



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 05:27 PM UTC

PDB ID : 6IYO / pdb_00006iyo
Title : Crystal Structure of the acyltransferase domain from the second module of the salinomycin polyketide synthase
Authors : Zhang, F.; Zheng, J.
Deposited on : 2018-12-17
Resolution : 2.20 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

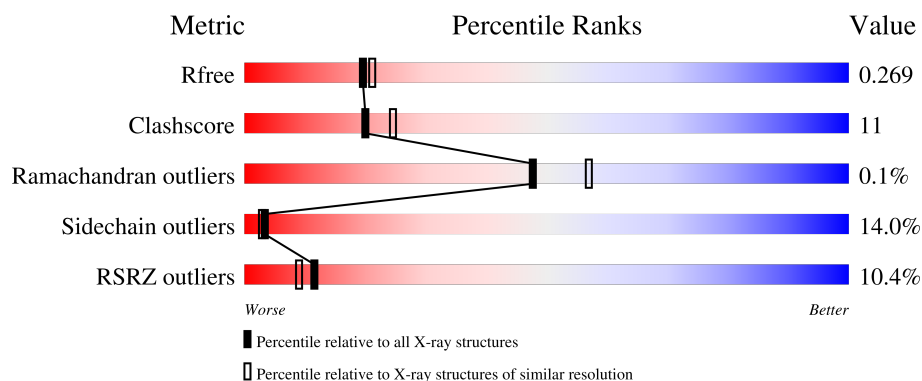
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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	6164 (2.20-2.20)
Clashscore	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)
RSRZ outliers	180081	6166 (2.20-2.20)

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	463	6% 70% 17% • 9%
1	B	463	13% 65% 19% 5% 10%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 6268 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 Type I modular polyketide synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	421	Total	C	N	O	S	0	0	0
			3148	1974	578	588	8			
1	B	415	Total	C	N	O	S	0	0	0
			3084	1930	567	579	8			

There are 42 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-40	MET	-	initiating methionine	UNP H1ZZT3
A	-39	GLY	-	expression tag	UNP H1ZZT3
A	-38	SER	-	expression tag	UNP H1ZZT3
A	-37	SER	-	expression tag	UNP H1ZZT3
A	-36	HIS	-	expression tag	UNP H1ZZT3
A	-35	HIS	-	expression tag	UNP H1ZZT3
A	-34	HIS	-	expression tag	UNP H1ZZT3
A	-33	HIS	-	expression tag	UNP H1ZZT3
A	-32	HIS	-	expression tag	UNP H1ZZT3
A	-31	HIS	-	expression tag	UNP H1ZZT3
A	-30	SER	-	expression tag	UNP H1ZZT3
A	-29	SER	-	expression tag	UNP H1ZZT3
A	-28	GLY	-	expression tag	UNP H1ZZT3
A	-27	LEU	-	expression tag	UNP H1ZZT3
A	-26	VAL	-	expression tag	UNP H1ZZT3
A	-25	PRO	-	expression tag	UNP H1ZZT3
A	-24	ARG	-	expression tag	UNP H1ZZT3
A	-23	GLY	-	expression tag	UNP H1ZZT3
A	-22	SER	-	expression tag	UNP H1ZZT3
A	-21	HIS	-	expression tag	UNP H1ZZT3
A	-20	MET	-	expression tag	UNP H1ZZT3
B	-40	MET	-	initiating methionine	UNP H1ZZT3
B	-39	GLY	-	expression tag	UNP H1ZZT3
B	-38	SER	-	expression tag	UNP H1ZZT3
B	-37	SER	-	expression tag	UNP H1ZZT3

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-36	HIS	-	expression tag	UNP H1ZZT3
B	-35	HIS	-	expression tag	UNP H1ZZT3
B	-34	HIS	-	expression tag	UNP H1ZZT3
B	-33	HIS	-	expression tag	UNP H1ZZT3
B	-32	HIS	-	expression tag	UNP H1ZZT3
B	-31	HIS	-	expression tag	UNP H1ZZT3
B	-30	SER	-	expression tag	UNP H1ZZT3
B	-29	SER	-	expression tag	UNP H1ZZT3
B	-28	GLY	-	expression tag	UNP H1ZZT3
B	-27	LEU	-	expression tag	UNP H1ZZT3
B	-26	VAL	-	expression tag	UNP H1ZZT3
B	-25	PRO	-	expression tag	UNP H1ZZT3
B	-24	ARG	-	expression tag	UNP H1ZZT3
B	-23	GLY	-	expression tag	UNP H1ZZT3
B	-22	SER	-	expression tag	UNP H1ZZT3
B	-21	HIS	-	expression tag	UNP H1ZZT3
B	-20	MET	-	expression tag	UNP H1ZZT3

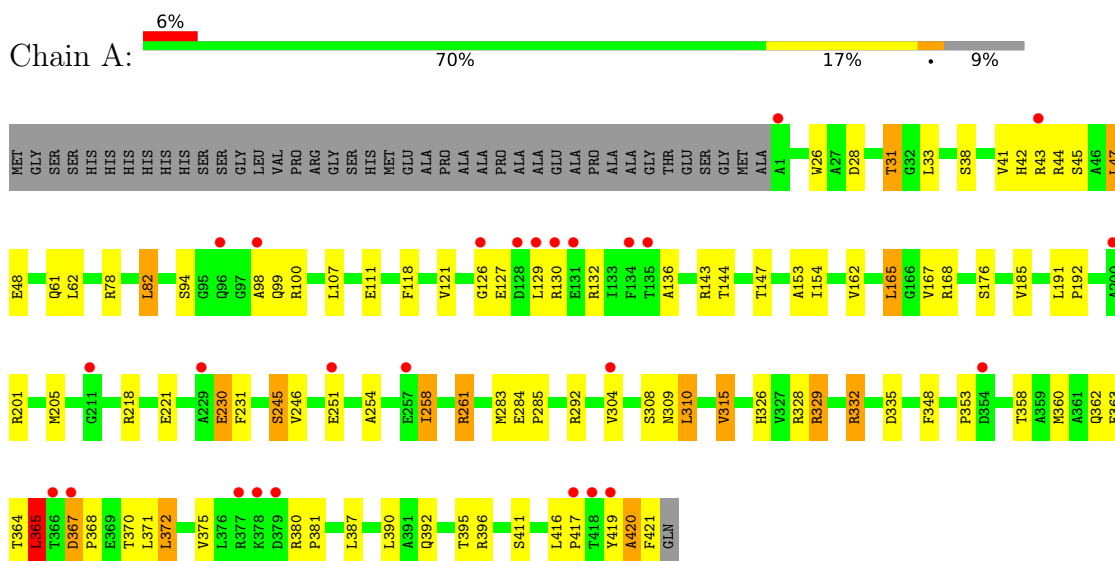
- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	25	Total O 25 25	0	0
2	B	11	Total O 11 11	0	0

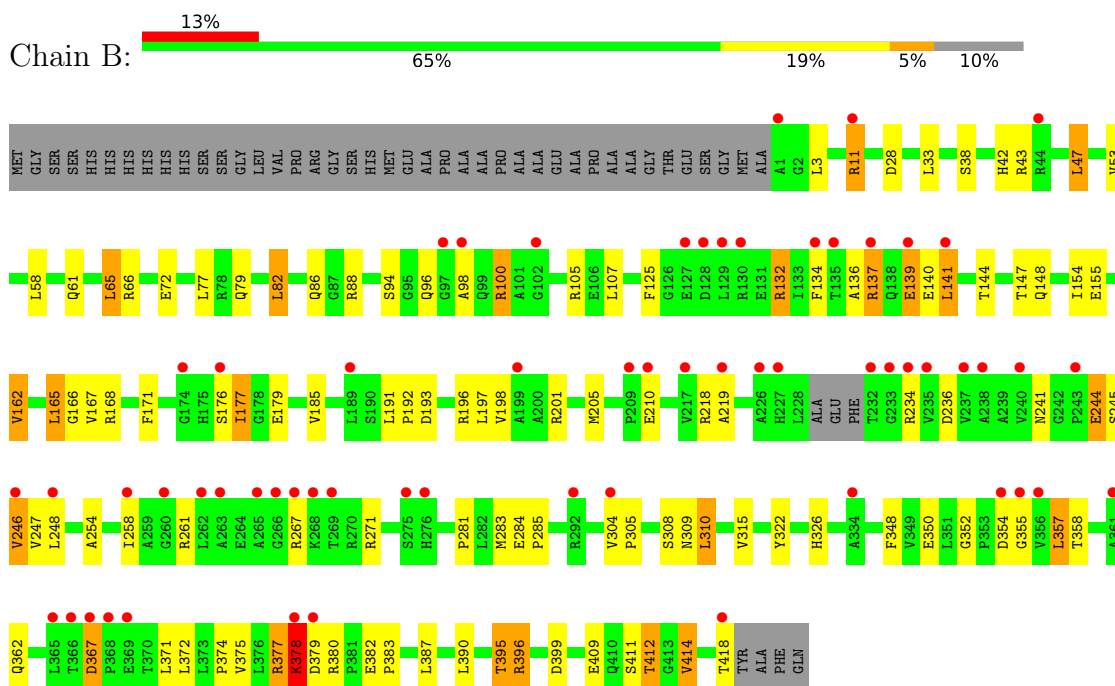
3 Residue-property plots

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: Type I modular polyketide synthase



- Molecule 1: Type I modular polyketide synthase



4 Data and refinement statistics

Property	Value	Source
Space group	P 2 21 21	Depositor
Cell constants a, b, c, α , β , γ	49.09Å 73.37Å 248.00Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.20 50.00 – 2.20	Depositor EDS
% Data completeness (in resolution range)	90.7 (50.00-2.20) 90.8 (50.00-2.20)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.06 (at 2.20Å)	Xtriage
Refinement program	REFMAC 5.8.0073	Depositor
R, R_{free}	0.219 , 0.260 0.231 , 0.269	Depositor DCC
R_{free} test set	2111 reflections (4.51%)	wwPDB-VP
Wilson B-factor (Å ²)	40.2	Xtriage
Anisotropy	0.129	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 26.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	6268	wwPDB-VP
Average B, all atoms (Å ²)	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.63% 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](#)

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	0.75	0/3208	0.89	9/4361 (0.2%)
1	B	0.67	0/3139	0.90	8/4267 (0.2%)
All	All	0.71	0/6347	0.90	17/8628 (0.2%)

There are no bond length outliers.

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	365	LEU	N-CA-C	8.78	120.62	111.14
1	A	364	THR	N-CA-C	7.21	118.93	111.14
1	B	136	ALA	N-CA-C	6.88	119.70	110.35
1	A	367	ASP	CA-C-N	6.53	126.30	119.05
1	A	367	ASP	C-N-CA	6.53	126.30	119.05
1	B	42	HIS	N-CA-C	6.31	118.23	111.36
1	A	258	ILE	CB-CA-C	-5.99	104.30	111.97
1	B	245	SER	N-CA-C	5.86	118.80	109.24
1	A	94	SER	N-CA-C	5.66	118.05	110.35
1	A	315	VAL	CB-CA-C	-5.62	103.51	111.21
1	A	129	LEU	N-CA-C	5.60	117.38	111.28
1	B	352	GLY	CA-C-N	5.45	125.10	119.05
1	B	352	GLY	C-N-CA	5.45	125.10	119.05
1	A	99	GLN	N-CA-C	5.39	118.05	110.23
1	B	378	LYS	N-CA-C	-5.38	101.71	110.20
1	B	47	LEU	N-CA-C	5.33	118.00	111.82
1	B	241	ASN	N-CA-C	5.28	117.03	111.28

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	3148	0	3103	59	0
1	B	3084	0	3043	87	0
2	A	25	0	0	1	0
2	B	11	0	0	0	0
All	All	6268	0	6146	141	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 (141) 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:137:ARG:HH21	1:B:139:GLU:HB2	0.99	1.12
1:B:137:ARG:NH2	1:B:139:GLU:HB2	1.84	0.91
1:A:165:LEU:HD23	1:A:390:LEU:HD11	1.54	0.88
1:B:165:LEU:HD23	1:B:390:LEU:HD11	1.56	0.87
1:A:367:ASP:OD1	1:A:368:PRO:HD2	1.74	0.87
1:B:100:ARG:NH2	1:B:378:LYS:CB	2.40	0.85
1:B:308:SER:HB2	1:B:315:VAL:HG13	1.59	0.84
1:A:26:TRP:CH2	1:A:31:THR:HG21	2.15	0.81
1:B:137:ARG:HH21	1:B:139:GLU:CB	1.90	0.81
1:B:411:SER:O	1:B:414:VAL:HG13	1.80	0.81
1:B:137:ARG:HD3	1:B:139:GLU:HB2	1.63	0.79
1:B:137:ARG:HD3	1:B:139:GLU:CB	2.13	0.78
1:A:362:GLN:HG3	1:A:372:LEU:HD13	1.66	0.75
1:B:100:ARG:HH22	1:B:378:LYS:CA	1.99	0.75
1:A:417:PRO:HG2	1:A:420:ALA:HB2	1.68	0.74
1:A:348:PHE:HB2	1:A:372:LEU:HD23	1.70	0.73
1:A:201:ARG:O	1:A:205:MET:HG2	1.91	0.71
1:B:201:ARG:O	1:B:205:MET:HG2	1.91	0.71
1:B:219:ALA:N	1:B:244:GLU:O	2.24	0.70
1:A:308:SER:HB2	1:A:315:VAL:CG2	2.22	0.69
1:A:118:PHE:CE2	1:A:130:ARG:HG3	2.28	0.69
1:A:118:PHE:HE2	1:A:130:ARG:HG3	1.57	0.68
1:B:348:PHE:HB2	1:B:372:LEU:HD23	1.74	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:98:ALA:HB1	1:A:353:PRO:HG2	1.76	0.66
1:A:326:HIS:HD2	2:A:510:HOH:O	1.79	0.66
1:B:125:PHE:HZ	1:B:198:VAL:HG11	1.61	0.65
1:B:132:ARG:HH11	1:B:132:ARG:HG3	1.60	0.65
1:B:105:ARG:NH1	1:B:134:PHE:O	2.31	0.64
1:B:162:VAL:HG13	1:B:167:VAL:HB	1.80	0.64
1:B:100:ARG:NH2	1:B:378:LYS:CA	2.60	0.63
1:B:137:ARG:HG3	1:B:140:GLU:H	1.63	0.63
1:B:367:ASP:OD1	1:B:367:ASP:N	2.30	0.63
1:A:126:GLY:O	1:A:127:GLU:HG2	1.98	0.63
1:B:98:ALA:HB1	1:B:354:ASP:OD2	1.98	0.62
1:A:82:LEU:HD23	1:A:82:LEU:N	2.14	0.62
1:A:308:SER:HB2	1:A:315:VAL:HG23	1.81	0.62
1:B:100:ARG:NH2	1:B:378:LYS:HB3	2.16	0.61
1:A:205:MET:HB3	1:A:283:MET:HE1	1.81	0.61
1:A:362:GLN:CG	1:A:372:LEU:HD13	2.30	0.61
1:B:350:GLU:OE1	1:B:358:THR:HG23	2.01	0.61
1:A:254:ALA:O	1:A:258:ILE:HG12	2.01	0.61
1:B:205:MET:HB3	1:B:283:MET:HE1	1.83	0.61
1:B:100:ARG:HH22	1:B:378:LYS:CB	2.09	0.60
1:B:350:GLU:CD	1:B:357:LEU:HB2	2.26	0.60
1:B:100:ARG:NH2	1:B:378:LYS:HA	2.16	0.60
1:B:125:PHE:CZ	1:B:198:VAL:CG1	2.85	0.60
1:A:417:PRO:O	1:A:420:ALA:HB3	2.02	0.60
1:A:419:TYR:C	1:A:421:PHE:H	2.10	0.59
1:A:230:GLU:OE1	1:A:261:ARG:NH1	2.37	0.58
1:A:41:VAL:HG23	1:A:42:HIS:CD2	2.39	0.58
1:B:177:ILE:HG12	1:B:177:ILE:O	2.03	0.58
1:B:100:ARG:NH2	1:B:378:LYS:HB2	2.17	0.57
1:A:38:SER:O	1:A:42:HIS:HD2	1.86	0.57
1:A:231:PHE:CD2	1:A:258:ILE:HD11	2.41	0.55
1:A:176:SER:H	1:A:309:ASN:HD21	1.55	0.55
1:B:82:LEU:N	1:B:82:LEU:HD23	2.21	0.55
1:A:162:VAL:HG22	1:A:167:VAL:HB	1.89	0.54
1:B:308:SER:HB2	1:B:315:VAL:CG1	2.36	0.54
1:B:125:PHE:CZ	1:B:198:VAL:HG11	2.42	0.54
1:A:41:VAL:CG2	1:A:42:HIS:CD2	2.90	0.54
1:B:125:PHE:CE1	1:B:198:VAL:CG1	2.91	0.54
1:B:350:GLU:OE2	1:B:357:LEU:HB2	2.07	0.53
1:A:47:LEU:HB3	1:B:11:ARG:HD3	1.91	0.53
1:A:309:ASN:HD22	1:A:326:HIS:HE1	1.55	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:284:GLU:N	1:B:285:PRO:CD	2.71	0.53
1:B:132:ARG:HG3	1:B:132:ARG:NH1	2.23	0.53
1:A:132:ARG:O	1:A:136:ALA:CB	2.57	0.53
1:B:246:VAL:CG2	1:B:247:VAL:N	2.72	0.53
1:B:411:SER:O	1:B:414:VAL:CG1	2.56	0.53
1:B:176:SER:H	1:B:309:ASN:HD21	1.55	0.53
1:B:139:GLU:HA	1:B:139:GLU:OE2	2.08	0.52
1:A:411:SER:HB3	1:B:38:SER:HB2	1.89	0.52
1:A:176:SER:H	1:A:309:ASN:ND2	2.08	0.51
1:A:48:GLU:HB2	1:B:11:ARG:HH21	1.75	0.51
1:A:332:ARG:NH2	1:A:335:ASP:OD2	2.44	0.50
1:A:284:GLU:N	1:A:285:PRO:CD	2.74	0.50
1:A:308:SER:HB2	1:A:315:VAL:HG22	1.93	0.50
1:B:137:ARG:HD3	1:B:139:GLU:H	1.76	0.50
1:B:409:GLU:O	1:B:412:THR:HG22	2.12	0.50
1:B:409:GLU:O	1:B:412:THR:CG2	2.60	0.49
1:A:61:GLN:HA	1:A:61:GLN:OE1	2.13	0.49
1:A:419:TYR:C	1:A:421:PHE:N	2.70	0.49
1:B:176:SER:H	1:B:309:ASN:ND2	2.10	0.49
1:B:350:GLU:OE1	1:B:355:GLY:HA2	2.12	0.49
1:B:148:GLN:HA	1:B:177:ILE:HD12	1.95	0.49
1:B:246:VAL:HG23	1:B:247:VAL:N	2.28	0.49
1:A:348:PHE:CB	1:A:372:LEU:HD23	2.41	0.48
1:A:132:ARG:O	1:A:136:ALA:HB2	2.13	0.48
1:B:100:ARG:HH21	1:B:378:LYS:CB	2.21	0.48
1:A:231:PHE:CD2	1:A:258:ILE:CD1	2.97	0.48
1:B:362:GLN:OE1	1:B:372:LEU:HD12	2.14	0.48
1:A:358:THR:HG23	1:A:372:LEU:HB3	1.97	0.47
1:B:100:ARG:HH21	1:B:378:LYS:HB2	1.79	0.47
1:A:221:GLU:OE2	1:A:332:ARG:NH1	2.48	0.47
1:B:137:ARG:HE	1:B:137:ARG:HB2	1.55	0.47
1:B:236:ASP:HB2	1:B:281:PRO:HD3	1.96	0.47
1:A:328:ARG:HG3	1:A:329:ARG:HD3	1.98	0.46
1:A:165:LEU:CD2	1:A:390:LEU:HD11	2.35	0.46
1:B:137:ARG:HD3	1:B:139:GLU:N	2.30	0.46
1:B:165:LEU:CD2	1:B:390:LEU:HD11	2.36	0.46
1:B:309:ASN:HD22	1:B:326:HIS:HE1	1.62	0.45
1:A:360:MET:O	1:A:363:GLU:HB2	2.16	0.45
1:B:144:THR:HA	1:B:147:THR:HB	1.98	0.45
1:B:61:GLN:HA	1:B:61:GLN:OE1	2.17	0.45
1:B:53:VAL:HG21	1:B:65:LEU:HD13	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:191:LEU:HB3	1:A:192:PRO:HD3	1.98	0.45
1:A:417:PRO:O	1:A:420:ALA:CB	2.65	0.45
1:B:141:LEU:HD23	1:B:141:LEU:HA	1.81	0.44
1:B:191:LEU:HB3	1:B:192:PRO:HD3	1.99	0.44
1:A:38:SER:HB2	1:B:411:SER:HB3	1.98	0.44
1:A:121:VAL:HG11	1:A:153:ALA:HA	1.99	0.44
1:A:380:ARG:HB3	1:A:381:PRO:HD2	2.00	0.44
1:A:78:ARG:NH2	1:A:392:GLN:NE2	2.66	0.43
1:B:382:GLU:N	1:B:383:PRO:CD	2.81	0.43
1:A:365:LEU:HD12	1:A:365:LEU:HA	1.81	0.43
1:B:197:LEU:C	1:B:197:LEU:HD23	2.44	0.43
1:B:94:SER:O	1:B:155:GLU:OE2	2.37	0.43
1:B:166:GLY:HA2	1:B:168:ARG:NH2	2.33	0.43
1:B:355:GLY:HA3	1:B:374:PRO:HB3	2.00	0.43
1:A:245:SER:HB2	1:A:363:GLU:OE1	2.18	0.43
1:B:171:PHE:CD2	1:B:305:PRO:HB2	2.54	0.43
1:B:377:ARG:HD2	1:B:380:ARG:HG3	2.01	0.42
1:A:221:GLU:CD	1:A:332:ARG:HH12	2.25	0.42
1:A:416:LEU:HD23	1:A:421:PHE:HZ	1.85	0.42
1:B:193:ASP:HA	1:B:196:ARG:NH2	2.34	0.42
1:B:100:ARG:O	1:B:100:ARG:HG2	2.11	0.42
1:B:179:GLU:OE1	1:B:322:TYR:OH	2.29	0.42
1:A:44:ARG:O	1:B:11:ARG:NH2	2.52	0.42
1:B:362:GLN:OE1	1:B:372:LEU:CD1	2.67	0.42
1:B:137:ARG:HD3	1:B:139:GLU:CA	2.50	0.42
1:B:210:GLU:N	1:B:210:GLU:OE1	2.52	0.42
1:B:218:ARG:HG3	1:B:244:GLU:CD	2.44	0.42
1:A:310:LEU:HD12	1:A:310:LEU:HA	1.94	0.41
1:B:137:ARG:CD	1:B:139:GLU:HB2	2.43	0.41
1:B:219:ALA:HB2	1:B:267:ARG:HD3	2.01	0.41
1:B:254:ALA:O	1:B:258:ILE:HG12	2.20	0.41
1:A:144:THR:HA	1:A:147:THR:HB	2.03	0.41
1:B:310:LEU:HD12	1:B:310:LEU:HA	1.95	0.41
1:B:205:MET:HE2	1:B:283:MET:CE	2.51	0.40
1:B:377:ARG:HD2	1:B:380:ARG:CG	2.50	0.40
1:B:395:THR:HG22	1:B:396:ARG:HG2	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	419/463 (90%)	416 (99%)	2 (0%)	1 (0%)	43	51
1	B	411/463 (89%)	402 (98%)	9 (2%)	0	100	100
All	All	830/926 (90%)	818 (99%)	11 (1%)	1 (0%)	48	57

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	420	ALA

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	303/337 (90%)	268 (88%)	35 (12%)	5	5
1	B	297/337 (88%)	248 (84%)	49 (16%)	2	2
All	All	600/674 (89%)	516 (86%)	84 (14%)	3	3

All (84) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	28	ASP
1	A	31	THR
1	A	33	LEU
1	A	43	ARG
1	A	45	SER

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Mol	Chain	Res	Type
1	A	47	LEU
1	A	62	LEU
1	A	82	LEU
1	A	100	ARG
1	A	107	LEU
1	A	111	GLU
1	A	143	ARG
1	A	154	ILE
1	A	165	LEU
1	A	168	ARG
1	A	185	VAL
1	A	218	ARG
1	A	230	GLU
1	A	245	SER
1	A	246	VAL
1	A	251	GLU
1	A	261	ARG
1	A	292	ARG
1	A	304	VAL
1	A	310	LEU
1	A	329	ARG
1	A	332	ARG
1	A	365	LEU
1	A	370	THR
1	A	371	LEU
1	A	372	LEU
1	A	375	VAL
1	A	387	LEU
1	A	395	THR
1	A	396	ARG
1	B	3	LEU
1	B	11	ARG
1	B	28	ASP
1	B	33	LEU
1	B	43	ARG
1	B	47	LEU
1	B	58	LEU
1	B	65	LEU
1	B	66	ARG
1	B	72	GLU
1	B	77	LEU
1	B	79	GLN

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Mol	Chain	Res	Type
1	B	82	LEU
1	B	86	GLN
1	B	88	ARG
1	B	96	GLN
1	B	100	ARG
1	B	107	LEU
1	B	132	ARG
1	B	137	ARG
1	B	139	GLU
1	B	141	LEU
1	B	154	ILE
1	B	162	VAL
1	B	165	LEU
1	B	177	ILE
1	B	185	VAL
1	B	234	ARG
1	B	244	GLU
1	B	246	VAL
1	B	248	LEU
1	B	261	ARG
1	B	271	ARG
1	B	304	VAL
1	B	310	LEU
1	B	357	LEU
1	B	367	ASP
1	B	371	LEU
1	B	375	VAL
1	B	377	ARG
1	B	378	LYS
1	B	379	ASP
1	B	387	LEU
1	B	395	THR
1	B	396	ARG
1	B	399	ASP
1	B	412	THR
1	B	414	VAL
1	B	418	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	42	HIS

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Mol	Chain	Res	Type
1	A	79	GLN
1	A	309	ASN
1	A	326	HIS
1	A	392	GLN
1	B	42	HIS
1	B	49	HIS
1	B	309	ASN
1	B	326	HIS

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](#)

There are no ligands in this entry.

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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	421/463 (90%)	0.35	26 (6%) 26 23	25, 39, 68, 90	0
1	B	415/463 (89%)	0.94	61 (14%) 6 4	25, 56, 97, 132	0
All	All	836/926 (90%)	0.65	87 (10%) 11 9	25, 46, 88, 132	0

All (87) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	354	ASP	6.5
1	A	379	ASP	5.6
1	A	251	GLU	5.0
1	B	275	SER	4.9
1	B	369	GLU	4.7
1	B	139	GLU	4.7
1	B	98	ALA	4.2
1	B	232	THR	4.1
1	A	98	ALA	4.0
1	A	366	THR	4.0
1	A	135	THR	3.9
1	A	378	LYS	3.8
1	B	355	GLY	3.7
1	B	174	GLY	3.7
1	A	354	ASP	3.6
1	B	130	ARG	3.6
1	B	137	ARG	3.6
1	B	233	GLY	3.5
1	A	418	THR	3.4
1	B	258	ILE	3.4
1	B	418	THR	3.3
1	B	227	HIS	3.3
1	B	219	ALA	3.3
1	B	97	GLY	3.2

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Mol	Chain	Res	Type	RSRZ
1	B	237	VAL	3.2
1	B	368	PRO	3.2
1	A	131	GLU	3.1
1	B	367	ASP	3.1
1	B	267	ARG	3.1
1	B	176	SER	3.0
1	B	1	ALA	3.0
1	A	304	VAL	2.9
1	A	257	GLU	2.9
1	B	135	THR	2.9
1	B	248	LEU	2.8
1	B	292	ARG	2.8
1	B	356	VAL	2.8
1	B	127	GLU	2.8
1	B	262	LEU	2.8
1	B	238	ALA	2.8
1	B	269	THR	2.7
1	A	126	GLY	2.7
1	B	379	ASP	2.7
1	B	361	ALA	2.6
1	B	235	VAL	2.6
1	A	43	ARG	2.6
1	A	134	PHE	2.6
1	B	226	ALA	2.6
1	A	367	ASP	2.6
1	A	211	GLY	2.5
1	A	96	GLN	2.5
1	B	378	LYS	2.5
1	B	240	VAL	2.4
1	A	130	ARG	2.4
1	A	1	ALA	2.4
1	A	200	ALA	2.4
1	B	102	GLY	2.4
1	B	246	VAL	2.4
1	B	304	VAL	2.4
1	B	189	LEU	2.4
1	B	243	PRO	2.3
1	B	263	ALA	2.3
1	B	366	THR	2.3
1	A	419	TYR	2.3
1	B	334	ALA	2.3
1	B	44	ARG	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	209	PRO	2.3
1	B	268	LYS	2.3
1	B	128	ASP	2.2
1	A	377	ARG	2.2
1	B	260	GLY	2.2
1	B	134	PHE	2.2
1	B	217	VAL	2.2
1	A	417	PRO	2.2
1	B	234	ARG	2.2
1	A	229	ALA	2.2
1	B	365	LEU	2.2
1	A	128	ASP	2.1
1	B	276	HIS	2.1
1	B	11	ARG	2.1
1	B	141	LEU	2.1
1	B	210	GLU	2.1
1	B	129	LEU	2.1
1	B	199	ALA	2.0
1	B	266	GLY	2.0
1	B	265	ALA	2.0
1	A	129	LEU	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](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.