36	1.40
2	C	601	JXV	C6-C4	-2.08	1.36	1.40
2	B	601	JXV	C14-N12	2.05	1.37	1.33

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	601	JXV	N16-C14-N12	-6.14	119.00	128.60
2	A	601	JXV	N16-C14-N12	-6.06	119.12	128.60
2	C	601	JXV	N16-C14-N12	-6.01	119.20	128.60
2	D	601	JXV	N16-C14-N12	-5.88	119.41	128.60
2	A	601	JXV	C9-O7-C6	4.79	121.92	113.65
2	A	601	JXV	O8-C4-C6	-4.71	117.81	122.03
2	B	601	JXV	C9-O7-C6	4.63	121.64	113.65
2	C	601	JXV	C9-O7-C6	4.62	121.62	113.65
2	C	601	JXV	C14-N16-C11	4.56	121.92	115.74
2	D	601	JXV	C9-O7-C6	4.32	121.09	113.65
2	B	601	JXV	C14-N16-C11	4.30	121.57	115.74
2	D	601	JXV	C14-N16-C11	4.19	121.41	115.74
2	B	601	JXV	O8-C4-C6	-3.81	118.62	122.03
2	A	601	JXV	C14-N16-C11	3.71	120.76	115.74
2	B	601	JXV	C10-O8-C4	3.69	120.02	113.65
2	D	601	JXV	O8-C4-C6	-3.62	118.79	122.03
2	C	601	JXV	O8-C4-C6	-3.61	118.80	122.03
2	C	601	JXV	C10-O8-C4	2.92	118.69	113.65
2	D	601	JXV	C10-O8-C4	2.92	118.69	113.65

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	601	JXV	O26-C19-C18	2.88	116.32	108.58
2	A	601	JXV	C3-C1-C11	-2.75	116.94	121.28
2	B	601	JXV	O26-C19-C18	2.71	115.86	108.58
2	B	601	JXV	C3-C1-C11	-2.64	117.11	121.28
2	A	601	JXV	O8-C4-C2	2.50	120.89	117.05
2	C	601	JXV	C3-C1-C11	-2.38	117.53	121.28
2	A	601	JXV	N17-C13-N12	2.23	120.32	116.95
2	B	601	JXV	N17-C13-N12	2.23	120.31	116.95
2	B	601	JXV	O8-C4-C2	2.12	120.31	117.05
2	C	601	JXV	C15-C11-N16	-2.10	119.42	122.16
2	D	601	JXV	C15-C11-N16	-2.01	119.55	122.16

There are no chirality outliers.

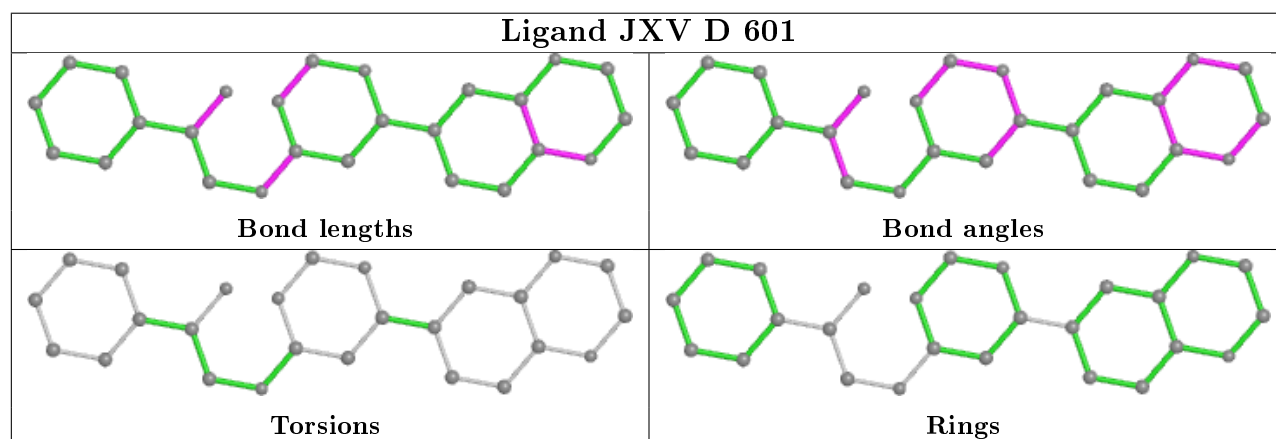
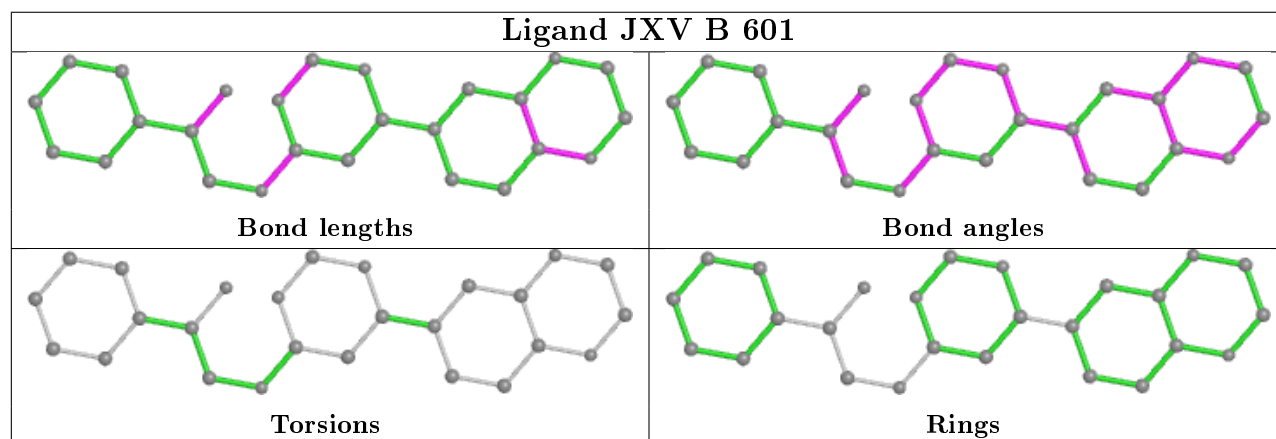
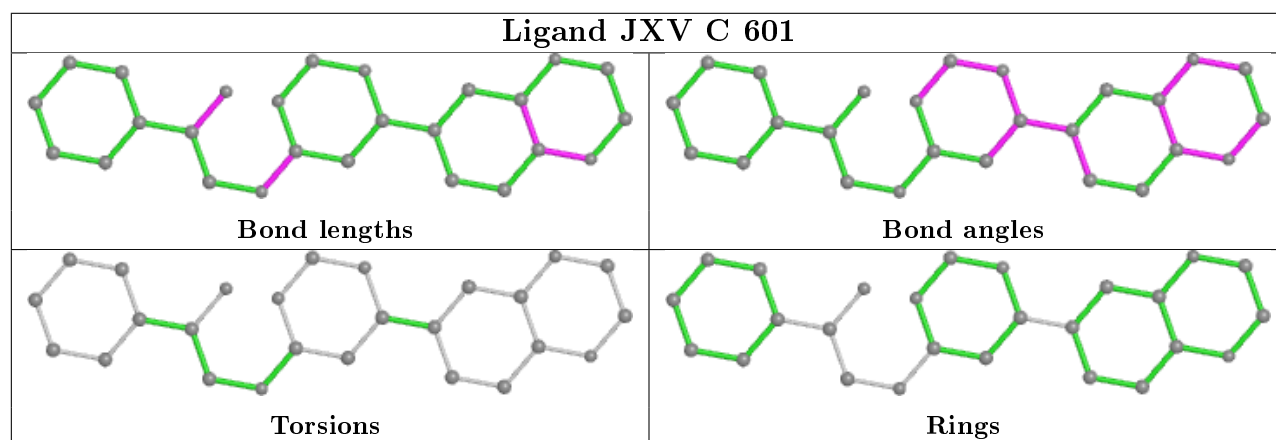
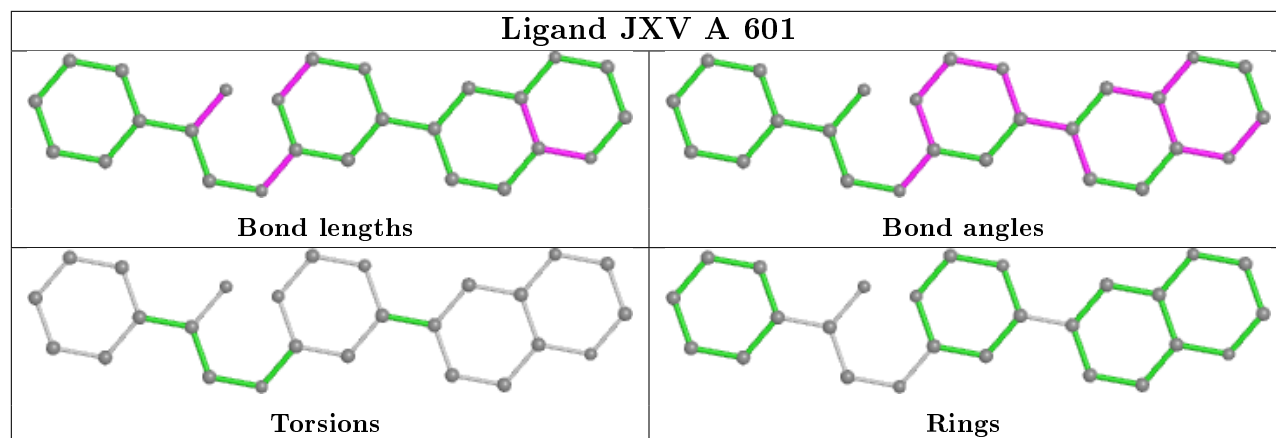
There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	601	JXV	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 than 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.



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, 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	543/580 (93%)	-0.03	9 (1%) 70 67	40, 57, 88, 118	19 (3%)
1	B	542/580 (93%)	-0.02	5 (0%) 84 82	38, 64, 85, 102	22 (4%)
1	C	542/580 (93%)	-0.15	14 (2%) 56 51	39, 59, 86, 101	26 (4%)
1	D	542/580 (93%)	-0.08	10 (1%) 68 65	40, 66, 93, 111	20 (3%)
All	All	2169/2320 (93%)	-0.07	38 (1%) 68 65	38, 62, 88, 118	87 (4%)

All (38) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	476	GLY	4.4
1	A	425	LEU	3.9
1	D	126	SER	3.5
1	C	417	LEU	3.3
1	D	406	LEU	3.3
1	C	406	LEU	3.1
1	D	413	TRP	3.0
1	C	74	LEU	3.0
1	D	522	LEU	2.8
1	A	277	GLN	2.8
1	C	574	PRO	2.8
1	A	421	LEU	2.8
1	A	32	THR	2.8
1	D	33	GLY	2.8
1	B	426	PHE	2.7
1	A	132	GLY	2.7
1	C	392	PHE	2.7
1	D	574	PRO	2.6
1	B	403	ASP	2.6
1	C	413	TRP	2.6
1	D	403	ASP	2.6

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Mol	Chain	Res	Type	RSRZ
1	C	414	PHE	2.5
1	A	417	LEU	2.5
1	A	403	ASP	2.5
1	D	414	PHE	2.4
1	C	78	PRO	2.4
1	C	425	LEU	2.3
1	A	426	PHE	2.3
1	C	77	LEU	2.3
1	C	76	THR	2.2
1	D	277	GLN	2.2
1	C	426	PHE	2.2
1	B	530	ILE	2.1
1	B	64	LEU	2.1
1	A	414	PHE	2.1
1	C	411	PRO	2.0
1	C	389	LEU	2.0
1	D	64	LEU	2.0

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

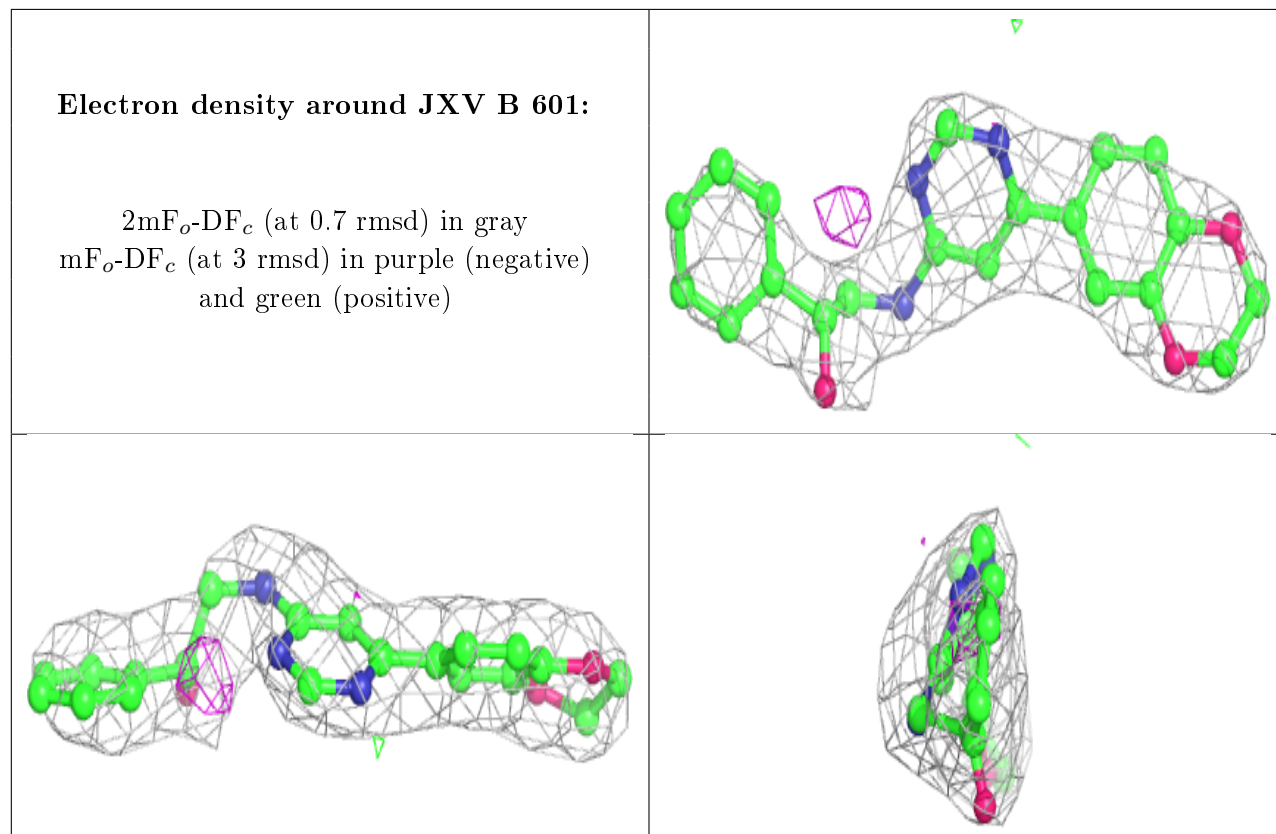
6.4 Ligands ⓘ

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	JXV	B	601	26/26	0.90	0.36	71,76,83,85	0
2	JXV	C	601	26/26	0.91	0.21	57,68,74,77	0
2	JXV	D	601	26/26	0.91	0.24	70,77,87,90	0
2	JXV	A	601	26/26	0.92	0.23	47,61,71,78	0

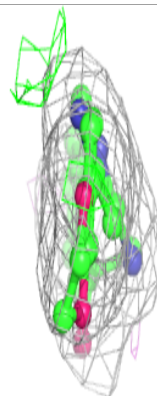
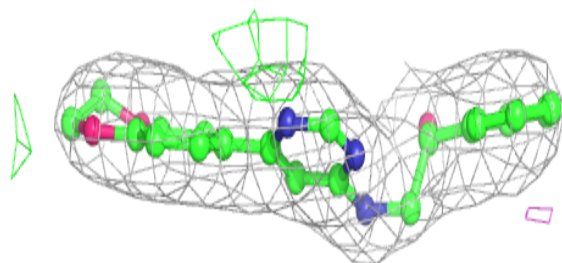
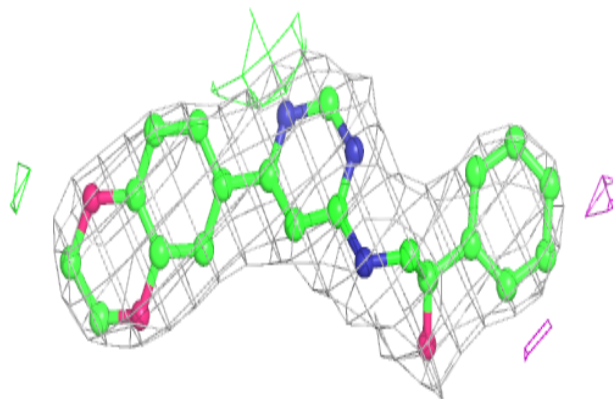
The following is a graphical depiction of the model fit to experimental electron density of all

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.

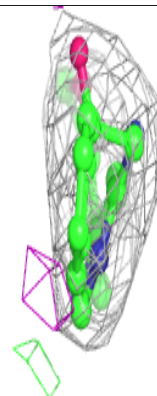
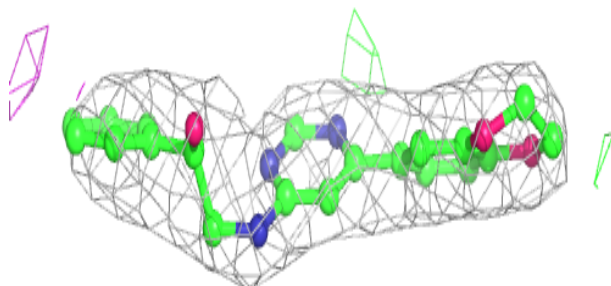
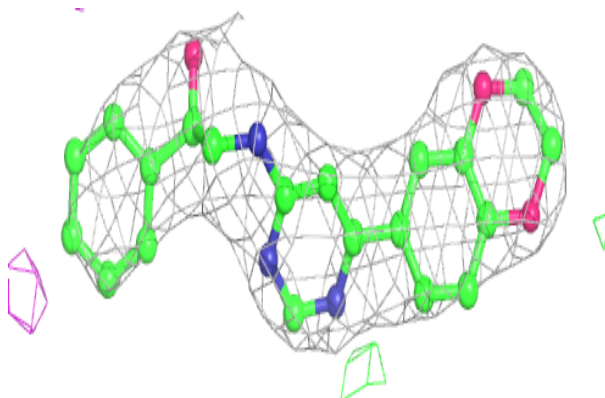


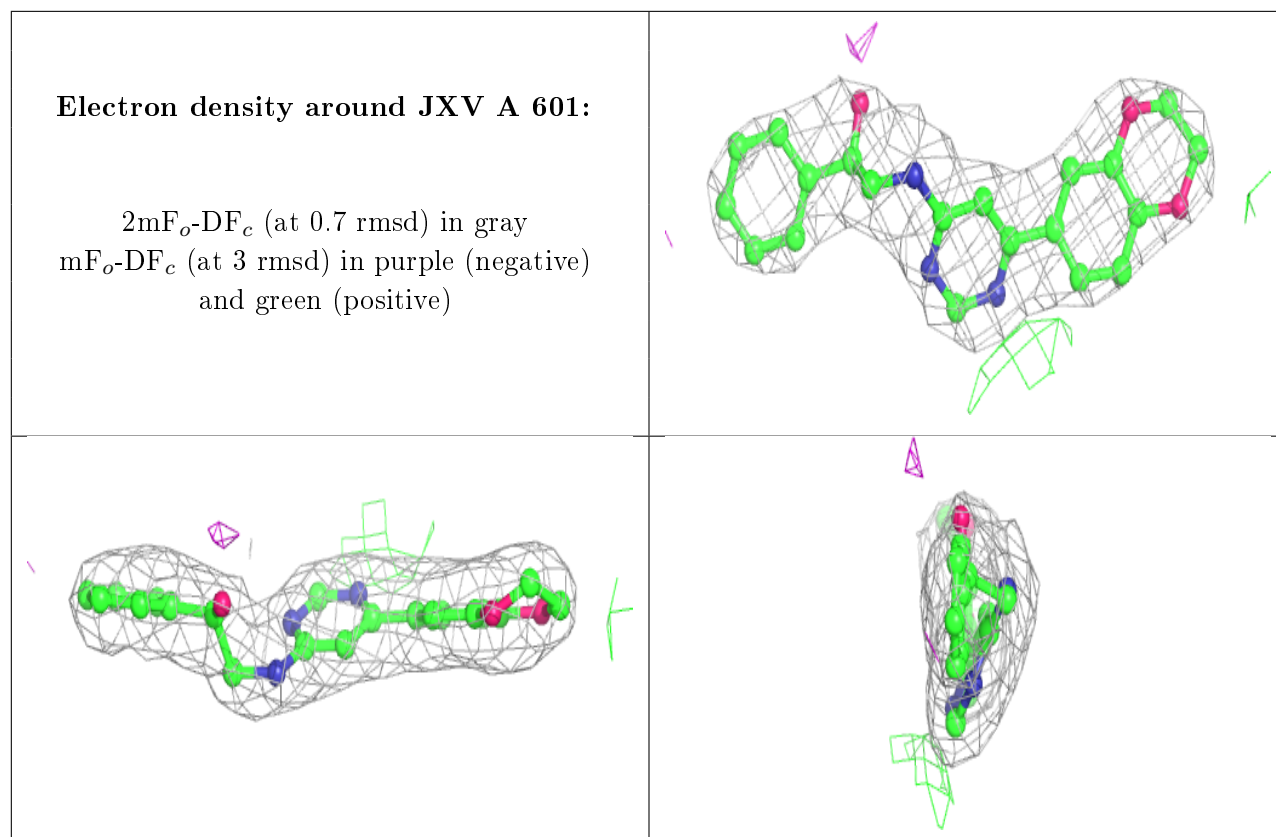
Electron density around JXV C 601:

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

**Electron density around JXV D 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.