



# Full wwPDB X-ray Structure Validation Report ⓘ

Jun 9, 2025 – 12:16 PM EDT

PDB ID : 9NOM / pdb\_00009nom  
Title : Structure of the NIS synthetase NcdF from nocardichelin biosynthesis  
Authors : Fisk, M.B.; Gulick, A.M.  
Deposited on : 2025-03-10  
Resolution : 2.87 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](mailto: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 Phenix2.0rc1  
Mogul : 2022.3.0, CSD as543be (2022)  
Xtriage (Phenix) : 2.0rc1  
EDS : 3.0  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
CCP4 : 9.0.006 (Gargrove)  
Density-Fitness : 1.0.12  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.43.1

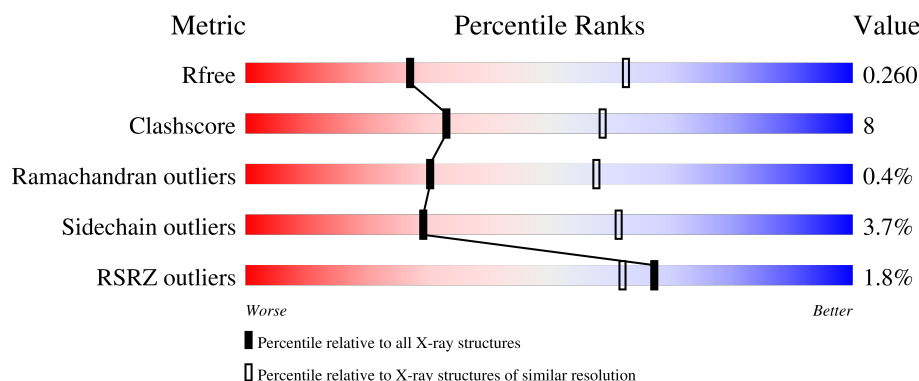
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.87 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))
$R_{free}$	164625	3316 (2.90-2.86)
Clashscore	180529	3609 (2.90-2.86)
Ramachandran outliers	177936	3529 (2.90-2.86)
Sidechain outliers	177891	3532 (2.90-2.86)
RSRZ outliers	164620	3319 (2.90-2.86)

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  $\geq 3$ , 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	612	
1	B	612	

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	MLI	A	701	-	-	X	-

## 2 Entry composition [i](#)

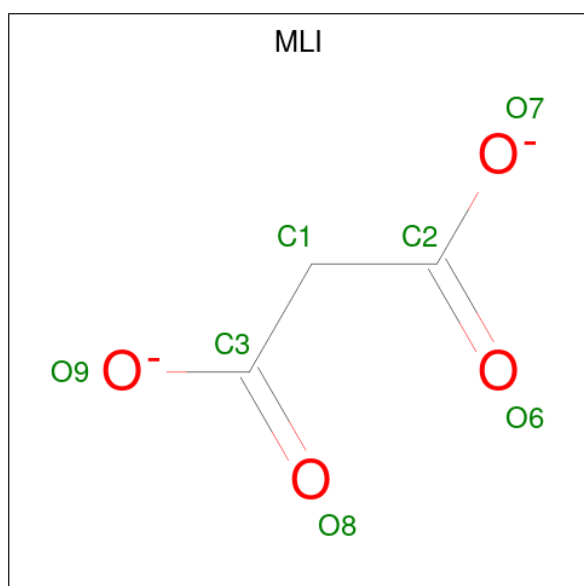
There are 2 unique types of molecules in this entry. The entry contains 9027 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 NcdF, a non-ribosomal independent siderophore synthetase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	574	Total	C	N	O	S	0	1	0
			4501	2862	792	829	18			
1	B	580	Total	C	N	O	S	0	0	0
			4512	2874	784	836	18			

- Molecule 2 is MALONATE ION (CCD ID: MLI) (formula:  $C_3H_2O_4$ ).

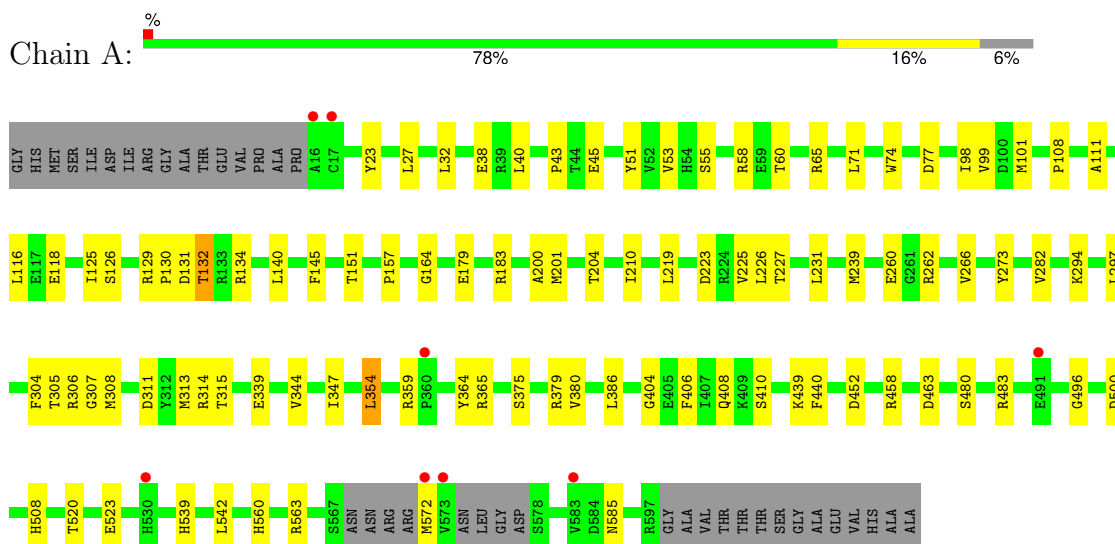


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			7	3	4		
2	B	1	Total	C	O	0	0
			7	3	4		

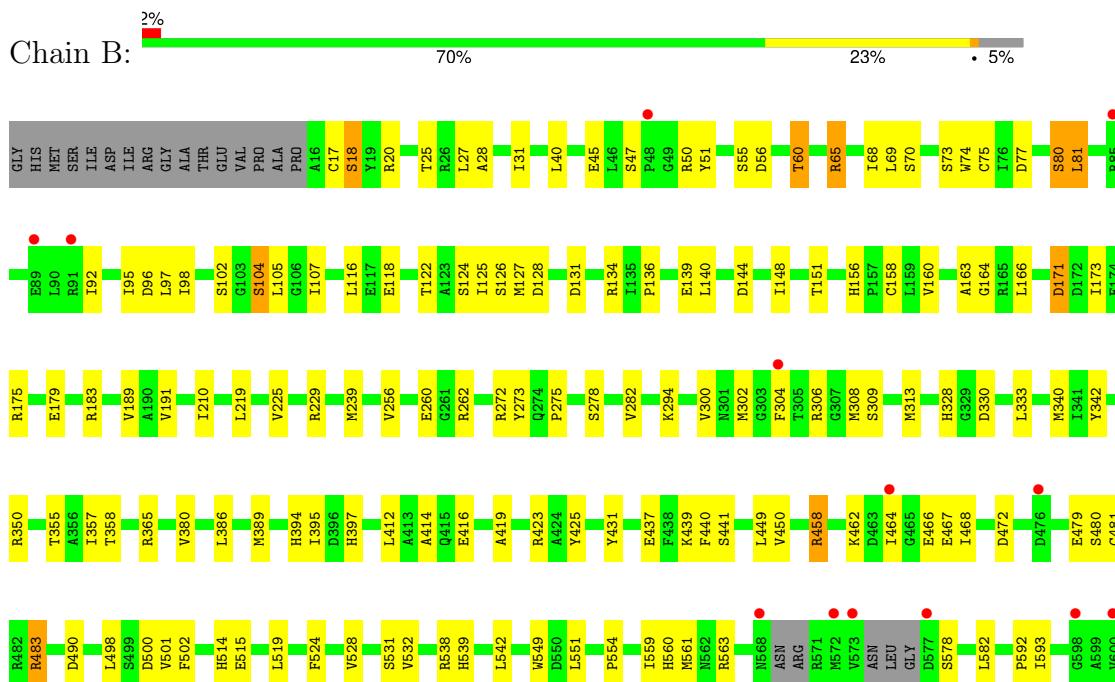
### 3 Residue-property plots

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: NcdF, a non-ribosomal independent siderophore synthetase



- Molecule 1: NcdF, a non-ribosomal independent siderophore synthetase



THR  
THR  
THR  
SER  
GLY  
ALA  
GLU  
VAL  
HIS  
ALA  
ALA

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	84.54Å 118.81Å 168.20Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.70 – 2.87 50.70 – 2.87	Depositor EDS
% Data completeness (in resolution range)	99.7 (50.70-2.87) 90.4 (50.70-2.87)	Depositor EDS
$R_{merge}$	0.33	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.00 (at 2.86Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, $R_{free}$	0.203 , 0.261 0.203 , 0.260	Depositor DCC
$R_{free}$ test set	19005 reflections (47.23%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	43.4	Xtriage
Anisotropy	0.484	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 47.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	9027	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.68% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

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

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.39	0/4610	0.59	0/6278
1	B	0.36	0/4621	0.56	0/6299
All	All	0.37	0/9231	0.58	0/12577

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	4501	0	4356	61	1
1	B	4512	0	4347	77	1
2	A	7	0	2	3	0
2	B	7	0	2	1	0
All	All	9027	0	8707	137	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 8.

All (137) 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:B:539:HIS:HB3	1:B:542:LEU:HD12	1.63	0.79
1:B:18:SER:OG	1:B:131:ASP:OD2	2.06	0.74
1:B:260:GLU:OE1	1:B:262:ARG:NH2	2.24	0.71
1:B:389:MET:HG3	1:B:449:LEU:HD11	1.73	0.69
1:A:304:PHE:HE1	1:A:572:MET:HB2	1.58	0.69
1:A:305:THR:HG22	1:A:307:GLY:H	1.58	0.68
1:B:490:ASP:OD1	1:B:549:TRP:NE1	2.19	0.68
1:B:28:ALA:HA	1:B:31:ILE:HD12	1.75	0.67
1:B:439:LYS:NZ	1:B:500:ASP:OD2	2.30	0.65
1:B:20:ARG:NH1	1:B:128:ASP:OD1	2.29	0.65
1:A:520:THR:N	1:A:523:GLU:OE1	2.25	0.65
1:A:210:ILE:HG23	1:A:219:LEU:HD11	1.80	0.61
1:A:43:PRO:HB3	1:A:53:VAL:HG23	1.81	0.61
1:B:342:TYR:HA	1:B:464:ILE:HD11	1.84	0.60
1:A:38:GLU:OE1	1:A:560:HIS:HB3	2.02	0.60
1:A:404:GLY:O	1:A:408:GLN:HG3	2.02	0.59
1:A:539:HIS:HB3	1:A:542:LEU:HD12	1.83	0.59
1:A:354:LEU:HD22	1:A:364:TYR:HB3	1.83	0.59
1:B:95:ILE:HD12	1:B:95:ILE:H	1.67	0.59
1:B:68:ILE:HD11	1:B:74:TRP:CE3	2.38	0.58
1:B:440:PHE:CE2	1:B:468:ILE:HD12	2.39	0.58
1:B:134:ARG:HB3	1:B:397:HIS:ND1	2.19	0.58
1:B:308:MET:HB3	1:B:313:MET:HE3	1.84	0.58
1:A:201:MET:HE2	1:A:344:VAL:HG12	1.84	0.57
1:A:273:TYR:HB3	1:A:282:VAL:HB	1.85	0.57
1:B:273:TYR:HB3	1:B:282:VAL:HB	1.86	0.57
1:B:414:ALA:HB1	1:B:519:LEU:HB2	1.86	0.57
1:B:25:THR:HG23	1:B:92:ILE:HG21	1.87	0.56
1:B:136:PRO:HG2	1:B:139:GLU:HG3	1.87	0.56
1:B:578:SER:O	1:B:582:LEU:HD12	2.05	0.56
1:B:45:GLU:HB2	1:B:51:TYR:CD2	2.40	0.56
1:A:380:VAL:HG11	1:A:386:LEU:HD21	1.89	0.55
1:B:140:LEU:HD11	1:B:151:THR:HG21	1.87	0.54
1:B:498:LEU:O	1:B:502:PHE:HB2	2.07	0.54
1:B:210:ILE:HG23	1:B:219:LEU:HD11	1.90	0.54
1:A:294:LYS:CE	2:A:701:MLI:H12	2.39	0.52
1:A:116:LEU:HD12	1:B:357:ILE:HD13	1.90	0.52
1:B:333:LEU:HD13	1:B:431:TYR:CD2	2.45	0.52
1:A:294:LYS:HE2	2:A:701:MLI:H12	1.91	0.52
1:A:311:ASP:HA	1:A:314:ARG:NH1	2.25	0.51
1:A:40:LEU:HD21	1:A:563:ARG:HG2	1.93	0.51
1:B:171:ASP:O	1:B:175:ARG:HG3	2.10	0.51

Continued on next page...

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:239:MET:HE3	1:A:347:ILE:HG23	1.92	0.51
1:B:302:MET:C	1:B:304:PHE:H	2.19	0.51
1:A:45:GLU:HG3	1:A:51:TYR:CE2	2.45	0.51
1:B:69:LEU:HB2	1:B:73:SER:HB3	1.93	0.51
1:A:201:MET:HE2	1:A:344:VAL:HA	1.92	0.50
1:B:56:ASP:OD1	1:B:104:SER:OG	2.30	0.50
1:B:166:LEU:HB2	1:B:300:VAL:HB	1.94	0.50
1:A:260:GLU:OE1	1:A:262:ARG:NH1	2.42	0.50
1:B:183:ARG:O	1:B:183:ARG:HG2	2.10	0.49
1:B:462:LYS:O	1:B:464:ILE:HG12	2.12	0.49
1:A:225:VAL:HG11	1:A:266:VAL:HA	1.94	0.49
1:A:201:MET:CE	1:A:344:VAL:HG12	2.43	0.48
1:A:308:MET:HB3	1:A:313:MET:HE3	1.94	0.48
1:B:225:VAL:O	1:B:229:ARG:HG3	2.13	0.48
1:A:439:LYS:NZ	1:A:440:PHE:O	2.45	0.48
1:A:129:ARG:NH2	1:A:179:GLU:HB2	2.28	0.48
1:A:304:PHE:CE1	1:A:572:MET:HB2	2.42	0.48
1:A:55:SER:HA	1:A:101:MET:CE	2.44	0.48
1:B:156:HIS:CE1	1:B:158:CYS:HB2	2.49	0.47
1:A:131:ASP:HA	1:A:134:ARG:HG3	1.95	0.47
1:B:191:VAL:HG21	1:B:239:MET:HE3	1.96	0.47
1:A:55:SER:HB3	1:A:60:THR:HB	1.96	0.47
1:A:496:GLY:O	1:A:500:ASP:HB2	2.14	0.47
1:B:440:PHE:CE2	1:B:464:ILE:HG22	2.51	0.46
1:B:275:PRO:HA	1:B:282:VAL:HG12	1.95	0.46
1:B:437:GLU:CD	1:B:472:ASP:HB2	2.39	0.46
1:A:223:ASP:O	1:A:227:THR:HG23	2.16	0.46
1:B:118:GLU:HG3	1:B:164:GLY:HA3	1.98	0.46
1:B:419:ALA:O	1:B:423:ARG:HG3	2.15	0.46
1:A:125:ILE:HD13	1:A:125:ILE:HA	1.61	0.46
1:B:116:LEU:HD23	1:B:116:LEU:HA	1.83	0.46
1:B:412:LEU:HB3	1:B:416:GLU:HB3	1.98	0.45
1:B:440:PHE:CZ	1:B:468:ILE:HD12	2.51	0.45
1:A:359:ARG:C	1:A:365:ARG:HH21	2.23	0.45
1:A:27:LEU:HD23	1:A:27:LEU:HA	1.53	0.45
1:A:58:ARG:HA	1:A:58:ARG:HD2	1.69	0.45
1:B:125:ILE:HG12	1:B:179:GLU:OE2	2.17	0.45
1:B:55:SER:HB3	1:B:60:THR:HB	1.99	0.45
1:B:20:ARG:NH1	1:B:127:MET:HE3	2.32	0.45
1:B:183:ARG:HA	1:B:273:TYR:O	2.16	0.45
1:B:479:GLU:C	1:B:481:CYS:H	2.24	0.45

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:65:ARG:NH2	1:A:77:ASP:OD2	2.48	0.44
1:A:406:PHE:O	1:A:410:SER:HB3	2.18	0.44
1:B:105:LEU:HB3	1:B:107:ILE:HG13	1.99	0.44
1:B:528:VAL:O	1:B:532:VAL:HG23	2.17	0.44
1:B:75:CYS:SG	1:B:515:GLU:HB3	2.58	0.44
1:A:108:PRO:O	1:A:111:ALA:N	2.40	0.44
1:A:71:LEU:HD23	1:A:71:LEU:HA	1.89	0.44
1:A:130:PRO:HB2	1:A:132:THR:CG2	2.48	0.44
1:B:81:LEU:HB3	1:B:92:ILE:HG13	2.00	0.43
1:B:340:MET:HE3	1:B:340:MET:HB2	1.81	0.43
1:A:463:ASP:CG	2:A:701:MLI:H11	2.43	0.43
1:B:380:VAL:HG11	1:B:386:LEU:HD21	2.00	0.43
1:A:118:GLU:HG3	1:A:164:GLY:HA3	2.01	0.43
1:A:200:ALA:HB1	1:A:204:THR:HB	2.00	0.43
1:B:122:THR:HA	1:B:163:ALA:HB3	2.00	0.43
1:A:32:LEU:HA	1:A:32:LEU:HD23	1.63	0.43
1:B:70:SER:HB3	1:B:592:PRO:HB3	2.00	0.43
1:B:524:PHE:O	1:B:528:VAL:HG23	2.19	0.43
1:B:538:ARG:HG2	1:B:538:ARG:O	2.19	0.43
1:A:297:LEU:O	1:A:306:ARG:HB2	2.18	0.42
1:A:339:GLU:OE1	1:A:458:ARG:NH1	2.52	0.42
1:B:441:SER:OG	1:B:467:GLU:OE1	2.29	0.42
1:A:226:LEU:HD12	1:A:231:LEU:HD12	1.99	0.42
1:B:50:ARG:HD2	1:B:65:ARG:HB3	2.02	0.42
1:A:99:VAL:HG22	1:A:116:LEU:HD11	2.01	0.42
1:B:144:ASP:O	1:B:148:ILE:HG13	2.20	0.42
1:B:219:LEU:HA	1:B:219:LEU:HD23	1.59	0.42
1:B:134:ARG:HB3	1:B:397:HIS:CE1	2.54	0.42
1:B:466:GLU:HA	1:B:483:ARG:NH2	2.35	0.42
1:B:560:HIS:HB3	1:B:563:ARG:HG3	2.01	0.42
1:A:140:LEU:HD11	1:A:151:THR:HG21	2.02	0.42
1:A:226:LEU:HD12	1:A:226:LEU:HA	1.73	0.42
1:A:315:THR:OG1	1:A:483:ARG:NH2	2.45	0.42
1:B:306:ARG:NH1	1:B:306:ARG:HG2	2.35	0.41
1:A:23:TYR:CD1	1:A:126:SER:HB3	2.55	0.41
1:B:40:LEU:HD23	1:B:563:ARG:NH1	2.35	0.41
1:B:309:SER:HA	1:B:365:ARG:O	2.21	0.41
1:B:358:THR:O	1:B:365:ARG:NH2	2.54	0.41
1:B:69:LEU:HD11	1:B:514:HIS:HD2	1.85	0.41
1:A:38:GLU:O	1:A:563:ARG:NH1	2.53	0.41
1:A:125:ILE:HD12	1:A:179:GLU:HG3	2.03	0.41

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:77:ASP:HB3	1:B:80:SER:HB3	2.02	0.41
1:B:559:ILE:HG22	1:B:561:MET:HE2	2.01	0.41
1:A:239:MET:HB3	1:A:347:ILE:HD13	2.03	0.41
1:B:294:LYS:NZ	2:B:701:MLI:H11	2.35	0.41
1:B:425:TYR:OH	1:B:501:VAL:HG13	2.21	0.41
1:A:43:PRO:HG2	1:A:74:TRP:CH2	2.56	0.41
1:A:130:PRO:HB2	1:A:132:THR:HG23	2.02	0.41
1:B:394:HIS:C	1:B:395:ILE:HG13	2.46	0.41
1:B:551:LEU:O	1:B:593:ILE:HD11	2.21	0.41
1:A:157:PRO:HB2	1:A:508:HIS:CD2	2.56	0.41
1:B:450:VAL:HB	1:B:458:ARG:HG2	2.03	0.40
1:A:116:LEU:HD23	1:A:116:LEU:HA	1.85	0.40
1:A:183:ARG:HA	1:A:273:TYR:O	2.21	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:A:452:ASP:O	1:B:272:ARG:NH2[4_445]	2.19	0.01

## 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	569/612 (93%)	537 (94%)	31 (5%)	1 (0%)	44	71
1	B	574/612 (94%)	530 (92%)	41 (7%)	3 (0%)	25	53
All	All	1143/1224 (93%)	1067 (93%)	72 (6%)	4 (0%)	30	63

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	145	PHE
1	B	328	HIS
1	B	330	ASP
1	B	554	PRO

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	464/509 (91%)	457 (98%)	7 (2%)	60	84
1	B	462/509 (91%)	435 (94%)	27 (6%)	17	43
All	All	926/1018 (91%)	892 (96%)	34 (4%)	29	61

All (34) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	98	ILE
1	A	132	THR
1	A	354	LEU
1	A	375	SER
1	A	379	ARG
1	A	480	SER
1	A	585	ASN
1	B	17	CYS
1	B	18	SER
1	B	27	LEU
1	B	47	SER
1	B	60	THR
1	B	65	ARG
1	B	80	SER
1	B	81	LEU
1	B	96	ASP
1	B	97	LEU
1	B	98	ILE
1	B	102	SER
1	B	104	SER

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	B	124	SER
1	B	126	SER
1	B	160	VAL
1	B	171	ASP
1	B	173	ILE
1	B	189	VAL
1	B	256	VAL
1	B	278	SER
1	B	350	ARG
1	B	355	THR
1	B	458	ARG
1	B	480	SER
1	B	483	ARG
1	B	531	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	195	ASN
1	A	277	GLN
1	A	408	GLN
1	A	443	HIS
1	B	37	HIS
1	B	146	GLN
1	B	276	GLN
1	B	277	GLN
1	B	514	HIS
1	B	548	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 oligosaccharides in this entry.

## 5.6 Ligand geometry

2 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	B	701	-	6,6,6	1.39	0	7,7,7	0.95	0
2	MLI	A	701	-	6,6,6	1.30	0	7,7,7	1.01	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	MLI	B	701	-	-	4/4/4/4	-
2	MLI	A	701	-	-	2/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	701	MLI	C3-C1-C2-O6
2	A	701	MLI	C3-C1-C2-O7
2	B	701	MLI	C3-C1-C2-O7
2	B	701	MLI	C2-C1-C3-O9
2	B	701	MLI	C3-C1-C2-O6
2	B	701	MLI	C2-C1-C3-O8

There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	701	MLI	1	0
2	A	701	MLI	3	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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	574/612 (93%)	-0.09	8 (1%) 73 68	21, 43, 63, 81	1 (0%)
1	B	580/612 (94%)	0.18	13 (2%) 62 56	31, 50, 73, 87	0
All	All	1154/1224 (94%)	0.05	21 (1%) 67 62	21, 46, 70, 87	1 (0%)

All (21) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	577	ASP	3.8
1	A	573	VAL	3.7
1	B	573	VAL	3.4
1	B	600	VAL	3.4
1	A	530[A]	HIS	2.9
1	B	89	GLU	2.8
1	A	16	ALA	2.7
1	B	85	ARG	2.6
1	B	464	ILE	2.6
1	B	568	ASN	2.4
1	A	583	VAL	2.3
1	A	360	PRO	2.3
1	A	572	MET	2.2
1	B	304	PHE	2.2
1	B	48	PRO	2.1
1	B	476	ASP	2.1
1	A	491	GLU	2.1
1	B	598	GLY	2.1
1	B	572	MET	2.0
1	B	91	ARG	2.0
1	A	17	CYS	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 monosaccharides 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<sup>th</sup> 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( $\text{\AA}^2$ )	Q<0.9
2	MLI	B	701	7/7	0.77	0.15	42,53,58,63	0
2	MLI	A	701	7/7	0.78	0.15	45,54,62,65	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.