



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 11:21 AM UTC

PDB ID : 7YLQ / pdb_00007ylq
Title : Crystal structure of Microcystinase C from *Sphingomonas* sp. ACM-3962 at 2.6 Å resolution
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Deposited on : 2022-07-26
Resolution : 2.68 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
Xtriage (Phenix)	:	2.0
EDS	:	3.0
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

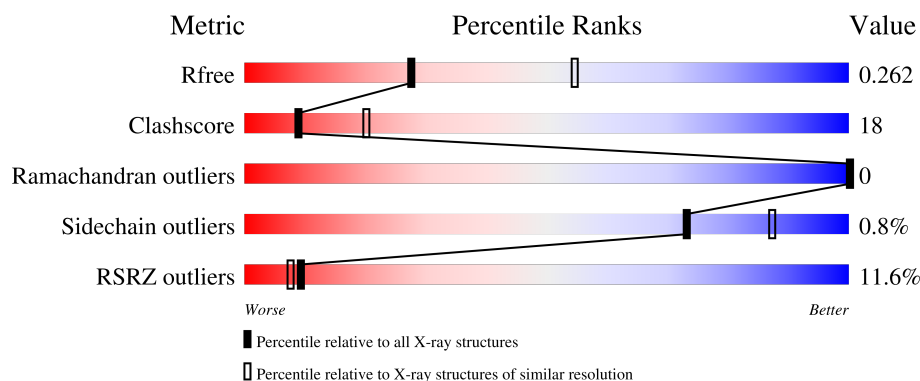
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.68 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	5070 (2.70-2.66)
Clashscore	190562	5409 (2.70-2.66)
Ramachandran outliers	187476	5324 (2.70-2.66)
Sidechain outliers	187428	5324 (2.70-2.66)
RSRZ outliers	180081	5070 (2.70-2.66)

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 $\leq 5\%$. 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	512	3% 71% 23% 6%
1	B	512	19% 53% 39% 8%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 7379 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 Microcystinase C.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	480	Total	C	N	O	S	0	2	0
			3688	2316	663	689	20			
1	B	471	Total	C	N	O	S	0	0	0
			3597	2261	643	672	21			

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	508	LEU	-	expression tag	UNP Q93CA6
A	509	GLU	-	expression tag	UNP Q93CA6
A	510	HIS	-	expression tag	UNP Q93CA6
A	511	HIS	-	expression tag	UNP Q93CA6
A	512	HIS	-	expression tag	UNP Q93CA6
B	508	LEU	-	expression tag	UNP Q93CA6
B	509	GLU	-	expression tag	UNP Q93CA6
B	510	HIS	-	expression tag	UNP Q93CA6
B	511	HIS	-	expression tag	UNP Q93CA6
B	512	HIS	-	expression tag	UNP Q93CA6

- Molecule 2 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	2	Total	Zn	0	0
			2	2		
2	B	1	Total	Zn	0	0
			1	1		

- Molecule 3 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	Ca	0	0
			1	1		

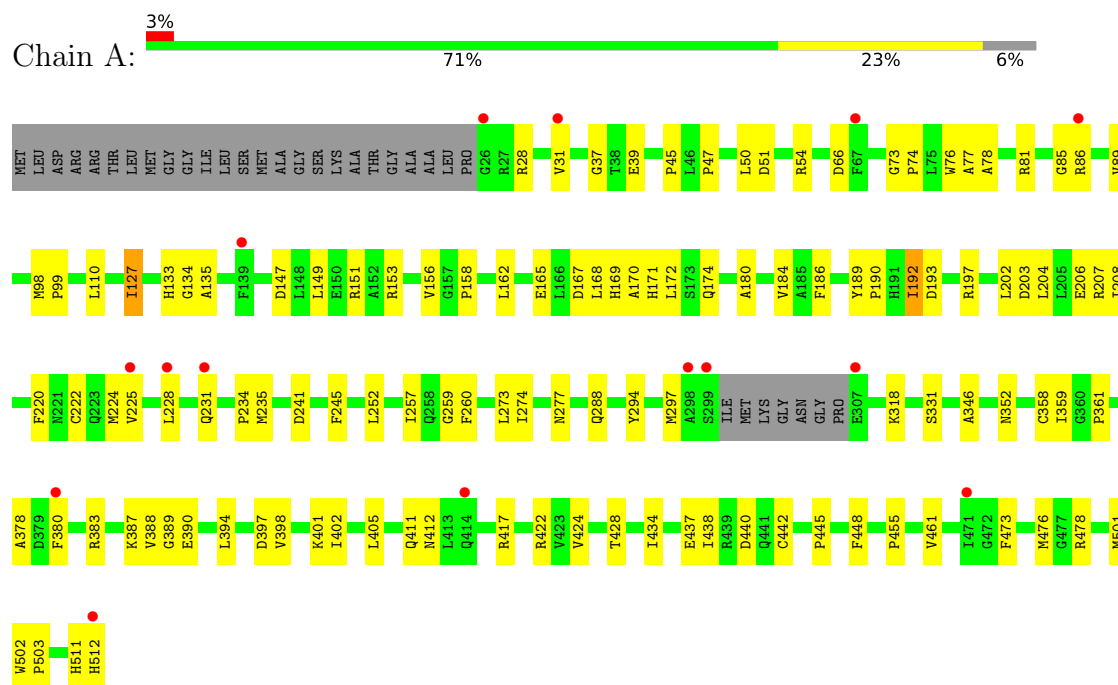
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	69	Total 69	O 69	0	0
4	B	21	Total 21	O 21	0	0

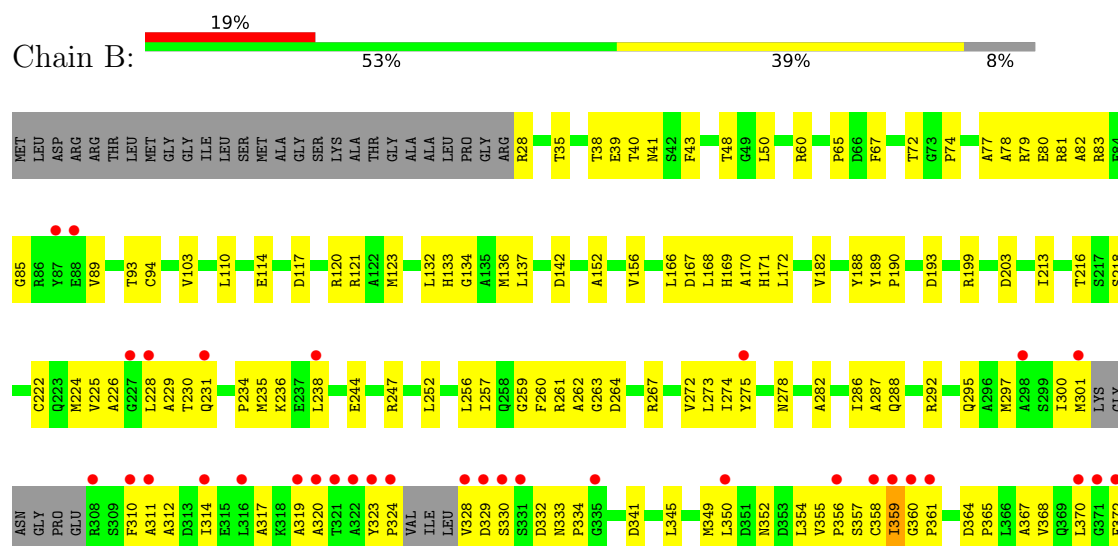
3 Residue-property plots [i](#)

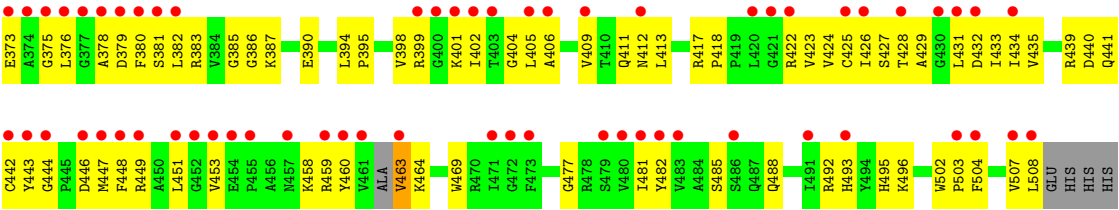
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Microcystinase C



• Molecule 1: Microcystinase C





4 Data and refinement statistics

Property	Value	Source
Space group	P 61 2 2	Depositor
Cell constants a, b, c, α , β , γ	138.43Å 138.43Å 275.57Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	48.83 – 2.68 48.83 – 2.68	Depositor EDS
% Data completeness (in resolution range)	99.8 (48.83-2.68) 99.8 (48.83-2.68)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.13 (at 2.69Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.231 , 0.264 0.232 , 0.262	Depositor DCC
R_{free} test set	2202 reflections (4.94%)	wwPDB-VP
Wilson B-factor (Å ²)	59.4	Xtriage
Anisotropy	0.561	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 45.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	7379	wwPDB-VP
Average B, all atoms (Å ²)	72.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.99% 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: ZN, CA

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	0.77	1/3763 (0.0%)	1.09	2/5098 (0.0%)
1	B	0.79	0/3667	1.07	2/4964 (0.0%)
All	All	0.78	1/7430 (0.0%)	1.08	4/10062 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	127	ILE	C-N	-5.49	1.26	1.33

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	375	GLY	CA-C-O	-6.25	117.92	122.23
1	A	192	ILE	N-CA-C	-5.69	107.95	113.53
1	A	259	GLY	CA-C-O	-5.37	118.28	122.52
1	B	259	GLY	CA-C-O	-5.30	118.33	122.52

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	3688	0	3639	93	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	3597	0	3559	184	0
2	A	2	0	0	0	0
2	B	1	0	0	0	0
3	B	1	0	0	0	0
4	A	69	0	0	17	0
4	B	21	0	0	9	0
All	All	7379	0	7198	268	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 18.

All (268) 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:381:SER:HA	1:B:399:ARG:HA	1.42	1.00
1:B:432:ASP:HB2	4:B:706:HOH:O	1.65	0.95
1:B:234:PRO:HG2	1:B:297:MET:HG2	1.52	0.91
1:B:376:LEU:HA	1:B:402:ILE:HD11	1.52	0.90
1:A:228[A]:LEU:HD21	1:A:234:PRO:HD2	1.55	0.87
1:A:478:ARG:HG3	4:A:862:HOH:O	1.75	0.84
1:B:394:LEU:HD12	1:B:395:PRO:HD2	1.62	0.81
1:A:172:LEU:HD12	1:A:257:ILE:HG13	1.63	0.81
1:B:378:ALA:H	1:B:402:ILE:HG13	1.45	0.81
1:B:323:TYR:HB3	1:B:324:PRO:HD3	1.64	0.80
1:B:38:THR:HG22	1:B:136:MET:HG3	1.65	0.79
1:B:35:THR:HG21	1:B:72:THR:HG22	1.65	0.78
1:B:311:ALA:O	1:B:314:ILE:HG12	1.84	0.78
1:A:422:ARG:HD3	4:A:812:HOH:O	1.84	0.78
1:B:43:PHE:CE1	1:B:492:ARG:HB3	2.21	0.75
1:B:352:ASN:HB2	1:B:354:LEU:HG	1.67	0.75
1:A:445:PRO:HD2	4:A:855:HOH:O	1.86	0.74
1:B:361:PRO:HD2	1:B:464:LYS:HB2	1.70	0.74
1:B:300:ILE:HD12	1:B:300:ILE:H	1.53	0.73
1:A:47:PRO:HB2	1:B:373:GLU:HG2	1.70	0.72
1:A:383:ARG:NE	4:A:803:HOH:O	2.24	0.71
1:B:28:ARG:NH2	1:B:85:GLY:HA2	2.06	0.71
1:B:244:GLU:OE2	1:B:247:ARG:NH2	2.24	0.69
1:A:234:PRO:HG2	1:A:297:MET:HE3	1.73	0.69
1:B:358:CYS:SG	1:B:458:LYS:HG3	2.33	0.69
1:B:359:ILE:CG2	1:B:433:ILE:HA	2.23	0.69
1:B:349:MET:HE2	1:B:431:LEU:HD22	1.75	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:447:MET:HG3	1:B:448:PHE:H	1.57	0.67
1:A:169:HIS:CE1	4:A:810:HOH:O	2.48	0.67
1:B:368:VAL:HG23	1:B:435:VAL:HG12	1.78	0.66
1:A:39:GLU:HG3	1:A:133:HIS:NE2	2.10	0.65
1:B:234:PRO:HG2	1:B:297:MET:CG	2.26	0.65
1:B:379:ASP:HA	1:B:401:LYS:HA	1.79	0.65
1:B:381:SER:CA	1:B:399:ARG:HA	2.22	0.65
1:B:50:LEU:HD11	1:B:110:LEU:HD23	1.79	0.65
1:A:39:GLU:HG3	1:A:133:HIS:CE1	2.32	0.64
1:B:231:GLN:O	1:B:236:LYS:HD2	1.98	0.64
1:B:345:LEU:HB3	4:B:707:HOH:O	1.96	0.64
1:A:153:ARG:HH11	1:A:158:PRO:HA	1.63	0.64
1:B:402:ILE:HA	1:B:426:ILE:HA	1.80	0.64
1:A:511:HIS:O	1:A:512:HIS:HB2	1.96	0.63
1:B:376:LEU:CA	1:B:402:ILE:HD11	2.26	0.63
1:B:453:VAL:HG13	1:B:458:LYS:HE3	1.81	0.63
1:B:359:ILE:HG21	1:B:433:ILE:HG23	1.81	0.63
1:B:439:ARG:NE	4:B:702:HOH:O	2.25	0.63
1:B:310:PHE:O	1:B:314:ILE:HG23	1.99	0.62
1:A:31:VAL:HG22	1:A:127:ILE:HB	1.80	0.62
1:A:174:GLN:HB3	4:A:859:HOH:O	1.99	0.62
1:B:349:MET:HE3	1:B:357:SER:HB2	1.81	0.61
1:B:359:ILE:HG21	1:B:433:ILE:HA	1.81	0.61
1:A:422:ARG:CD	4:A:812:HOH:O	2.46	0.61
1:B:441:GLN:HE21	1:B:443:TYR:HE1	1.45	0.61
1:A:47:PRO:HD3	1:B:370:LEU:HD22	1.83	0.61
1:B:256:LEU:HD23	1:B:272:VAL:HG13	1.82	0.61
1:B:350:LEU:HD21	1:B:431:LEU:HD23	1.81	0.61
1:B:507:VAL:O	1:B:508:LEU:C	2.43	0.61
1:B:412:ASN:HB2	1:B:417:ARG:NH1	2.17	0.60
1:A:405:LEU:CD2	1:A:424:VAL:HG22	2.32	0.60
1:B:80:GLU:HG2	1:B:83:ARG:HH12	1.67	0.60
1:A:172:LEU:N	4:A:802:HOH:O	2.22	0.59
1:B:40:THR:HG21	1:B:137:LEU:HB2	1.83	0.59
1:A:228[A]:LEU:HD23	1:A:235:MET:HB2	1.83	0.59
1:A:390:GLU:HA	1:B:383:ARG:HH12	1.67	0.59
1:B:355:VAL:HA	1:B:356:PRO:C	2.28	0.59
1:A:45:PRO:HG2	1:A:388:VAL:HG12	1.86	0.58
1:B:189:TYR:HA	1:B:190:PRO:C	2.28	0.58
1:A:412:ASN:HB2	1:A:417:ARG:NH1	2.18	0.58
1:A:501:MET:HE1	4:A:816:HOH:O	2.02	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:328:VAL:HG23	1:B:330:SER:H	1.69	0.58
1:A:153:ARG:HA	1:A:156:VAL:HG22	1.84	0.57
1:B:171:HIS:HE2	1:B:260:PHE:HB3	1.68	0.57
1:B:171:HIS:HB3	1:B:267:ARG:HG3	1.85	0.57
1:B:361:PRO:HD3	1:B:442:CYS:HB2	1.85	0.57
1:B:350:LEU:CD2	1:B:431:LEU:HD23	2.35	0.56
1:A:411:GLN:O	1:A:417:ARG:HA	2.05	0.56
1:B:81:ARG:HH21	1:B:199:ARG:HB3	1.71	0.56
1:A:135:ALA:HA	1:A:171:HIS:CD2	2.41	0.56
1:B:235:MET:HE1	1:B:238:LEU:HD23	1.86	0.56
1:B:228:LEU:HD12	1:B:229:ALA:O	2.06	0.55
1:B:172:LEU:HD22	1:B:257:ILE:HG13	1.87	0.55
1:B:264:ASP:CG	1:B:495:HIS:H	2.14	0.55
1:B:446:ASP:HA	1:B:449:ARG:HD2	1.88	0.55
1:B:297:MET:HA	1:B:300:ILE:HD13	1.89	0.55
1:A:318:LYS:HE2	1:A:352:ASN:HB3	1.88	0.55
1:B:332:ASP:OD2	1:B:341:ASP:N	2.41	0.54
1:B:359:ILE:HG23	1:B:360:GLY:N	2.20	0.54
1:B:406:ALA:HB1	1:B:409:VAL:HG23	1.89	0.54
1:A:390:GLU:HA	1:B:383:ARG:NH1	2.22	0.54
1:B:442:CYS:HB3	1:B:463:VAL:HG13	1.89	0.54
1:A:358:CYS:SG	1:A:461:VAL:HG13	2.48	0.54
1:B:228:LEU:HD11	1:B:235:MET:HB2	1.88	0.54
1:A:380:PHE:HE1	1:A:402:ILE:HD11	1.73	0.54
1:B:381:SER:HA	1:B:399:ARG:CA	2.29	0.53
1:B:35:THR:HG22	4:B:720:HOH:O	2.09	0.53
1:A:172:LEU:HD11	1:A:273:LEU:HD22	1.91	0.53
1:B:168:LEU:HD21	1:B:189:TYR:HB2	1.90	0.53
1:B:167:ASP:OD1	1:B:168:LEU:N	2.42	0.53
1:A:31:VAL:HA	1:A:127:ILE:O	2.08	0.52
1:A:383:ARG:NH1	1:B:390:GLU:HA	2.25	0.52
1:B:38:THR:CG2	1:B:136:MET:HG3	2.36	0.52
1:B:447:MET:HG3	1:B:448:PHE:N	2.22	0.52
1:B:171:HIS:CD2	4:B:718:HOH:O	2.63	0.52
1:B:235:MET:HE3	1:B:238:LEU:HB3	1.90	0.52
1:A:45:PRO:HD2	4:A:835:HOH:O	2.09	0.52
1:B:354:LEU:O	1:B:357:SER:HB3	2.09	0.52
1:B:359:ILE:HG22	1:B:433:ILE:HA	1.91	0.52
1:B:216:THR:HG23	1:B:278:ASN:HA	1.91	0.52
1:B:404:GLY:N	1:B:425:CYS:HB3	2.25	0.52
1:A:134:GLY:HA3	1:A:170:ALA:HB1	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:77:ALA:O	1:A:81:ARG:HG3	2.11	0.51
1:A:361:PRO:HD3	1:A:442:CYS:HB2	1.92	0.51
1:B:230:THR:O	1:B:236:LYS:HG2	2.11	0.51
1:B:132:LEU:HB2	1:B:166:LEU:HD23	1.92	0.51
1:A:220:PHE:CE2	1:A:288:GLN:HG3	2.45	0.51
1:A:387:LYS:HD2	1:B:387:LYS:HB3	1.92	0.51
1:B:355:VAL:HB	1:B:356:PRO:HA	1.94	0.50
1:B:355:VAL:HG12	1:B:357:SER:OG	2.11	0.50
1:B:394:LEU:HD12	1:B:395:PRO:CD	2.37	0.50
1:B:333:ASN:HD22	1:B:334:PRO:HD2	1.77	0.50
1:B:81:ARG:NH1	1:B:203:ASP:OD1	2.45	0.50
1:B:431:LEU:HD12	1:B:432:ASP:N	2.27	0.50
1:B:188:TYR:HA	1:B:230:THR:HG21	1.94	0.50
1:B:264:ASP:CG	1:B:496:LYS:H	2.19	0.50
1:B:193:ASP:OD1	1:B:193:ASP:N	2.45	0.49
1:B:485:SER:O	1:B:488:GLN:HG3	2.13	0.49
1:B:493:HIS:O	4:B:701:HOH:O	2.20	0.49
1:A:389:GLY:O	1:B:383:ARG:NH1	2.46	0.49
1:B:418:PRO:HB2	1:B:440:ASP:OD2	2.12	0.49
4:A:803:HOH:O	1:B:386:GLY:C	2.55	0.48
1:A:99:PRO:HB3	4:A:839:HOH:O	2.13	0.48
1:B:261:ARG:HG3	1:B:504:PHE:HZ	1.78	0.48
1:B:367:ALA:HB3	1:B:435:VAL:HG11	1.96	0.48
1:B:469:TRP:H	1:B:469:TRP:CD1	2.32	0.48
1:B:48:THR:O	1:B:103:VAL:HA	2.14	0.48
1:B:426:ILE:CG2	1:B:433:ILE:HB	2.43	0.48
1:A:165:GLU:HA	1:A:184:VAL:O	2.13	0.48
1:B:169:HIS:HE1	1:B:189:TYR:CD1	2.32	0.48
1:B:79:ARG:O	1:B:82:ALA:HB3	2.14	0.48
1:B:282:ALA:O	1:B:286:ILE:HG13	2.13	0.48
1:A:81:ARG:NH2	1:A:203:ASP:OD1	2.47	0.47
1:B:426:ILE:HG23	1:B:433:ILE:HB	1.96	0.47
1:A:422:ARG:NH1	4:A:812:HOH:O	2.43	0.47
1:A:455:PRO:HB2	1:A:476:MET:HE1	1.96	0.47
1:A:189:TYR:HA	1:A:190:PRO:C	2.38	0.47
1:B:41:ASN:OD1	1:B:262:ALA:HB1	2.14	0.47
1:B:300:ILE:HD12	1:B:300:ILE:N	2.26	0.47
1:A:149:LEU:HD13	1:A:180:ALA:HB2	1.95	0.47
1:B:300:ILE:H	1:B:300:ILE:CD1	2.27	0.46
1:A:235:MET:HE1	1:A:294:TYR:CE2	2.50	0.46
1:A:167:ASP:OD1	1:A:168:LEU:N	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:65:PRO:HB2	1:B:67:PHE:CD2	2.50	0.46
1:B:323:TYR:CB	1:B:324:PRO:HD3	2.42	0.46
1:B:349:MET:CE	1:B:357:SER:HB2	2.46	0.46
1:B:442:CYS:SG	1:B:447:MET:SD	3.11	0.46
1:B:288:GLN:O	1:B:292:ARG:HG3	2.16	0.46
1:B:370:LEU:HD12	1:B:382:LEU:CD1	2.45	0.46
1:B:451:LEU:O	1:B:453:VAL:HG23	2.16	0.46
1:A:383:ARG:NH2	4:A:803:HOH:O	2.49	0.46
1:B:171:HIS:HE1	1:B:263:GLY:HA3	1.81	0.46
1:B:213:ILE:HD12	1:B:252:LEU:HD21	1.97	0.46
1:A:331:SER:OG	4:A:801:HOH:O	2.20	0.46
1:A:387:LYS:O	1:B:387:LYS:HE2	2.16	0.46
1:A:437:GLU:HG3	1:A:438:ILE:HG13	1.98	0.45
1:B:234:PRO:CG	1:B:297:MET:HG2	2.35	0.45
1:A:383:ARG:HH12	1:B:390:GLU:HA	1.81	0.45
1:B:428:THR:OG1	1:B:429:ALA:N	2.48	0.45
1:B:502:TRP:CG	1:B:503:PRO:HA	2.51	0.45
1:B:319:ALA:O	1:B:320:ALA:HB3	2.16	0.45
1:A:193:ASP:O	1:A:197:ARG:HG2	2.17	0.45
1:B:365:PRO:O	1:B:368:VAL:HB	2.17	0.45
1:B:323:TYR:O	1:B:459:ARG:HA	2.16	0.45
1:A:153:ARG:NH1	1:A:158:PRO:HA	2.30	0.45
1:A:378:ALA:O	1:A:401:LYS:HA	2.17	0.45
1:A:383:ARG:HG3	1:A:397:ASP:OD1	2.17	0.45
1:B:260:PHE:CE2	1:B:262:ALA:HB3	2.51	0.45
1:B:481:ILE:N	1:B:481:ILE:HD12	2.32	0.45
1:B:35:THR:HG23	1:B:94:CYS:SG	2.57	0.45
1:B:169:HIS:HE1	1:B:189:TYR:CE1	2.35	0.45
1:A:37:GLY:HA2	4:A:846:HOH:O	2.16	0.45
1:A:153:ARG:HH21	1:A:162:LEU:HB3	1.82	0.44
1:B:380:PHE:C	1:B:399:ARG:HG2	2.41	0.44
1:A:412:ASN:HB2	1:A:417:ARG:HH11	1.82	0.44
1:A:442:CYS:SG	1:A:473:PHE:HE2	2.40	0.44
1:A:73:GLY:N	1:A:74:PRO:CD	2.80	0.44
1:B:123:MET:HE3	1:B:123:MET:HB3	1.90	0.44
1:B:274:ILE:HD13	1:B:287:ALA:HA	1.98	0.44
1:A:398:VAL:HG13	1:A:428:THR:HG21	2.00	0.44
1:B:134:GLY:HA3	1:B:170:ALA:HB1	2.00	0.44
1:B:379:ASP:OD2	1:B:399:ARG:NH1	2.51	0.44
1:B:117:ASP:OD1	1:B:120:ARG:NH1	2.51	0.44
1:A:66:ASP:O	1:A:76:TRP:HH2	2.01	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:405:LEU:HD23	1:A:424:VAL:HG22	2.00	0.44
1:B:372:PHE:HZ	1:B:406:ALA:O	2.01	0.43
1:A:190:PRO:HD3	1:A:231:GLN:OE1	2.18	0.43
1:A:361:PRO:HG2	1:A:440:ASP:O	2.18	0.43
1:B:77:ALA:O	1:B:81:ARG:HG3	2.18	0.43
1:B:235:MET:O	1:B:236:LYS:C	2.62	0.43
1:B:449:ARG:C	1:B:451:LEU:N	2.76	0.43
1:B:152:ALA:O	1:B:156:VAL:HG22	2.18	0.43
1:B:216:THR:CG2	1:B:278:ASN:HA	2.48	0.43
1:B:120:ARG:NH1	1:B:121:ARG:HG3	2.33	0.43
1:A:50:LEU:HD11	1:A:110:LEU:HD13	2.01	0.43
1:A:204:LEU:O	1:A:208:ILE:HG13	2.19	0.43
1:B:372:PHE:CD1	1:B:405:LEU:HD22	2.53	0.43
1:A:167:ASP:HA	1:A:186:PHE:CD2	2.53	0.42
1:B:444:GLY:O	1:B:447:MET:HG2	2.19	0.42
1:A:222:CYS:HB2	1:A:224:MET:HG2	2.01	0.42
1:A:81:ARG:HD3	1:A:86:ARG:HH21	1.85	0.42
1:B:93:THR:OG1	1:B:114:GLU:OE2	2.34	0.42
1:B:404:GLY:CA	1:B:425:CYS:HB3	2.50	0.42
1:B:231:GLN:C	1:B:236:LYS:HD2	2.44	0.42
1:B:364:ASP:O	1:B:365:PRO:C	2.62	0.42
1:B:385:GLY:O	1:B:387:LYS:HG2	2.20	0.42
1:B:142:ASP:C	4:B:704:HOH:O	2.63	0.42
1:B:381:SER:HA	1:B:398:VAL:O	2.19	0.42
1:A:51:ASP:OD1	1:A:54:ARG:NH2	2.52	0.42
1:A:434:ILE:HG13	1:A:448:PHE:CD1	2.54	0.42
1:B:74:PRO:HD2	4:B:720:HOH:O	2.20	0.42
1:B:225:VAL:HG13	1:B:225:VAL:O	2.19	0.42
1:A:193:ASP:HB2	1:A:197:ARG:NH1	2.35	0.42
1:A:228[A]:LEU:CD2	1:A:234:PRO:HD2	2.37	0.42
1:B:311:ALA:O	1:B:312:ALA:C	2.62	0.42
1:A:346:ALA:HB2	1:A:359:ILE:HD13	2.01	0.42
1:B:225:VAL:O	1:B:226:ALA:HB2	2.19	0.42
1:A:147:ASP:OD1	1:A:151:ARG:NE	2.48	0.42
1:B:80:GLU:HA	1:B:83:ARG:NH1	2.35	0.42
1:B:103:VAL:HG21	1:B:136:MET:HE3	2.02	0.42
1:A:225:VAL:HG13	1:A:225:VAL:O	2.20	0.41
1:A:241:ASP:O	1:A:245:PHE:HD1	2.02	0.41
1:B:224:MET:HE3	1:B:502:TRP:CE3	2.55	0.41
1:B:228:LEU:CD1	1:B:235:MET:HB2	2.49	0.41
1:A:260:PHE:HZ	4:A:839:HOH:O	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:317:ALA:O	1:B:460:TYR:HE2	2.03	0.41
1:B:411:GLN:O	1:B:418:PRO:HD2	2.20	0.41
1:B:182:VAL:HG23	1:B:275:TYR:CE1	2.55	0.41
1:B:361:PRO:CD	1:B:464:LYS:HB2	2.45	0.41
1:B:382:LEU:N	1:B:398:VAL:O	2.52	0.41
1:B:404:GLY:HA3	1:B:425:CYS:HB3	2.02	0.41
1:B:439:ARG:CD	4:B:702:HOH:O	2.66	0.41
1:A:28:ARG:HH12	1:A:85:GLY:C	2.28	0.41
1:A:78:ALA:HB1	1:A:89:VAL:HG12	2.03	0.41
1:B:324:PRO:HG2	1:B:477:GLY:HA2	2.03	0.41
1:B:28:ARG:CZ	1:B:85:GLY:HA2	2.50	0.41
1:B:328:VAL:HG21	1:B:482:TYR:CD2	2.56	0.41
1:B:406:ALA:HB3	1:B:423:VAL:HB	2.03	0.41
1:B:405:LEU:HD23	1:B:424:VAL:HG22	2.02	0.41
1:B:413:LEU:HD22	1:B:443:TYR:CE1	2.56	0.41
1:B:218:SER:O	1:B:273:LEU:HD12	2.21	0.41
1:B:328:VAL:HG23	1:B:330:SER:N	2.32	0.41
1:B:368:VAL:HG11	1:B:422:ARG:HB3	2.03	0.41
1:B:448:PHE:O	1:B:453:VAL:HB	2.21	0.41
1:A:98:MET:HE3	1:A:98:MET:HB2	1.86	0.41
1:A:502:TRP:CG	1:A:503:PRO:HA	2.56	0.41
1:B:222:CYS:HA	1:B:295:GLN:HE21	1.86	0.41
1:B:328:VAL:O	1:B:329:ASP:C	2.62	0.41
1:A:274:ILE:HD13	1:A:274:ILE:HA	1.88	0.40
1:B:78:ALA:HB1	1:B:89:VAL:HG12	2.03	0.40
1:B:359:ILE:CG2	1:B:360:GLY:N	2.83	0.40
1:B:376:LEU:HA	1:B:402:ILE:CD1	2.35	0.40
1:A:203:ASP:O	1:A:207:ARG:HG3	2.21	0.40
1:B:39:GLU:HG3	1:B:133:HIS:CE1	2.56	0.40
1:B:60:ARG:NH1	1:B:114:GLU:OE2	2.54	0.40
1:A:502:TRP:HA	1:A:503:PRO:HA	1.82	0.40
1:A:252:LEU:HD11	1:A:277:ASN:HB2	2.02	0.40
1:A:383:ARG:NH1	1:A:397:ASP:OD1	2.54	0.40
1:B:317:ALA:O	1:B:460:TYR:CE2	2.75	0.40
1:B:434:ILE:HD12	1:B:451:LEU:HG	2.03	0.40
1:A:202:LEU:O	1:A:206:GLU:HG3	2.22	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	478/512 (93%)	465 (97%)	13 (3%)	0	100	100
1	B	463/512 (90%)	437 (94%)	26 (6%)	0	100	100
All	All	941/1024 (92%)	902 (96%)	39 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	380/400 (95%)	378 (100%)	2 (0%)	81	91
1	B	371/400 (93%)	367 (99%)	4 (1%)	65	83
All	All	751/800 (94%)	745 (99%)	6 (1%)	73	87

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	192	ILE
1	A	394	LEU
1	B	301	MET
1	B	359	ILE
1	B	427	SER
1	B	463	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13)

such sidechains are listed below:

Mol	Chain	Res	Type
1	A	223	GLN
1	A	278	ASN
1	A	468	GLN
1	A	488	GLN
1	A	493	HIS
1	A	510	HIS
1	B	109	GLN
1	B	333	ASN
1	B	352	ASN
1	B	408	ASN
1	B	414	GLN
1	B	441	GLN
1	B	487	GLN

5.3.3 RNA [i](#)

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](#)

Of 4 ligands modelled in this entry, 4 are monoatomic - leaving 0 for Mogul analysis.

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.

No monomer is involved in short contacts.

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	480/512 (93%)	0.27	15 (3%)	51	47	28, 56, 88, 124	2 (0%)
1	B	471/512 (91%)	0.97	95 (20%)	3	2	47, 81, 136, 197	1 (0%)
All	All	951/1024 (92%)	0.61	110 (11%)	9	7	28, 64, 127, 197	3 (0%)

All (110) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	360	GLY	7.4
1	A	228[A]	LEU	5.8
1	B	400	GLY	5.7
1	B	451	LEU	5.6
1	B	324	PRO	5.5
1	B	508	LEU	5.3
1	B	461	VAL	5.2
1	B	377	GLY	5.1
1	A	512	HIS	4.9
1	B	359	ILE	4.7
1	B	378	ALA	4.5
1	A	139	PHE	4.5
1	B	328	VAL	4.4
1	B	376	LEU	4.4
1	A	299	SER	4.4
1	B	358	CYS	4.1
1	B	463	VAL	4.0
1	B	442	CYS	3.9
1	B	491	ILE	3.9
1	B	405	LEU	3.8
1	B	425	CYS	3.7
1	B	382	LEU	3.6
1	B	308	ARG	3.6
1	B	319	ALA	3.6

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Mol	Chain	Res	Type	RSRZ
1	A	298	ALA	3.5
1	B	228	LEU	3.4
1	B	402	ILE	3.4
1	B	380	PHE	3.3
1	B	471	ILE	3.3
1	B	481	ILE	3.3
1	A	471	ILE	3.3
1	A	26	GLY	3.2
1	B	453	VAL	3.2
1	B	379	ASP	3.1
1	B	323	TYR	3.1
1	B	403	THR	3.1
1	B	480	VAL	3.1
1	B	231	GLN	3.1
1	B	473	PHE	3.1
1	B	482	TYR	3.0
1	B	361	PRO	3.0
1	B	373	GLU	3.0
1	B	483	VAL	3.0
1	A	307	GLU	3.0
1	B	426	ILE	2.9
1	B	310	PHE	2.9
1	B	460	TYR	2.9
1	B	381	SER	2.9
1	A	231	GLN	2.8
1	B	431	LEU	2.8
1	B	434	ILE	2.8
1	B	455	PRO	2.8
1	B	331	SER	2.8
1	B	316	LEU	2.8
1	A	414	GLN	2.7
1	B	406	ALA	2.7
1	B	472	GLY	2.7
1	B	374	ALA	2.7
1	B	356	PRO	2.7
1	B	238	LEU	2.6
1	B	371	GLY	2.6
1	B	370	LEU	2.6
1	B	503	PRO	2.6
1	B	372	PHE	2.6
1	B	448	PHE	2.5
1	B	428	THR	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	504	PHE	2.5
1	B	447	MET	2.5
1	B	486	SER	2.5
1	B	452	GLY	2.5
1	B	320	ALA	2.5
1	B	449	ARG	2.5
1	B	479	SER	2.4
1	B	314	ILE	2.4
1	B	375	GLY	2.4
1	A	225	VAL	2.4
1	B	420	LEU	2.4
1	A	31	VAL	2.4
1	B	330	SER	2.3
1	A	86	ARG	2.3
1	B	322	ALA	2.3
1	B	329	ASP	2.3
1	B	399	ARG	2.3
1	B	88	GLU	2.3
1	B	401	LYS	2.3
1	B	421	GLY	2.3
1	B	301	MET	2.3
1	B	430	GLY	2.3
1	B	444	GLY	2.3
1	B	275	TYR	2.2
1	B	493	HIS	2.2
1	B	443	TYR	2.2
1	B	457	ASN	2.2
1	B	227	GLY	2.2
1	B	422	ARG	2.2
1	B	409	VAL	2.2
1	B	454	GLU	2.1
1	B	311	ALA	2.1
1	B	321	THR	2.1
1	B	87	TYR	2.1
1	A	380	PHE	2.1
1	A	67	PHE	2.1
1	B	432	ASP	2.1
1	B	507	VAL	2.1
1	B	446	ASP	2.0
1	B	459	ARG	2.0
1	B	298	ALA	2.0
1	B	350	LEU	2.0

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Mol	Chain	Res	Type	RSRZ
1	B	335	GLY	2.0
1	B	412	ASN	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 oligosaccharides 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, 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($\text{\AA}^2$)	Q<0.9
3	CA	B	602	1/1	0.85	0.17	101,101,101,101	0
2	ZN	B	601	1/1	0.90	0.09	71,71,71,71	1
2	ZN	A	702	1/1	0.95	0.08	90,90,90,90	0
2	ZN	A	701	1/1	0.97	0.06	53,53,53,53	1

6.5 Other polymers [i](#)

There are no such residues in this entry.