Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 05:43 PM GMT

PDB ID	:	4JAT
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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

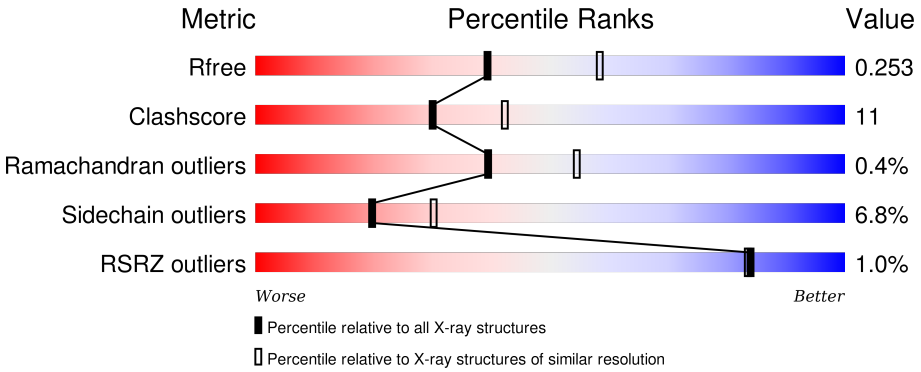
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

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 2.42 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}	91344	3386 (2.44-2.40)
Clashscore	102246	3897 (2.44-2.40)
Ramachandran outliers	100387	3837 (2.44-2.40)
Sidechain outliers	100360	3838 (2.44-2.40)
RSRZ outliers	91569	3396 (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 on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. 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	81% 16%
1	B	353	% 79% 19%
1	C	353	% 73% 24%
1	D	353	% 71% 24%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	PLM	A	400	-	-	-	X
2	PLM	B	400	-	-	-	X
2	PLM	C	400	-	-	-	X
2	PLM	D	400	-	-	-	X

2 Entry composition

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.

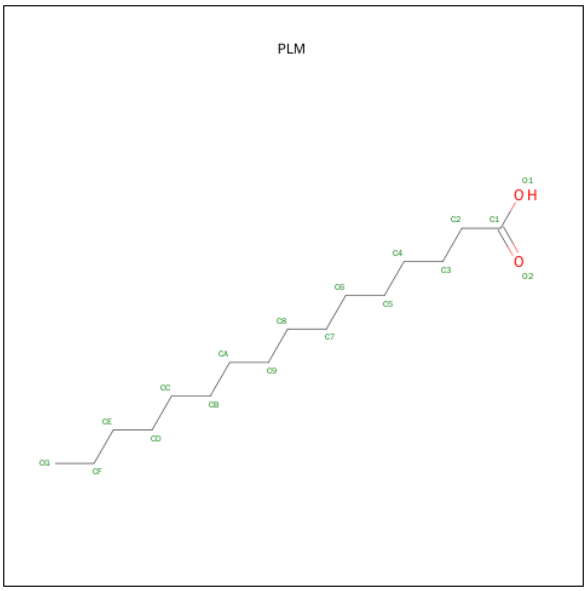
- Molecule 1 is a protein called Alpha-pyrone synthesis polyketide synthase-like Pks11.

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 (three-letter code: 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.

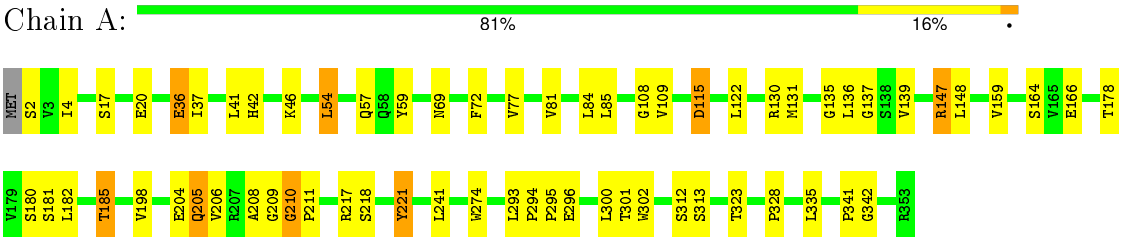
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	69	Total O 69 69	0	0
3	B	83	Total O 83 83	0	0
3	C	71	Total O 71 71	0	0
3	D	71	Total O 71 71	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

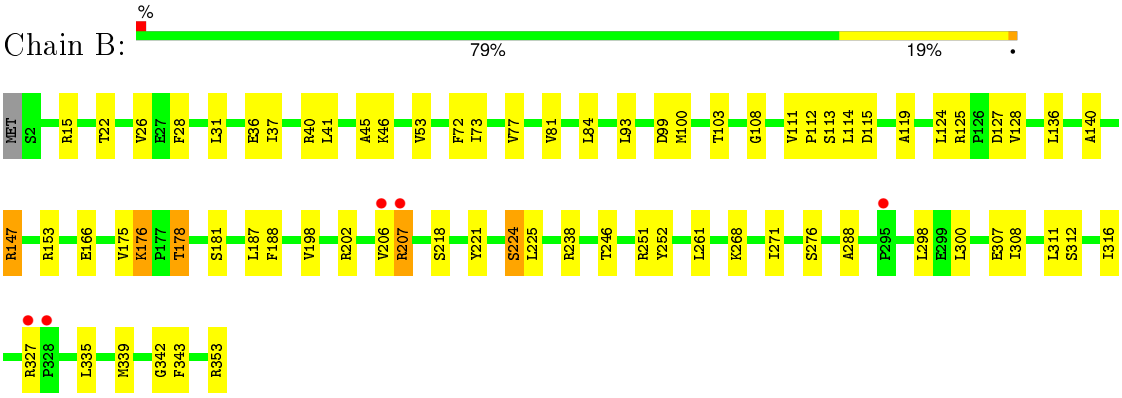
- Molecule 1: Alpha-pyrone synthesis polyketide synthase-like Pks11

Chain A:



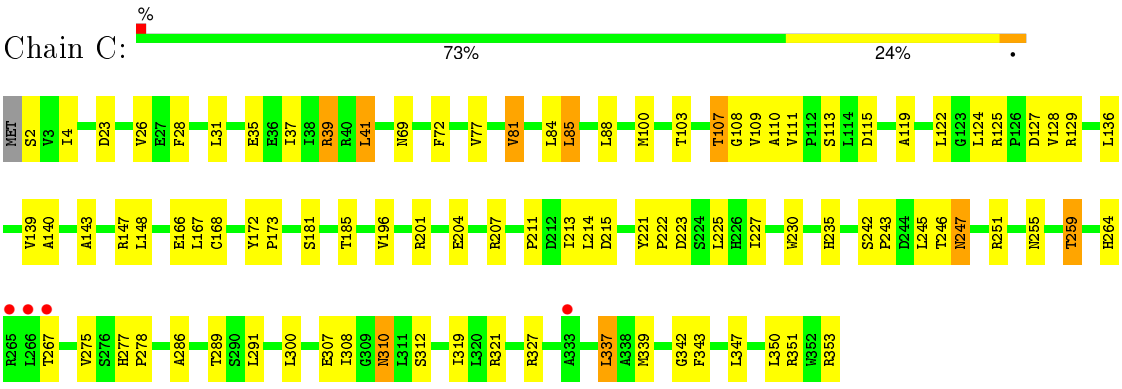
- Molecule 1: Alpha-pyrone synthesis polyketide synthase-like Pks11

Chain B:



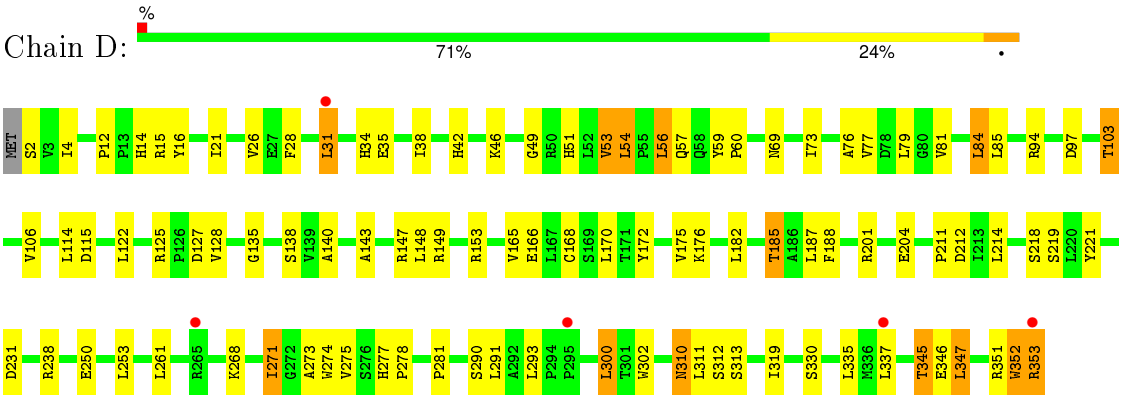
- Molecule 1: Alpha-pyrone synthesis polyketide synthase-like Pks11

Chain C:



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

Chain D:


%
71%
24%
MET S2 V3 I4 P12 P13 H14 R15 Y16 I21 V26 E27 F28 L31 H34 E35 I38 H42 K46 G49 R50 B51 L52 V53 L54 P55 L56 Q57 Q58 Y59 P60 N69 I73 A76 V77 D78 L79 G80 V81 L84 L85 R94 D97 T103
V106 L114 D115 L122 R125 P126 D127 V128 G135 S138 V139 A140 A143 R147 L148 R149 R153 V165 E166 L167 C168 S169 L170 T171 Y172 V175 K176 L182 T185 A186 L187 F188 R201 E204 P211 D212 I213 L214 S218 S219 L220 Y221
D231 R238 E250 L253 L261 R265 K268 T271 G272 A273 W274 V275 S276 H277 P278 P281 S290 L291 A292 L293 P294 P295 L300 T301 W302 N310 L311 S312 S313 I319 S330 L335 M336 L337 T345 E346 L347 R351 W352 R353

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 43.59 – 2.43	Depositor EDS
% Data completeness (in resolution range)	96.5 (37.65-2.42) 96.2 (43.59-2.43)	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 0.196 , 0.253	Depositor DCC
R_{free} test set	2541 reflections (5.10%)	DCC
Wilson B-factor (Å^2)	44.2	Xtriage
Anisotropy	0.216	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 42.8	EDS
Estimated twinning fraction	0.014 for h,-k,-h-l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Outliers	1 of 49843 reflections (0.002%)	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, 0.375 respectively for untwinned datasets, and 0.333, 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	0.45	0/2695	0.53	0/3671
1	B	0.41	0/2695	0.54	0/3671
1	C	0.43	0/2695	0.53	0/3671
1	D	0.45	0/2695	0.56	0/3671
All	All	0.43	0/10780	0.54	0/14684

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	2642	0	2675	40	0
1	B	2642	0	2675	49	0
1	C	2642	0	2675	69	0
1	D	2642	0	2675	86	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	238	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 11.

All (238) 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:C:69:ASN:HD21	1:C:109:VAL:H	1.17	0.88
1:B:166:GLU:HG3	1:B:312:SER:HB3	1.52	0.88
1:D:26:VAL:HG11	1:D:35:GLU:HG3	1.56	0.87
1:B:28:PHE:HB2	1:B:31:LEU:HD12	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:D:42:HIS:NE2	1:D:185:THR:HG23	2.08	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:124:LEU:HB3	1:C:128:VAL:HG21	1.74	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
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:C:246:THR:HG23	1:C:286:ALA:HB2	1.79	0.62
1:B:45:ALA:HB1	1:B:187:LEU:HD23	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:C:310:ASN:HD22	1:C:310:ASN:C	2.02	0.61
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:212:ASP:OD2	1:D:351:ARG:NH2	2.35	0.59
1:D:94:ARG:HB3	1:D:94:ARG:CZ	2.31	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:D:103:THR:HG21	1:D:114:LEU:HB2	1.85	0.58
1:C:289:THR:O	1:C:291:LEU:O	2.22	0.58
1:B:119:ALA:HA	1:B:124:LEU:HG	1.86	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:330:SER:OG	1:D:353:ARG:CB	2.41	0.57
1:D:310:ASN:HD22	1:D:311:LEU:N	2.02	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:C:143:ALA:O	1:C:147:ARG:HG2	2.06	0.54
1:B:308:ILE:HD12	1:B:311:LEU:CD2	2.38	0.54
1:A:166:GLU:HG3	1:A:312:SER:HB3	1.89	0.54
1:C:247:ASN:C	1:C:247:ASN:ND2	2.60	0.54
1:B:22:THR:O	1:B:26:VAL:HG13	2.08	0.54
1:D:46:LYS:HD3	1:D:302:TRP:CZ3	2.43	0.53
1:B:188:PHE:CZ	2:B:400:PLM:H31	2.43	0.53
1:B:77:VAL:O	1:B:81:VAL:HG23	2.07	0.53
1:B:206:VAL:O	1:B:206:VAL:HG12	2.06	0.53
1:C:227:ILE:CG2	1:C:245:LEU:HD13	2.39	0.53
1:D:26:VAL:O	1:D:26:VAL:HG12	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:310:ASN:HD22	1:D:312:SER:H	1.57	0.52
1:D:214:LEU:HD11	1:D:351:ARG:HB2	1.92	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:C:35:GLU:CD	1:C:39:ARG:HH11	2.13	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:B:36:GLU:HG2	1:B:40:ARG:NH1	2.27	0.49
1:B:15:ARG:NH2	1:B:307:GLU:O	2.39	0.49
1:D:46:LYS:HD3	1:D:302:TRP:HZ3	1.77	0.49
1:B:84:LEU:O	1:B:84:LEU:HD12	2.12	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:46:LYS:HD2	1:A:302:TRP:HZ3	1.78	0.49
1:B:93:LEU:HD21	1:B:206:VAL:HG11	1.94	0.49
1:A:115:ASP:OD2	1:A:130:ARG:HB3	2.13	0.49
1:D:310:ASN:HD22	1:D:310:ASN:C	2.16	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:D:274:TRP:CZ3	1:D:335:LEU:HD23	2.48	0.49
1:C:247:ASN:ND2	1:C:251:ARG:HD3	2.28	0.49
1:B:125:ARG:O	1:B:128:VAL:HG23	2.13	0.49
1:D:271:ILE:HD11	1:D:274:TRP:CD1	2.47	0.48
1:D:149:ARG:NH2	1:D:153:ARG:HH11	2.11	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: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:HA	1:B:147:ARG:HD3	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:D:353:ARG:O	1:D:353:ARG:HD3	2.15	0.46
1:C:275:VAL:HG13	1:C:319:ILE:HG22	1.96	0.46
1:C:185:THR:HA	2:C:400:PLM:HB2	1.96	0.46
1:C:307:GLU:HG3	1:C:308:ILE:HG23	1.97	0.46
1:D:166:GLU:CG	1:D:312:SER:HB3	2.43	0.46
1:D:221:TYR:HD1	1:D:221:TYR:N	2.12	0.46
1:B:225:LEU:HD23	1:B:342:GLY:O	2.14	0.46
1:C:353:ARG:HG3	1:C:353:ARG:HH11	1.80	0.46
1:A:323:THR:O	1:A:328:PRO:HD3	2.14	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:4:ILE:HB	1:D:211:PRO:HD2	1.97	0.45
1:B:224:SER:OG	1:B:343:PHE:HB3	2.15	0.45
1:B:73:ILE:O	1:B:77:VAL:HG23	2.16	0.45
1:B:111:VAL:HA	1:B:112:PRO:C	2.36	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:A:57:GLN:CD	1:A:57:GLN:H	2.20	0.45
1:D:300:LEU:HA	1:D:300:LEU:HD12	1.86	0.45
1:D:253:LEU:HD11	1:D:337:LEU:HD11	1.97	0.45
1:D:69:ASN:O	1:D:73:ILE:HG13	2.17	0.45
1:A:178:THR:O	1:A:182:LEU:HG	2.16	0.45
1:C:107:THR:CG2	1:C:107:THR:O	2.64	0.44
1:D:15:ARG:NH1	1:D:49:GLY:HA3	2.32	0.44
1:A:147:ARG:NH2	1:C:129:ARG:HG2	2.32	0.44
1:C:107:THR:HG23	1:C:107:THR:O	2.17	0.44
1:C:72:PHE:CZ	1:C:108:GLY:HA3	2.51	0.44
1:A:85:LEU:HA	1:A:85:LEU:HD23	1.84	0.44
1:A:217:ARG:HD3	3:A:528:HOH:O	2.17	0.44
1:B:46:LYS:HA	1:B:46:LYS:HD3	1.87	0.44
1:C:277:HIS:HA	1:C:278:PRO:HD3	1.70	0.44
1:A:131:MET:HG2	1:A:131:MET:O	2.17	0.43
1:C:213:ILE:HA	1:C:350:LEU:HD23	1.99	0.43
1:B:218:SER:O	1:D:127:ASP:HA	2.18	0.43
1:D:271:ILE:C	1:D:271:ILE:HD12	2.39	0.43
1:C:172:TYR:N	1:C:173:PRO:CD	2.81	0.43
1:D:94:ARG:O	1:D:97:ASP:HB2	2.19	0.43
1:B:37:ILE:O	1:B:41:LEU:HG	2.18	0.43
1:C:215:ASP:OD2	1:C:264:HIS:HE1	2.02	0.43
1:B:268:LYS:HB2	1:B:268:LYS:HE3	1.43	0.43
1:A:137:GLY:O	1:A:313:SER:HB3	2.17	0.43
1:B:238:ARG:HD2	3:B:560:HOH:O	2.16	0.43
1:D:85:LEU:HG	1:D:122:LEU:HD21	2.00	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:D:26:VAL:CG1	1:D:35:GLU:CB	2.96	0.43
1:A:274:TRP:CZ3	1:A:335:LEU:HD23	2.54	0.43
1:D:271:ILE:O	1:D:271:ILE:HG13	2.18	0.43
1:D:103:THR:HG22	3:D:543:HOH:O	2.18	0.43
1:D:277:HIS:ND1	1:D:278:PRO:HD2	2.34	0.43
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4:ILE:HB	1:A:211:PRO:HD2	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:C:72:PHE:CD1	1:C:108:GLY:HA3	2.54	0.42
1:A:180:SER:HB2	1:A:241:LEU:HB3	2.02	0.42
1:D:188:PHE:CZ	2:D:400:PLM:H31	2.55	0.42
1:B:124:LEU:HB3	1:B:128:VAL:HG21	2.00	0.42
1:C:110:ALA:O	1:C:113:SER:HA	2.20	0.42
1:B:288:ALA:HB2	1:B:298:LEU:HD12	2.02	0.42
1:D:261:LEU:HA	1:D:261:LEU:HD23	1.82	0.42
1:D:15:ARG:HB2	1:D:51:HIS:CD2	2.54	0.42
1:A:221:TYR:CD1	1:A:221:TYR:N	2.87	0.42
1:B:221:TYR:N	1:B:221:TYR:CD1	2.88	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:D:59:TYR:N	1:D:60:PRO:CD	2.82	0.42
1:B:72:PHE:CE2	1:B:108:GLY:HA3	2.55	0.42
1:D:140:ALA:HB3	1:D:313:SER:CB	2.50	0.41
1:D:53:VAL:HG13	1:D:54:LEU:HD13	2.01	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:206:VAL:HG23	1:A:208:ALA:N	2.36	0.41
1:A:36:GLU:HG3	1:A:37:ILE:N	2.35	0.41
2:A:400:PLM:H71	2:A:400:PLM:H41	1.79	0.41
1:C:221:TYR:HA	1:C:222:PRO:HD3	1.85	0.41
1:D:271:ILE:HD12	1:D:273:ALA:N	2.19	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:A:17:SER:O	1:A:20:GLU:HB2	2.21	0.41
1:D:218:SER:HA	1:D:346:GLU:OE1	2.21	0.41
1:C:337:LEU:HB2	1:C:347:LEU:CD2	2.51	0.41
1:B:136:LEU:HB2	1:B:140:ALA:HB2	2.03	0.41
1:C:242:SER:HA	1:C:243:PRO:HD3	1.91	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:268:LYS:HE2	1:D:268:LYS:HB3	1.84	0.40
1:D:176:LYS:HD2	1:D:176:LYS:HA	1.71	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:218:SER:O	1:C:127:ASP:HA	2.21	0.40
1:D:201:ARG:HE	1:D:204:GLU:CD	2.25	0.40
1:B:271:ILE:HD12	1:B:335:LEU:HB2	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	350/353 (99%)	338 (97%)	10 (3%)	2 (1%)	30	41
1	B	350/353 (99%)	334 (95%)	15 (4%)	1 (0%)	46	62
1	C	350/353 (99%)	337 (96%)	12 (3%)	1 (0%)	46	62
1	D	350/353 (99%)	335 (96%)	14 (4%)	1 (0%)	46	62
All	All	1400/1412 (99%)	1344 (96%)	51 (4%)	5 (0%)	39	54

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%)	264 (94%)	16 (6%)	25	39
1	B	280/281 (100%)	264 (94%)	16 (6%)	25	39
1	C	280/281 (100%)	257 (92%)	23 (8%)	14	21
1	D	280/281 (100%)	259 (92%)	21 (8%)	17	26
All	All	1120/1124 (100%)	1044 (93%)	76 (7%)	20	30

All (76) 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	185	THR
1	A	204	GLU
1	A	205	GLN
1	A	221	TYR
1	A	300	LEU
1	A	301	THR
1	B	53	VAL
1	B	100	MET
1	B	115	ASP
1	B	147	ARG
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	276	SER
1	B	300	LEU
1	B	316	ILE

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Mol	Chain	Res	Type
1	B	339	MET
1	B	353	ARG
1	C	2	SER
1	C	39	ARG
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	115	ASP
1	C	148	LEU
1	C	181	SER
1	C	204	GLU
1	C	207	ARG
1	C	223	ASP
1	C	235	HIS
1	C	247	ASN
1	C	259	THR
1	C	267	THR
1	C	300	LEU
1	C	310	ASN
1	C	321	ARG
1	C	337	LEU
1	C	339	MET
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
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	310	ASN

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Mol	Chain	Res	Type
1	D	345	THR
1	D	347	LEU
1	D	352	TRP
1	D	353	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	69	ASN
1	A	247	ASN
1	A	318	HIS
1	B	51	HIS
1	B	57	GLN
1	B	205	GLN
1	C	51	HIS
1	C	69	ASN
1	C	247	ASN
1	C	264	HIS
1	C	310	ASN
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

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	PLM	A	400	-	14,17,17	0.21	0	14,17,17	0.77	0
2	PLM	B	400	-	14,17,17	0.26	0	14,17,17	0.64	0
2	PLM	C	400	-	14,17,17	0.19	0	14,17,17	0.75	0
2	PLM	D	400	-	14,17,17	0.30	0	14,17,17	0.96	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	A	400	-	-	0/13/15/15	0/0/0/0
2	PLM	B	400	-	-	0/13/15/15	0/0/0/0
2	PLM	C	400	-	-	0/13/15/15	0/0/0/0
2	PLM	D	400	-	-	0/13/15/15	0/0/0/0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 11 short contacts:

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

5.7 Other polymers (i)

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%)	-0.34	0 100 100	22, 42, 56, 69	0
1	B	352/353 (99%)	-0.25	5 (1%) 78 77	22, 40, 57, 79	0
1	C	352/353 (99%)	-0.27	4 (1%) 82 82	22, 41, 58, 80	0
1	D	352/353 (99%)	-0.18	5 (1%) 78 77	22, 41, 57, 72	0
All	All	1408/1412 (99%)	-0.26	14 (0%) 84 83	22, 41, 57, 80	0

All (14) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	267	THR	4.4
1	B	206	VAL	4.0
1	C	265	ARG	3.3
1	D	353	ARG	2.9
1	C	333	ALA	2.9
1	B	207	ARG	2.8
1	B	327	ARG	2.6
1	B	295	PRO	2.5
1	C	266	LEU	2.5
1	D	295	PRO	2.3
1	D	265	ARG	2.3
1	D	337	LEU	2.2
1	B	328	PRO	2.1
1	D	31	LEU	2.1

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 (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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å^2)	Q<0.9
2	PLM	C	400	18/18	0.85	0.22	5.60	37,43,62,66	0
2	PLM	D	400	18/18	0.84	0.24	5.00	41,45,55,58	0
2	PLM	A	400	18/18	0.85	0.27	3.45	42,49,62,62	0
2	PLM	B	400	18/18	0.87	0.21	2.58	38,46,58,63	0

6.5 Other polymers (i)

There are no such residues in this entry.