



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 12:02 AM UTC

PDB ID : 9D2A / pdb_00009d2a
Title : Crystal structure of (+)-sabinene synthase from Thuja plicata: condition 3
Authors : Gaynes, M.N.; Christianson, D.W.
Deposited on : 2024-08-08
Resolution : 2.21 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
Mogul	:	2022.3.0, CSD as543be (2022)
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

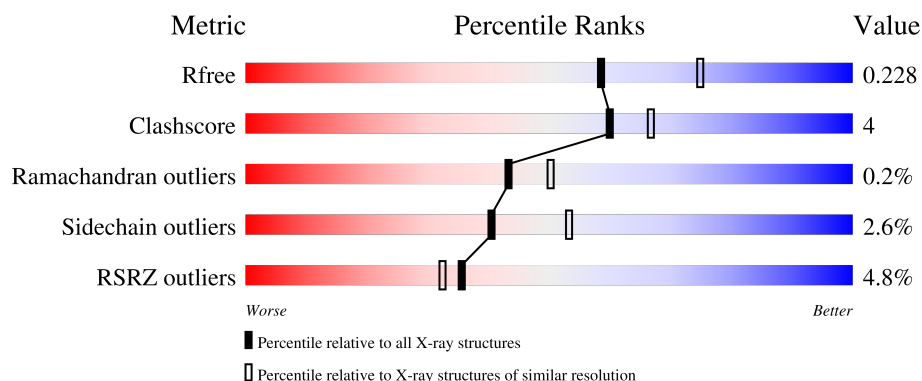
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

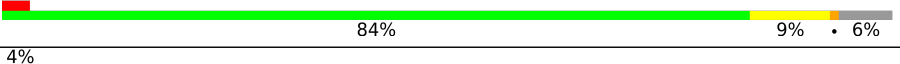
The reported resolution of this entry is 2.21 Å.

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	7682 (2.24-2.20)
Clashscore	190562	8402 (2.24-2.20)
Ramachandran outliers	187476	8303 (2.24-2.20)
Sidechain outliers	187428	8304 (2.24-2.20)
RSRZ outliers	180081	7683 (2.24-2.20)

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	554	
1	B	554	
1	C	554	
1	D	554	

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	EDO	B	701	-	-	X	-
3	CO	B	704	-	-	X	-

2 Entry composition [i](#)

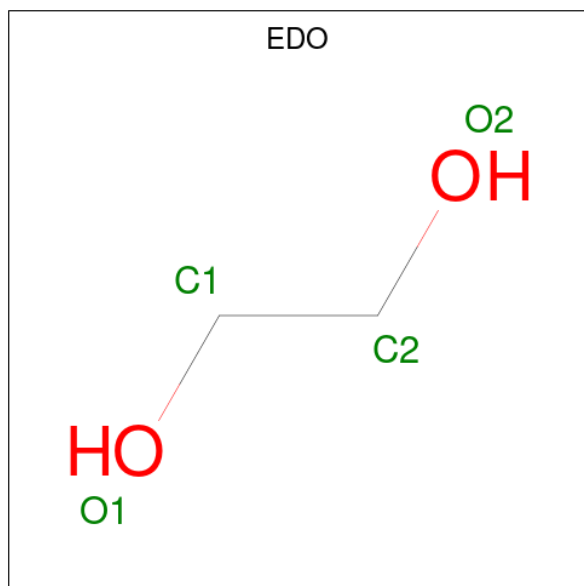
There are 4 unique types of molecules in this entry. The entry contains 16618 atoms, of which 0 are hydrogens and 0 are deuteriums.

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	C	512	Total	C	N	O	S	0	0	0
			4015	2560	676	759	20			
1	D	512	Total	C	N	O	S	0	0	0
			4003	2553	670	760	20			
1	A	513	Total	C	N	O	S	0	0	0
			4031	2572	678	760	21			
1	B	522	Total	C	N	O	S	0	0	0
			4133	2631	697	784	21			

- Molecule 2 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	C	1	Total	C	O	0	0
			4	2	2		
2	D	1	Total	C	O	0	0
			4	2	2		

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

- Molecule 3 is COBALT (II) ION (CCD ID: CO) (formula: Co).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	C	3	Total	Co	0	0
			3	3		
3	D	3	Total	Co	0	0
			3	3		
3	A	3	Total	Co	0	0
			3	3		
3	B	4	Total	Co	0	0
			4	4		

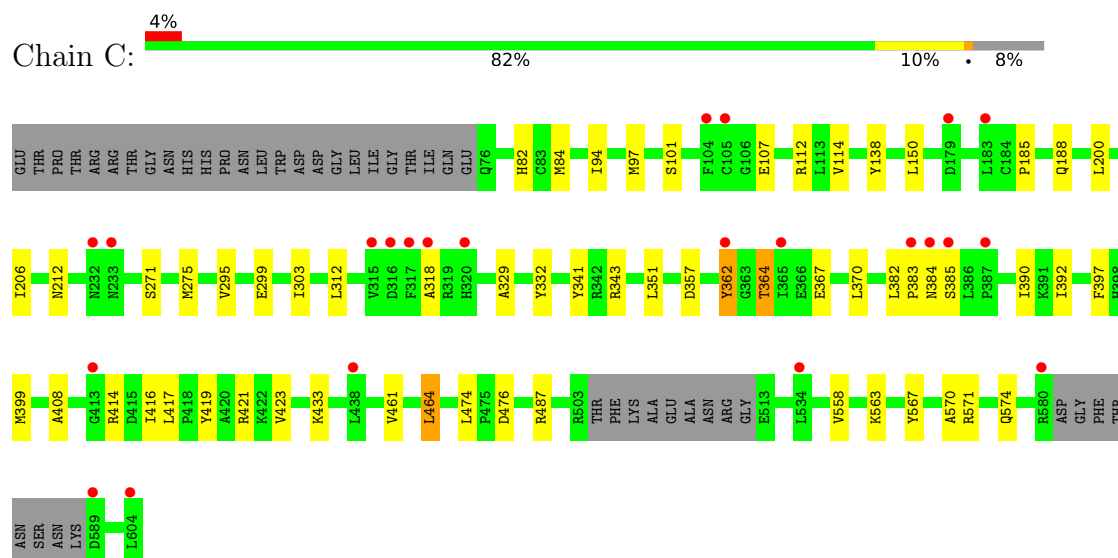
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	C	68	Total	O	0	0
			68	68		
4	D	88	Total	O	0	0
			88	88		
4	A	109	Total	O	0	0
			109	109		
4	B	138	Total	O	0	0
			138	138		

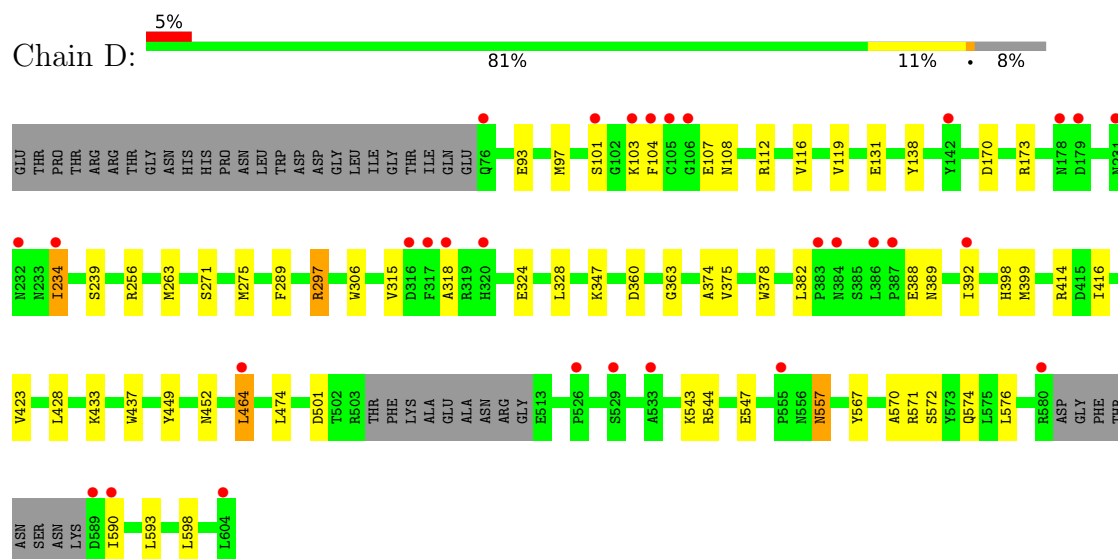
3 Residue-property plots [i](#)

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.

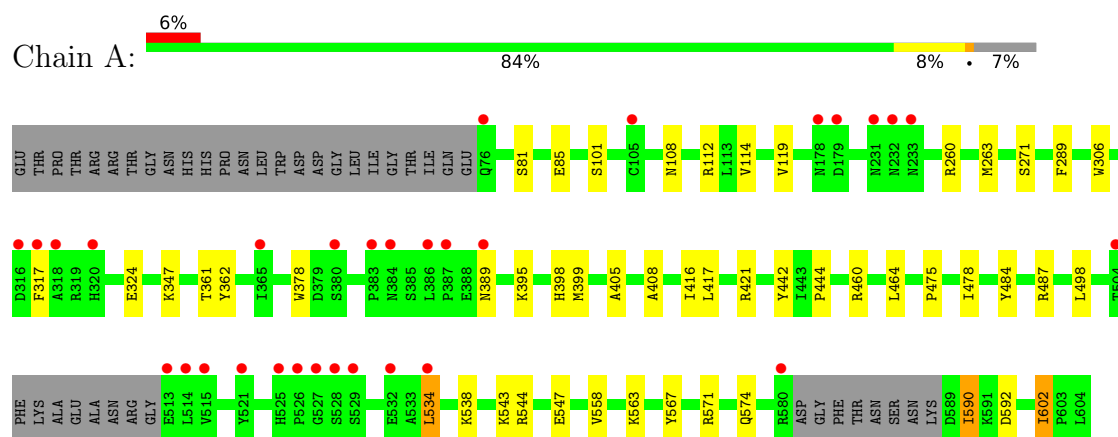
• Molecule 1: Sabinene synthase



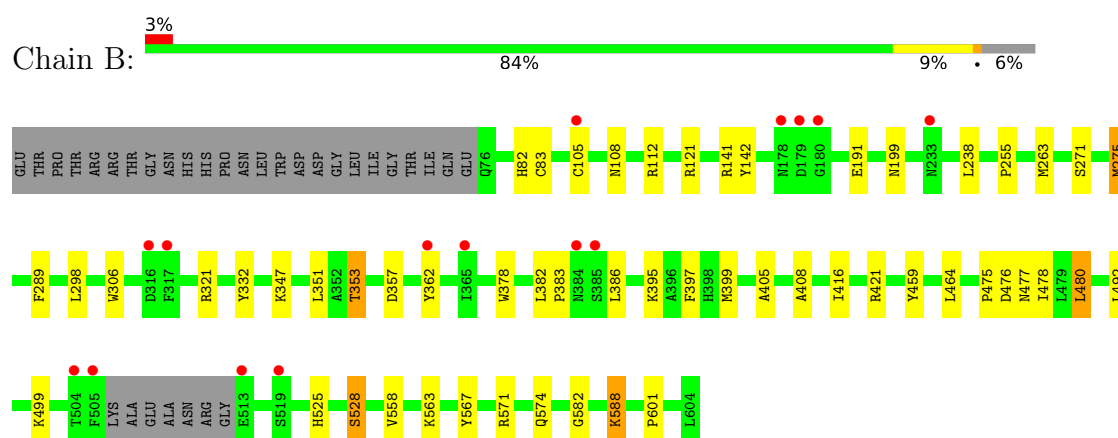
• Molecule 1: Sabinene synthase



• Molecule 1: Sabinene synthase



• Molecule 1: Sabinene synthase



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	274.48Å 90.77Å 193.94Å 90.00° 134.79° 90.00°	Depositor
Resolution (Å)	34.41 – 2.21 34.41 – 2.21	Depositor EDS
% Data completeness (in resolution range)	83.5 (34.41-2.21) 83.5 (34.41-2.21)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.83 (at 2.22Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.198 , 0.227 0.199 , 0.228	Depositor DCC
R_{free} test set	2002 reflections (1.18%)	wwPDB-VP
Wilson B-factor (Å ²)	42.2	Xtriage
Anisotropy	0.029	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 43.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.53$, $\langle L^2 \rangle = 0.37$	Xtriage
Estimated twinning fraction	0.033 for h+2*k,-h-l 0.000 for h,-k,-h-l 0.000 for -h-2*k,-k,l	Xtriage
F_o , F_c correlation	0.96	EDS
Total number of atoms	16618	wwPDB-VP
Average B, all atoms (Å ²)	49.0	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 39.69 % 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 3.0587e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹ Intensities estimated from amplitudes.

² 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: CO, EDO

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	0/4119	0.52	0/5597
1	B	0.39	0/4224	0.58	2/5734 (0.0%)
1	C	0.37	0/4102	0.55	0/5576
1	D	0.36	0/4089	0.54	0/5559
All	All	0.37	0/16534	0.55	2/22466 (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	B	601	PRO	CA-C-N	-5.69	117.81	123.04
1	B	601	PRO	C-N-CA	-5.69	117.81	123.04

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	4031	0	3805	27	0
1	B	4133	0	3930	36	0
1	C	4015	0	3791	36	0
1	D	4003	0	3775	35	0
2	A	4	0	6	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	8	0	12	5	0
2	C	4	0	6	0	0
2	D	4	0	6	0	0
3	A	3	0	0	0	0
3	B	4	0	0	2	0
3	C	3	0	0	0	0
3	D	3	0	0	0	0
4	A	109	0	0	2	0
4	B	138	0	0	5	0
4	C	68	0	0	1	0
4	D	88	0	0	3	0
All	All	16618	0	15331	135	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 4.

All (135) 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:423:VAL:HG21	1:D:464:LEU:HD22	1.41	1.01
1:B:82:HIS:HD2	4:B:801:HOH:O	1.42	1.00
1:B:83:CYS:HG	3:B:704:CO:CO	0.76	0.98
1:C:423:VAL:HG21	1:C:464:LEU:HD22	1.44	0.96
1:B:383:PRO:HG2	1:B:386:LEU:HD13	1.50	0.94
1:C:82:HIS:HD2	4:C:805:HOH:O	1.60	0.85
1:A:567:TYR:CE2	1:A:571:ARG:HD2	2.19	0.77
1:B:199:ASN:HD21	2:B:701:EDO:H11	1.51	0.76
1:A:574:GLN:NE2	4:A:801:HOH:O	2.20	0.74
1:D:101:SER:OG	1:D:112:ARG:HG2	1.88	0.74
1:D:315:VAL:HG12	1:D:318:ALA:H	1.55	0.71
1:C:364:THR:OG1	1:C:367:GLU:HG3	1.89	0.71
1:B:582:GLY:HA3	1:B:588:LYS:HD3	1.73	0.68
1:A:558:VAL:HB	1:A:563:LYS:HD2	1.74	0.67
1:B:405:ALA:HA	1:B:416:ILE:HD11	1.77	0.66
1:A:534:LEU:HD22	1:A:538:LYS:HE3	1.79	0.65
1:B:382:LEU:HB3	1:B:383:PRO:HD2	1.81	0.63
1:C:364:THR:HG23	1:C:367:GLU:CD	2.24	0.62
1:A:475:PRO:HG2	1:A:478:ILE:HD12	1.81	0.62
1:D:328:LEU:HD11	1:D:576:LEU:HD22	1.83	0.60
1:B:567:TYR:CE2	1:B:571:ARG:HD2	2.37	0.60
1:D:433:LYS:NZ	4:D:805:HOH:O	2.33	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:567:TYR:CE2	1:D:571:ARG:HD2	2.39	0.57
1:C:567:TYR:CE2	1:C:571:ARG:HD2	2.40	0.57
1:B:351:LEU:HD13	1:B:397:PHE:HA	1.86	0.57
1:B:83:CYS:SG	3:B:704:CO:CO	1.85	0.56
2:B:701:EDO:H21	4:B:826:HOH:O	2.05	0.55
1:A:378:TRP:CD2	1:A:421:ARG:HD3	2.41	0.55
1:A:108:ASN:O	1:A:112:ARG:HG3	2.07	0.55
1:B:199:ASN:HD21	2:B:701:EDO:C1	2.18	0.55
1:D:263:MET:HE1	1:D:289:PHE:HB2	1.89	0.54
1:B:459:TYR:OH	1:B:492:LEU:HD13	2.07	0.54
1:B:321:ARG:HD3	1:B:353:THR:HG21	1.89	0.52
1:B:191:GLU:HG3	1:B:238:LEU:HD22	1.92	0.52
1:C:364:THR:N	1:C:367:GLU:OE1	2.36	0.52
1:B:563:LYS:NZ	4:B:806:HOH:O	2.44	0.51
1:D:107:GLU:HA	1:D:138:TYR:OH	2.11	0.51
1:B:306:TRP:CD2	1:B:347:LYS:HD2	2.45	0.51
1:B:475:PRO:HD2	1:B:478:ILE:HB	1.92	0.51
1:B:525:HIS:O	1:B:528:SER:OG	2.23	0.51
1:B:476:ASP:O	1:B:480:LEU:HD13	2.10	0.51
1:D:306:TRP:CE2	1:D:347:LYS:HD3	2.45	0.51
1:C:364:THR:HG23	1:C:367:GLU:OE1	2.10	0.51
1:C:570:ALA:O	1:C:574:GLN:HG2	2.10	0.51
1:C:367:GLU:HA	1:C:370:LEU:HD12	1.93	0.50
1:D:398:HIS:HD2	4:D:845:HOH:O	1.95	0.50
1:B:306:TRP:CE2	1:B:347:LYS:HD2	2.46	0.50
1:B:82:HIS:CD2	4:B:801:HOH:O	2.32	0.50
1:C:351:LEU:HD13	1:C:397:PHE:HA	1.93	0.50
1:D:170:ASP:HA	1:D:173:ARG:HG3	1.93	0.49
1:B:499:LYS:HB2	1:B:574:GLN:HE22	1.77	0.49
1:C:295:VAL:O	1:C:299:GLU:HG3	2.13	0.49
1:C:558:VAL:HB	1:C:563:LYS:HD2	1.94	0.49
1:A:543:LYS:O	1:A:547:GLU:HG3	2.12	0.49
1:D:328:LEU:HD22	1:D:572:SER:HB2	1.96	0.48
1:B:395:LYS:HE2	1:B:399:MET:HE2	1.95	0.48
1:A:405:ALA:HA	1:A:416:ILE:HD11	1.96	0.48
1:D:433:LYS:HD3	1:D:437:TRP:CZ2	2.48	0.48
1:A:317:PHE:CE2	1:A:389:ASN:HB3	2.49	0.48
1:A:487:ARG:HG3	1:A:487:ARG:HH11	1.78	0.48
1:C:94:ILE:HG23	1:C:97:MET:HE2	1.96	0.48
1:B:141:ARG:NH2	1:B:142:TYR:OH	2.47	0.47
1:D:414:ARG:NH2	1:D:474:LEU:O	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:558:VAL:HB	1:B:563:LYS:HD2	1.94	0.47
1:B:347:LYS:HE2	4:B:863:HOH:O	2.14	0.47
1:C:84:MET:HE2	1:C:84:MET:HB3	1.74	0.47
1:A:378:TRP:HB2	1:A:421:ARG:NH1	2.31	0.46
1:C:417:LEU:O	1:C:421:ARG:HG3	2.16	0.46
1:B:199:ASN:ND2	2:B:701:EDO:H11	2.26	0.46
1:A:317:PHE:HE2	1:A:389:ASN:HB3	1.80	0.46
1:D:543:LYS:O	1:D:547:GLU:HG3	2.15	0.46
1:C:275:MET:HE3	1:C:275:MET:HB3	1.85	0.45
1:C:357:ASP:HB3	1:C:362:TYR:CE1	2.52	0.45
1:D:388:GLU:O	1:D:389:ASN:C	2.60	0.45
1:B:378:TRP:CD2	1:B:421:ARG:HD2	2.52	0.45
1:C:419:TYR:HE1	1:C:464:LEU:CD1	2.30	0.45
1:D:433:LYS:HD2	1:D:452:ASN:CG	2.42	0.45
1:D:93:GLU:O	1:D:97:MET:HG3	2.17	0.45
1:C:423:VAL:HG12	1:C:461:VAL:HG12	1.98	0.45
1:B:121:ARG:NH2	2:B:701:EDO:H12	2.32	0.45
1:D:375:VAL:HG21	1:D:428:LEU:HD11	1.99	0.44
1:B:588:LYS:HB2	1:B:588:LYS:HE3	1.57	0.44
1:D:103:LYS:O	1:D:104:PHE:C	2.60	0.44
1:A:324:GLU:HG2	1:A:590:ILE:CG2	2.47	0.44
1:A:398:HIS:HD2	4:A:841:HOH:O	2.01	0.44
1:C:408:ALA:HB3	1:C:416:ILE:HG12	1.99	0.44
1:C:419:TYR:CE1	1:C:464:LEU:HD11	2.53	0.44
1:C:357:ASP:HB3	1:C:362:TYR:HE1	1.82	0.44
1:A:417:LEU:O	1:A:421:ARG:HG3	2.17	0.43
1:B:275:MET:HB2	1:B:275:MET:HE2	1.54	0.43
1:D:275:MET:HB2	1:D:275:MET:HE2	1.74	0.43
1:C:312:LEU:HD23	1:C:392:ILE:HD12	2.00	0.43
1:D:360:ASP:OD1	1:D:360:ASP:C	2.61	0.43
1:B:263:MET:HE1	1:B:289:PHE:HB2	1.99	0.43
1:C:303:ILE:HD11	1:C:343:ARG:HA	2.01	0.43
1:D:234:ILE:CG2	1:D:239:SER:HB2	2.49	0.43
1:A:306:TRP:CE2	1:A:347:LYS:HD3	2.53	0.43
1:D:374:ALA:O	1:D:378:TRP:N	2.52	0.43
1:B:255:PRO:HD2	1:B:332:TYR:HB3	2.01	0.43
1:C:414:ARG:NH2	1:C:474:LEU:O	2.52	0.43
1:A:395:LYS:O	1:A:399:MET:HG3	2.19	0.42
1:D:131:GLU:H	1:D:131:GLU:CD	2.26	0.42
1:D:297:ARG:HG2	1:D:598:LEU:O	2.18	0.42
1:D:570:ALA:O	1:D:574:GLN:HG2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:433:LYS:HB2	1:C:433:LYS:HE3	1.45	0.42
1:D:112:ARG:O	1:D:116:VAL:HG23	2.19	0.42
1:B:357:ASP:HB3	1:B:362:TYR:CE2	2.54	0.42
1:C:150:LEU:HD11	1:C:200:LEU:HD13	2.02	0.42
1:C:329:ALA:HA	1:C:332:TYR:CE1	2.55	0.42
1:C:185:PRO:HB2	1:C:188:GLN:HG3	2.01	0.42
1:D:234:ILE:HD12	1:D:234:ILE:HA	1.66	0.42
1:B:408:ALA:HB3	1:B:416:ILE:HG12	2.01	0.41
1:C:341:TYR:C	1:C:341:TYR:CD1	2.98	0.41
1:D:449:TYR:OH	1:D:501:ASP:OD2	2.29	0.41
1:A:408:ALA:HB3	1:A:416:ILE:HG12	2.02	0.41
1:C:101:SER:OG	1:C:112:ARG:HG2	2.20	0.41
1:A:590:ILE:HD13	1:A:590:ILE:HA	1.72	0.41
1:A:442:TYR:HE1	1:A:444:PRO:HB3	1.84	0.41
1:C:107:GLU:HA	1:C:138:TYR:OH	2.21	0.41
1:C:382:LEU:HB3	1:C:383:PRO:HD2	2.01	0.41
1:D:382:LEU:HD23	1:D:382:LEU:HA	1.91	0.41
1:A:263:MET:HE1	1:A:289:PHE:HB2	2.02	0.41
1:A:498:LEU:HD23	1:A:498:LEU:HA	1.93	0.41
1:C:487:ARG:HD2	1:C:487:ARG:HA	1.82	0.41
1:D:108:ASN:O	1:D:112:ARG:HG3	2.21	0.41
1:A:260:ARG:CZ	1:A:602:ILE:HD12	2.51	0.41
1:C:382:LEU:HD23	1:C:382:LEU:HA	1.85	0.41
1:A:81:SER:O	1:A:85:GLU:HG3	2.21	0.41
1:A:317:PHE:HB2	1:A:362:TYR:CZ	2.55	0.41
1:C:367:GLU:HG3	1:C:367:GLU:H	1.64	0.40
1:D:324:GLU:HG2	1:D:590:ILE:HG13	2.02	0.40
1:A:460:ARG:CZ	1:A:484:TYR:HB3	2.51	0.40
1:B:108:ASN:O	1:B:112:ARG:HG3	2.21	0.40
1:D:256:ARG:HG3	4:D:841:HOH:O	2.21	0.40
1:D:557:ASN:OD1	1:D:557:ASN:N	2.48	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	507/554 (92%)	494 (97%)	12 (2%)	1 (0%)	43	50
1	B	518/554 (94%)	497 (96%)	21 (4%)	0	100	100
1	C	506/554 (91%)	488 (96%)	16 (3%)	2 (0%)	30	33
1	D	506/554 (91%)	487 (96%)	18 (4%)	1 (0%)	43	50
All	All	2037/2216 (92%)	1966 (96%)	67 (3%)	4 (0%)	43	50

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	363	GLY
1	C	318	ALA
1	A	361	THR
1	C	384	ASN

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	408/487 (84%)	398 (98%)	10 (2%)	42	55
1	B	427/487 (88%)	417 (98%)	10 (2%)	44	58
1	C	407/487 (84%)	396 (97%)	11 (3%)	39	52
1	D	405/487 (83%)	394 (97%)	11 (3%)	39	52
All	All	1647/1948 (84%)	1605 (97%)	42 (3%)	40	53

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

Mol	Chain	Res	Type
1	C	114	VAL
1	C	206	ILE
1	C	212	ASN
1	C	271	SER

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Mol	Chain	Res	Type
1	C	362	TYR
1	C	364	THR
1	C	385	SER
1	C	390	ILE
1	C	399	MET
1	C	464	LEU
1	C	476	ASP
1	D	119	VAL
1	D	234	ILE
1	D	271	SER
1	D	297	ARG
1	D	392	ILE
1	D	399	MET
1	D	416	ILE
1	D	464	LEU
1	D	544	ARG
1	D	557	ASN
1	D	593	LEU
1	A	101	SER
1	A	114	VAL
1	A	119	VAL
1	A	271	SER
1	A	464	LEU
1	A	534	LEU
1	A	544	ARG
1	A	590	ILE
1	A	592	ASP
1	A	602	ILE
1	B	105	CYS
1	B	271	SER
1	B	275	MET
1	B	298	LEU
1	B	353	THR
1	B	464	LEU
1	B	477	ASN
1	B	480	LEU
1	B	528	SER
1	B	588	LYS

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

Mol	Chain	Res	Type
1	C	120	GLN
1	C	163	ASN
1	C	398	HIS
1	C	402	ASN
1	C	489	ASN
1	C	525	HIS
1	D	120	GLN
1	D	163	ASN
1	D	489	ASN
1	D	550	GLN
1	A	120	GLN
1	A	163	ASN
1	B	129	GLN
1	B	574	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 18 ligands modelled in this entry, 13 are monoatomic - leaving 5 for Mogul analysis.

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	EDO	A	701	-	3,3,3	0.88	0	2,2,2	0.34	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	EDO	B	702	-	3,3,3	0.78	0	2,2,2	0.66	0
2	EDO	B	701	-	3,3,3	0.83	0	2,2,2	0.14	0
2	EDO	D	701	-	3,3,3	0.74	0	2,2,2	0.41	0
2	EDO	C	701	-	3,3,3	0.84	0	2,2,2	0.25	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	EDO	A	701	-	-	0/1/1/1	-
2	EDO	B	702	-	-	0/1/1/1	-
2	EDO	B	701	-	-	1/1/1/1	-
2	EDO	D	701	-	-	1/1/1/1	-
2	EDO	C	701	-	-	1/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	701	EDO	O1-C1-C2-O2
2	C	701	EDO	O1-C1-C2-O2
2	B	701	EDO	O1-C1-C2-O2

There are no ring outliers.

1 monomer is involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	701	EDO	5	0

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	513/554 (92%)	0.09	31 (6%) 27 25	27, 47, 77, 95	0
1	B	522/554 (94%)	-0.04	15 (2%) 53 51	27, 44, 69, 92	0
1	C	512/554 (92%)	0.22	23 (4%) 38 35	28, 51, 81, 97	0
1	D	512/554 (92%)	0.23	30 (5%) 28 25	31, 49, 79, 99	0
All	All	2059/2216 (92%)	0.12	99 (4%) 35 32	27, 48, 78, 99	0

All (99) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	105	CYS	4.7
1	C	105	CYS	4.4
1	D	604	LEU	4.0
1	D	178	ASN	3.8
1	D	101	SER	3.8
1	D	589	ASP	3.8
1	C	362	TYR	3.7
1	B	179	ASP	3.6
1	B	317	PHE	3.6
1	A	527	GLY	3.5
1	C	320	HIS	3.5
1	C	317	PHE	3.4
1	C	315	VAL	3.4
1	D	384	ASN	3.4
1	A	178	ASN	3.3
1	D	320	HIS	3.3
1	A	316	ASP	3.2
1	C	438	LEU	3.2
1	C	232	ASN	3.2
1	A	320	HIS	3.2
1	D	234	ILE	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	528	SER	3.2
1	B	385	SER	3.1
1	C	589	ASP	3.1
1	C	387	PRO	2.9
1	A	387	PRO	2.9
1	C	179	ASP	2.9
1	B	519	SER	2.9
1	C	104	PHE	2.9
1	B	504	THR	2.9
1	A	383	PRO	2.9
1	A	384	ASN	2.9
1	B	316	ASP	2.9
1	B	505	PHE	2.8
1	D	529	SER	2.8
1	B	365	ILE	2.7
1	A	529	SER	2.7
1	C	534	LEU	2.7
1	D	386	LEU	2.7
1	B	513	GLU	2.7
1	D	103	LYS	2.6
1	B	105	CYS	2.6
1	D	590	ILE	2.6
1	C	384	ASN	2.6
1	A	504	THR	2.6
1	C	604	LEU	2.5
1	A	514	LEU	2.5
1	D	533	ALA	2.5
1	A	179	ASP	2.5
1	C	318	ALA	2.5
1	A	232	ASN	2.5
1	A	534	LEU	2.5
1	A	76	GLN	2.5
1	D	179	ASP	2.5
1	D	76	GLN	2.5
1	A	386	LEU	2.4
1	C	233	ASN	2.4
1	D	231	ASN	2.4
1	A	231	ASN	2.4
1	C	365	ILE	2.4
1	A	521	TYR	2.4
1	D	526	PRO	2.4
1	D	104	PHE	2.4

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Mol	Chain	Res	Type	RSRZ
1	D	580	ARG	2.4
1	B	233	ASN	2.4
1	C	383	PRO	2.4
1	A	105	CYS	2.4
1	A	513	GLU	2.3
1	D	232	ASN	2.3
1	B	384	ASN	2.3
1	D	142	TYR	2.3
1	B	178	ASN	2.3
1	D	106	GLY	2.3
1	C	385	SER	2.3
1	A	365	ILE	2.3
1	D	317	PHE	2.2
1	D	464	LEU	2.2
1	A	515	VAL	2.2
1	A	317	PHE	2.2
1	C	580	ARG	2.2
1	D	555	PRO	2.2
1	A	580	ARG	2.2
1	A	532	GLU	2.1
1	B	362	TYR	2.1
1	D	392	ILE	2.1
1	C	413	GLY	2.1
1	D	318	ALA	2.1
1	A	318	ALA	2.1
1	C	183	LEU	2.1
1	D	316	ASP	2.1
1	A	526	PRO	2.1
1	A	380	SER	2.1
1	C	316	ASP	2.1
1	A	233	ASN	2.1
1	B	180	GLY	2.1
1	D	383	PRO	2.0
1	A	525	HIS	2.0
1	A	389	ASN	2.0
1	D	387	PRO	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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(Å ²)	Q<0.9
3	CO	B	706	1/1	0.62	0.32	163,163,163,163	0
2	EDO	B	702	4/4	0.83	0.19	50,53,59,67	0
2	EDO	D	701	4/4	0.84	0.21	57,66,70,73	0
2	EDO	C	701	4/4	0.85	0.25	58,62,67,78	0
3	CO	D	703	1/1	0.87	0.12	100,100,100,100	0
2	EDO	B	701	4/4	0.89	0.17	41,42,52,61	0
3	CO	D	702	1/1	0.89	0.12	104,104,104,104	0
3	CO	C	704	1/1	0.90	0.15	127,127,127,127	0
3	CO	A	704	1/1	0.90	0.11	89,89,89,89	0
3	CO	B	705	1/1	0.90	0.09	112,112,112,112	0
2	EDO	A	701	4/4	0.90	0.16	52,56,62,69	0
3	CO	B	704	1/1	0.91	0.09	80,80,80,80	0
3	CO	C	702	1/1	0.92	0.08	85,85,85,85	0
3	CO	D	704	1/1	0.92	0.09	90,90,90,90	0
3	CO	A	703	1/1	0.93	0.09	95,95,95,95	0
3	CO	A	702	1/1	0.95	0.07	82,82,82,82	0
3	CO	C	703	1/1	0.95	0.07	84,84,84,84	0
3	CO	B	703	1/1	0.98	0.05	73,73,73,73	0

6.5 Other polymers [i](#)

There are no such residues in this entry.