



Full wwPDB X-ray Structure Validation Report ⓘ

May 4, 2026 – 06:10 PM JST

PDB ID : 9KA1 / pdb_00009ka1
Title : Crystal structure of bicyclogermacrene synthase mutant I290V/I385C/V434C/L454C/V476W/L558I
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Deposited on : 2024-10-28
Resolution : 2.30 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

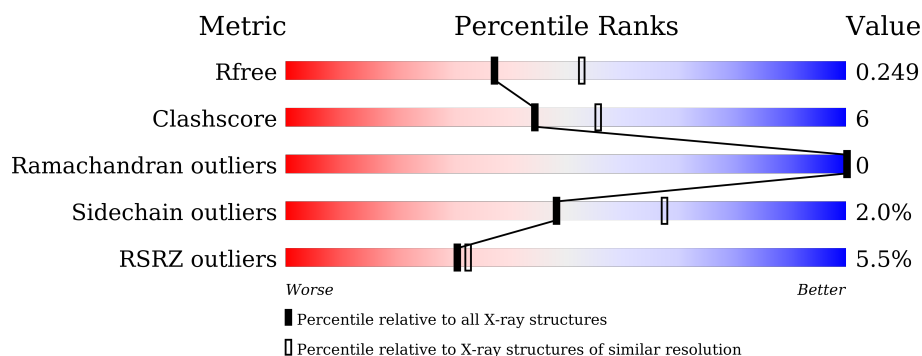
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (2.30-2.30)

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	565	<div> <div>5%</div> <div> <div></div> <div>76%</div> <div>13%</div> <div>•</div> <div>11%</div> </div> </div>
1	B	565	<div> <div>5%</div> <div> <div></div> <div>75%</div> <div>16%</div> <div>•</div> <div>9%</div> </div> </div>

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 8706 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 Bicyclogermacrene synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	504	Total	C	N	O	S	0	1	0
			4201	2687	705	788	21			
1	B	513	Total	C	N	O	S	0	1	0
			4278	2734	720	803	21			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	290	VAL	ILE	engineered mutation	UNP J7LMP2
A	385	CYS	ILE	engineered mutation	UNP J7LMP2
A	434	CYS	VAL	engineered mutation	UNP J7LMP2
A	454	CYS	LEU	engineered mutation	UNP J7LMP2
A	476	TRP	VAL	engineered mutation	UNP J7LMP2
A	558	ILE	LEU	engineered mutation	UNP J7LMP2
B	290	VAL	ILE	engineered mutation	UNP J7LMP2
B	385	CYS	ILE	engineered mutation	UNP J7LMP2
B	434	CYS	VAL	engineered mutation	UNP J7LMP2
B	454	CYS	LEU	engineered mutation	UNP J7LMP2
B	476	TRP	VAL	engineered mutation	UNP J7LMP2
B	558	ILE	LEU	engineered mutation	UNP J7LMP2

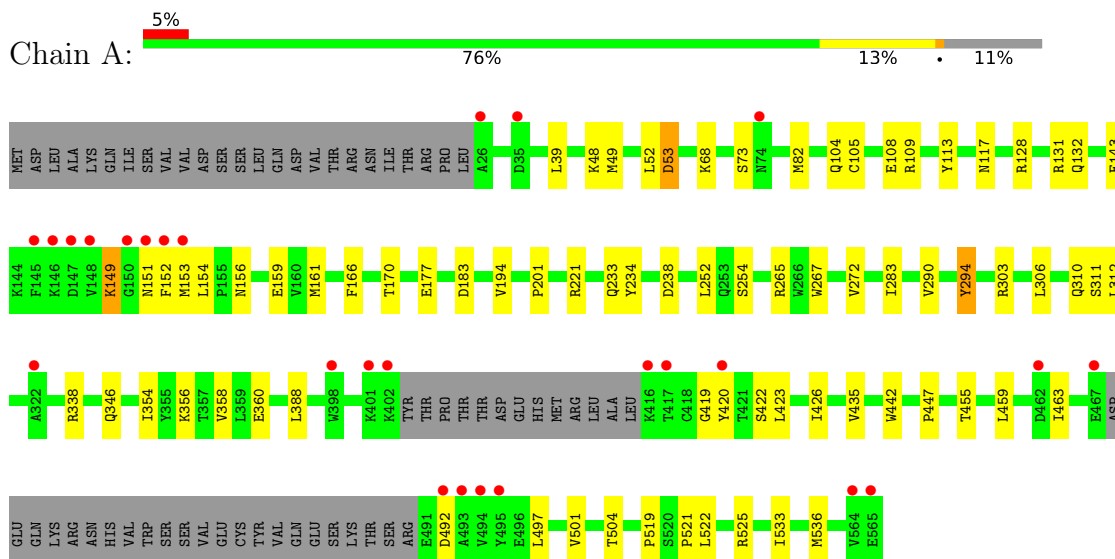
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	107	Total	O	0	0
			107	107		
2	B	120	Total	O	0	0
			120	120		

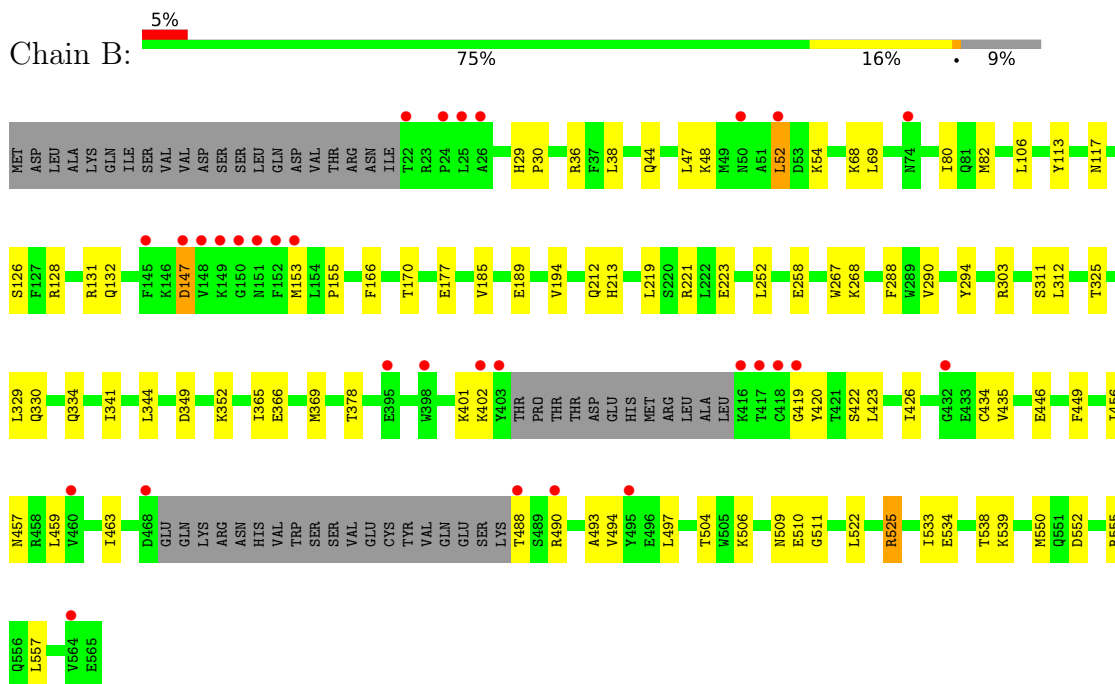
3 Residue-property plots

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: Bicyclogermacrene synthase



• Molecule 1: Bicyclogermacrene synthase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	58.34Å 90.94Å 233.97Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	31.37 – 2.30 31.37 – 2.30	Depositor EDS
% Data completeness (in resolution range)	95.4 (31.37-2.30) 95.5 (31.37-2.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.11 (at 2.29Å)	Xtriage
Refinement program	PHENIX (1.20.1_4487: ???)	Depositor
R, R_{free}	0.217 , 0.247 0.219 , 0.249	Depositor DCC
R_{free} test set	2000 reflections (3.54%)	wwPDB-VP
Wilson B-factor (Å ²)	35.1	Xtriage
Anisotropy	0.860	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 43.3	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	8706	wwPDB-VP
Average B, all atoms (Å ²)	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.71% 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	0.28	0/4298	0.47	0/5806
1	B	0.30	1/4377 (0.0%)	0.46	0/5914
All	All	0.29	1/8675 (0.0%)	0.46	0/11720

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	446	GLU	C-O	-7.78	1.20	1.23

There are no bond angle outliers.

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	4201	0	4081	47	1
1	B	4278	0	4157	53	1
2	A	107	0	0	4	0
2	B	120	0	0	1	0
All	All	8706	0	8238	100	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 6.

All (100) 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:221:ARG:HG2	1:B:557:LEU:HD21	1.60	0.84
1:A:338:ARG:HH21	1:A:346:GLN:HE22	1.33	0.77
1:B:366:GLU:HG3	1:B:378:THR:HG21	1.70	0.74
1:A:131:ARG:NH2	1:A:177:GLU:OE2	2.22	0.71
1:B:128:ARG:O	1:B:132:GLN:HG2	1.95	0.66
1:A:356:LYS:O	1:A:360:GLU:HG3	1.94	0.66
1:A:455:THR:O	1:A:459:LEU:HG	1.96	0.66
1:B:552:ASP:OD1	1:B:555:ARG:NH2	2.28	0.66
1:A:152:PHE:HD2	1:A:154:LEU:H	1.44	0.65
1:A:39:LEU:O	1:A:265:ARG:NH2	2.30	0.64
1:B:490:ARG:O	1:B:494:VAL:HG23	1.98	0.63
1:A:149:LYS:HE3	1:A:159:GLU:HG3	1.80	0.63
1:A:312:LEU:HD13	1:A:358:VAL:HG22	1.80	0.62
1:A:132:GLN:HG3	2:A:606:HOH:O	2.00	0.61
1:B:131:ARG:NH2	1:B:177:GLU:OE2	2.30	0.61
1:B:185:VAL:O	1:B:189:GLU:HG2	2.01	0.60
1:B:153:MET:O	1:B:155:PRO:HD3	2.01	0.60
1:B:493:ALA:O	1:B:497:LEU:HD23	2.01	0.60
1:B:401:LYS:HD2	1:B:402:LYS:O	2.02	0.59
1:A:221:ARG:HD2	2:A:625:HOH:O	2.03	0.57
1:A:294:TYR:CD2	1:A:525:ARG:HD2	2.39	0.57
1:A:442:TRP:CE2	1:A:447:PRO:HG3	2.39	0.57
1:A:128:ARG:O	1:A:132:GLN:HG2	2.03	0.56
1:A:104:GLN:HG3	1:A:108:GLU:OE2	2.08	0.54
1:B:435:VAL:HG13	1:B:522:LEU:HD21	1.90	0.54
1:B:80:ILE:HG13	1:B:106:LEU:HD13	1.90	0.54
1:B:459:LEU:O	1:B:463:ILE:HG13	2.08	0.54
1:A:166:PHE:O	1:A:170:THR:HG23	2.09	0.53
1:B:349:ASP:HA	1:B:352:LYS:HD2	1.91	0.53
1:A:455:THR:HG22	1:A:459:LEU:HD11	1.91	0.52
1:B:349:ASP:HA	1:B:352:LYS:CD	2.40	0.52
1:A:49:MET:HA	1:A:49:MET:HE2	1.93	0.50
1:B:456:ILE:HG13	1:B:504:THR:HG21	1.93	0.50
1:B:538:THR:C	1:B:539:LYS:HD2	2.36	0.50
1:A:420:TYR:CZ	1:A:533:ILE:HD11	2.47	0.50
1:A:267:TRP:CZ3	1:A:311:SER:HB3	2.47	0.49
1:B:166:PHE:O	1:B:170:THR:HG23	2.11	0.49
1:A:338:ARG:NH2	1:A:346:GLN:HE22	2.04	0.49
1:B:463:ILE:HG23	1:B:494:VAL:HG13	1.94	0.49
1:B:221:ARG:HG2	1:B:557:LEU:CD2	2.39	0.49
1:A:151:ASN:HD21	1:A:156:ASN:H	1.60	0.49
1:A:283:ILE:HG22	2:A:632:HOH:O	2.11	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:420:TYR:OH	1:B:457:ASN:ND2	2.45	0.49
1:B:69:LEU:HG	1:B:82:MET:HE2	1.95	0.48
1:B:506:LYS:O	1:B:510:GLU:HG3	2.13	0.48
1:B:68:LYS:CB	1:B:82:MET:HE1	2.44	0.47
1:B:509:ASN:ND2	2:B:610:HOH:O	2.47	0.47
1:B:48:LYS:HG2	1:B:258:GLU:HG3	1.97	0.47
1:A:68:LYS:NZ	1:A:238:ASP:OD2	2.40	0.47
1:A:105:CYS:HA	1:A:109:ARG:HH21	1.80	0.47
1:B:147:ASP:N	1:B:147:ASP:OD1	2.46	0.47
1:B:221:ARG:NH2	1:B:252:LEU:HB3	2.29	0.47
1:A:290:VAL:HG12	1:A:303:ARG:HG2	1.97	0.47
1:A:442:TRP:NE1	1:A:447:PRO:HG3	2.30	0.46
1:B:47:LEU:HD23	1:B:47:LEU:HA	1.76	0.46
1:A:497:LEU:O	1:A:501:VAL:HG23	2.15	0.46
1:B:288:PHE:CE2	1:B:557:LEU:HD12	2.50	0.46
1:B:422:SER:O	1:B:426:ILE:HG12	2.16	0.46
1:A:131:ARG:HH22	1:A:177:GLU:CD	2.21	0.46
1:B:365:ILE:O	1:B:369:MET:HG2	2.15	0.46
1:B:29:HIS:ND1	1:B:30:PRO:O	2.45	0.46
1:A:53:ASP:OD1	1:A:53:ASP:N	2.45	0.45
1:B:38:LEU:HD11	1:B:268:LYS:HD2	1.98	0.45
1:A:166:PHE:CE2	1:A:183:ASP:HB3	2.51	0.45
1:B:525:ARG:HD3	1:B:525:ARG:HA	1.54	0.45
1:B:344:LEU:HD23	1:B:344:LEU:HA	1.58	0.45
1:B:341:ILE:HD12	1:B:341:ILE:HA	1.78	0.45
1:B:288:PHE:CD1	1:B:550:MET:HE1	2.52	0.44
1:A:48:LYS:NZ	2:A:608:HOH:O	2.49	0.44
1:B:267:TRP:CZ3	1:B:311:SER:HB3	2.53	0.44
1:A:519:PRO:HB2	1:A:521:PRO:HD2	1.99	0.44
1:B:52:LEU:HD22	1:B:52:LEU:HA	1.82	0.44
1:B:330:GLN:O	1:B:334:GLN:HG3	2.17	0.43
1:B:449:PHE:CD1	1:B:511:GLY:HA3	2.53	0.43
1:B:325:THR:O	1:B:329:LEU:HG	2.19	0.43
1:B:44:GLN:HB3	1:B:258:GLU:OE2	2.18	0.43
1:A:422:SER:O	1:A:426:ILE:HG12	2.19	0.43
1:A:354:ILE:O	1:A:358:VAL:HG23	2.20	0.42
1:A:252:LEU:HD12	1:A:252:LEU:HA	1.81	0.42
1:B:290:VAL:HG12	1:B:303:ARG:HG2	2.00	0.42
1:A:153:MET:HE2	1:A:153:MET:HB3	1.88	0.42
1:B:219:LEU:O	1:B:223:GLU:HG2	2.20	0.42
1:A:82:MET:HE2	1:A:82:MET:HB2	1.88	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:113:TYR:O	1:B:117:ASN:HB2	2.19	0.42
1:B:420:TYR:CZ	1:B:533:ILE:HD11	2.55	0.41
1:A:161:MET:HE3	1:A:234:TYR:HE2	1.85	0.41
1:A:306:LEU:O	1:A:310:GLN:HB2	2.21	0.41
1:A:459:LEU:O	1:A:463:ILE:HG13	2.19	0.41
1:A:536:MET:HE2	1:A:536:MET:HB3	1.65	0.41
1:A:113:TYR:O	1:A:117:ASN:HB2	2.21	0.41
1:B:80:ILE:HD11	1:B:126:SER:HA	2.02	0.41
1:A:525:ARG:HA	1:A:525:ARG:HD3	1.73	0.41
1:A:310:GLN:HG3	1:A:423:LEU:HD21	2.02	0.40
1:B:212:GLN:O	1:B:213:HIS:CG	2.74	0.40
1:A:435:VAL:HG22	1:A:522:LEU:HD11	2.03	0.40
1:A:388:LEU:HD13	1:A:419:GLY:HA2	2.04	0.40
1:B:54:LYS:HD3	1:B:54:LYS:HA	1.73	0.40
1:B:419:GLY:O	1:B:423:LEU:HG	2.21	0.40
1:A:201:PRO:HB3	1:A:233:GLN:HB2	2.04	0.40
1:B:312:LEU:HD13	1:B:312:LEU:HA	1.90	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:143:GLU:OE2	1:B:36:ARG:NH2[1_565]	2.12	0.08

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	499/565 (88%)	481 (96%)	18 (4%)	0	100	100
1	B	508/565 (90%)	497 (98%)	11 (2%)	0	100	100
All	All	1007/1130 (89%)	978 (97%)	29 (3%)	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	457/515 (89%)	447 (98%)	10 (2%)	45	65
1	B	466/515 (90%)	458 (98%)	8 (2%)	53	72
All	All	923/1030 (90%)	905 (98%)	18 (2%)	48	67

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	52	LEU
1	A	53	ASP
1	A	73	SER
1	A	149	LYS
1	A	194	VAL
1	A	254	SER
1	A	272	VAL
1	A	294	TYR
1	A	492	ASP
1	A	504	THR
1	B	52	LEU
1	B	147	ASP
1	B	194	VAL
1	B	294	TYR
1	B	434	CYS
1	B	488	THR
1	B	525	ARG
1	B	534	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	41	ASN

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Mol	Chain	Res	Type
1	A	46	GLN
1	A	208	HIS
1	A	213	HIS
1	A	346	GLN
1	A	457	ASN
1	A	551	GLN
1	B	50	ASN
1	B	132	GLN
1	B	171	HIS
1	B	457	ASN
1	B	551	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 ⓘ

There are no ligands in this entry.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	504/565 (89%)	0.38	26 (5%) 33 34	17, 43, 85, 122	1 (0%)
1	B	513/565 (90%)	0.42	30 (5%) 29 31	16, 43, 88, 125	1 (0%)
All	All	1017/1130 (90%)	0.40	56 (5%) 30 32	16, 43, 87, 125	2 (0%)

All (56) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	419	GLY	6.6
1	B	418	CYS	5.2
1	A	148	VAL	5.1
1	B	417	THR	4.9
1	B	25	LEU	4.9
1	B	152	PHE	4.8
1	B	403	TYR	4.7
1	B	148	VAL	4.6
1	B	488	THR	4.2
1	B	24	PRO	4.2
1	B	416	LYS	3.7
1	B	153	MET	3.5
1	A	417	THR	3.4
1	B	151	ASN	3.3
1	B	460	VAL	3.3
1	A	152	PHE	3.2
1	B	395	GLU	3.1
1	B	402	LYS	3.1
1	B	468	ASP	3.1
1	A	26	ALA	3.1
1	A	150	GLY	3.0
1	B	26	ALA	3.0
1	A	153	MET	3.0
1	A	565	GLU	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	146	LYS	2.9
1	B	22	THR	2.9
1	A	322	ALA	2.9
1	B	564	VAL	2.9
1	B	398	TRP	2.8
1	A	494	VAL	2.8
1	A	147	ASP	2.7
1	B	74	ASN	2.7
1	A	398	TRP	2.7
1	A	145	PHE	2.7
1	A	416	LYS	2.7
1	B	432	GLY	2.6
1	A	420	TYR	2.6
1	A	564	VAL	2.6
1	A	74	ASN	2.5
1	A	401	LYS	2.5
1	B	495	TYR	2.4
1	A	493	ALA	2.4
1	B	52	LEU	2.3
1	A	467	GLU	2.3
1	A	151	ASN	2.3
1	B	149	LYS	2.3
1	A	35	ASP	2.3
1	B	50	ASN	2.3
1	B	147	ASP	2.2
1	A	462	ASP	2.2
1	A	402	LYS	2.2
1	A	492	ASP	2.1
1	A	495	TYR	2.1
1	B	490	ARG	2.1
1	B	150	GLY	2.0
1	B	145	PHE	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.