



Full wwPDB X-ray Structure Validation Report ⓘ

May 15, 2020 – 04:06 am BST

PDB ID : 3OV3
Title : G211F mutant of curcumin synthase 1 from *Curcuma longa*
Authors : Katsuyama, Y.; Miyazono, K.; Tanokura, M.; Ohnishi, Y.; Horinouchi, S.
Deposited on : 2010-09-15
Resolution : 2.50 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
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

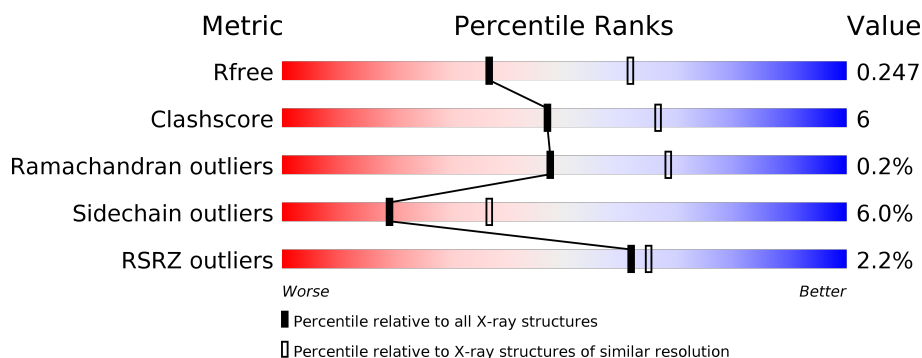
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	393	<div> <div>2%</div> <div> <div></div> <div>83%</div> <div>13%</div> <div>..</div> </div> </div>
1	B	393	<div> <div>3%</div> <div> <div></div> <div>84%</div> <div>13%</div> <div>..</div> </div> </div>
1	C	393	<div> <div>2%</div> <div> <div></div> <div>84%</div> <div>14%</div> <div>..</div> </div> </div>
1	D	393	<div> <div>2%</div> <div> <div></div> <div>82%</div> <div>16%</div> <div>..</div> </div> </div>

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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	MLI	A	396	-	-	X	-
2	MLI	C	395	-	-	X	-
2	MLI	D	394	-	-	X	-
2	MLI	D	395	-	-	X	-

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 12494 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.

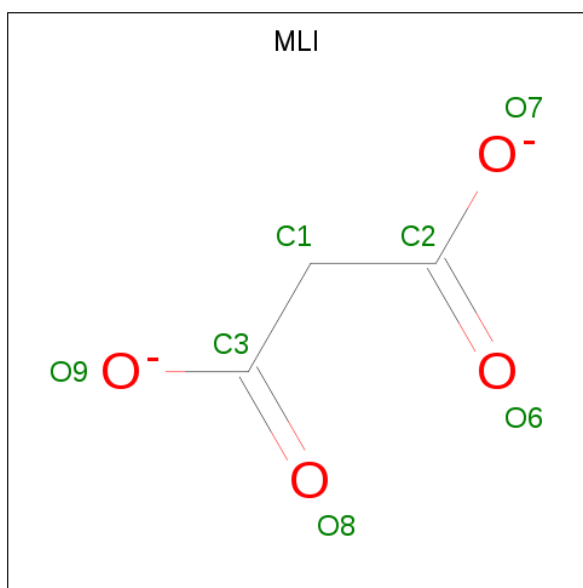
- Molecule 1 is a protein called Curcumin synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	387	Total	C	N	O	S	0	0	0
			3023	1921	532	554	16			
1	B	389	Total	C	N	O	S	0	0	0
			3039	1931	535	557	16			
1	C	391	Total	C	N	O	S	0	0	0
			3059	1943	541	559	16			
1	D	389	Total	C	N	O	S	0	0	0
			3039	1931	535	557	16			

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	211	PHE	GLY	ENGINEERED MUTATION	UNP C0SVZ6
A	390	HIS	-	EXPRESSION TAG	UNP C0SVZ6
A	391	HIS	-	EXPRESSION TAG	UNP C0SVZ6
A	392	HIS	-	EXPRESSION TAG	UNP C0SVZ6
A	393	HIS	-	EXPRESSION TAG	UNP C0SVZ6
B	211	PHE	GLY	ENGINEERED MUTATION	UNP C0SVZ6
B	390	HIS	-	EXPRESSION TAG	UNP C0SVZ6
B	391	HIS	-	EXPRESSION TAG	UNP C0SVZ6
B	392	HIS	-	EXPRESSION TAG	UNP C0SVZ6
B	393	HIS	-	EXPRESSION TAG	UNP C0SVZ6
C	211	PHE	GLY	ENGINEERED MUTATION	UNP C0SVZ6
C	390	HIS	-	EXPRESSION TAG	UNP C0SVZ6
C	391	HIS	-	EXPRESSION TAG	UNP C0SVZ6
C	392	HIS	-	EXPRESSION TAG	UNP C0SVZ6
C	393	HIS	-	EXPRESSION TAG	UNP C0SVZ6
D	211	PHE	GLY	ENGINEERED MUTATION	UNP C0SVZ6
D	390	HIS	-	EXPRESSION TAG	UNP C0SVZ6
D	391	HIS	-	EXPRESSION TAG	UNP C0SVZ6
D	392	HIS	-	EXPRESSION TAG	UNP C0SVZ6
D	393	HIS	-	EXPRESSION TAG	UNP C0SVZ6

- Molecule 2 is MALONATE ION (three-letter code: MLI) (formula: $C_3H_2O_4$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C O 7 3 4	0	0
2	A	1	Total C O 7 3 4	0	0
2	A	1	Total C O 7 3 4	0	0
2	A	1	Total C O 7 3 4	0	0
2	A	1	Total C O 7 3 4	0	0
2	C	1	Total C O 7 3 4	0	0
2	C	1	Total C O 7 3 4	0	0
2	C	1	Total C O 7 3 4	0	0
2	D	1	Total C O 7 3 4	0	0
2	D	1	Total C O 7 3 4	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	62	Total O 62 62	0	0

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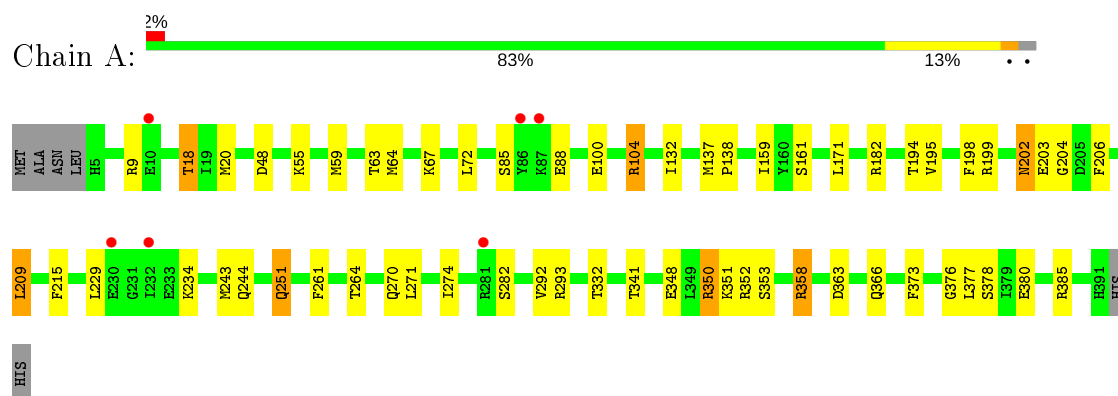
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	66	Total 66	O 66	0	0
3	C	79	Total 79	O 79	0	0
3	D	57	Total 57	O 57	0	0

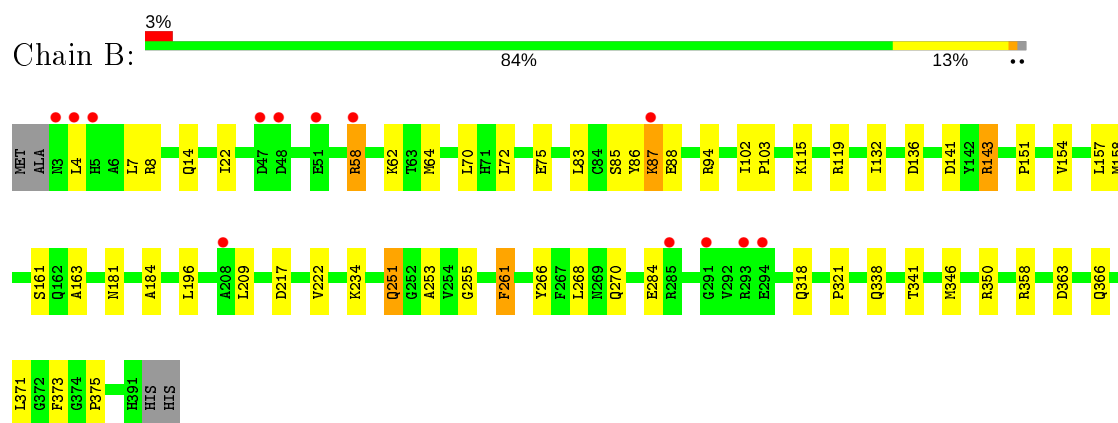
3 Residue-property plots [i](#)

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.

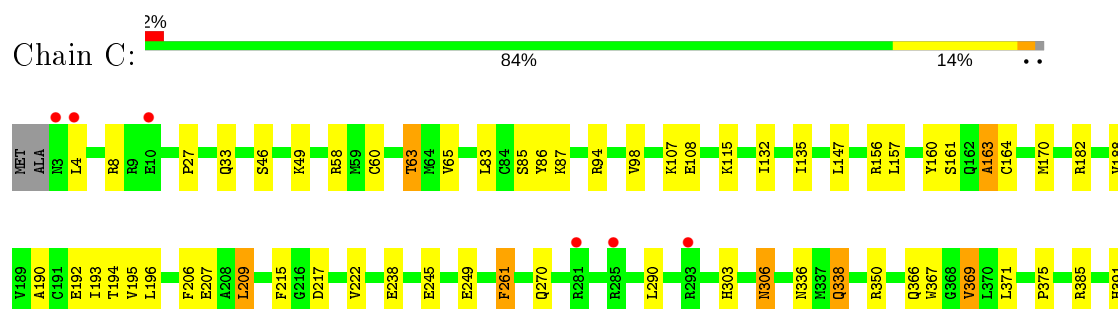
• Molecule 1: Curcumin synthase



• Molecule 1: Curcumin synthase

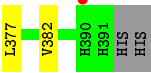
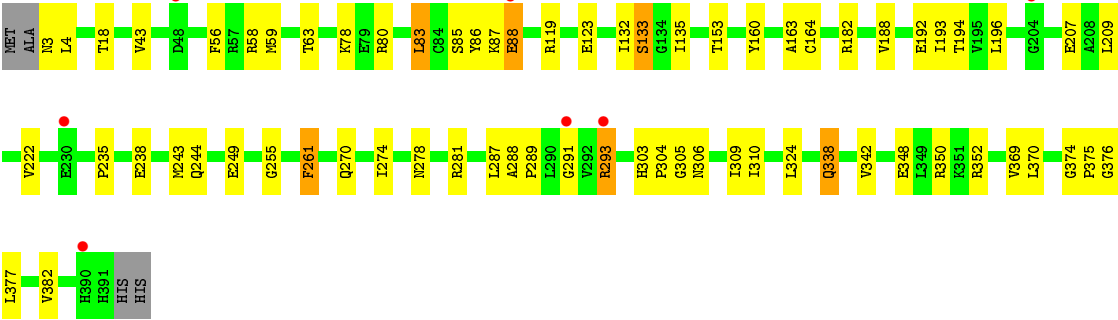
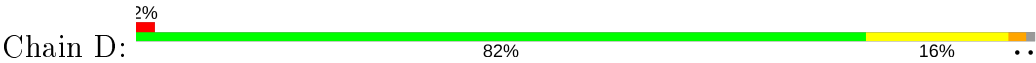


• Molecule 1: Curcumin synthase





● Molecule 1: Curcumin synthase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	76.70Å 116.36Å 221.24Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.90 – 2.50 19.90 – 2.50	Depositor EDS
% Data completeness (in resolution range)	98.4 (19.90-2.50) 98.4 (19.90-2.50)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.96 (at 2.50Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, R_{free}	0.192 , 0.247 0.192 , 0.247	Depositor DCC
R_{free} test set	3451 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å ²)	37.4	Xtriage
Anisotropy	0.148	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 42.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	12494	wwPDB-VP
Average B, all atoms (Å ²)	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.70% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: MLI

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	0.70	0/3088	0.75	0/4178
1	B	0.62	0/3104	0.69	1/4200 (0.0%)
1	C	0.69	0/3126	0.71	0/4230
1	D	0.66	0/3104	0.71	0/4200
All	All	0.67	0/12422	0.72	1/16808 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	119	ARG	NE-CZ-NH2	-5.36	117.62	120.30

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	3023	0	3022	34	0
1	B	3039	0	3039	30	0
1	C	3059	0	3053	42	0
1	D	3039	0	3039	48	0
2	A	35	0	10	4	0
2	C	21	0	6	9	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	14	0	4	9	0
3	A	62	0	0	0	0
3	B	66	0	0	3	0
3	C	79	0	0	1	0
3	D	57	0	0	0	0
All	All	12494	0	12173	150	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 6.

All (150) 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:C:194:THR:HA	2:C:395:MLI:C1	1.71	1.20
1:C:194:THR:HA	2:C:395:MLI:H12	1.20	1.10
1:D:306:ASN:HD22	2:D:394:MLI:H11	1.18	1.06
1:D:194:THR:HA	2:D:395:MLI:H12	1.42	1.01
1:B:251:GLN:H	1:B:251:GLN:HE21	1.05	0.93
1:D:163:ALA:HB3	1:D:375:PRO:HD2	1.51	0.93
1:D:119:ARG:NH2	1:D:123:GLU:HG3	1.88	0.88
1:C:194:THR:HA	2:C:395:MLI:H11	1.56	0.86
1:C:193:ILE:O	2:C:395:MLI:H11	1.75	0.85
1:D:306:ASN:ND2	2:D:394:MLI:H11	1.92	0.84
1:C:194:THR:CA	2:C:395:MLI:H12	2.04	0.82
1:A:251:GLN:HE21	1:A:251:GLN:H	1.27	0.81
1:A:366:GLN:HE21	1:A:385:ARG:HD2	1.47	0.79
1:C:163:ALA:HB3	1:C:375:PRO:HD2	1.64	0.79
1:D:348:GLU:OE2	1:D:352:ARG:HD2	1.83	0.78
1:D:194:THR:HA	2:D:395:MLI:C1	2.14	0.77
1:B:251:GLN:H	1:B:251:GLN:NE2	1.82	0.77
1:A:353:SER:HA	1:A:358:ARG:HG3	1.73	0.70
1:C:156:ARG:H	1:D:244:GLN:NE2	1.90	0.69
1:C:87:LYS:HG2	1:C:261:PHE:CD2	2.29	0.68
1:C:194:THR:CA	2:C:395:MLI:C1	2.64	0.66
1:A:18:THR:CG2	1:A:20:MET:HG3	2.25	0.66
1:C:63:THR:HG23	1:C:65:VAL:H	1.61	0.66
1:A:358:ARG:HD2	1:A:363:ASP:OD1	1.96	0.65
1:C:192:GLU:HG3	1:C:338:GLN:HB2	1.78	0.65
1:C:182:ARG:HD3	3:C:462:HOH:O	1.97	0.65
1:A:194:THR:HA	2:A:396:MLI:H12	1.78	0.64
1:B:22:ILE:HG12	1:B:346:MET:CE	2.28	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:58:ARG:HG2	3:B:454:HOH:O	1.98	0.63
1:A:244:GLN:NE2	1:A:380:GLU:OE2	2.32	0.62
1:D:119:ARG:HH21	1:D:123:GLU:HG3	1.64	0.62
1:A:274:ILE:HG12	2:A:397:MLI:H12	1.82	0.62
1:D:194:THR:CA	2:D:395:MLI:H12	2.24	0.62
1:D:288:ALA:N	1:D:289:PRO:HD2	2.15	0.61
1:B:251:GLN:HE21	1:B:251:GLN:N	1.88	0.61
1:B:85:SER:OG	1:B:88:GLU:HB2	2.01	0.61
1:D:119:ARG:NH2	1:D:123:GLU:CG	2.63	0.60
1:C:86:TYR:O	1:C:87:LYS:HG3	2.03	0.59
1:D:342:VAL:HG21	1:D:370:LEU:HD21	1.84	0.58
1:C:33:GLN:HE21	1:C:63:THR:HG21	1.69	0.58
1:A:85:SER:OG	1:A:88:GLU:HB2	2.03	0.58
1:B:163:ALA:HB3	1:B:375:PRO:HD2	1.86	0.58
1:C:366:GLN:HE21	1:C:385:ARG:HD2	1.69	0.57
1:C:196:LEU:HB2	2:C:395:MLI:O9	2.04	0.57
1:C:170:MET:HE1	1:C:190:ALA:HB2	1.87	0.57
1:A:72:LEU:HG	1:A:195:VAL:HG22	1.86	0.56
1:B:87:LYS:HG3	1:B:261:PHE:CD2	2.40	0.56
1:B:64:MET:HE3	3:B:457:HOH:O	2.05	0.56
1:D:291:GLY:O	1:D:293:ARG:NH1	2.39	0.55
1:B:4:LEU:O	1:B:8:ARG:HB2	2.06	0.54
1:C:193:ILE:C	2:C:395:MLI:H11	2.28	0.54
1:C:60:CYS:O	1:C:63:THR:HG22	2.08	0.54
1:D:18:THR:HG22	1:D:238:GLU:HG2	1.92	0.53
1:A:198:PHE:CD1	1:A:198:PHE:C	2.82	0.52
1:B:83:LEU:HD11	1:B:94:ARG:HG2	1.91	0.52
1:A:48:ASP:HA	2:A:398:MLI:H11	1.91	0.52
1:A:202:ASN:ND2	1:A:204:GLY:H	2.09	0.51
1:B:132:ILE:HA	1:B:161:SER:HA	1.93	0.51
1:D:193:ILE:O	2:D:395:MLI:H12	2.10	0.51
1:C:63:THR:CG2	1:C:65:VAL:H	2.23	0.51
1:D:376:GLY:N	1:D:377:LEU:HA	2.25	0.51
1:D:87:LYS:HD2	1:D:261:PHE:CD2	2.46	0.51
1:C:306:ASN:HD22	1:C:306:ASN:C	2.14	0.50
1:C:196:LEU:HB2	2:C:395:MLI:C3	2.41	0.50
1:B:141:ASP:HB3	1:B:158:MET:HB2	1.93	0.50
1:C:163:ALA:HB3	1:C:375:PRO:CD	2.39	0.50
1:C:94:ARG:O	1:C:98:VAL:HG22	2.11	0.50
1:D:193:ILE:C	2:D:395:MLI:H12	2.33	0.49
1:D:374:GLY:O	1:D:377:LEU:HD12	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:181:ASN:HB2	1:B:184:ALA:HB2	1.95	0.49
1:B:70:LEU:HA	1:B:217:ASP:OD2	2.13	0.49
1:B:358:ARG:HG3	1:B:363:ASP:HA	1.94	0.49
1:A:18:THR:HG22	1:A:20:MET:HG3	1.95	0.48
1:C:206:PHE:O	1:C:209:LEU:HB2	2.14	0.48
1:A:206:PHE:O	1:A:209:LEU:HB2	2.13	0.48
1:A:100:GLU:O	1:A:104:ARG:HD3	2.14	0.48
1:D:188:VAL:HB	1:D:222:VAL:HG22	1.96	0.48
1:D:163:ALA:CB	1:D:375:PRO:HD2	2.33	0.48
1:D:86:TYR:CD2	1:D:87:LYS:HG2	2.49	0.47
1:B:22:ILE:CD1	1:B:346:MET:HE3	2.43	0.47
1:C:290:LEU:HD13	1:C:367:TRP:CD2	2.49	0.47
1:B:102:ILE:HB	1:B:103:PRO:HD3	1.96	0.47
1:C:156:ARG:H	1:D:244:GLN:HE22	1.59	0.47
1:B:163:ALA:HB3	1:B:375:PRO:CD	2.45	0.47
1:B:222:VAL:HG11	1:B:346:MET:HE1	1.97	0.47
1:C:132:ILE:HA	1:C:161:SER:HA	1.96	0.47
1:D:59:MET:O	1:D:63:THR:HG23	2.15	0.47
1:B:94:ARG:HD3	1:B:196:LEU:HA	1.98	0.46
1:D:261:PHE:CD1	1:D:261:PHE:C	2.89	0.46
1:A:132:ILE:HA	1:A:161:SER:HA	1.98	0.46
1:D:192:GLU:HG3	1:D:338:GLN:HB2	1.97	0.46
1:A:9:ARG:HB3	1:A:9:ARG:NH2	2.30	0.46
1:A:182:ARG:HG2	1:A:182:ARG:HH11	1.80	0.46
1:A:59:MET:O	1:A:63:THR:HG23	2.16	0.46
1:A:376:GLY:N	1:A:377:LEU:HA	2.30	0.45
1:D:261:PHE:C	1:D:261:PHE:HD1	2.19	0.45
1:C:369:VAL:CG2	1:C:371:LEU:HD13	2.46	0.45
1:D:304:PRO:HB3	1:D:310:ILE:HD11	1.97	0.45
1:D:370:LEU:HB3	1:D:382:VAL:HB	1.97	0.45
1:A:194:THR:HA	2:A:396:MLI:C1	2.46	0.45
1:B:253:ALA:HA	1:B:268:LEU:HD12	1.98	0.45
1:D:338:GLN:NE2	2:D:395:MLI:O8	2.50	0.45
1:D:287:LEU:HD21	1:D:369:VAL:HG22	1.98	0.45
1:C:238:GLU:OE1	1:D:4:LEU:HD23	2.17	0.45
1:A:194:THR:HG21	1:A:215:PHE:HB3	1.98	0.44
1:A:64:MET:O	1:A:332:THR:HG23	2.17	0.44
1:A:373:PHE:HA	1:A:378:SER:O	2.18	0.44
1:C:135:ILE:HG12	1:C:160:TYR:CD2	2.53	0.44
1:D:133:SER:HB3	1:D:196:LEU:HD12	1.99	0.44
1:B:151:PRO:HD2	1:B:154:VAL:CG2	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:86:TYR:CE2	1:B:87:LYS:HD2	2.53	0.43
1:C:391:HIS:C	1:C:393:HIS:H	2.20	0.43
1:C:83:LEU:CD2	1:C:94:ARG:HG2	2.48	0.43
1:A:159:ILE:HD12	1:B:157:LEU:HD11	2.01	0.43
1:C:188:VAL:HB	1:C:222:VAL:CG2	2.48	0.43
1:D:85:SER:OG	1:D:88:GLU:HB2	2.18	0.43
1:D:86:TYR:CZ	1:D:87:LYS:HE2	2.54	0.43
1:C:27:PRO:HG2	1:C:217:ASP:HB2	2.00	0.43
1:A:171:LEU:HD23	1:A:171:LEU:HA	1.84	0.42
1:B:136:ASP:OD2	1:B:143:ARG:NH2	2.51	0.42
1:A:202:ASN:HD22	1:A:203:GLU:N	2.17	0.42
1:B:115:LYS:NZ	3:B:435:HOH:O	2.49	0.42
1:C:107:LYS:HD3	1:C:147:LEU:HB3	2.01	0.42
1:D:56:PHE:CD1	1:D:59:MET:HE2	2.54	0.42
1:B:255:GLY:HA3	1:B:266:TYR:CZ	2.55	0.42
1:A:137:MET:HA	1:A:138:PRO:C	2.38	0.42
1:D:274:ILE:O	1:D:278:ASN:ND2	2.48	0.42
1:D:164:CYS:HB3	1:D:303:HIS:CE1	2.54	0.42
1:A:293:ARG:HA	1:A:293:ARG:HD2	1.87	0.41
1:D:255:GLY:HA2	1:D:375:PRO:HG3	2.01	0.41
1:A:376:GLY:HA3	1:A:377:LEU:C	2.41	0.41
1:D:18:THR:HB	1:D:235:PRO:HB3	2.03	0.41
1:D:306:ASN:OD1	1:D:309:ILE:HG13	2.19	0.41
1:C:366:GLN:HG2	1:C:367:TRP:CD1	2.56	0.41
1:A:348:GLU:OE2	1:A:352:ARG:NE	2.54	0.41
1:D:80:ARG:HB2	1:D:83:LEU:HD22	2.02	0.41
1:D:135:ILE:HA	1:D:160:TYR:CZ	2.56	0.41
1:D:163:ALA:HB3	1:D:375:PRO:CD	2.37	0.41
1:D:288:ALA:N	1:D:289:PRO:CD	2.84	0.41
1:B:75:GLU:H	1:B:75:GLU:CD	2.23	0.41
1:C:164:CYS:HB3	1:C:303:HIS:CE1	2.55	0.41
1:C:94:ARG:HD3	1:C:196:LEU:HA	2.03	0.41
1:C:215:PHE:HD1	1:C:336:ASN:HB3	1.85	0.41
1:A:350:ARG:HD2	1:A:351:LYS:N	2.36	0.40
1:C:193:ILE:HG22	1:C:195:VAL:HG23	2.02	0.40
1:C:46:SER:HB3	1:C:49:LYS:HD2	2.03	0.40
1:D:135:ILE:HG12	1:D:160:TYR:CD2	2.56	0.40
1:A:198:PHE:CD1	1:A:199:ARG:N	2.89	0.40
1:B:72:LEU:HA	1:B:72:LEU:HD23	1.95	0.40
1:D:132:ILE:HB	2:D:395:MLI:O8	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	385/393 (98%)	369 (96%)	16 (4%)	0	100	100
1	B	387/393 (98%)	373 (96%)	14 (4%)	0	100	100
1	C	389/393 (99%)	369 (95%)	19 (5%)	1 (0%)	41	61
1	D	387/393 (98%)	370 (96%)	15 (4%)	2 (0%)	29	48
All	All	1548/1572 (98%)	1481 (96%)	64 (4%)	3 (0%)	47	68

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	207	GLU
1	C	163	ALA
1	D	305	GLY

5.3.2 Protein sidechains

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	314/319 (98%)	295 (94%)	19 (6%)	18	36
1	B	316/319 (99%)	296 (94%)	20 (6%)	18	34
1	C	318/319 (100%)	300 (94%)	18 (6%)	20	39
1	D	316/319 (99%)	297 (94%)	19 (6%)	19	37
All	All	1264/1276 (99%)	1188 (94%)	76 (6%)	19	37

All (76) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	18	THR
1	A	55	LYS
1	A	67	LYS
1	A	104	ARG
1	A	202	ASN
1	A	209	LEU
1	A	229	LEU
1	A	234	LYS
1	A	243	MET
1	A	251	GLN
1	A	261	PHE
1	A	264	THR
1	A	270	GLN
1	A	271	LEU
1	A	282	SER
1	A	292	VAL
1	A	341	THR
1	A	350	ARG
1	A	358	ARG
1	B	7	LEU
1	B	14	GLN
1	B	58	ARG
1	B	62	LYS
1	B	87	LYS
1	B	143	ARG
1	B	209	LEU
1	B	234	LYS
1	B	251	GLN
1	B	261	PHE
1	B	270	GLN
1	B	284	GLU
1	B	318	GLN
1	B	321	PRO
1	B	338	GLN
1	B	341	THR
1	B	350	ARG
1	B	366	GLN
1	B	371	LEU
1	B	373	PHE
1	C	4	LEU
1	C	8	ARG
1	C	58	ARG
1	C	63	THR

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Mol	Chain	Res	Type
1	C	85	SER
1	C	108	GLU
1	C	115	LYS
1	C	157	LEU
1	C	207	GLU
1	C	209	LEU
1	C	245	GLU
1	C	249	GLU
1	C	261	PHE
1	C	270	GLN
1	C	306	ASN
1	C	338	GLN
1	C	350	ARG
1	C	369	VAL
1	D	3	ASN
1	D	43	VAL
1	D	58	ARG
1	D	78	LYS
1	D	83	LEU
1	D	88	GLU
1	D	133	SER
1	D	153	THR
1	D	182	ARG
1	D	209	LEU
1	D	243	MET
1	D	249	GLU
1	D	261	PHE
1	D	270	GLN
1	D	281	ARG
1	D	293	ARG
1	D	324	LEU
1	D	338	GLN
1	D	350	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	50	GLN
1	A	155	ASN
1	A	202	ASN
1	A	251	GLN
1	A	366	GLN

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Mol	Chain	Res	Type
1	B	202	ASN
1	B	251	GLN
1	B	270	GLN
1	B	366	GLN
1	B	391	HIS
1	C	11	GLN
1	C	202	ASN
1	C	270	GLN
1	C	306	ASN
1	C	366	GLN
1	D	3	ASN
1	D	202	ASN
1	D	244	GLN
1	D	303	HIS
1	D	338	GLN

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 ⓘ

10 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	MLI	A	396	-	0,6,6	0.00	-	0,7,7	0.00	-
2	MLI	C	395	-	0,6,6	0.00	-	0,7,7	0.00	-
2	MLI	A	395	-	0,6,6	0.00	-	0,7,7	0.00	-
2	MLI	A	398	-	0,6,6	0.00	-	0,7,7	0.00	-
2	MLI	A	394	-	0,6,6	0.00	-	0,7,7	0.00	-
2	MLI	D	394	-	0,6,6	0.00	-	0,7,7	0.00	-
2	MLI	C	394	-	0,6,6	0.00	-	0,7,7	0.00	-
2	MLI	A	397	-	0,6,6	0.00	-	0,7,7	0.00	-
2	MLI	D	395	-	0,6,6	0.00	-	0,7,7	0.00	-
2	MLI	C	396	-	0,6,6	0.00	-	0,7,7	0.00	-

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	MLI	A	396	-	-	0/0/4/4	-
2	MLI	C	395	-	-	0/0/4/4	-
2	MLI	A	395	-	-	0/0/4/4	-
2	MLI	A	398	-	-	0/0/4/4	-
2	MLI	A	394	-	-	0/0/4/4	-
2	MLI	D	394	-	-	0/0/4/4	-
2	MLI	C	394	-	-	0/0/4/4	-
2	MLI	A	397	-	-	0/0/4/4	-
2	MLI	D	395	-	-	0/0/4/4	-
2	MLI	C	396	-	-	0/0/4/4	-

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.

6 monomers are involved in 22 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	396	MLI	2	0
2	C	395	MLI	9	0
2	A	398	MLI	1	0
2	D	394	MLI	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	397	MLI	1	0
2	D	395	MLI	7	0

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	387/393 (98%)	-0.45	6 (1%) 72 74	20, 30, 50, 74	0
1	B	389/393 (98%)	-0.26	13 (3%) 46 50	22, 38, 72, 90	0
1	C	391/393 (99%)	-0.37	8 (2%) 65 68	21, 31, 55, 81	0
1	D	389/393 (98%)	-0.30	7 (1%) 68 71	21, 35, 61, 74	0
All	All	1556/1572 (98%)	-0.34	34 (2%) 62 65	20, 33, 63, 90	0

All (34) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	393	HIS	6.3
1	C	281	ARG	4.3
1	D	293	ARG	4.0
1	B	3	ASN	4.0
1	C	3	ASN	3.8
1	C	285	ARG	3.7
1	B	293	ARG	3.6
1	B	291	GLY	3.6
1	B	48	ASP	3.6
1	C	293	ARG	3.5
1	C	392	HIS	3.5
1	D	230	GLU	3.2
1	D	204	GLY	3.1
1	B	285	ARG	3.0
1	B	58	ARG	2.8
1	C	4	LEU	2.7
1	B	4	LEU	2.6
1	B	51	GLU	2.4
1	B	5	HIS	2.3
1	B	294	GLU	2.3
1	A	230	GLU	2.2

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Mol	Chain	Res	Type	RSRZ
1	D	88	GLU	2.2
1	B	47	ASP	2.2
1	D	48	ASP	2.2
1	A	281	ARG	2.2
1	D	390	HIS	2.2
1	A	87	LYS	2.1
1	B	208	ALA	2.1
1	A	232	ILE	2.1
1	C	10	GLU	2.1
1	B	87	LYS	2.1
1	A	86	TYR	2.0
1	D	291	GLY	2.0
1	A	10	GLU	2.0

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	MLI	C	396	7/7	0.60	0.29	75,75,76,76	0
2	MLI	C	394	7/7	0.62	0.34	67,70,71,71	0
2	MLI	A	394	7/7	0.80	0.19	65,66,67,67	0
2	MLI	D	395	7/7	0.81	0.25	51,52,56,60	0
2	MLI	A	395	7/7	0.81	0.22	58,60,62,62	0
2	MLI	A	398	7/7	0.86	0.28	57,59,60,61	0
2	MLI	D	394	7/7	0.90	0.18	82,83,83,84	0
2	MLI	A	397	7/7	0.91	0.25	69,69,73,73	0
2	MLI	A	396	7/7	0.94	0.24	45,47,50,50	0
2	MLI	C	395	7/7	0.96	0.17	53,55,56,58	0

6.5 Other polymers ⓘ

There are no such residues in this entry.