



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 10:32 PM UTC

PDB ID : 9D28 / pdb_00009d28
Title : Crystal structure of (+)-sabinene synthase from Thuja plicata
Authors : Gaynes, M.N.; Christianson, D.W.
Deposited on : 2024-08-08
Resolution : 2.32 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

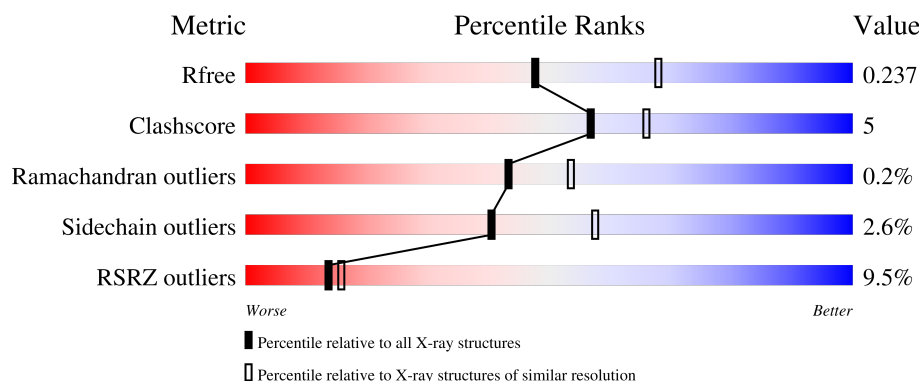
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.32 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	7754 (2.34-2.30)
Clashscore	190562	8383 (2.34-2.30)
Ramachandran outliers	187476	8303 (2.34-2.30)
Sidechain outliers	187428	8303 (2.34-2.30)
RSRZ outliers	180081	7760 (2.34-2.30)

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	554	8% 81% 11% 7%
1	B	554	10% 81% 10% 7%
1	C	554	8% 81% 12% 6%
1	D	554	9% 83% 9% 7%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 16245 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 Sabinene synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	515	Total	C	N	O	S	0	0	0
			3995	2541	674	760	20			
1	A	515	Total	C	N	O	S	0	0	0
			3987	2537	671	759	20			
1	C	522	Total	C	N	O	S	0	0	0
			4073	2596	686	771	20			
1	D	515	Total	C	N	O	S	0	0	0
			3995	2548	671	756	20			

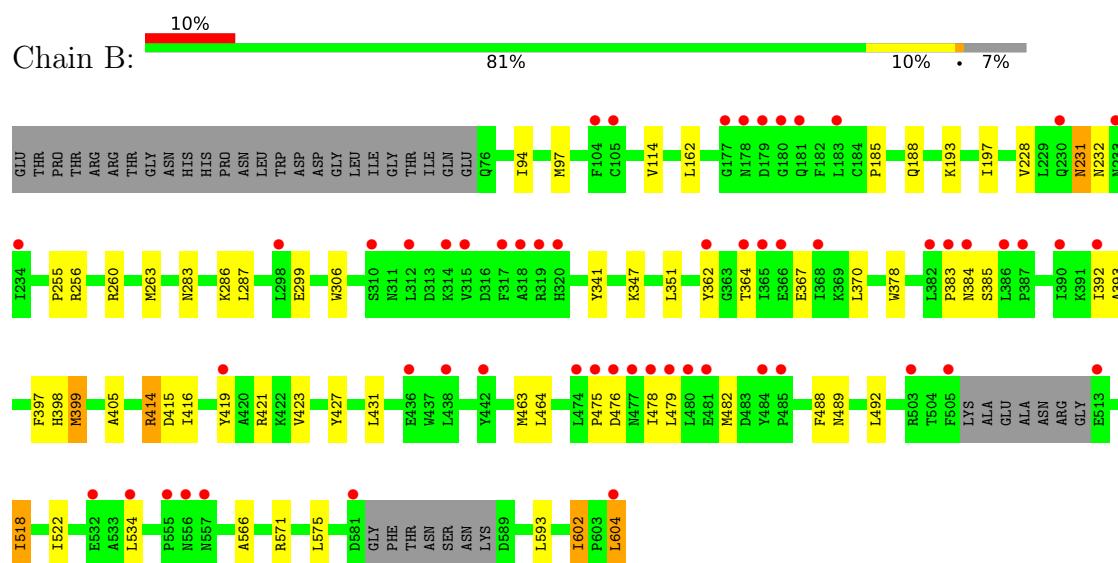
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	36	Total	O	0	0
			36	36		
2	A	38	Total	O	0	0
			38	38		
2	C	72	Total	O	0	0
			72	72		
2	D	49	Total	O	0	0
			49	49		

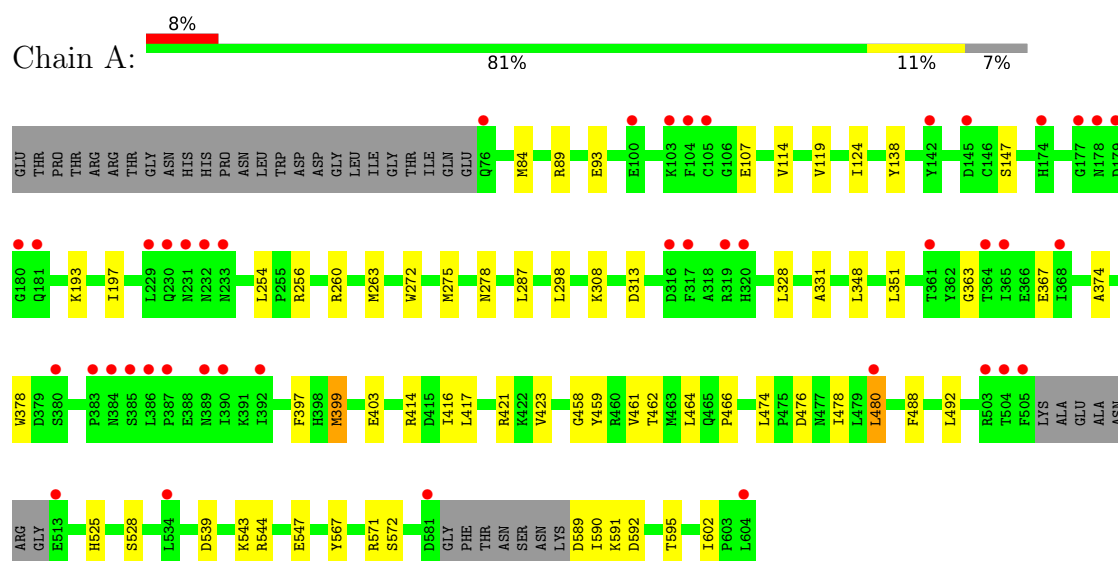
3 Residue-property plots

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: Sabinene synthase

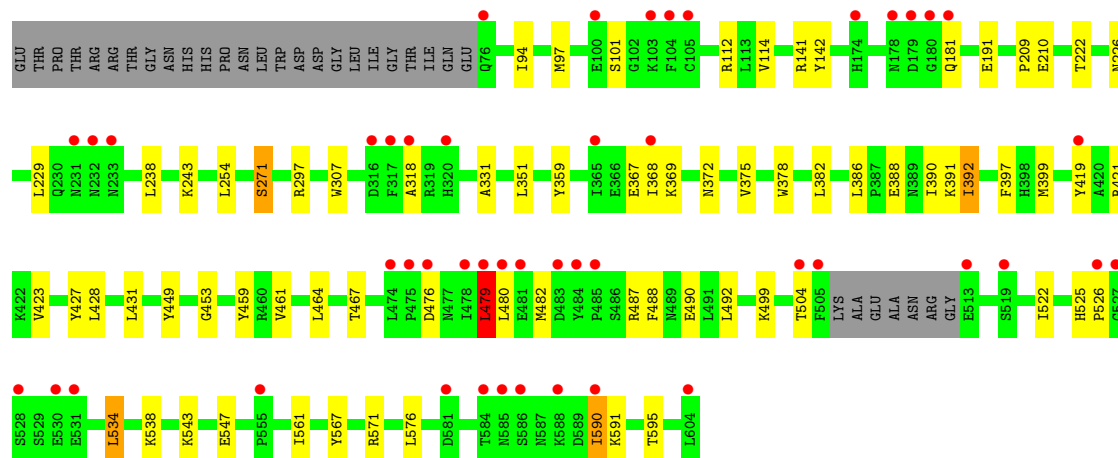


• Molecule 1: Sabinene synthase



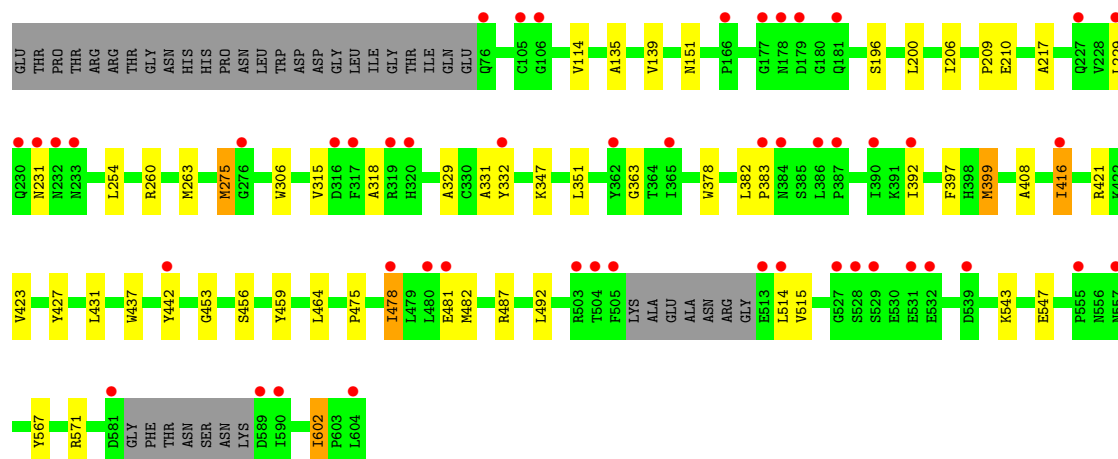
• Molecule 1: Sabinene synthase

Chain C: 



• Molecule 1: Sabinene synthase

Chain D: 



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	273.29Å 89.81Å 194.52Å 90.00° 134.89° 90.00°	Depositor
Resolution (Å)	96.81 – 2.32 96.81 – 2.32	Depositor EDS
% Data completeness (in resolution range)	99.0 (96.81-2.32) 98.8 (96.81-2.32)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.50 (at 2.32Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.213 , 0.235 0.214 , 0.237	Depositor DCC
R_{free} test set	1989 reflections (1.38%)	wwPDB-VP
Wilson B-factor (Å ²)	50.7	Xtriage
Anisotropy	0.617	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 46.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.029 for -h-2*1,k,h+1 0.000 for h,-k,-h-l 0.000 for h+2*1,-k,-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	16245	wwPDB-VP
Average B, all atoms (Å ²)	60.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 39.16 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 3.3075e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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	0.36	0/4073	0.53	0/5544
1	B	0.40	0/4082	0.59	0/5554
1	C	0.40	0/4163	0.57	1/5663 (0.0%)
1	D	0.41	0/4082	0.60	1/5556 (0.0%)
All	All	0.39	0/16400	0.57	2/22317 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	479	LEU	N-CA-C	-5.99	104.87	111.82
1	D	482	MET	N-CA-C	-5.31	106.74	113.43

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	3987	0	3694	32	0
1	B	3995	0	3714	35	0
1	C	4073	0	3824	44	0
1	D	3995	0	3720	33	0
2	A	38	0	0	2	0
2	B	36	0	0	2	0
2	C	72	0	0	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	49	0	0	0	0
All	All	16245	0	14952	144	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 5.

All (144) 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:D:315:VAL:HG23	1:D:392:ILE:HD11	1.44	0.98
1:B:423:VAL:HG21	1:B:464:LEU:HD22	1.51	0.92
1:D:423:VAL:HG21	1:D:464:LEU:HD22	1.55	0.88
1:A:423:VAL:HG21	1:A:464:LEU:HD22	1.56	0.87
1:D:315:VAL:HG12	1:D:318:ALA:H	1.41	0.86
1:C:423:VAL:HG21	1:C:464:LEU:HD22	1.60	0.82
1:C:419:TYR:CZ	1:C:479:LEU:HD11	2.21	0.75
1:D:315:VAL:CG2	1:D:392:ILE:HD11	2.20	0.69
1:B:351:LEU:HD13	1:B:397:PHE:HA	1.75	0.68
1:D:382:LEU:HB3	1:D:383:PRO:HD2	1.77	0.66
1:D:315:VAL:HG12	1:D:318:ALA:N	2.09	0.64
1:C:94:ILE:HA	1:C:97:MET:HE2	1.78	0.64
1:A:544:ARG:NH1	1:A:547:GLU:OE2	2.29	0.63
1:D:567:TYR:CE2	1:D:571:ARG:HD2	2.33	0.62
1:C:567:TYR:CE2	1:C:571:ARG:HD2	2.35	0.62
1:C:367:GLU:HG2	1:C:386:LEU:HD22	1.81	0.62
1:D:378:TRP:CD2	1:D:421:ARG:HD3	2.36	0.61
1:B:94:ILE:HA	1:B:97:MET:HE2	1.82	0.61
1:B:185:PRO:HG2	1:B:188:GLN:HG3	1.83	0.60
1:C:386:LEU:O	1:C:391:LYS:HD2	2.02	0.60
1:A:567:TYR:CE2	1:A:571:ARG:HD2	2.38	0.59
1:A:351:LEU:HD13	1:A:397:PHE:HA	1.85	0.58
1:D:351:LEU:HD13	1:D:397:PHE:HA	1.85	0.58
1:C:419:TYR:CE1	1:C:479:LEU:HD11	2.40	0.56
1:C:476:ASP:HA	1:C:479:LEU:HD22	1.88	0.56
1:C:141:ARG:NH2	1:C:142:TYR:OH	2.38	0.56
1:A:417:LEU:O	1:A:421:ARG:HG3	2.07	0.55
1:A:589:ASP:HA	1:A:592:ASP:OD2	2.06	0.55
1:C:487:ARG:NH1	1:C:490:GLU:OE1	2.32	0.55
1:C:191:GLU:HG3	1:C:238:LEU:HD22	1.88	0.55
1:C:369:LYS:HA	1:C:372:ASN:HB2	1.88	0.54
1:C:382:LEU:HB3	1:C:386:LEU:HD12	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:475:PRO:HD2	1:D:478:ILE:HB	1.89	0.54
1:C:222:THR:O	1:C:226:ASN:ND2	2.41	0.54
1:D:329:ALA:HA	1:D:332:TYR:CE1	2.43	0.52
1:A:328:LEU:HD22	1:A:572:SER:HB2	1.91	0.52
1:A:193:LYS:O	1:A:197:ILE:HG12	2.11	0.51
1:C:378:TRP:CD2	1:C:421:ARG:HD2	2.46	0.51
1:D:487:ARG:NH2	1:D:547:GLU:OE1	2.44	0.50
1:B:383:PRO:C	1:B:385:SER:H	2.19	0.50
1:D:543:LYS:O	1:D:547:GLU:HG3	2.11	0.50
1:C:399:MET:HA	1:C:399:MET:HE2	1.92	0.50
1:C:423:VAL:HG12	1:C:461:VAL:HG12	1.93	0.50
1:D:254:LEU:HD13	1:D:331:ALA:HB3	1.93	0.50
1:B:405:ALA:HA	1:B:416:ILE:HD11	1.92	0.49
1:D:200:LEU:HD11	1:D:217:ALA:HB1	1.94	0.49
1:D:437:TRP:HE3	1:D:515:VAL:HG11	1.77	0.49
1:B:463:MET:HE3	1:B:566:ALA:HB2	1.94	0.49
1:B:482:MET:O	1:B:489:ASN:HB2	2.12	0.49
1:C:351:LEU:HD13	1:C:397:PHE:HA	1.94	0.49
1:B:283:ASN:O	1:B:287:LEU:HG	2.13	0.49
1:C:101:SER:HB3	1:C:112:ARG:HG2	1.95	0.48
1:B:518:ILE:O	1:B:522:ILE:HG12	2.14	0.48
1:D:229:LEU:C	1:D:231:ASN:H	2.20	0.48
1:D:442:TYR:C	1:D:514:LEU:HD21	2.38	0.48
1:C:419:TYR:CE2	1:C:479:LEU:HD21	2.49	0.48
1:A:260:ARG:CZ	1:A:602:ILE:HD12	2.44	0.48
1:A:275:MET:HA	1:A:275:MET:HE3	1.96	0.48
1:C:591:LYS:O	1:C:595:THR:HG23	2.14	0.47
1:C:427:TYR:CZ	1:C:431:LEU:HD11	2.49	0.47
1:A:591:LYS:O	1:A:595:THR:HG23	2.14	0.47
1:A:107:GLU:HA	1:A:138:TYR:OH	2.14	0.47
1:A:414:ARG:NH2	1:A:474:LEU:O	2.46	0.47
1:C:209:PRO:O	1:C:210:GLU:HB2	2.14	0.47
1:B:399:MET:HA	1:B:399:MET:HE2	1.97	0.47
1:C:479:LEU:HD23	1:C:480:LEU:N	2.30	0.47
1:D:427:TYR:CZ	1:D:431:LEU:HD11	2.50	0.47
1:B:419:TYR:CZ	1:B:479:LEU:HD13	2.50	0.47
1:D:442:TYR:O	1:D:514:LEU:HD21	2.15	0.47
1:A:275:MET:O	2:A:701:HOH:O	2.21	0.46
1:C:467:THR:HG21	1:C:482:MET:HE1	1.96	0.46
1:D:209:PRO:O	1:D:210:GLU:HB2	2.14	0.46
1:A:89:ARG:HD2	1:A:93:GLU:OE2	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:256:ARG:HG3	2:A:713:HOH:O	2.14	0.46
1:C:543:LYS:O	1:C:547:GLU:HG3	2.15	0.46
1:B:228:VAL:O	1:B:231:ASN:O	2.33	0.46
1:A:272:TRP:CZ3	1:A:278:ASN:HB3	2.51	0.46
1:C:487:ARG:NH2	1:C:547:GLU:OE1	2.46	0.46
1:C:488:PHE:CE2	1:C:492:LEU:HD11	2.50	0.46
1:C:388:GLU:O	1:C:392:ILE:HG23	2.16	0.46
1:C:499:LYS:NZ	2:C:707:HOH:O	2.49	0.46
1:C:534:LEU:HD23	1:C:534:LEU:HA	1.71	0.45
1:B:414:ARG:HG3	1:B:415:ASP:O	2.16	0.45
1:A:89:ARG:O	1:A:93:GLU:HG3	2.15	0.45
1:C:534:LEU:HD22	1:C:538:LYS:HE2	1.97	0.45
1:B:286:LYS:HB3	1:B:604:LEU:HD23	1.99	0.45
1:B:378:TRP:HB2	1:B:421:ARG:NH2	2.31	0.45
1:A:476:ASP:O	1:A:480:LEU:HG	2.16	0.45
1:C:419:TYR:O	1:C:423:VAL:HG23	2.17	0.45
1:B:475:PRO:O	1:B:478:ILE:N	2.47	0.45
1:A:458:GLY:O	1:A:462:THR:HG23	2.17	0.45
1:D:275:MET:HE2	1:D:275:MET:HB2	1.85	0.44
1:B:260:ARG:CZ	1:B:602:ILE:HD12	2.47	0.44
1:A:374:ALA:O	1:A:378:TRP:N	2.50	0.44
1:B:378:TRP:HB2	1:B:421:ARG:CZ	2.47	0.44
1:C:271:SER:OG	2:C:701:HOH:O	2.21	0.44
1:B:392:ILE:HG13	1:B:393:ALA:N	2.32	0.43
1:A:263:MET:SD	1:A:602:ILE:HD13	2.57	0.43
1:A:399:MET:HE2	1:A:399:MET:HA	1.98	0.43
1:A:525:HIS:O	1:A:528:SER:OG	2.24	0.43
1:D:378:TRP:CE3	1:D:421:ARG:HD3	2.53	0.43
1:B:475:PRO:O	1:B:476:ASP:C	2.61	0.43
1:D:408:ALA:HB3	1:D:416:ILE:HG12	2.00	0.43
1:B:575:LEU:HD21	1:B:593:LEU:HD11	2.01	0.43
1:A:423:VAL:HG12	1:A:461:VAL:HG12	2.01	0.43
1:C:254:LEU:HD13	1:C:331:ALA:HB3	2.01	0.43
1:B:256:ARG:HG3	2:B:712:HOH:O	2.17	0.43
1:D:260:ARG:NH1	1:D:602:ILE:HD12	2.34	0.43
1:D:459:TYR:CD2	1:D:459:TYR:C	2.95	0.43
1:B:427:TYR:CZ	1:B:431:LEU:HD11	2.54	0.42
1:C:525:HIS:O	1:C:526:PRO:C	2.63	0.42
1:B:263:MET:SD	1:B:602:ILE:HD13	2.59	0.42
1:A:543:LYS:O	1:A:547:GLU:HG3	2.19	0.42
1:B:255:PRO:HD3	1:B:571:ARG:NH2	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:307:TRP:HH2	1:C:318:ALA:HB1	1.84	0.42
1:B:306:TRP:CD1	1:B:347:LYS:HE3	2.54	0.42
1:C:375:VAL:HG21	1:C:428:LEU:HD11	2.02	0.42
1:C:359:TYR:HA	1:C:368:ILE:HD11	2.01	0.42
1:D:151:ASN:HB2	1:D:196:SER:OG	2.20	0.42
1:D:453:GLY:HA2	1:D:456:SER:OG	2.20	0.42
1:D:306:TRP:CE2	1:D:347:LYS:HD2	2.54	0.42
1:B:299:GLU:HB3	2:B:702:HOH:O	2.20	0.41
1:B:341:TYR:CD1	1:B:341:TYR:C	2.98	0.41
1:B:488:PHE:CE2	1:B:492:LEU:HD11	2.55	0.41
1:A:459:TYR:CD2	1:A:459:TYR:C	2.98	0.41
1:D:263:MET:SD	1:D:602:ILE:HD13	2.61	0.41
1:D:459:TYR:OH	1:D:492:LEU:HD13	2.20	0.41
1:A:254:LEU:HD13	1:A:331:ALA:HB3	2.01	0.41
1:A:308:LYS:HA	1:A:313:ASP:OD2	2.21	0.41
1:A:348:LEU:HD12	1:A:466:PRO:HD3	2.02	0.41
1:C:297:ARG:HG2	2:C:763:HOH:O	2.19	0.41
1:C:449:TYR:O	1:C:453:GLY:N	2.50	0.41
1:C:229:LEU:HD22	1:C:243:LYS:HE3	2.02	0.41
1:B:351:LEU:HD23	1:B:351:LEU:HA	1.85	0.41
1:B:378:TRP:CD1	1:B:398:HIS:HE2	2.38	0.41
1:A:84:MET:HE3	1:A:84:MET:HB2	1.81	0.41
1:D:135:ALA:O	1:D:139:VAL:HG23	2.21	0.41
1:B:162:LEU:HD23	1:B:162:LEU:HA	1.92	0.40
1:B:364:THR:N	1:B:367:GLU:OE1	2.31	0.40
1:A:488:PHE:CE2	1:A:492:LEU:HD11	2.56	0.40
1:C:576:LEU:HD12	1:C:590:ILE:HG21	2.02	0.40
1:D:399:MET:HA	1:D:399:MET:HE2	2.04	0.40
1:B:193:LYS:O	1:B:197:ILE:HG12	2.21	0.40
1:C:459:TYR:OH	1:C:492:LEU:HD13	2.21	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	509/554 (92%)	491 (96%)	17 (3%)	1 (0%)	43	53
1	B	509/554 (92%)	488 (96%)	19 (4%)	2 (0%)	30	37
1	C	518/554 (94%)	493 (95%)	24 (5%)	1 (0%)	43	53
1	D	509/554 (92%)	487 (96%)	21 (4%)	1 (0%)	43	53
All	All	2045/2216 (92%)	1959 (96%)	81 (4%)	5 (0%)	43	53

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	232	ASN
1	B	384	ASN
1	A	363	GLY
1	C	590	ILE
1	D	363	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	394/487 (81%)	380 (96%)	14 (4%)	31	45
1	B	398/487 (82%)	388 (98%)	10 (2%)	42	59
1	C	411/487 (84%)	401 (98%)	10 (2%)	43	60
1	D	396/487 (81%)	388 (98%)	8 (2%)	48	66
All	All	1599/1948 (82%)	1557 (97%)	42 (3%)	40	57

All (42) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	114	VAL
1	B	231	ASN
1	B	362	TYR

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Mol	Chain	Res	Type
1	B	370	LEU
1	B	399	MET
1	B	414	ARG
1	B	518	ILE
1	B	534	LEU
1	B	602	ILE
1	B	604	LEU
1	A	114	VAL
1	A	119	VAL
1	A	124	ILE
1	A	147	SER
1	A	287	LEU
1	A	298	LEU
1	A	367	GLU
1	A	399	MET
1	A	403	GLU
1	A	416	ILE
1	A	478	ILE
1	A	480	LEU
1	A	539	ASP
1	A	590	ILE
1	C	114	VAL
1	C	181	GLN
1	C	271	SER
1	C	390	ILE
1	C	392	ILE
1	C	479	LEU
1	C	504	THR
1	C	522	ILE
1	C	534	LEU
1	C	561	ILE
1	D	114	VAL
1	D	206	ILE
1	D	275	MET
1	D	399	MET
1	D	416	ILE
1	D	478	ILE
1	D	481	GLU
1	D	602	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	82	HIS
1	B	120	GLN
1	B	134	GLN
1	B	163	ASN
1	B	311	ASN
1	B	525	HIS
1	A	398	HIS
1	A	489	ASN
1	A	525	HIS
1	C	525	HIS
1	D	120	GLN
1	D	163	ASN
1	D	212	ASN
1	D	231	ASN

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

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	515/554 (92%)	0.69	43 (8%) 17 19	41, 61, 86, 96	0
1	B	515/554 (92%)	0.78	56 (10%) 10 12	40, 62, 90, 99	0
1	C	522/554 (94%)	0.59	47 (9%) 15 17	37, 56, 82, 93	0
1	D	515/554 (92%)	0.74	50 (9%) 13 15	40, 59, 87, 104	0
All	All	2067/2216 (93%)	0.70	196 (9%) 14 16	37, 60, 87, 104	0

All (196) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	232	ASN	6.8
1	C	478	ILE	6.7
1	B	478	ILE	6.6
1	C	586	SER	6.3
1	D	505	PHE	6.0
1	D	317	PHE	5.7
1	C	505	PHE	5.7
1	C	180	GLY	5.5
1	C	179	ASP	5.3
1	D	105	CYS	5.1
1	A	505	PHE	4.9
1	A	178	ASN	4.8
1	B	581	ASP	4.7
1	C	316	ASP	4.7
1	C	479	LEU	4.7
1	B	476	ASP	4.6
1	D	581	ASP	4.6
1	C	483	ASP	4.6
1	A	504	THR	4.5
1	C	105	CYS	4.5
1	B	480	LEU	4.4

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Mol	Chain	Res	Type	RSRZ
1	A	76	GLN	4.3
1	B	105	CYS	4.3
1	C	481	GLU	4.3
1	B	505	PHE	4.3
1	D	320	HIS	4.2
1	C	484	TYR	4.0
1	D	514	LEU	4.0
1	D	513	GLU	4.0
1	B	179	ASP	4.0
1	A	581	ASP	3.9
1	D	590	ILE	3.9
1	A	320	HIS	3.9
1	C	476	ASP	3.8
1	B	604	LEU	3.8
1	A	604	LEU	3.8
1	B	320	HIS	3.7
1	B	319	ARG	3.7
1	D	233	ASN	3.7
1	D	178	ASN	3.6
1	A	179	ASP	3.6
1	D	529	SER	3.5
1	D	555	PRO	3.5
1	C	480	LEU	3.5
1	C	588	LYS	3.5
1	B	178	ASN	3.5
1	D	316	ASP	3.5
1	C	531	GLU	3.5
1	A	384	ASN	3.5
1	A	229	LEU	3.4
1	B	383	PRO	3.4
1	A	105	CYS	3.4
1	B	233	ASN	3.4
1	A	390	ILE	3.4
1	A	180	GLY	3.4
1	A	231	ASN	3.4
1	B	477	ASN	3.3
1	B	386	LEU	3.3
1	B	438	LEU	3.3
1	B	479	LEU	3.3
1	D	504	THR	3.3
1	D	230	GLN	3.3
1	D	383	PRO	3.3

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Mol	Chain	Res	Type	RSRZ
1	D	532	GLU	3.2
1	C	485	PRO	3.2
1	B	317	PHE	3.2
1	B	384	ASN	3.2
1	D	181	GLN	3.2
1	B	365	ILE	3.2
1	D	177	GLY	3.1
1	D	589	ASP	3.1
1	B	180	GLY	3.1
1	B	315	VAL	3.1
1	C	474	LEU	3.1
1	C	604	LEU	3.1
1	C	475	PRO	3.1
1	C	181	GLN	3.0
1	C	530	GLU	3.0
1	D	106	GLY	3.0
1	A	233	ASN	3.0
1	A	365	ILE	2.9
1	D	231	ASN	2.9
1	C	317	PHE	2.9
1	A	230	GLN	2.9
1	B	419	TYR	2.9
1	B	475	PRO	2.9
1	B	555	PRO	2.9
1	D	76	GLN	2.9
1	A	364	THR	2.9
1	A	383	PRO	2.8
1	C	419	TYR	2.8
1	A	386	LEU	2.8
1	C	178	ASN	2.8
1	B	503	ARG	2.8
1	B	442	TYR	2.8
1	D	229	LEU	2.8
1	A	503	ARG	2.8
1	A	316	ASP	2.8
1	D	384	ASN	2.8
1	B	474	LEU	2.8
1	C	513	GLU	2.8
1	A	103	LYS	2.8
1	D	387	PRO	2.8
1	B	534	LEU	2.7
1	A	534	LEU	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	557	ASN	2.7
1	B	382	LEU	2.7
1	D	503	ARG	2.7
1	B	364	THR	2.7
1	B	390	ILE	2.7
1	B	230	GLN	2.7
1	C	233	ASN	2.7
1	A	480	LEU	2.7
1	B	513	GLU	2.6
1	C	585	ASN	2.6
1	B	177	GLY	2.6
1	B	481	GLU	2.6
1	C	527	GLY	2.6
1	B	310	SER	2.6
1	B	234	ILE	2.5
1	A	380	SER	2.5
1	D	365	ILE	2.5
1	D	480	LEU	2.5
1	C	232	ASN	2.5
1	A	177	GLY	2.5
1	A	387	PRO	2.5
1	D	527	GLY	2.5
1	A	317	PHE	2.5
1	D	332	TYR	2.5
1	D	392	ILE	2.5
1	D	386	LEU	2.5
1	D	539	ASP	2.5
1	D	227	GLN	2.5
1	D	531	GLU	2.4
1	D	604	LEU	2.4
1	C	174	HIS	2.4
1	B	366	GLU	2.4
1	C	365	ILE	2.4
1	B	362	TYR	2.4
1	A	232	ASN	2.4
1	C	519	SER	2.4
1	C	528	SER	2.4
1	B	181	GLN	2.4
1	B	318	ALA	2.4
1	C	103	LYS	2.4
1	C	504	THR	2.4
1	A	104	PHE	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	556	ASN	2.3
1	A	145	ASP	2.3
1	C	318	ALA	2.3
1	B	104	PHE	2.3
1	D	416	ILE	2.3
1	B	392	ILE	2.3
1	A	142	TYR	2.3
1	D	528	SER	2.3
1	A	368	ILE	2.3
1	A	392	ILE	2.3
1	C	590	ILE	2.3
1	D	179	ASP	2.3
1	A	513	GLU	2.3
1	B	183	LEU	2.2
1	C	231	ASN	2.2
1	D	362	TYR	2.2
1	A	181	GLN	2.2
1	D	478	ILE	2.2
1	C	104	PHE	2.2
1	B	532	GLU	2.2
1	C	555	PRO	2.2
1	A	100	GLU	2.2
1	C	100	GLU	2.2
1	B	387	PRO	2.2
1	B	436	GLU	2.2
1	A	174	HIS	2.2
1	A	361	THR	2.2
1	D	442	TYR	2.1
1	D	481	GLU	2.1
1	D	319	ARG	2.1
1	B	368	ILE	2.1
1	D	390	ILE	2.1
1	A	389	ASN	2.1
1	B	298	LEU	2.1
1	C	368	ILE	2.1
1	D	166	PRO	2.1
1	C	76	GLN	2.1
1	D	557	ASN	2.1
1	C	526	PRO	2.1
1	D	276	GLY	2.1
1	A	385	SER	2.0
1	C	584	THR	2.0

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Mol	Chain	Res	Type	RSRZ
1	C	320	HIS	2.0
1	C	581	ASP	2.0
1	B	485	PRO	2.0
1	B	484	TYR	2.0
1	A	319	ARG	2.0
1	B	312	LEU	2.0
1	B	314	LYS	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.