Full wwPDB X-ray Structure Validation Report ⓘ

Mar 18, 2026 – 03:10 AM UTC

PDB ID	:	4JAT / pdb_00004jat
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	:	2013-02-19
Resolution	:	2.42 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:

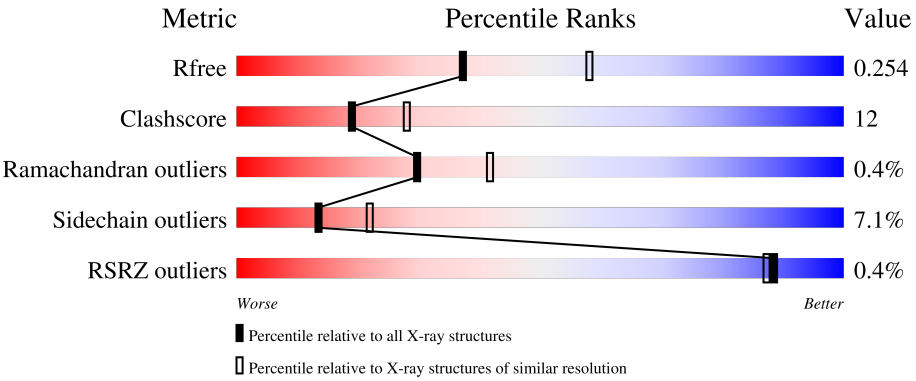
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

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 2.42 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}	180053	6062 (2.44-2.40)
Clashscore	190562	6562 (2.44-2.40)
Ramachandran outliers	187476	6481 (2.44-2.40)
Sidechain outliers	187428	6482 (2.44-2.40)
RSRZ outliers	180081	6066 (2.44-2.40)

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	353	79% 18% .
1	B	353	% 76% 21% .
1	C	353	72% 24% .
1	D	353	% 69% 27% .

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 10934 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.

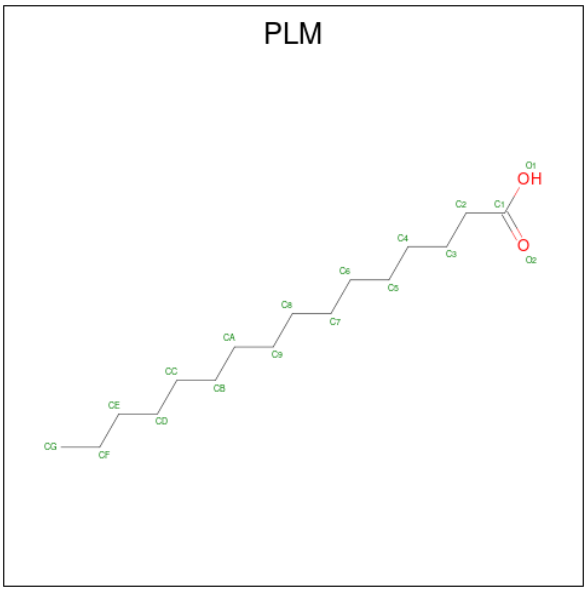
- Molecule 1 is a protein called Alpha-pyrone synthesis polyketide synthase-like Pks11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	352	Total	C	N	O	S	0	0	0
			2642	1671	469	495	7			
1	B	352	Total	C	N	O	S	0	0	0
			2642	1671	469	495	7			
1	C	352	Total	C	N	O	S	0	0	0
			2642	1671	469	495	7			
1	D	352	Total	C	N	O	S	0	0	0
			2642	1671	469	495	7			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	138	SER	CYS	engineered mutation	UNP O06587
B	138	SER	CYS	engineered mutation	UNP O06587
C	138	SER	CYS	engineered mutation	UNP O06587
D	138	SER	CYS	engineered mutation	UNP O06587

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



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

- Molecule 3 is water.

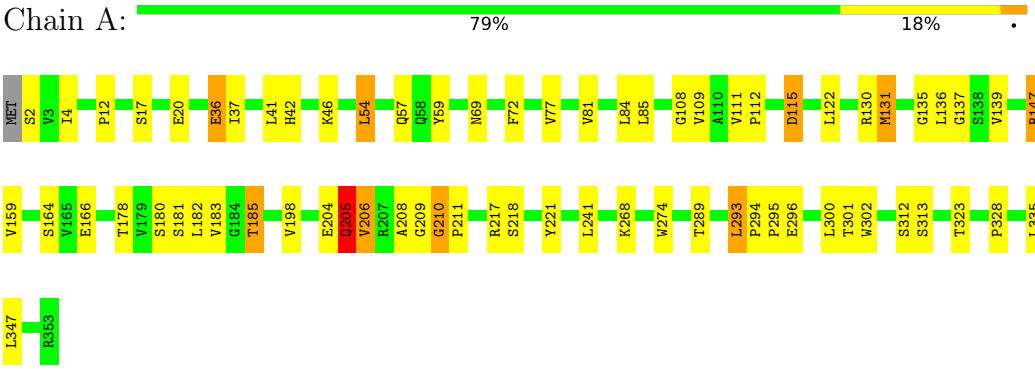
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	69	Total O 69 69	0	0
3	B	83	Total O 83 83	0	0
3	C	71	Total O 71 71	0	0
3	D	71	Total O 71 71	0	0

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.

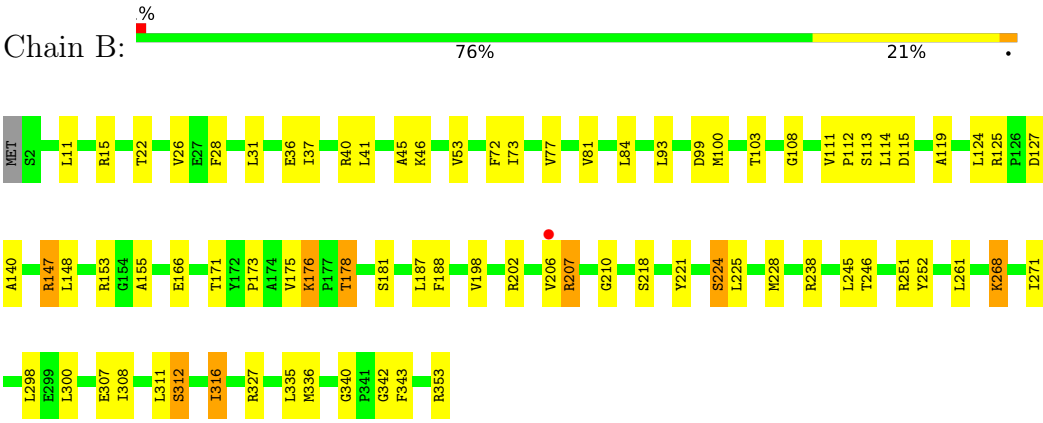
• Molecule 1: Alpha-pyrone synthesis polyketide synthase-like Pks11

Chain A:



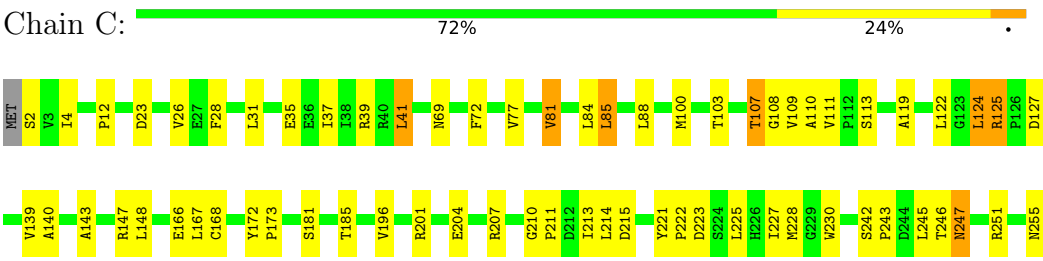
• Molecule 1: Alpha-pyrone synthesis polyketide synthase-like Pks11

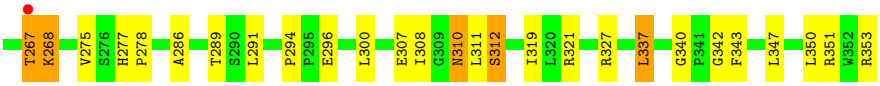
Chain B:



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

Chain C:

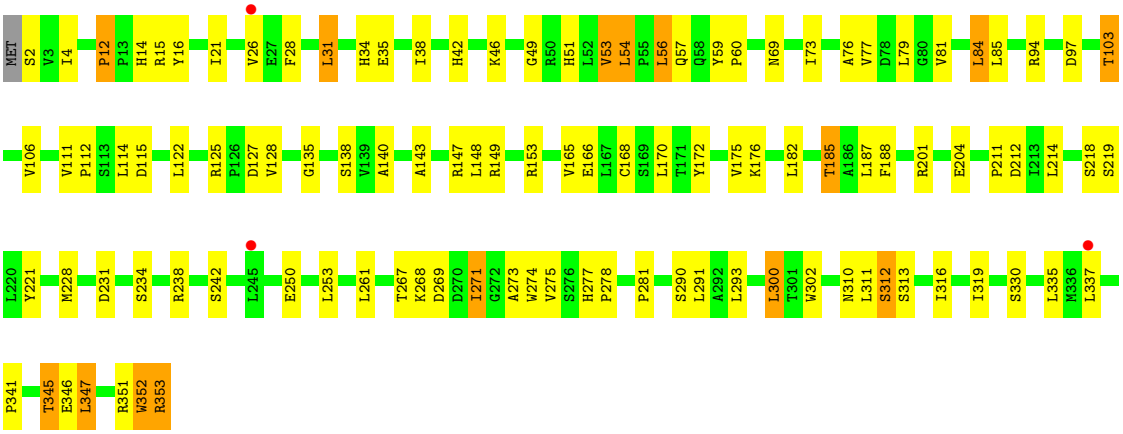




• Molecule 1: Alpha-pyrone synthesis polyketide synthase-like Pks11

Chain D:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	72.37Å 48.87Å 194.62Å 90.00° 97.95° 90.00°	Depositor
Resolution (Å)	37.65 – 2.42 37.65 – 2.43	Depositor EDS
% Data completeness (in resolution range)	96.5 (37.65-2.42) 96.1 (37.65-2.43)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.98 (at 2.42Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.196 , 0.276 0.199 , 0.254	Depositor DCC
R_{free} test set	2541 reflections (4.90%)	wwPDB-VP
Wilson B-factor (Å^2)	44.2	Xtriage
Anisotropy	0.216	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 35.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.014 for h,-k,-h-l	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	10934	wwPDB-VP
Average B, all atoms (Å^2)	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.11% 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: 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	0.66	4/2695 (0.1%)	0.85	4/3671 (0.1%)
1	B	0.58	1/2695 (0.0%)	0.86	5/3671 (0.1%)
1	C	0.58	1/2695 (0.0%)	0.87	6/3671 (0.2%)
1	D	0.61	1/2695 (0.0%)	0.88	5/3671 (0.1%)
All	All	0.61	7/10780 (0.1%)	0.87	20/14684 (0.1%)

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	206	VAL	C-O	-9.52	1.13	1.24
1	D	312	SER	C-O	-6.20	1.18	1.24
1	C	312	SER	C-O	-5.85	1.18	1.24
1	A	131	MET	C-O	-5.12	1.18	1.24
1	A	205	GLN	C-N	-5.09	1.27	1.34
1	B	11	LEU	C-O	-5.06	1.19	1.24
1	A	12	PRO	C-O	-5.05	1.20	1.24

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	234	SER	CA-C-O	7.49	128.57	120.10
1	B	155	ALA	CA-C-N	6.51	126.64	119.87
1	B	155	ALA	C-N-CA	6.51	126.64	119.87
1	C	12	PRO	CA-C-N	6.02	125.23	118.97
1	C	12	PRO	C-N-CA	6.02	125.23	118.97
1	D	242	SER	CA-C-N	5.93	125.55	119.56
1	D	242	SER	C-N-CA	5.93	125.55	119.56
1	A	293	LEU	CA-C-N	5.76	123.81	119.66
1	A	293	LEU	C-N-CA	5.76	123.81	119.66
1	A	155	ALA	CA-C-N	5.74	125.41	119.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	155	ALA	C-N-CA	5.74	125.41	119.56
1	B	312	SER	CB-CA-C	-5.64	110.09	116.63
1	B	210	GLY	CA-C-N	5.46	125.41	119.78
1	B	210	GLY	C-N-CA	5.46	125.41	119.78
1	C	125	ARG	CA-C-N	5.21	124.88	119.56
1	C	125	ARG	C-N-CA	5.21	124.88	119.56
1	D	12	PRO	CA-C-N	5.12	124.73	119.05
1	D	12	PRO	C-N-CA	5.12	124.73	119.05
1	C	210	GLY	CA-C-N	5.10	125.00	119.85
1	C	210	GLY	C-N-CA	5.10	125.00	119.85

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2642	0	2675	41	0
1	B	2642	0	2675	54	0
1	C	2642	0	2675	74	0
1	D	2642	0	2675	90	0
2	A	18	0	31	1	0
2	B	18	0	31	2	0
2	C	18	0	31	4	0
2	D	18	0	31	4	0
3	A	69	0	0	1	0
3	B	83	0	0	2	0
3	C	71	0	0	0	0
3	D	71	0	0	1	0
All	All	10934	0	10824	253	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 (253) 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:330:SER:OG	1:D:353:ARG:HB2	1.54	1.07
1:C:201:ARG:HD2	1:D:353:ARG:HG2	1.29	1.05
1:A:205:GLN:O	1:A:205:GLN:HG2	1.68	0.91
1:D:271:ILE:HD12	1:D:273:ALA:H	1.38	0.89
1:B:166:GLU:HG3	1:B:312:SER:HB3	1.52	0.88
1:C:69:ASN:HD21	1:C:109:VAL:H	1.17	0.88
1:B:28:PHE:HB2	1:B:31:LEU:HD12	1.56	0.87
1:D:26:VAL:HG11	1:D:35:GLU:HG3	1.56	0.87
1:D:337:LEU:HD13	1:D:347:LEU:HD11	1.54	0.86
1:C:28:PHE:HB2	1:C:31:LEU:HD12	1.59	0.84
1:D:26:VAL:HG11	1:D:35:GLU:CG	2.10	0.82
1:D:182:LEU:O	1:D:185:THR:HG22	1.80	0.82
1:C:107:THR:HG21	1:C:167:LEU:H	1.45	0.81
1:A:69:ASN:HD21	1:A:109:VAL:H	1.27	0.80
1:C:26:VAL:CG1	1:C:35:GLU:HB2	2.12	0.79
1:C:247:ASN:HD21	1:C:251:ARG:NH2	1.80	0.79
1:A:182:LEU:O	1:A:185:THR:HG22	1.82	0.79
1:D:166:GLU:HG3	1:D:312:SER:HB3	1.67	0.77
1:A:42:HIS:NE2	1:A:185:THR:HG23	2.00	0.77
1:A:205:GLN:O	1:A:205:GLN:CG	2.30	0.76
1:C:125:ARG:O	1:C:128:VAL:HG23	1.85	0.76
1:B:198:VAL:HG13	1:B:202:ARG:HB3	1.68	0.74
1:D:77:VAL:O	1:D:81:VAL:HG23	1.88	0.73
1:B:103:THR:HG21	1:B:114:LEU:HB2	1.71	0.71
1:C:166:GLU:HG3	1:C:312:SER:HB3	1.71	0.71
1:A:77:VAL:O	1:A:81:VAL:HG23	1.90	0.71
1:C:255:ASN:O	1:C:259:THR:HG23	1.92	0.69
1:B:36:GLU:HG2	1:B:40:ARG:HH11	1.58	0.68
1:B:224:SER:HB3	1:B:343:PHE:H	1.58	0.68
1:C:124:LEU:HB3	1:C:128:VAL:HG21	1.74	0.68
1:D:42:HIS:NE2	1:D:185:THR:HG23	2.08	0.68
1:C:310:ASN:C	1:C:310:ASN:HD22	2.02	0.68
1:C:26:VAL:HG11	1:C:35:GLU:HB2	1.75	0.67
1:C:310:ASN:HD22	1:C:312:SER:H	1.41	0.67
1:D:337:LEU:HD13	1:D:347:LEU:CD1	2.24	0.66
1:C:84:LEU:HD23	1:C:122:LEU:HD12	1.77	0.66
1:C:201:ARG:CD	1:D:353:ARG:HG2	2.17	0.65
1:D:337:LEU:CD1	1:D:347:LEU:HD11	2.24	0.65
1:C:26:VAL:HG13	1:C:35:GLU:HB2	1.78	0.65
1:C:247:ASN:HD21	1:C:251:ARG:HH21	1.41	0.64
1:C:107:THR:HG21	1:C:167:LEU:N	2.12	0.64
1:D:310:ASN:ND2	1:D:312:SER:H	1.96	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:337:LEU:CD1	1:D:347:LEU:CD1	2.76	0.64
1:C:28:PHE:CB	1:C:31:LEU:HD12	2.29	0.63
1:B:45:ALA:HB1	1:B:187:LEU:HD23	1.79	0.62
1:C:246:THR:HG23	1:C:286:ALA:HB2	1.79	0.62
1:C:72:PHE:CE1	1:C:108:GLY:HA3	2.35	0.62
1:D:143:ALA:O	1:D:147:ARG:HG2	2.00	0.62
1:C:77:VAL:O	1:C:81:VAL:HG13	2.00	0.62
1:D:352:TRP:O	1:D:353:ARG:HB3	1.99	0.61
1:C:225:LEU:HD23	1:C:342:GLY:O	2.00	0.61
1:A:178:THR:HG22	1:A:181:SER:HB2	1.82	0.61
1:D:219:SER:HB3	1:D:345:THR:HG22	1.83	0.61
1:C:278:PRO:HG3	1:C:319:ILE:HD11	1.82	0.60
1:D:28:PHE:CD1	1:D:60:PRO:HG3	2.36	0.60
1:D:94:ARG:HB3	1:D:94:ARG:CZ	2.31	0.59
1:D:212:ASP:OD2	1:D:351:ARG:NH2	2.35	0.59
1:B:308:ILE:HD12	1:B:311:LEU:HD22	1.83	0.59
1:C:119:ALA:HA	1:C:124:LEU:HG	1.83	0.59
1:B:28:PHE:CB	1:B:31:LEU:HD12	2.31	0.59
1:B:37:ILE:HG23	3:B:564:HOH:O	2.01	0.59
1:B:251:ARG:HG2	1:B:252:TYR:CE2	2.38	0.58
1:C:247:ASN:C	1:C:247:ASN:ND2	2.60	0.58
1:D:103:THR:HG21	1:D:114:LEU:HB2	1.85	0.58
1:B:119:ALA:HA	1:B:124:LEU:HG	1.86	0.58
1:C:289:THR:O	1:C:291:LEU:O	2.22	0.58
1:D:275:VAL:HG13	1:D:319:ILE:HG22	1.86	0.57
1:C:310:ASN:ND2	1:C:312:SER:H	2.01	0.57
1:C:37:ILE:HG12	1:C:41:LEU:HD22	1.85	0.57
1:D:231:ASP:HB3	1:D:238:ARG:HB3	1.86	0.57
1:D:310:ASN:HD22	1:D:311:LEU:N	2.02	0.57
1:D:330:SER:OG	1:D:353:ARG:CB	2.41	0.57
1:C:35:GLU:O	1:C:39:ARG:HG3	2.05	0.57
1:C:84:LEU:HD23	1:C:122:LEU:CD1	2.34	0.56
1:C:230:TRP:HH2	2:C:400:PLM:H62	1.71	0.56
1:C:35:GLU:CD	1:C:39:ARG:HH11	2.13	0.56
1:D:125:ARG:O	1:D:128:VAL:HG23	2.06	0.56
1:B:175:VAL:O	1:B:176:LYS:HG2	2.05	0.55
1:B:251:ARG:HG2	1:B:252:TYR:CZ	2.41	0.55
1:A:72:PHE:CE1	1:A:108:GLY:HA3	2.42	0.54
1:D:228:MET:HE2	1:D:341:PRO:HD3	1.88	0.54
1:C:143:ALA:O	1:C:147:ARG:HG2	2.06	0.54
1:A:166:GLU:HG3	1:A:312:SER:HB3	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:308:ILE:HD12	1:B:311:LEU:CD2	2.38	0.54
1:D:310:ASN:HD22	1:D:310:ASN:C	2.16	0.54
1:B:22:THR:O	1:B:26:VAL:HG13	2.08	0.54
1:B:188:PHE:CZ	2:B:400:PLM:H31	2.43	0.53
1:D:46:LYS:HD3	1:D:302:TRP:CZ3	2.43	0.53
1:B:77:VAL:O	1:B:81:VAL:HG23	2.07	0.53
1:B:206:VAL:HG12	1:B:206:VAL:O	2.06	0.53
1:C:227:ILE:CG2	1:C:245:LEU:HD13	2.39	0.53
1:D:26:VAL:HG12	1:D:26:VAL:O	2.08	0.53
1:B:307:GLU:HG3	1:B:308:ILE:HG23	1.91	0.53
1:D:34:HIS:O	1:D:38:ILE:HG13	2.09	0.52
1:B:178:THR:HG22	1:B:181:SER:H	1.74	0.52
1:A:135:GLY:HA3	1:C:113:SER:HB3	1.92	0.52
1:C:72:PHE:CE2	1:C:107:THR:HG22	2.45	0.52
1:D:214:LEU:HD11	1:D:351:ARG:HB2	1.92	0.52
1:D:310:ASN:HD22	1:D:312:SER:H	1.57	0.52
1:C:136:LEU:O	1:C:139:VAL:HG12	2.09	0.52
1:D:14:HIS:HB3	1:D:16:TYR:CE2	2.45	0.51
1:A:178:THR:HG23	1:A:181:SER:H	1.76	0.51
1:B:99:ASP:OD1	1:B:125:ARG:NH1	2.41	0.51
1:D:12:PRO:HG3	1:D:79:LEU:HD11	1.93	0.51
1:C:214:LEU:HD11	1:C:351:ARG:HB2	1.93	0.50
1:C:278:PRO:HG3	1:C:319:ILE:CD1	2.40	0.50
1:A:209:GLY:O	1:A:210:GLY:O	2.30	0.50
1:D:168:CYS:SG	2:D:400:PLM:H42	2.52	0.50
1:A:57:GLN:CD	1:A:57:GLN:H	2.20	0.49
1:B:15:ARG:NH2	1:B:307:GLU:O	2.39	0.49
1:B:36:GLU:HG2	1:B:40:ARG:NH1	2.27	0.49
1:B:84:LEU:O	1:B:84:LEU:HD12	2.12	0.49
1:D:46:LYS:HD3	1:D:302:TRP:HZ3	1.77	0.49
1:A:46:LYS:HD2	1:A:302:TRP:HZ3	1.78	0.49
1:A:178:THR:CG2	1:A:181:SER:HB2	2.42	0.49
1:C:245:LEU:HD11	1:C:343:PHE:CE1	2.47	0.49
1:B:93:LEU:HD21	1:B:206:VAL:HG11	1.94	0.49
1:B:111:VAL:HA	1:B:112:PRO:C	2.36	0.49
1:A:115:ASP:OD2	1:A:130:ARG:HB3	2.13	0.49
1:C:230:TRP:CH2	2:C:400:PLM:H62	2.48	0.49
1:D:250:GLU:HA	1:D:290:SER:OG	2.13	0.49
1:D:149:ARG:NH2	1:D:153:ARG:NH1	2.61	0.49
1:B:125:ARG:O	1:B:128:VAL:HG23	2.13	0.49
1:C:247:ASN:ND2	1:C:251:ARG:HD3	2.28	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:274:TRP:CZ3	1:D:335:LEU:HD23	2.48	0.49
1:D:149:ARG:NH2	1:D:153:ARG:HH11	2.11	0.48
1:D:271:ILE:HD11	1:D:274:TRP:CD1	2.47	0.48
1:D:185:THR:HA	2:D:400:PLM:HA2	1.96	0.48
1:D:291:LEU:HB2	1:D:293:LEU:HG	1.96	0.48
1:D:271:ILE:HD12	1:D:271:ILE:C	2.39	0.48
1:C:136:LEU:HB2	1:C:140:ALA:HB2	1.95	0.48
1:D:26:VAL:HG11	1:D:35:GLU:CB	2.42	0.48
1:A:159:VAL:HG22	1:A:198:VAL:HG12	1.96	0.47
1:D:221:TYR:CD1	1:D:221:TYR:N	2.82	0.47
1:A:46:LYS:HD2	1:A:302:TRP:CZ3	2.49	0.47
1:A:54:LEU:HB2	1:A:59:TYR:CZ	2.50	0.47
1:C:23:ASP:OD1	1:C:39:ARG:NH2	2.47	0.47
1:C:85:LEU:HD22	1:C:122:LEU:HD21	1.96	0.47
1:B:147:ARG:HD3	1:B:147:ARG:HA	1.54	0.47
1:B:113:SER:HB3	1:D:135:GLY:HA3	1.97	0.47
1:D:21:ILE:HA	1:D:56:LEU:HD21	1.97	0.47
1:D:172:TYR:HA	1:D:175:VAL:HG23	1.95	0.47
1:D:271:ILE:CD1	1:D:273:ALA:H	2.18	0.47
1:B:228:MET:HE3	1:B:340:GLY:HA2	1.96	0.46
1:D:353:ARG:O	1:D:353:ARG:HD3	2.15	0.46
1:C:185:THR:HA	2:C:400:PLM:HB2	1.96	0.46
1:C:275:VAL:HG13	1:C:319:ILE:HG22	1.96	0.46
1:C:307:GLU:HG3	1:C:308:ILE:HG23	1.97	0.46
1:B:225:LEU:HD23	1:B:342:GLY:O	2.14	0.46
1:D:166:GLU:CG	1:D:312:SER:HB3	2.43	0.46
1:D:221:TYR:N	1:D:221:TYR:HD1	2.12	0.46
1:A:323:THR:O	1:A:328:PRO:HD3	2.14	0.46
1:C:353:ARG:HG3	1:C:353:ARG:HH11	1.80	0.46
1:C:69:ASN:ND2	1:C:109:VAL:H	1.99	0.46
1:B:176:LYS:O	1:B:178:THR:N	2.44	0.46
1:A:81:VAL:HG13	1:A:122:LEU:HD21	1.98	0.46
1:D:15:ARG:HD2	1:D:51:HIS:CE1	2.51	0.46
1:B:206:VAL:O	1:B:207:ARG:HB2	2.16	0.45
1:D:4:ILE:HB	1:D:211:PRO:HD2	1.97	0.45
1:B:73:ILE:O	1:B:77:VAL:HG23	2.16	0.45
1:B:224:SER:OG	1:B:343:PHE:HB3	2.15	0.45
1:A:295:PRO:HG2	1:A:296:GLU:OE2	2.17	0.45
1:D:337:LEU:HD12	1:D:347:LEU:CD1	2.47	0.45
1:D:300:LEU:HD12	1:D:300:LEU:HA	1.86	0.45
1:D:69:ASN:O	1:D:73:ILE:HG13	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:253:LEU:HD11	1:D:337:LEU:HD11	1.97	0.45
1:D:201:ARG:HE	1:D:204:GLU:CD	2.25	0.45
1:A:178:THR:O	1:A:182:LEU:HG	2.16	0.45
1:A:147:ARG:NH2	1:C:129:ARG:HG2	2.32	0.44
1:C:107:THR:O	1:C:107:THR:CG2	2.64	0.44
1:D:15:ARG:NH1	1:D:49:GLY:HA3	2.32	0.44
1:A:85:LEU:HD23	1:A:85:LEU:HA	1.84	0.44
1:C:72:PHE:CZ	1:C:108:GLY:HA3	2.51	0.44
1:C:107:THR:O	1:C:107:THR:HG23	2.17	0.44
1:A:217:ARG:HD3	3:A:528:HOH:O	2.17	0.44
1:D:352:TRP:H	1:D:352:TRP:CD1	2.35	0.44
1:B:46:LYS:HA	1:B:46:LYS:HD3	1.87	0.44
1:C:310:ASN:C	1:C:310:ASN:ND2	2.73	0.44
1:C:277:HIS:HA	1:C:278:PRO:HD3	1.70	0.44
1:A:131:MET:O	1:A:131:MET:HG2	2.17	0.43
1:B:218:SER:O	1:D:127:ASP:HA	2.18	0.43
1:C:213:ILE:HA	1:C:350:LEU:HD23	1.99	0.43
1:C:172:TYR:N	1:C:173:PRO:CD	2.81	0.43
1:A:137:GLY:O	1:A:313:SER:HB3	2.17	0.43
1:B:37:ILE:O	1:B:41:LEU:HG	2.18	0.43
1:B:238:ARG:HD2	3:B:560:HOH:O	2.16	0.43
1:B:268:LYS:HB2	1:B:268:LYS:HE3	1.43	0.43
1:C:215:ASP:OD2	1:C:264:HIS:HE1	2.02	0.43
1:D:85:LEU:HG	1:D:122:LEU:HD21	2.00	0.43
1:D:94:ARG:O	1:D:97:ASP:HB2	2.19	0.43
1:D:140:ALA:HB3	1:D:313:SER:HB3	2.00	0.43
1:A:136:LEU:O	1:A:341:PRO:HD2	2.18	0.43
1:A:274:TRP:CZ3	1:A:335:LEU:HD23	2.54	0.43
1:D:26:VAL:CG1	1:D:35:GLU:CB	2.96	0.43
1:B:175:VAL:C	1:B:176:LYS:HG2	2.43	0.43
1:D:103:THR:HG22	3:D:543:HOH:O	2.18	0.43
1:D:271:ILE:O	1:D:271:ILE:HG13	2.18	0.43
1:D:277:HIS:ND1	1:D:278:PRO:HD2	2.34	0.43
1:A:4:ILE:HB	1:A:211:PRO:HD2	2.01	0.42
1:B:125:ARG:HD2	1:B:127:ASP:OD1	2.18	0.42
1:C:88:LEU:HD23	1:C:196:VAL:HG21	2.01	0.42
1:A:122:LEU:HA	1:A:122:LEU:HD23	1.71	0.42
1:D:26:VAL:CG1	1:D:35:GLU:HB2	2.48	0.42
1:D:46:LYS:HB2	1:D:281:PRO:HG3	2.02	0.42
1:A:293:LEU:HA	1:A:294:PRO:HD3	1.88	0.42
1:B:316:ILE:HG12	1:B:336:MET:HE2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:180:SER:HB2	1:A:241:LEU:HB3	2.02	0.42
1:C:72:PHE:CD1	1:C:108:GLY:HA3	2.54	0.42
1:B:124:LEU:HB3	1:B:128:VAL:HG21	2.00	0.42
1:B:288:ALA:HB2	1:B:298:LEU:HD12	2.02	0.42
1:C:110:ALA:O	1:C:113:SER:HA	2.20	0.42
1:D:188:PHE:CZ	2:D:400:PLM:H31	2.55	0.42
1:D:261:LEU:HD23	1:D:261:LEU:HA	1.82	0.42
1:A:221:TYR:N	1:A:221:TYR:CD1	2.87	0.42
1:B:221:TYR:N	1:B:221:TYR:CD1	2.88	0.42
1:D:15:ARG:HB2	1:D:51:HIS:CD2	2.54	0.42
1:B:166:GLU:CG	1:B:312:SER:HB3	2.37	0.42
1:B:188:PHE:CD2	2:B:400:PLM:H62	2.55	0.42
1:C:4:ILE:HB	1:C:211:PRO:HD2	2.02	0.42
1:A:135:GLY:HA2	1:C:111:VAL:HG22	2.02	0.42
1:C:228:MET:HE3	1:C:340:GLY:HA2	2.01	0.42
1:B:72:PHE:CE2	1:B:108:GLY:HA3	2.55	0.42
1:D:59:TYR:N	1:D:60:PRO:CD	2.82	0.42
1:D:53:VAL:HG13	1:D:54:LEU:HD13	2.01	0.41
1:D:140:ALA:HB3	1:D:313:SER:CB	2.50	0.41
1:D:26:VAL:HG13	1:D:35:GLU:HA	2.03	0.41
2:D:400:PLM:H81	2:D:400:PLM:H51	1.65	0.41
1:A:36:GLU:HG3	1:A:37:ILE:N	2.35	0.41
1:A:206:VAL:HG23	1:A:208:ALA:N	2.36	0.41
1:C:247:ASN:C	1:C:247:ASN:HD22	2.28	0.41
1:D:267:THR:C	1:D:269:ASP:N	2.78	0.41
2:A:400:PLM:H41	2:A:400:PLM:H71	1.79	0.41
1:C:294:PRO:HB2	1:C:296:GLU:CD	2.45	0.41
1:C:221:TYR:HA	1:C:222:PRO:HD3	1.85	0.41
1:A:17:SER:O	1:A:20:GLU:HB2	2.21	0.41
1:B:136:LEU:HB2	1:B:140:ALA:HB2	2.03	0.41
1:B:245:LEU:HD23	1:B:245:LEU:C	2.46	0.41
1:C:242:SER:HA	1:C:243:PRO:HD3	1.91	0.41
1:C:337:LEU:HB2	1:C:347:LEU:CD2	2.51	0.41
1:D:31:LEU:HD12	1:D:31:LEU:HA	1.88	0.41
1:D:76:ALA:HA	1:D:165:VAL:HG11	2.01	0.41
1:D:218:SER:HA	1:D:346:GLU:OE1	2.21	0.41
1:D:271:ILE:HD12	1:D:273:ALA:N	2.19	0.41
1:A:111:VAL:HA	1:A:112:PRO:C	2.46	0.41
1:D:84:LEU:HA	1:D:84:LEU:HD23	1.83	0.41
1:C:168:CYS:HB3	2:C:400:PLM:H71	2.02	0.40
1:D:111:VAL:HA	1:D:112:PRO:C	2.45	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:268:LYS:HE2	1:D:268:LYS:HB3	1.84	0.40
1:A:218:SER:O	1:C:127:ASP:HA	2.21	0.40
1:D:176:LYS:HD2	1:D:176:LYS:HA	1.71	0.40
1:B:171:THR:C	1:B:173:PRO:HD2	2.46	0.40
1:B:271:ILE:HD12	1:B:335:LEU:HB2	2.03	0.40
1:C:267:THR:O	1:C:268:LYS:C	2.65	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	350/353 (99%)	338 (97%)	10 (3%)	2 (1%)	21	30
1	B	350/353 (99%)	334 (95%)	15 (4%)	1 (0%)	36	49
1	C	350/353 (99%)	337 (96%)	12 (3%)	1 (0%)	36	49
1	D	350/353 (99%)	335 (96%)	14 (4%)	1 (0%)	36	49
All	All	1400/1412 (99%)	1344 (96%)	51 (4%)	5 (0%)	30	42

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	210	GLY
1	C	327	ARG
1	D	106	VAL
1	B	327	ARG
1	A	342	GLY

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%)	261 (93%)	19 (7%)	14	24
1	B	280/281 (100%)	263 (94%)	17 (6%)	17	28
1	C	280/281 (100%)	258 (92%)	22 (8%)	11	18
1	D	280/281 (100%)	259 (92%)	21 (8%)	12	20
All	All	1120/1124 (100%)	1041 (93%)	79 (7%)	13	22

All (79) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	SER
1	A	36	GLU
1	A	41	LEU
1	A	54	LEU
1	A	84	LEU
1	A	115	ASP
1	A	139	VAL
1	A	147	ARG
1	A	148	LEU
1	A	164	SER
1	A	183	VAL
1	A	185	THR
1	A	204	GLU
1	A	205	GLN
1	A	268	LYS
1	A	289	THR
1	A	300	LEU
1	A	301	THR
1	A	347	LEU
1	B	53	VAL
1	B	100	MET
1	B	115	ASP
1	B	147	ARG
1	B	148	LEU

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Mol	Chain	Res	Type
1	B	153	ARG
1	B	176	LYS
1	B	178	THR
1	B	207	ARG
1	B	224	SER
1	B	246	THR
1	B	261	LEU
1	B	268	LYS
1	B	276	SER
1	B	300	LEU
1	B	316	ILE
1	B	353	ARG
1	C	2	SER
1	C	41	LEU
1	C	81	VAL
1	C	85	LEU
1	C	100	MET
1	C	103	THR
1	C	107	THR
1	C	124	LEU
1	C	148	LEU
1	C	181	SER
1	C	204	GLU
1	C	207	ARG
1	C	223	ASP
1	C	247	ASN
1	C	259	THR
1	C	267	THR
1	C	268	LYS
1	C	300	LEU
1	C	310	ASN
1	C	311	LEU
1	C	321	ARG
1	C	337	LEU
1	D	2	SER
1	D	31	LEU
1	D	53	VAL
1	D	54	LEU
1	D	56	LEU
1	D	57	GLN
1	D	84	LEU
1	D	103	THR

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Mol	Chain	Res	Type
1	D	115	ASP
1	D	138	SER
1	D	148	LEU
1	D	170	LEU
1	D	185	THR
1	D	187	LEU
1	D	271	ILE
1	D	300	LEU
1	D	316	ILE
1	D	345	THR
1	D	347	LEU
1	D	352	TRP
1	D	353	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	57	GLN
1	A	69	ASN
1	A	235	HIS
1	A	247	ASN
1	A	318	HIS
1	B	34	HIS
1	B	57	GLN
1	B	58	GLN
1	B	205	GLN
1	C	51	HIS
1	C	57	GLN
1	C	69	ASN
1	C	247	ASN
1	C	264	HIS
1	C	310	ASN
1	D	14	HIS
1	D	51	HIS
1	D	310	ASN

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 oligosaccharides in this entry.

5.6 Ligand geometry (i)

4 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	PLM	D	400	-	17,17,17	0.69	1 (5%)	17,17,17	0.98	0
2	PLM	A	400	-	17,17,17	0.53	0	17,17,17	1.07	1 (5%)
2	PLM	B	400	-	17,17,17	0.60	1 (5%)	17,17,17	1.23	2 (11%)
2	PLM	C	400	-	17,17,17	0.60	0	17,17,17	0.87	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
2	PLM	D	400	-	-	10/15/15/15	-
2	PLM	A	400	-	-	10/15/15/15	-
2	PLM	B	400	-	-	10/15/15/15	-
2	PLM	C	400	-	-	6/15/15/15	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	400	PLM	O1-C1	-2.40	1.22	1.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	400	PLM	O1-C1	-2.16	1.23	1.30

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	400	PLM	C3-C2-C1	-3.28	105.95	114.51
2	B	400	PLM	O2-C1-C2	-2.59	114.88	123.09
2	A	400	PLM	O2-C1-C2	-2.51	115.14	123.09

There are no chirality outliers.

All (36) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	400	PLM	C5-C6-C7-C8
2	D	400	PLM	C3-C4-C5-C6
2	A	400	PLM	C4-C5-C6-C7
2	A	400	PLM	C6-C7-C8-C9
2	B	400	PLM	C1-C2-C3-C4
2	D	400	PLM	C8-C9-CA-CB
2	C	400	PLM	C8-C9-CA-CB
2	C	400	PLM	C7-C8-C9-CA
2	D	400	PLM	CC-CD-CE-CF
2	B	400	PLM	CC-CD-CE-CF
2	A	400	PLM	CB-CC-CD-CE
2	A	400	PLM	CA-CB-CC-CD
2	B	400	PLM	C3-C4-C5-C6
2	B	400	PLM	C5-C6-C7-C8
2	C	400	PLM	C6-C7-C8-C9
2	B	400	PLM	CA-CB-CC-CD
2	D	400	PLM	CD-CE-CF-CG
2	C	400	PLM	CC-CD-CE-CF
2	D	400	PLM	CA-CB-CC-CD
2	C	400	PLM	C1-C2-C3-C4
2	D	400	PLM	C1-C2-C3-C4
2	C	400	PLM	C2-C3-C4-C5
2	B	400	PLM	C7-C8-C9-CA
2	D	400	PLM	C9-CA-CB-CC
2	A	400	PLM	C5-C6-C7-C8
2	B	400	PLM	C4-C5-C6-C7
2	B	400	PLM	C9-CA-CB-CC
2	A	400	PLM	O1-C1-C2-C3
2	A	400	PLM	C9-CA-CB-CC

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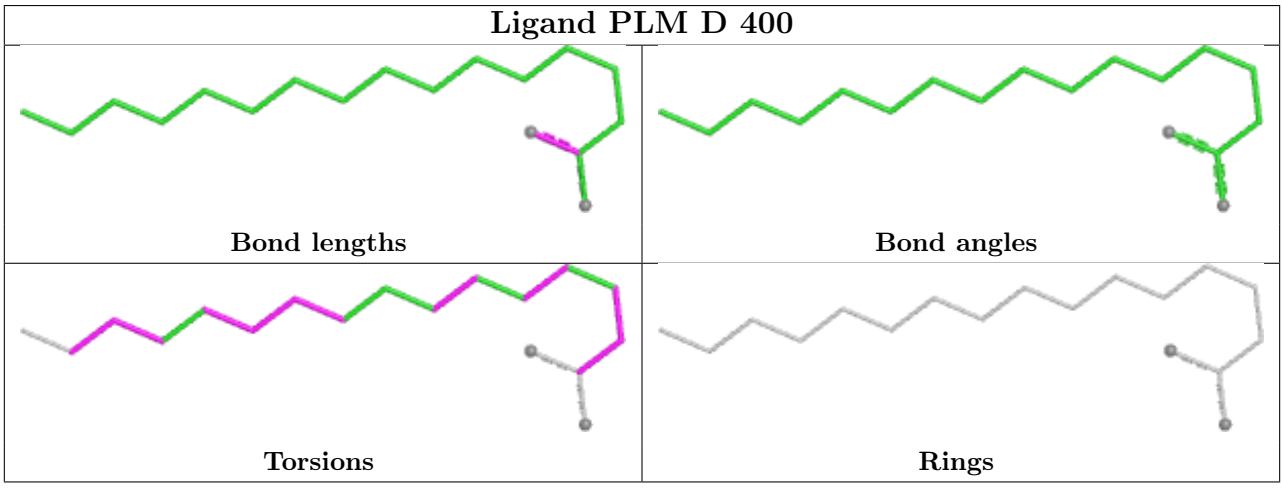
Mol	Chain	Res	Type	Atoms
2	A	400	PLM	C2-C3-C4-C5
2	D	400	PLM	O1-C1-C2-C3
2	B	400	PLM	O1-C1-C2-C3
2	D	400	PLM	O2-C1-C2-C3
2	A	400	PLM	O2-C1-C2-C3
2	A	400	PLM	CC-CD-CE-CF
2	B	400	PLM	O2-C1-C2-C3

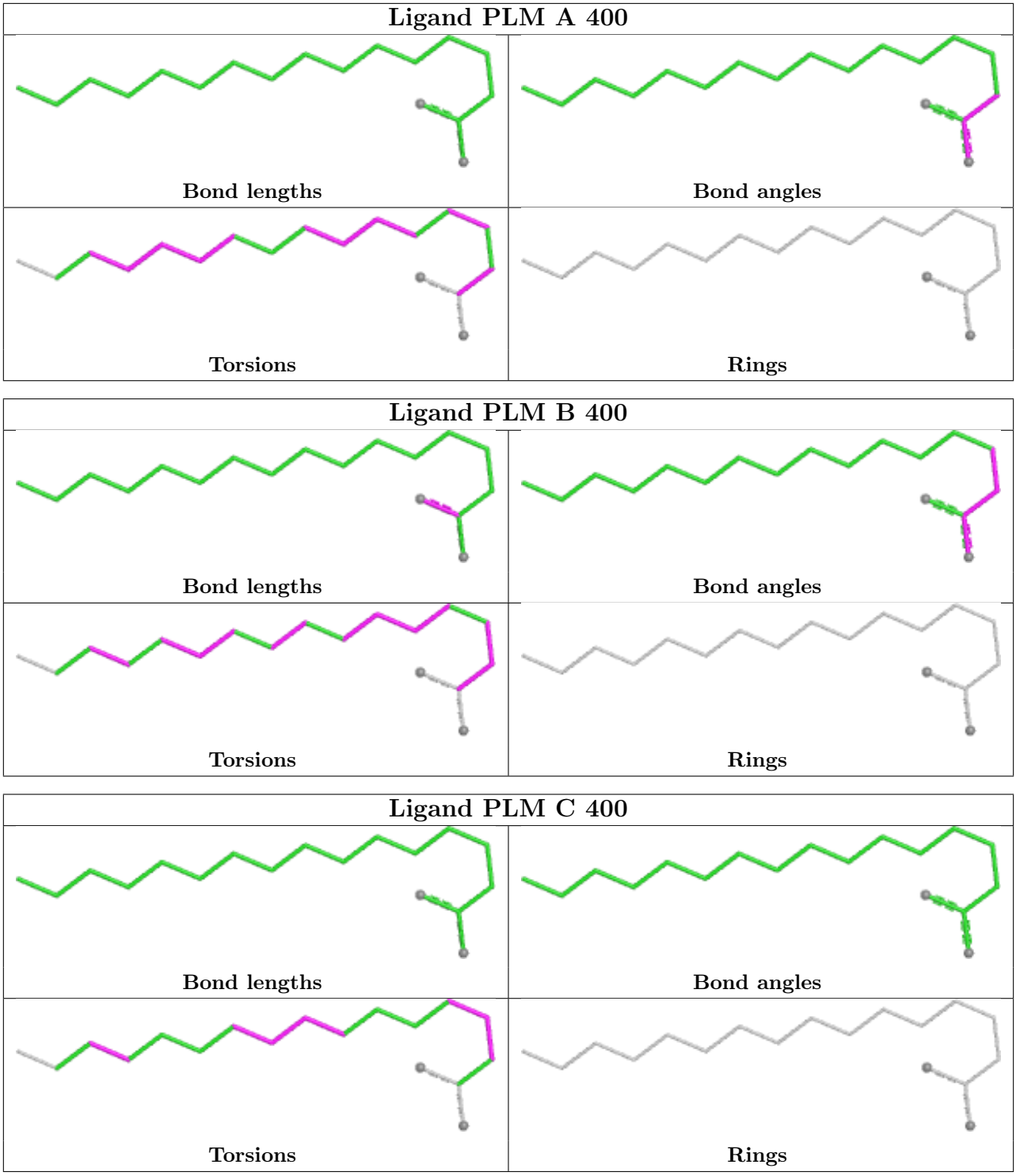
There are no ring outliers.

4 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	400	PLM	4	0
2	A	400	PLM	1	0
2	B	400	PLM	2	0
2	C	400	PLM	4	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.





5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	352/353 (99%)	-0.18	0	100	100	22, 42, 56, 69	0
1	B	352/353 (99%)	-0.13	2 (0%)	85	84	22, 40, 57, 79	0
1	C	352/353 (99%)	-0.13	1 (0%)	90	88	22, 41, 58, 80	0
1	D	352/353 (99%)	-0.09	3 (0%)	81	79	22, 41, 57, 72	0
All	All	1408/1412 (99%)	-0.13	6 (0%)	88	87	22, 41, 57, 80	0

All (6) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	206	VAL	3.4
1	D	337	LEU	2.9
1	D	26	VAL	2.8
1	D	245	LEU	2.5
1	C	267	THR	2.3
1	B	128	VAL	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 oligosaccharides 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,

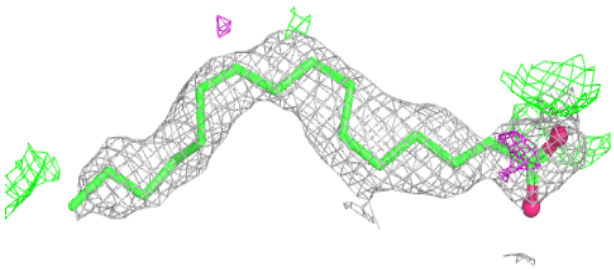
median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

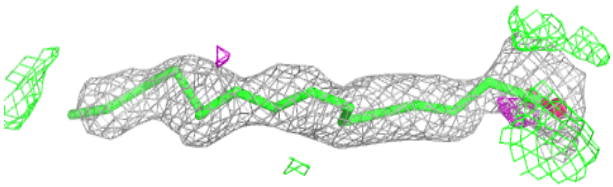
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	PLM	A	400	18/18	0.76	0.16	42,49,62,62	0
2	PLM	B	400	18/18	0.83	0.15	38,46,58,63	0
2	PLM	C	400	18/18	0.83	0.14	37,43,62,66	0
2	PLM	D	400	18/18	0.86	0.13	41,45,55,58	0

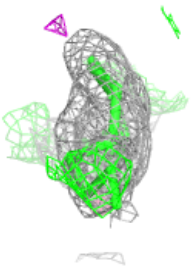
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around 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)

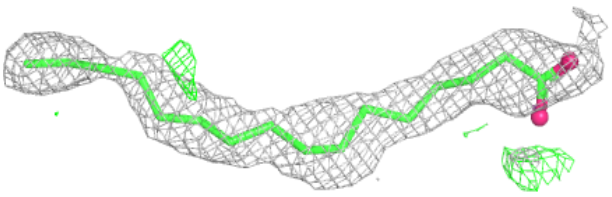


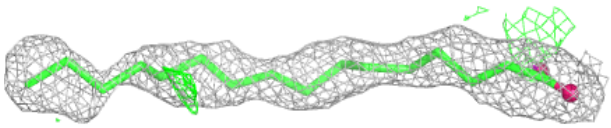


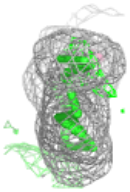


Electron density around PLM B 400:

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

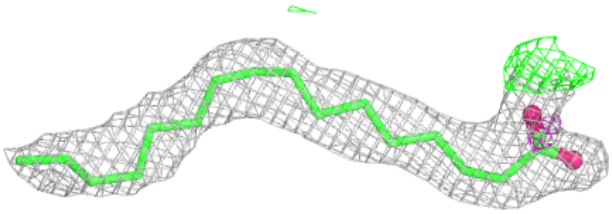


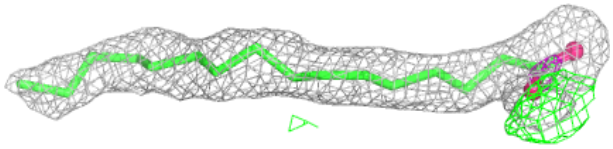


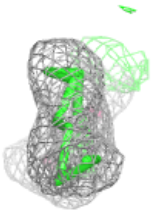


Electron density around PLM C 400:

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

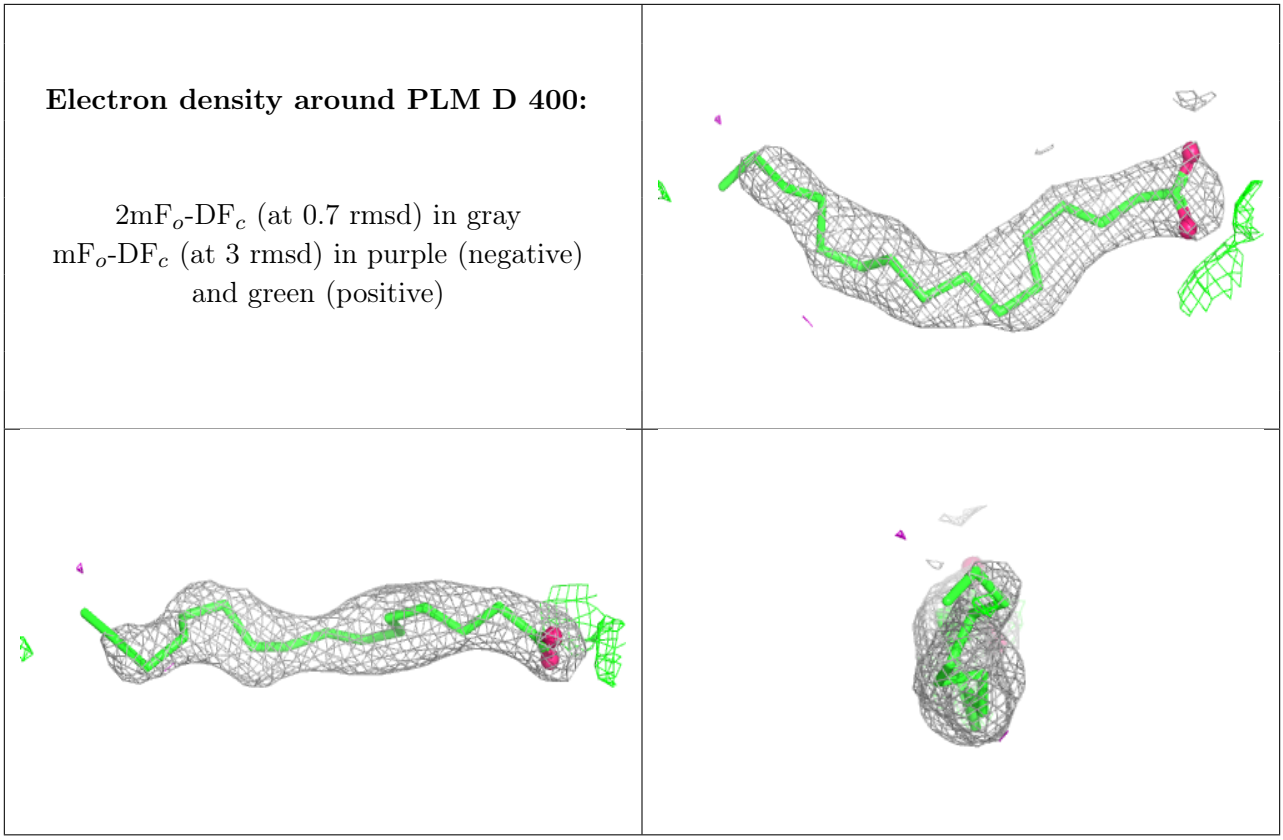






Electron density around PLM D 400:

$2mF_o$-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.