Full wwPDB X-ray Structure Validation Report ⓘ

May 23, 2020 – 12:22 am BST

PDB ID	:	4JAO
Title	:	Crystal Structure of Mycobacterium tuberculosis PKS11 Reveals Intermediates in the Synthesis of Methyl-branched Alkylpyrones
Authors	:	Gokulan, K.; Sacchettini, J.C.; Mycobacterium Tuberculosis Structural Proteomics Project (XMTB)
Deposited on	:	2013-02-18
Resolution	:	2.05 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:

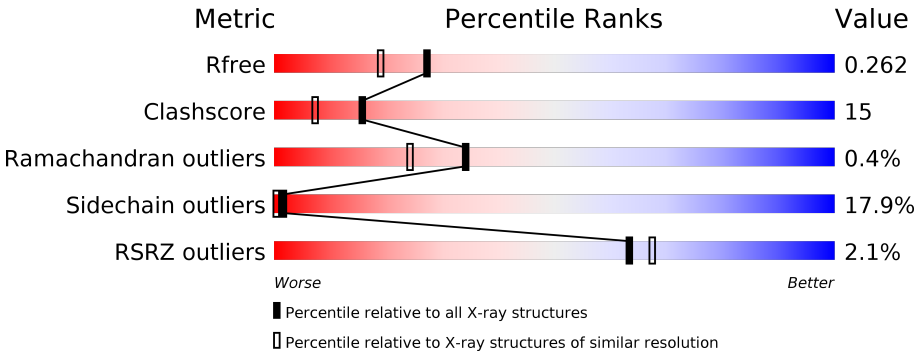
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.05 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	1692 (2.04-2.04)
Clashscore	141614	1773 (2.04-2.04)
Ramachandran outliers	138981	1752 (2.04-2.04)
Sidechain outliers	138945	1752 (2.04-2.04)
RSRZ outliers	127900	1672 (2.04-2.04)

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 <=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	353	3% 60% 31% 7%
1	B	353	% 65% 27% 7%
1	C	353	3% 66% 26% 8%
1	D	353	2% 64% 28% 8%

2 Entry composition

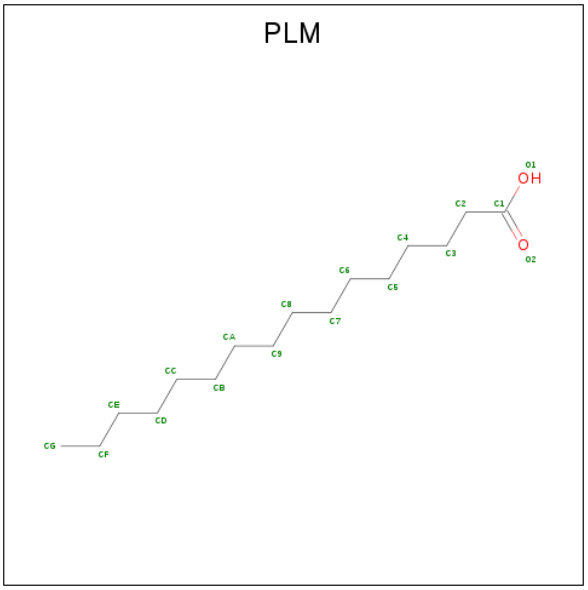
There are 4 unique types of molecules in this entry. The entry contains 11027 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Alpha-pyrone synthesis polyketide synthase-like Pks11.

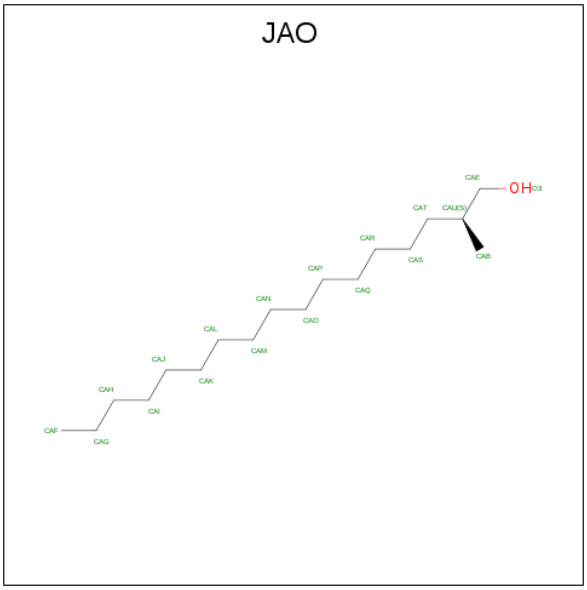
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	D	352	Total	C	N	O	S	0	0	0
			2642	1671	469	494	8			
1	C	352	Total	C	N	O	S	0	0	0
			2642	1671	469	494	8			
1	B	352	Total	C	N	O	S	0	0	0
			2642	1671	469	494	8			
1	A	352	Total	C	N	O	S	0	0	0
			2642	1671	469	494	8			

- Molecule 2 is PALMITIC ACID (three-letter code: PLM) (formula: $C_{16}H_{32}O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	D	1	Total	C	O	0	0
			18	16	2		
2	A	1	Total	C	O	0	0
			18	16	2		

- Molecule 3 is (2S)-2-methylheptadecan-1-ol (three-letter code: JAO) (formula: $C_{18}H_{38}O$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	C	1	Total C O 19 18 1	0	0
3	B	1	Total C O 19 18 1	0	0

- Molecule 4 is water.

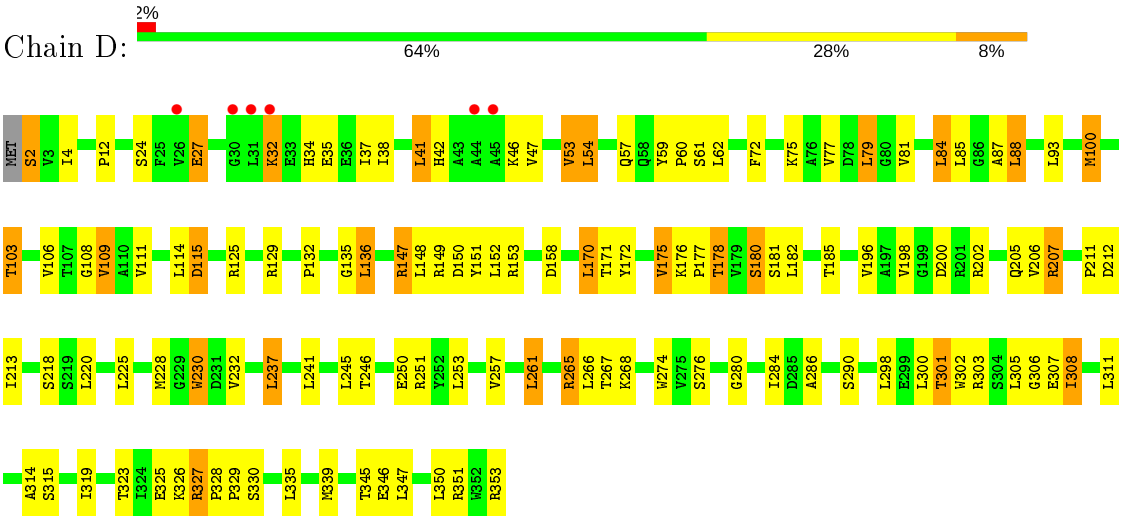
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	D	88	Total O 88 88	0	0
4	C	87	Total O 87 87	0	0
4	B	114	Total O 114 114	0	0
4	A	96	Total O 96 96	0	0

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.

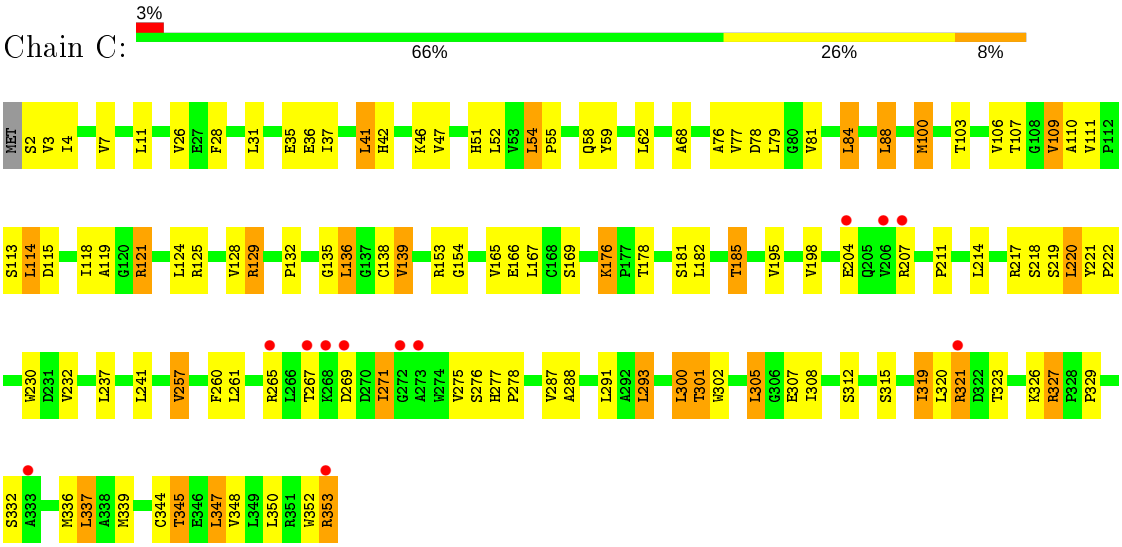
- Molecule 1: Alpha-pyrone synthesis polyketide synthase-like Pks11

Chain D:



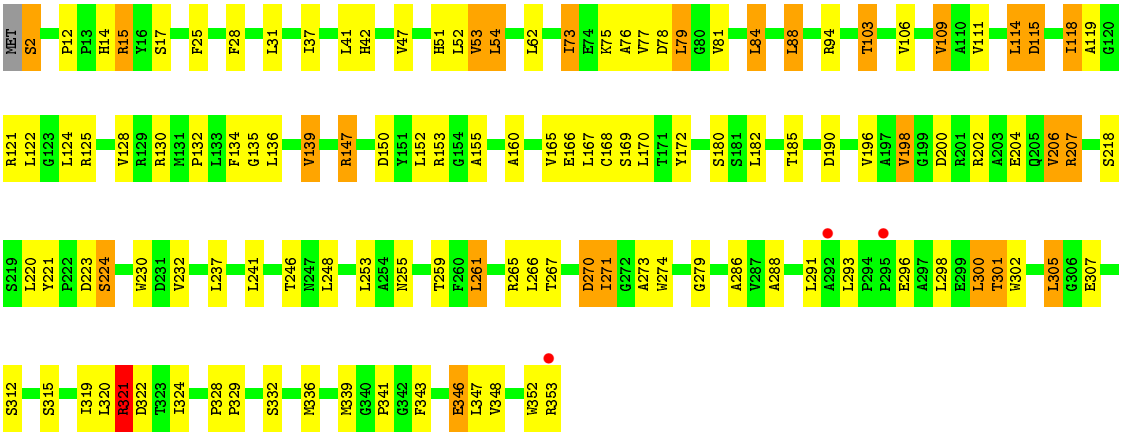
- Molecule 1: Alpha-pyrone synthesis polyketide synthase-like Pks11

Chain C:



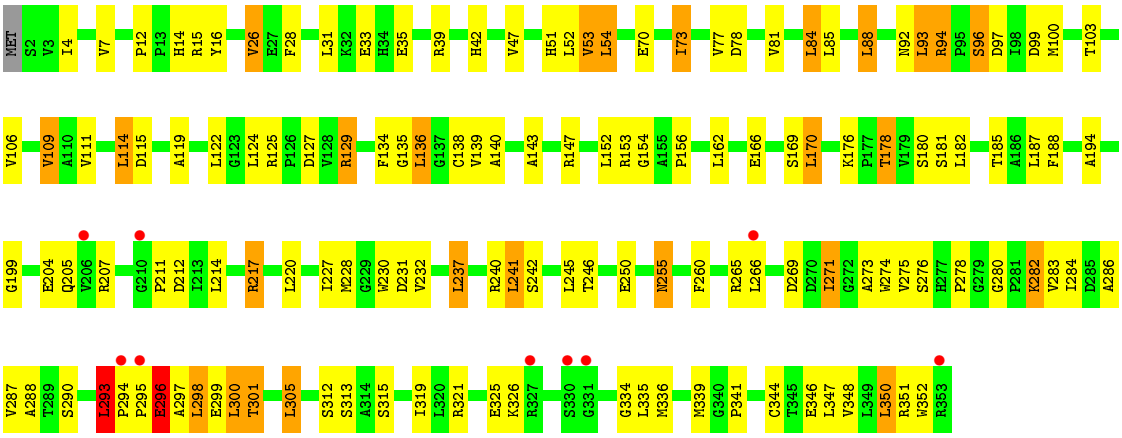
- Molecule 1: Alpha-pyrone synthesis polyketide synthase-like Pks11

Chain B:



- Molecule 1: Alpha-pyrone synthesis polyketide synthase-like Pks11

Chain A:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	71.12Å 48.43Å 189.69Å 90.00° 97.25° 90.00°	Depositor
Resolution (Å)	47.04 – 2.05 47.04 – 2.04	Depositor EDS
% Data completeness (in resolution range)	77.0 (47.04-2.05) 77.0 (47.04-2.04)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.20 (at 2.05Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.2_869)	Depositor
R, R_{free}	0.211 , 0.271 0.208 , 0.262	Depositor DCC
R_{free} test set	3158 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å^2)	35.7	Xtriage
Anisotropy	0.153	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 34.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	11027	wwPDB-VP
Average B, all atoms (Å^2)	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.81% 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: JAO, PLM

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	0.63	2/2695 (0.1%)	0.73	3/3671 (0.1%)
1	B	0.53	0/2695	0.69	1/3671 (0.0%)
1	C	0.55	2/2695 (0.1%)	0.63	1/3671 (0.0%)
1	D	0.50	0/2695	0.61	0/3671
All	All	0.55	4/10780 (0.0%)	0.66	5/14684 (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	1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	346	GLU	CD-OE1	-6.15	1.18	1.25
1	C	166	GLU	CD-OE2	-5.31	1.19	1.25
1	C	166	GLU	CD-OE1	-5.11	1.20	1.25
1	A	295	PRO	N-CD	5.09	1.54	1.47

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	321	ARG	NE-CZ-NH1	-6.58	117.01	120.30
1	A	293	LEU	C-N-CD	5.81	140.61	128.40
1	A	12	PRO	C-N-CD	5.74	140.44	128.40
1	A	294	PRO	C-N-CD	5.70	140.37	128.40
1	C	176	LYS	C-N-CD	5.16	139.23	128.40

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	296	GLU	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	2642	0	2675	93	0
1	B	2642	0	2674	86	0
1	C	2642	0	2673	76	1
1	D	2642	0	2675	83	1
2	A	18	0	31	5	0
2	D	18	0	31	4	0
3	B	19	0	35	4	0
3	C	19	0	35	2	0
4	A	96	0	0	3	0
4	B	114	0	0	2	0
4	C	87	0	0	4	0
4	D	88	0	0	2	0
All	All	11027	0	10829	315	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 15.

All (315) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:288:ALA:HA	1:A:293:LEU:HD11	1.37	1.07
1:C:353:ARG:HG3	1:C:353:ARG:HH11	1.35	0.89
1:D:135:GLY:HA2	1:C:111:VAL:HG22	1.57	0.85
1:D:136:LEU:HD13	1:C:132:PRO:HG2	1.59	0.84
1:B:84:LEU:HD12	1:B:118:ILE:HD11	1.61	0.83
1:C:28:PHE:HB2	1:C:31:LEU:HD12	1.60	0.81
1:A:288:ALA:HA	1:A:293:LEU:CD1	2.13	0.79
1:C:336:MET:HB2	1:C:348:VAL:HB	1.68	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:296:GLU:HB3	1:A:299:GLU:HB2	1.67	0.75
1:A:119:ALA:HA	1:A:124:LEU:HG	1.69	0.74
1:D:218:SER:OG	1:D:346:GLU:OE2	2.04	0.74
1:B:135:GLY:HA2	1:A:111:VAL:HG22	1.71	0.71
1:C:307:GLU:HG3	1:C:308:ILE:HG23	1.73	0.71
1:D:109:VAL:HG22	1:C:232:VAL:HG21	1.73	0.71
1:B:53:VAL:HG22	1:B:75:LYS:HG2	1.72	0.70
1:C:332:SER:HG	1:C:352:TRP:HD1	1.38	0.70
1:C:321:ARG:NH2	4:C:569:HOH:O	2.23	0.70
1:B:111:VAL:HG22	1:A:135:GLY:HA2	1.72	0.70
1:C:28:PHE:CB	1:C:31:LEU:HD12	2.21	0.70
1:A:214:LEU:HD11	1:A:351:ARG:HB2	1.74	0.68
1:B:28:PHE:HB2	1:B:31:LEU:HD12	1.75	0.68
1:A:14:HIS:HB3	1:A:16:TYR:CE2	2.29	0.67
1:D:153:ARG:HD3	1:C:154:GLY:O	1.95	0.67
1:A:103:THR:HG21	1:A:114:LEU:HB3	1.75	0.67
1:C:107:THR:HG21	1:C:167:LEU:H	1.61	0.66
1:B:15:ARG:HG2	1:B:51:HIS:CE1	2.31	0.66
1:D:206:VAL:O	1:D:207:ARG:HG2	1.97	0.65
1:A:230:TRP:CH2	2:A:400:PLM:H52	2.31	0.65
1:B:224:SER:HB3	1:B:343:PHE:H	1.60	0.65
1:B:198:VAL:HG13	1:B:202:ARG:HB3	1.79	0.65
1:C:28:PHE:HB2	1:C:31:LEU:CD1	2.26	0.65
1:B:109:VAL:HG22	1:A:232:VAL:HG21	1.78	0.65
1:C:182:LEU:O	1:C:185:THR:HG22	1.97	0.64
1:C:11:LEU:HD13	1:C:51:HIS:CE1	2.33	0.64
1:D:27:GLU:OE1	1:D:32:LYS:NZ	2.30	0.64
1:A:250:GLU:HA	1:A:290:SER:OG	1.98	0.63
1:B:166:GLU:HG3	1:B:312:SER:HB3	1.80	0.63
1:B:169:SER:HA	3:B:401:JAO:H15	1.81	0.63
1:A:212:ASP:OD2	1:A:351:ARG:NH2	2.31	0.62
1:D:182:LEU:O	1:D:185:THR:HG22	1.98	0.62
1:D:228:MET:HG3	1:D:241:LEU:HD12	1.81	0.62
1:C:107:THR:HG21	1:C:167:LEU:N	2.13	0.62
1:C:321:ARG:NH1	4:C:544:HOH:O	2.33	0.62
1:C:219:SER:HB3	1:C:345:THR:HG22	1.82	0.62
1:C:353:ARG:CG	1:C:353:ARG:HH11	2.10	0.62
1:B:301:THR:HB	1:B:319:ILE:HD13	1.81	0.61
1:C:106:VAL:O	1:C:230:TRP:NE1	2.27	0.61
1:B:232:VAL:HG21	1:A:109:VAL:HG22	1.82	0.61
1:A:73:ILE:O	1:A:77:VAL:HG13	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:42:HIS:NE2	1:A:185:THR:HG23	2.17	0.60
1:D:42:HIS:NE2	1:D:185:THR:HG23	2.16	0.60
1:C:276:SER:HB3	1:C:301:THR:HG21	1.84	0.60
1:D:115:ASP:OD1	1:D:132:PRO:HB3	2.02	0.60
1:D:111:VAL:HG22	1:C:135:GLY:HA2	1.82	0.60
1:A:78:ASP:HA	1:A:81:VAL:HG22	1.83	0.60
1:B:139:VAL:HG22	1:B:346:GLU:HB2	1.83	0.60
1:A:178:THR:HG22	1:A:181:SER:H	1.67	0.59
1:C:47:VAL:HG22	1:C:305:LEU:HD22	1.84	0.59
1:C:353:ARG:HG3	1:C:353:ARG:NH1	2.14	0.59
1:D:232:VAL:HG21	1:C:109:VAL:HG22	1.86	0.58
1:B:207:ARG:HH21	1:B:207:ARG:HG2	1.68	0.57
1:A:15:ARG:HD3	1:A:51:HIS:CE1	2.39	0.57
1:A:271:ILE:HD11	1:A:274:TRP:CG	2.39	0.57
1:A:288:ALA:CA	1:A:293:LEU:HD11	2.25	0.57
1:D:135:GLY:CA	1:C:111:VAL:HG22	2.31	0.57
1:D:274:TRP:CZ3	1:D:335:LEU:HD23	2.39	0.57
1:B:114:LEU:O	1:B:118:ILE:HG23	2.05	0.57
1:B:134:PHE:HB3	1:A:134:PHE:HB3	1.86	0.57
1:B:147:ARG:NH1	1:B:150:ASP:OD2	2.36	0.57
1:D:106:VAL:HG11	2:D:400:PLM:H32	1.86	0.57
1:D:212:ASP:OD1	1:D:353:ARG:NH2	2.38	0.57
1:B:182:LEU:O	1:B:185:THR:HG22	2.05	0.56
1:B:155:ALA:HB2	1:A:153:ARG:NH1	2.20	0.56
1:C:4:ILE:HD12	1:C:211:PRO:HG2	1.87	0.56
1:C:59:TYR:CE1	1:C:169:SER:HB3	2.39	0.56
1:A:182:LEU:O	1:A:185:THR:HG22	2.05	0.56
1:B:47:VAL:HG22	1:B:305:LEU:HD22	1.87	0.55
1:D:100:MET:HB2	1:D:129:ARG:HB2	1.88	0.55
1:D:12:PRO:HG3	1:D:79:LEU:HD21	1.88	0.55
1:C:257:VAL:HG11	1:C:291:LEU:HD22	1.88	0.55
1:B:106:VAL:HG22	1:B:230:TRP:HE1	1.72	0.55
1:B:84:LEU:HD22	1:B:88:LEU:HD22	1.88	0.55
1:B:106:VAL:HG22	1:B:230:TRP:NE1	2.22	0.55
1:A:53:VAL:HG13	1:A:54:LEU:HD13	1.88	0.55
1:C:119:ALA:HA	1:C:124:LEU:HG	1.87	0.55
1:D:106:VAL:O	1:D:230:TRP:NE1	2.32	0.55
1:A:246:THR:HG23	1:A:286:ALA:HB2	1.88	0.54
1:C:107:THR:CG2	1:C:167:LEU:H	2.19	0.54
1:B:77:VAL:O	1:B:81:VAL:HG13	2.07	0.54
1:A:271:ILE:HD11	1:A:274:TRP:CD2	2.42	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:155:ALA:HB2	1:A:153:ARG:HH11	1.70	0.54
1:C:220:LEU:HD23	1:C:344:CYS:HB3	1.89	0.54
1:D:47:VAL:HA	1:D:306:GLY:HA2	1.90	0.54
1:D:206:VAL:C	1:D:207:ARG:HG2	2.26	0.54
1:D:230:TRP:CH2	2:D:400:PLM:H52	2.42	0.54
1:A:14:HIS:HB2	1:A:52:LEU:O	2.07	0.54
1:B:125:ARG:HG2	4:B:561:HOH:O	2.07	0.54
1:B:255:ASN:O	1:B:259:THR:HG23	2.09	0.53
1:C:78:ASP:HB3	1:C:121:ARG:HH11	1.71	0.53
1:A:70:GLU:O	1:A:73:ILE:HG13	2.08	0.53
1:A:275:VAL:O	1:A:336:MET:HA	2.08	0.53
1:A:271:ILE:HD11	1:A:274:TRP:CD1	2.44	0.53
1:A:255:ASN:N	1:A:255:ASN:OD1	2.42	0.53
1:B:266:LEU:HD22	1:B:270:ASP:HB3	1.90	0.53
1:B:328:PRO:HG2	1:B:352:TRP:CD2	2.44	0.53
1:D:198:VAL:HG13	1:D:202:ARG:HB3	1.91	0.53
1:C:42:HIS:NE2	1:C:185:THR:HG23	2.24	0.52
1:C:312:SER:OG	3:C:401:JAO:H36	2.09	0.52
1:D:93:LEU:HD21	1:D:206:VAL:HG22	1.91	0.52
1:A:274:TRP:CD1	1:A:297:ALA:HB1	2.45	0.52
1:B:273:ALA:HB3	1:B:352:TRP:CZ2	2.44	0.52
1:A:280:GLY:O	1:A:284:ILE:HG13	2.10	0.52
1:A:232:VAL:HG22	1:A:237:LEU:HD12	1.91	0.52
1:A:301:THR:HG22	1:A:319:ILE:HG21	1.91	0.52
1:A:28:PHE:HB2	1:A:31:LEU:HD12	1.92	0.51
1:B:246:THR:HG23	1:B:286:ALA:HB2	1.92	0.51
1:B:230:TRP:HH2	3:B:401:JAO:H25	1.75	0.51
1:B:207:ARG:HH21	1:B:207:ARG:CG	2.23	0.51
1:C:124:LEU:HB3	1:C:128:VAL:HG11	1.93	0.51
1:D:265:ARG:HG2	1:A:154:GLY:HA2	1.92	0.51
1:A:125:ARG:NE	1:A:127:ASP:OD1	2.32	0.51
1:A:136:LEU:O	1:A:139:VAL:HG12	2.10	0.51
1:B:271:ILE:HG13	1:B:271:ILE:O	2.08	0.51
1:B:329:PRO:HB2	1:B:332:SER:HB3	1.92	0.51
1:A:26:VAL:HG22	1:A:35:GLU:HA	1.92	0.51
1:D:77:VAL:O	1:D:81:VAL:HG13	2.11	0.51
1:D:230:TRP:CD2	1:D:237:LEU:HB3	2.46	0.51
1:B:130:ARG:NH2	1:A:344:CYS:SG	2.84	0.50
1:A:140:ALA:HB3	1:A:313:SER:HB3	1.93	0.50
1:C:84:LEU:HD22	1:C:88:LEU:HD13	1.94	0.50
1:C:353:ARG:CG	1:C:353:ARG:NH1	2.73	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:228:MET:HB3	1:A:241:LEU:HD23	1.93	0.50
1:A:106:VAL:O	1:A:230:TRP:NE1	2.41	0.50
1:A:85:LEU:HD11	1:A:122:LEU:HD21	1.94	0.50
1:B:168:CYS:HB3	3:B:401:JAO:H24	1.94	0.50
1:B:88:LEU:HD13	1:B:196:VAL:HG21	1.93	0.50
1:B:15:ARG:NH2	1:B:307:GLU:O	2.44	0.50
1:C:37:ILE:HG12	1:C:41:LEU:HD22	1.94	0.50
1:D:172:TYR:HA	1:D:175:VAL:HG13	1.94	0.50
1:B:119:ALA:HA	1:B:124:LEU:HG	1.94	0.49
1:C:110:ALA:O	1:C:113:SER:HA	2.13	0.49
1:D:125:ARG:HG2	4:D:585:HOH:O	2.11	0.49
1:C:77:VAL:O	1:C:81:VAL:HG13	2.13	0.49
1:A:162:LEU:O	1:A:194:ALA:HA	2.13	0.49
1:D:301:THR:HB	1:D:319:ILE:HD13	1.94	0.49
1:B:73:ILE:O	1:B:77:VAL:HG13	2.13	0.48
1:C:329:PRO:HB2	1:C:332:SER:HB3	1.95	0.48
1:D:230:TRP:CE2	1:D:237:LEU:HB3	2.48	0.48
1:D:307:GLU:HG3	1:D:308:ILE:HD13	1.94	0.48
1:D:103:THR:HG21	1:D:114:LEU:HB2	1.95	0.48
1:B:221:TYR:HD2	1:B:248:LEU:HD13	1.77	0.48
1:C:76:ALA:HA	1:C:165:VAL:HG11	1.95	0.48
1:A:99:ASP:O	1:A:129:ARG:HG2	2.14	0.48
1:D:311:LEU:HB3	1:D:314:ALA:HB3	1.95	0.48
1:B:84:LEU:HD12	1:B:118:ILE:CD1	2.40	0.48
1:C:320:LEU:HA	1:C:323:THR:HG22	1.95	0.48
1:D:136:LEU:HD13	1:C:132:PRO:CG	2.37	0.48
1:C:347:LEU:HD22	4:C:562:HOH:O	2.14	0.48
1:B:78:ASP:OD1	1:B:121:ARG:NH1	2.37	0.47
1:C:288:ALA:HA	1:C:293:LEU:HB2	1.96	0.47
1:C:54:LEU:HB2	1:C:59:TYR:CZ	2.49	0.47
1:D:276:SER:HB3	1:D:301:THR:HG21	1.97	0.47
1:A:188:PHE:CG	2:A:400:PLM:H62	2.50	0.47
1:B:42:HIS:NE2	1:B:185:THR:HG23	2.29	0.47
1:B:14:HIS:HB2	1:B:52:LEU:O	2.14	0.47
1:B:291:LEU:HB2	1:B:293:LEU:HG	1.96	0.47
1:B:341:PRO:CG	3:B:401:JAO:H3	2.44	0.47
1:A:273:ALA:HB3	1:A:352:TRP:HE1	1.79	0.47
1:A:217:ARG:HB3	1:A:217:ARG:HH21	1.80	0.47
1:D:178:THR:HG22	1:D:181:SER:H	1.80	0.47
1:D:53:VAL:HG13	1:D:54:LEU:HD13	1.96	0.47
1:B:53:VAL:HG13	1:B:54:LEU:HD13	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:296:GLU:HA	1:A:298:LEU:H	1.79	0.47
1:B:84:LEU:HD13	1:B:122:LEU:HD12	1.96	0.47
1:C:81:VAL:HG12	1:C:118:ILE:HG23	1.96	0.47
1:A:92:ASN:ND2	4:A:532:HOH:O	2.48	0.47
1:D:153:ARG:NH2	1:A:204:GLU:OE2	2.49	0.46
1:B:221:TYR:CD2	1:B:248:LEU:HD13	2.50	0.46
1:A:14:HIS:HB3	1:A:16:TYR:CZ	2.50	0.46
1:D:4:ILE:HD12	1:D:211:PRO:HG2	1.96	0.46
1:B:106:VAL:O	1:B:230:TRP:NE1	2.38	0.46
1:B:336:MET:HB2	1:B:348:VAL:HB	1.98	0.46
1:A:138:CYS:HB2	1:A:339:MET:O	2.16	0.46
1:D:53:VAL:HG22	1:D:75:LYS:HD2	1.98	0.46
1:A:274:TRP:CZ3	1:A:335:LEU:HD23	2.51	0.46
1:D:135:GLY:HA2	1:C:111:VAL:CG2	2.39	0.46
1:C:11:LEU:HD13	1:C:51:HIS:ND1	2.31	0.45
1:C:59:TYR:CZ	1:C:169:SER:HB3	2.52	0.45
1:D:250:GLU:HA	1:D:290:SER:OG	2.17	0.45
1:D:84:LEU:HD22	1:D:88:LEU:HD22	1.98	0.45
1:A:78:ASP:HB2	4:A:553:HOH:O	2.16	0.45
1:C:136:LEU:O	1:C:139:VAL:HG12	2.17	0.45
1:D:232:VAL:HG11	1:C:109:VAL:HG13	1.99	0.45
1:B:169:SER:OG	1:B:190:ASP:OD2	2.29	0.45
1:B:53:VAL:CG2	1:B:75:LYS:HG2	2.44	0.45
1:A:283:VAL:O	1:A:287:VAL:HG12	2.17	0.45
2:A:400:PLM:H72	2:A:400:PLM:HA1	1.65	0.45
1:D:147:ARG:NH1	1:D:150:ASP:OD2	2.50	0.45
1:D:151:TYR:OH	1:D:158:ASP:OD2	2.32	0.45
1:D:106:VAL:CG1	2:D:400:PLM:H32	2.46	0.45
1:A:334:GLY:N	1:A:350:LEU:O	2.42	0.45
1:B:12:PRO:HG3	1:B:79:LEU:HD21	1.99	0.45
1:A:336:MET:HB2	1:A:348:VAL:HB	1.99	0.45
1:B:139:VAL:CG2	1:B:346:GLU:HB2	2.46	0.45
1:C:271:ILE:HG13	1:C:271:ILE:O	2.17	0.45
1:A:106:VAL:HG22	1:A:230:TRP:NE1	2.33	0.44
1:A:182:LEU:HA	1:A:185:THR:HG22	2.00	0.44
1:B:288:ALA:HB2	1:B:298:LEU:HD12	1.99	0.44
1:D:232:VAL:HG22	1:D:237:LEU:HD12	1.99	0.44
1:D:46:LYS:HD2	1:D:302:TRP:CZ3	2.52	0.44
1:D:54:LEU:HD22	1:D:170:LEU:HD11	1.99	0.44
1:A:125:ARG:HG2	4:A:593:HOH:O	2.16	0.44
1:D:147:ARG:HA	1:D:147:ARG:HD3	1.56	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:320:LEU:O	1:B:324:ILE:HG13	2.17	0.44
1:B:218:SER:O	1:A:127:ASP:HA	2.17	0.44
1:C:217:ARG:HB2	1:C:260:PHE:CD1	2.53	0.44
1:B:15:ARG:HG2	1:B:51:HIS:NE2	2.33	0.44
1:D:2:SER:N	1:D:200:ASP:OD1	2.51	0.44
1:A:143:ALA:O	1:A:147:ARG:HG2	2.17	0.44
1:A:271:ILE:HD11	1:A:274:TRP:CE2	2.53	0.44
1:D:150:ASP:OD2	1:C:129:ARG:HD3	2.16	0.44
1:D:280:GLY:O	1:D:284:ILE:HG13	2.17	0.44
1:B:321:ARG:HG3	1:B:322:ASP:N	2.31	0.44
1:D:153:ARG:HG2	1:D:153:ARG:O	2.17	0.44
1:A:122:LEU:HA	1:A:122:LEU:HD23	1.88	0.43
1:B:152:LEU:HD11	1:B:160:ALA:HB3	2.00	0.43
1:C:100:MET:HB2	1:C:129:ARG:HB2	2.00	0.43
1:A:106:VAL:HG22	1:A:230:TRP:HE1	1.82	0.43
1:C:62:LEU:HD11	1:C:68:ALA:HA	1.99	0.43
1:D:24:SER:HB3	1:D:57:GLN:HE22	1.83	0.43
1:D:212:ASP:HB2	1:D:351:ARG:HB3	1.99	0.43
1:A:273:ALA:HB3	1:A:352:TRP:NE1	2.33	0.43
1:A:94:ARG:HG3	1:A:96:SER:HB3	2.01	0.43
1:A:166:GLU:HG3	1:A:312:SER:HB3	2.01	0.43
1:D:230:TRP:HA	1:D:230:TRP:CE3	2.54	0.43
1:A:282:LYS:HG2	1:A:282:LYS:H	1.48	0.43
1:A:94:ARG:HB3	1:A:94:ARG:HE	1.37	0.43
1:D:257:VAL:HG23	1:D:261:LEU:HD22	2.01	0.43
1:D:330:SER:OG	1:D:353:ARG:OXT	2.27	0.43
1:D:246:THR:HG23	1:D:286:ALA:HB2	2.00	0.43
1:C:176:LYS:HA	1:C:176:LYS:HD3	1.80	0.43
1:D:103:THR:HB	1:D:115:ASP:OD1	2.18	0.43
1:D:149:ARG:HD3	4:D:567:HOH:O	2.18	0.43
1:A:170:LEU:HA	1:A:170:LEU:HD12	1.86	0.43
1:D:109:VAL:HG13	1:C:232:VAL:HG11	2.01	0.43
1:C:26:VAL:HG13	1:C:35:GLU:HB2	2.00	0.43
1:D:38:ILE:HG12	1:D:182:LEU:HD22	2.00	0.43
1:B:81:VAL:HG22	4:B:543:HOH:O	2.18	0.43
1:C:114:LEU:HD12	1:C:114:LEU:HA	1.88	0.43
1:C:138:CYS:HB3	1:C:277:HIS:CE1	2.53	0.43
1:B:169:SER:O	1:B:172:TYR:HB2	2.19	0.42
1:C:125:ARG:NH1	4:C:507:HOH:O	2.51	0.42
1:D:72:PHE:HA	1:D:170:LEU:HD23	2.01	0.42
1:A:140:ALA:HB3	1:A:313:SER:CB	2.48	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:52:LEU:HD22	1:C:169:SER:OG	2.18	0.42
1:D:261:LEU:HB3	1:D:266:LEU:O	2.19	0.42
1:A:4:ILE:HD12	1:A:211:PRO:HG2	2.01	0.42
1:D:4:ILE:HG13	1:D:213:ILE:HD11	2.01	0.42
1:B:25:PHE:CE2	1:B:185:THR:HG21	2.54	0.42
1:D:37:ILE:HG12	1:D:41:LEU:HD22	2.01	0.42
1:D:136:LEU:HA	1:D:136:LEU:HD12	1.90	0.42
1:D:323:THR:O	1:D:328:PRO:HD3	2.19	0.42
1:A:217:ARG:HB2	1:A:260:PHE:CD1	2.55	0.42
1:A:230:TRP:HH2	2:A:400:PLM:H52	1.82	0.42
1:D:268:LYS:HB2	1:D:268:LYS:HZ2	1.84	0.42
1:A:176:LYS:HA	1:A:176:LYS:HD2	1.84	0.42
1:A:276:SER:OG	1:A:301:THR:HG21	2.20	0.42
1:A:47:VAL:HG22	1:A:305:LEU:HD22	2.02	0.42
1:B:293:LEU:HD23	1:B:293:LEU:HA	1.88	0.42
1:A:103:THR:HG21	1:A:114:LEU:CB	2.48	0.42
1:A:84:LEU:O	1:A:88:LEU:HB2	2.20	0.42
1:C:221:TYR:HA	1:C:222:PRO:HD3	1.94	0.41
1:D:147:ARG:HH12	1:C:129:ARG:HG2	1.84	0.41
1:D:171:THR:OG1	2:D:400:PLM:H81	2.19	0.41
1:D:59:TYR:N	1:D:60:PRO:HD2	2.35	0.41
1:B:206:VAL:O	1:B:207:ARG:C	2.58	0.41
1:B:261:LEU:HB3	1:B:266:LEU:O	2.20	0.41
1:D:329:PRO:HD3	1:B:265:ARG:NH1	2.35	0.41
1:D:34:HIS:CE1	1:D:177:PRO:HB2	2.56	0.41
1:A:231:ASP:OD1	1:A:240:ARG:NH2	2.50	0.41
1:A:93:LEU:HD12	1:A:97:ASP:OD2	2.21	0.41
1:B:79:LEU:HD23	1:B:167:LEU:HD21	2.02	0.41
1:B:2:SER:N	1:B:200:ASP:OD2	2.53	0.41
1:B:300:LEU:HD12	1:B:300:LEU:HA	1.86	0.41
1:C:275:VAL:HG13	1:C:319:ILE:HG13	2.02	0.41
1:A:77:VAL:O	1:A:81:VAL:HG13	2.20	0.41
1:B:81:VAL:HG12	1:B:118:ILE:HB	2.03	0.41
1:B:76:ALA:HA	1:B:165:VAL:HG11	2.02	0.41
1:B:182:LEU:HA	1:B:185:THR:HG22	2.03	0.41
1:B:288:ALA:HA	1:B:293:LEU:HB2	2.03	0.41
1:D:85:LEU:HD23	1:D:85:LEU:HA	1.72	0.41
1:B:271:ILE:HD11	1:B:274:TRP:CG	2.56	0.41
1:C:7:VAL:HG12	1:C:195:VAL:HG22	2.03	0.41
1:C:300:LEU:HD12	1:C:300:LEU:HA	1.83	0.41
1:C:78:ASP:HA	1:C:81:VAL:HG22	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:72:PHE:CD2	1:D:108:GLY:HA3	2.56	0.41
1:C:301:THR:HG22	1:C:319:ILE:HD13	2.02	0.41
1:B:328:PRO:HB2	1:B:352:TRP:CD1	2.56	0.41
1:B:103:THR:HG22	1:B:132:PRO:HA	2.02	0.40
1:B:207:ARG:CG	1:B:207:ARG:NH2	2.80	0.40
1:B:79:LEU:HD12	1:B:79:LEU:HA	1.86	0.40
1:C:88:LEU:HD12	1:C:88:LEU:HA	1.89	0.40
1:A:300:LEU:HA	1:A:300:LEU:HD12	1.74	0.40
1:D:106:VAL:HG22	1:D:230:TRP:NE1	2.36	0.40
1:A:156:PRO:HA	1:A:199:GLY:HA3	2.03	0.40
1:B:15:ARG:HH21	1:B:51:HIS:CE1	2.39	0.40
1:B:266:LEU:HA	1:B:266:LEU:HD23	1.93	0.40
1:C:287:VAL:HG21	1:C:337:LEU:HD21	2.03	0.40
1:C:55:PRO:HD2	1:C:58:GLN:OE1	2.22	0.40
1:A:136:LEU:O	1:A:341:PRO:HD2	2.21	0.40
1:B:115:ASP:OD2	1:B:130:ARG:HB3	2.21	0.40
1:A:169:SER:HA	2:A:400:PLM:HC1	2.04	0.40
1:A:227:ILE:HA	1:A:242:SER:HB3	2.04	0.40
3:C:401:JAO:H35	3:C:401:JAO:H1	1.83	0.40
1:D:87:ALA:HB1	1:D:196:VAL:HG23	2.04	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:180:SER:OG	1:C:36:GLU:OE1[2_656]	1.84	0.36

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	350/353 (99%)	342 (98%)	7 (2%)	1 (0%)	41 31

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	B	350/353 (99%)	335 (96%)	14 (4%)	1 (0%)	41 31
1	C	350/353 (99%)	335 (96%)	13 (4%)	2 (1%)	25 15
1	D	350/353 (99%)	335 (96%)	14 (4%)	1 (0%)	41 31
All	All	1400/1412 (99%)	1347 (96%)	48 (3%)	5 (0%)	34 24

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	278	PRO
1	D	327	ARG
1	C	327	ARG
1	B	279	GLY
1	C	278	PRO

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	280/281 (100%)	232 (83%)	48 (17%)	2 0
1	B	280/281 (100%)	230 (82%)	50 (18%)	2 0
1	C	280/281 (100%)	229 (82%)	51 (18%)	1 0
1	D	280/281 (100%)	229 (82%)	51 (18%)	1 0
All	All	1120/1124 (100%)	920 (82%)	200 (18%)	2 0

All (200) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	2	SER
1	D	27	GLU
1	D	32	LYS
1	D	35	GLU
1	D	41	LEU
1	D	53	VAL

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Mol	Chain	Res	Type
1	D	54	LEU
1	D	61	SER
1	D	62	LEU
1	D	79	LEU
1	D	84	LEU
1	D	88	LEU
1	D	100	MET
1	D	103	THR
1	D	109	VAL
1	D	115	ASP
1	D	136	LEU
1	D	147	ARG
1	D	148	LEU
1	D	152	LEU
1	D	170	LEU
1	D	175	VAL
1	D	176	LYS
1	D	178	THR
1	D	180	SER
1	D	205	GLN
1	D	207	ARG
1	D	220	LEU
1	D	225	LEU
1	D	230	TRP
1	D	237	LEU
1	D	245	LEU
1	D	251	ARG
1	D	253	LEU
1	D	261	LEU
1	D	265	ARG
1	D	267	THR
1	D	298	LEU
1	D	300	LEU
1	D	301	THR
1	D	303	ARG
1	D	305	LEU
1	D	308	ILE
1	D	315	SER
1	D	325	GLU
1	D	326	LYS
1	D	327	ARG
1	D	339	MET

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Mol	Chain	Res	Type
1	D	345	THR
1	D	347	LEU
1	D	350	LEU
1	C	2	SER
1	C	3	VAL
1	C	41	LEU
1	C	46	LYS
1	C	54	LEU
1	C	79	LEU
1	C	84	LEU
1	C	88	LEU
1	C	100	MET
1	C	103	THR
1	C	109	VAL
1	C	114	LEU
1	C	115	ASP
1	C	121	ARG
1	C	129	ARG
1	C	136	LEU
1	C	139	VAL
1	C	153	ARG
1	C	178	THR
1	C	181	SER
1	C	185	THR
1	C	198	VAL
1	C	204	GLU
1	C	207	ARG
1	C	214	LEU
1	C	218	SER
1	C	220	LEU
1	C	237	LEU
1	C	241	LEU
1	C	257	VAL
1	C	261	LEU
1	C	265	ARG
1	C	267	THR
1	C	269	ASP
1	C	271	ILE
1	C	293	LEU
1	C	300	LEU
1	C	301	THR
1	C	302	TRP

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Mol	Chain	Res	Type
1	C	305	LEU
1	C	315	SER
1	C	319	ILE
1	C	321	ARG
1	C	326	LYS
1	C	327	ARG
1	C	337	LEU
1	C	339	MET
1	C	345	THR
1	C	347	LEU
1	C	350	LEU
1	C	353	ARG
1	B	2	SER
1	B	15	ARG
1	B	17	SER
1	B	37	ILE
1	B	41	LEU
1	B	53	VAL
1	B	54	LEU
1	B	62	LEU
1	B	73	ILE
1	B	79	LEU
1	B	84	LEU
1	B	88	LEU
1	B	94	ARG
1	B	103	THR
1	B	109	VAL
1	B	114	LEU
1	B	115	ASP
1	B	118	ILE
1	B	128	VAL
1	B	136	LEU
1	B	139	VAL
1	B	147	ARG
1	B	153	ARG
1	B	170	LEU
1	B	180	SER
1	B	198	VAL
1	B	204	GLU
1	B	206	VAL
1	B	207	ARG
1	B	220	LEU

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Mol	Chain	Res	Type
1	B	223	ASP
1	B	224	SER
1	B	237	LEU
1	B	241	LEU
1	B	253	LEU
1	B	261	LEU
1	B	267	THR
1	B	270	ASP
1	B	271	ILE
1	B	296	GLU
1	B	300	LEU
1	B	301	THR
1	B	302	TRP
1	B	305	LEU
1	B	315	SER
1	B	321	ARG
1	B	339	MET
1	B	346	GLU
1	B	347	LEU
1	B	353	ARG
1	A	7	VAL
1	A	26	VAL
1	A	33	GLU
1	A	39	ARG
1	A	53	VAL
1	A	54	LEU
1	A	73	ILE
1	A	84	LEU
1	A	88	LEU
1	A	93	LEU
1	A	94	ARG
1	A	96	SER
1	A	100	MET
1	A	109	VAL
1	A	114	LEU
1	A	115	ASP
1	A	129	ARG
1	A	136	LEU
1	A	152	LEU
1	A	170	LEU
1	A	178	THR
1	A	180	SER

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Mol	Chain	Res	Type
1	A	187	LEU
1	A	205	GLN
1	A	207	ARG
1	A	217	ARG
1	A	220	LEU
1	A	237	LEU
1	A	241	LEU
1	A	245	LEU
1	A	255	ASN
1	A	265	ARG
1	A	266	LEU
1	A	269	ASP
1	A	271	ILE
1	A	282	LYS
1	A	293	LEU
1	A	296	GLU
1	A	298	LEU
1	A	300	LEU
1	A	301	THR
1	A	305	LEU
1	A	315	SER
1	A	321	ARG
1	A	325	GLU
1	A	326	LYS
1	A	347	LEU
1	A	350	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	D	57	GLN
1	B	51	HIS
1	A	51	HIS

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 carbohydrates in this entry.

5.6 Ligand geometry (i)

4 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	JAO	B	401	1	18,18,18	0.95	1 (5%)	18,18,18	0.84	0
2	PLM	A	400	-	14,17,17	0.46	0	13,17,17	1.26	3 (23%)
2	PLM	D	400	-	14,17,17	0.39	0	13,17,17	0.81	0
3	JAO	C	401	1	18,18,18	0.93	1 (5%)	18,18,18	0.80	0

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	JAO	B	401	1	-	12/17/17/17	-
2	PLM	A	400	-	-	0/13/15/15	-
2	PLM	D	400	-	-	0/13/15/15	-
3	JAO	C	401	1	-	9/17/17/17	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	401	JAO	O3-CAE	-3.85	1.26	1.42
3	B	401	JAO	O3-CAE	-3.79	1.26	1.42

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	400	PLM	C7-C6-C5	2.33	126.27	114.42
2	A	400	PLM	C9-C8-C7	-2.08	103.86	114.42
2	A	400	PLM	C8-C7-C6	2.03	124.75	114.42

There are no chirality outliers.

All (21) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	401	JAO	O3-CAE-CAU-CAB
3	C	401	JAO	O3-CAE-CAU-CAB
3	B	401	JAO	CAS-CAT-CAU-CAB
3	C	401	JAO	CAS-CAT-CAU-CAB
3	C	401	JAO	CAQ-CAR-CAS-CAT
3	B	401	JAO	CAJ-CAK-CAL-CAM
3	C	401	JAO	CAM-CAN-CAO-CAP
3	B	401	JAO	CAH-CAI-CAJ-CAK
3	B	401	JAO	CAN-CAO-CAP-CAQ
3	B	401	JAO	CAG-CAH-CAI-CAJ
3	B	401	JAO	CAQ-CAR-CAS-CAT
3	B	401	JAO	CAF-CAG-CAH-CAI
3	B	401	JAO	CAM-CAN-CAO-CAP
3	C	401	JAO	CAF-CAG-CAH-CAI
3	B	401	JAO	O3-CAE-CAU-CAT
3	C	401	JAO	CAH-CAI-CAJ-CAK
3	C	401	JAO	CAP-CAQ-CAR-CAS
3	C	401	JAO	CAJ-CAK-CAL-CAM
3	C	401	JAO	CAN-CAO-CAP-CAQ
3	B	401	JAO	CAS-CAT-CAU-CAE
3	B	401	JAO	CAP-CAQ-CAR-CAS

There are no ring outliers.

4 monomers are involved in 15 short contacts:

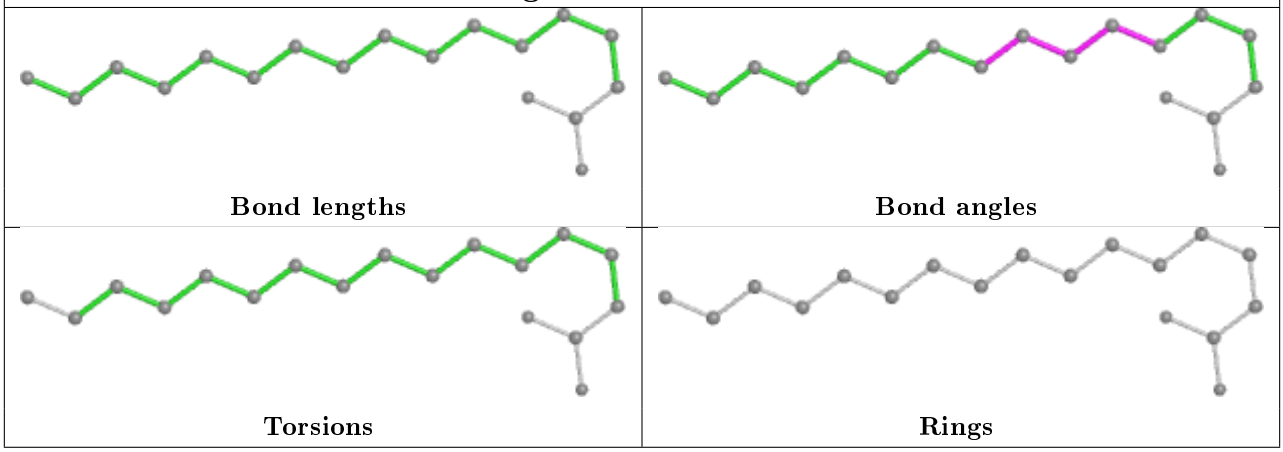
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	401	JAO	4	0
2	A	400	PLM	5	0
2	D	400	PLM	4	0
3	C	401	JAO	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In

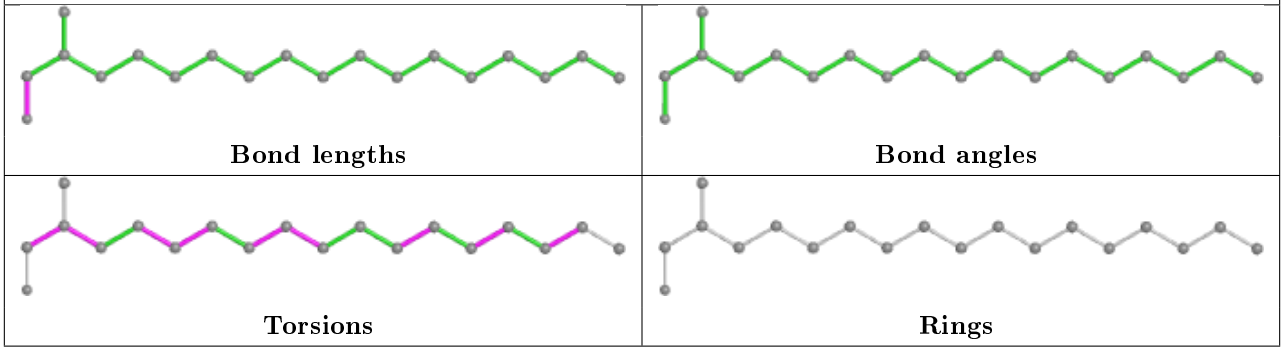
addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

Ligand JAO B 401

Ligand PLM A 400



Ligand JAO C 401



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	352/353 (99%)	0.13	9 (2%) 56 60	26, 39, 55, 71	0
1	B	352/353 (99%)	0.05	3 (0%) 84 86	23, 35, 55, 68	0
1	C	352/353 (99%)	0.13	12 (3%) 45 49	30, 43, 59, 72	0
1	D	352/353 (99%)	0.03	6 (1%) 70 73	31, 41, 56, 66	0
All	All	1408/1412 (99%)	0.08	30 (2%) 63 67	23, 40, 57, 72	0

All (30) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	267	THR	5.7
1	A	294	PRO	4.3
1	C	206	VAL	4.1
1	C	273	ALA	4.0
1	C	207	ARG	3.7
1	A	327	ARG	3.0
1	C	204	GLU	2.9
1	C	272	GLY	2.9
1	C	265	ARG	2.9
1	D	31	LEU	2.8
1	B	295	PRO	2.7
1	C	333	ALA	2.6
1	C	353	ARG	2.6
1	D	32	LYS	2.4
1	D	44	ALA	2.3
1	A	331	GLY	2.3
1	B	353	ARG	2.3
1	A	353	ARG	2.3
1	A	210	GLY	2.3
1	A	330	SER	2.3
1	D	30	GLY	2.3

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Mol	Chain	Res	Type	RSRZ
1	C	268	LYS	2.2
1	C	269	ASP	2.1
1	A	295	PRO	2.1
1	A	266	LEU	2.1
1	D	45	ALA	2.0
1	C	321	ARG	2.0
1	B	292	ALA	2.0
1	D	26	VAL	2.0
1	A	206	VAL	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 carbohydrates in this entry.

6.4 Ligands (i)

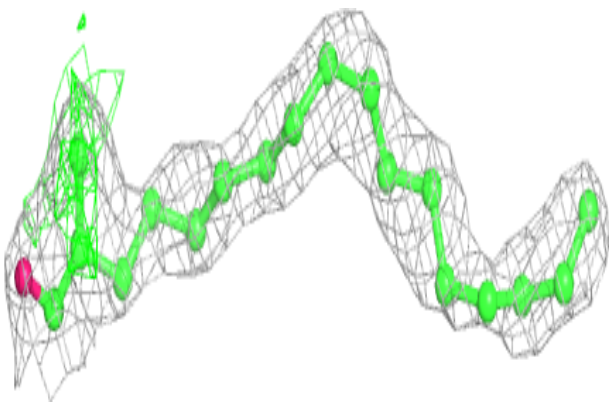
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

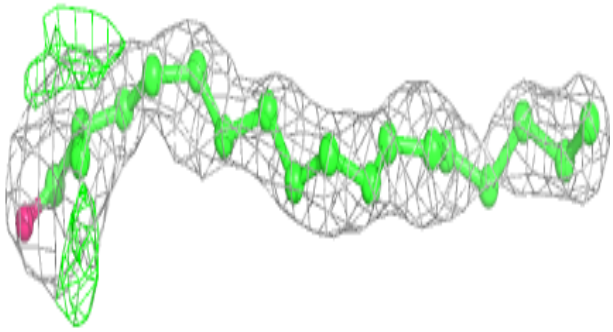
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	JAO	C	401	19/19	0.84	0.16	37,41,51,52	0
2	PLM	D	400	18/18	0.86	0.19	38,46,49,50	0
2	PLM	A	400	18/18	0.86	0.14	36,38,44,47	0
3	JAO	B	401	19/19	0.91	0.14	31,33,39,44	0

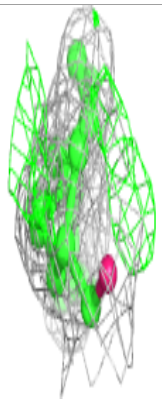
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around JAO 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)

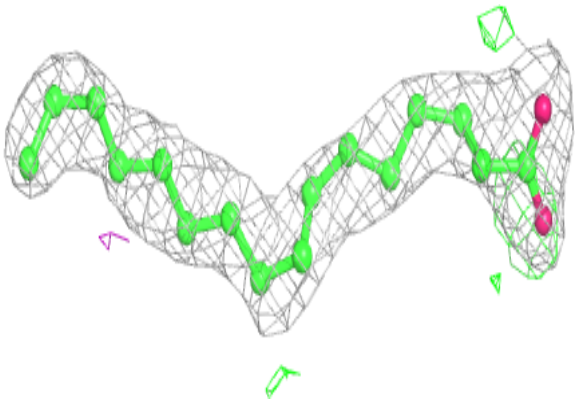


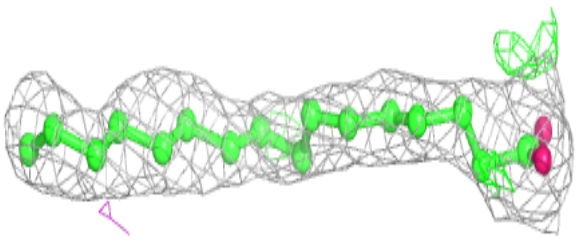


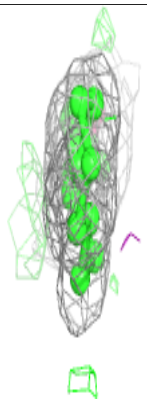


Electron density around PLM A 400:

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

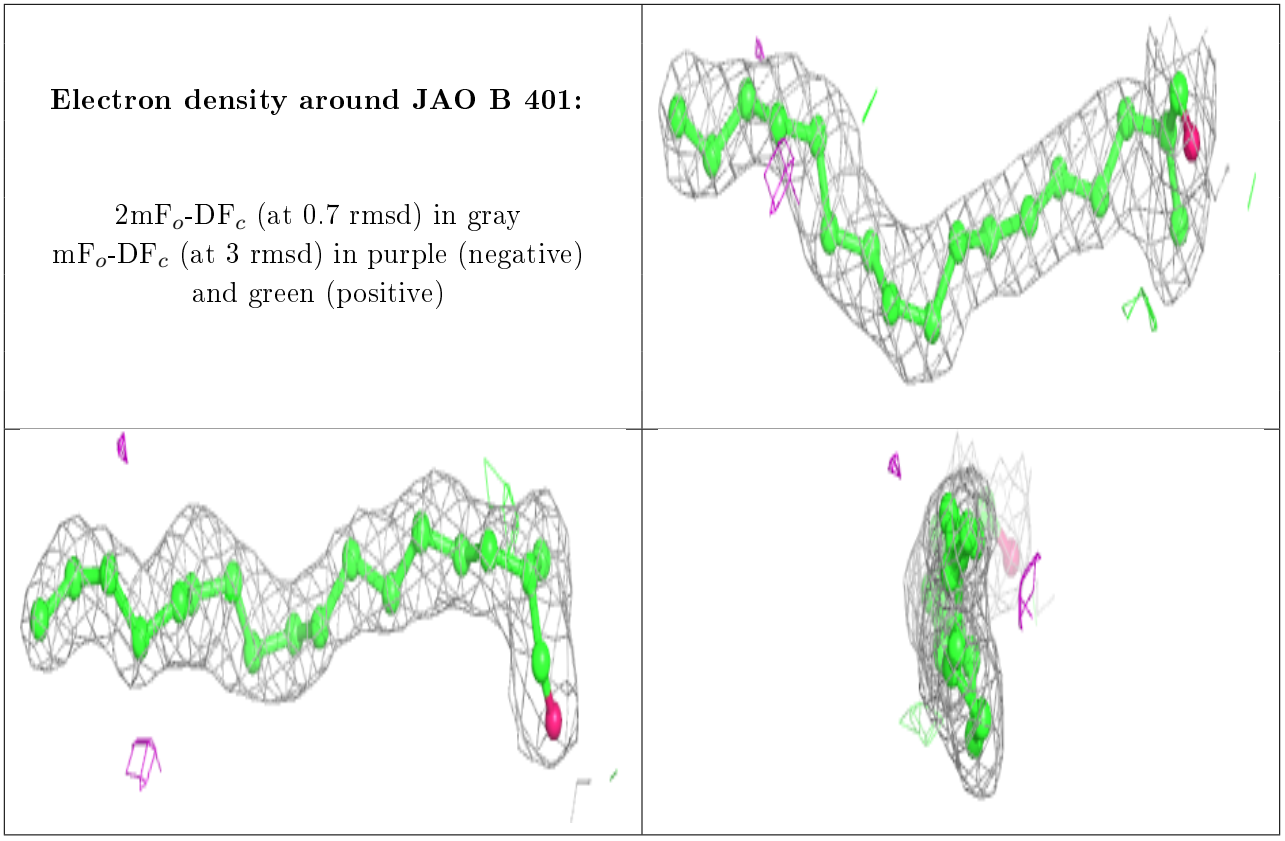






Electron density around JAO B 401:

$2mF_o$-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

There are no such residues in this entry.