



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 01:54 AM UTC

PDB ID : 3N0F / pdb_00003n0f
Title : Crystal Structure of Isoprene Synthase from Grey Poplar Leaves (*Populus x canescens*)
Authors : Koksai, M.; Christianson, D.W.
Deposited on : 2010-05-13
Resolution : 2.70 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

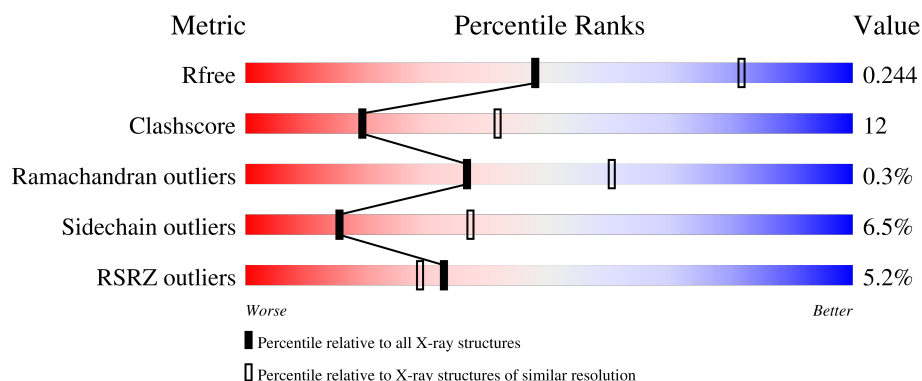
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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	3538 (2.70-2.70)
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (2.70-2.70)

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	555	5% 69% 24% • •
1	B	555	5% 70% 24% • •

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 8976 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 Isoprene synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	531	Total	C	N	O	S	0	0	0
			4326	2757	731	826	12			
1	B	531	Total	C	N	O	S	0	0	0
			4326	2757	731	826	12			

There are 30 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	41	MET	-	expression tag	UNP Q9AR86
A	42	ARG	-	expression tag	UNP Q9AR86
A	43	GLY	-	expression tag	UNP Q9AR86
A	44	SER	-	expression tag	UNP Q9AR86
A	45	HIS	-	expression tag	UNP Q9AR86
A	46	HIS	-	expression tag	UNP Q9AR86
A	47	HIS	-	expression tag	UNP Q9AR86
A	48	HIS	-	expression tag	UNP Q9AR86
A	49	HIS	-	expression tag	UNP Q9AR86
A	50	HIS	-	expression tag	UNP Q9AR86
A	51	GLY	-	expression tag	UNP Q9AR86
A	52	SER	-	expression tag	UNP Q9AR86
A	59	ASP	ASN	engineered mutation	UNP Q9AR86
A	308	ARG	LYS	engineered mutation	UNP Q9AR86
A	533	TRP	CYS	engineered mutation	UNP Q9AR86
B	41	MET	-	expression tag	UNP Q9AR86
B	42	ARG	-	expression tag	UNP Q9AR86
B	43	GLY	-	expression tag	UNP Q9AR86
B	44	SER	-	expression tag	UNP Q9AR86
B	45	HIS	-	expression tag	UNP Q9AR86
B	46	HIS	-	expression tag	UNP Q9AR86
B	47	HIS	-	expression tag	UNP Q9AR86
B	48	HIS	-	expression tag	UNP Q9AR86
B	49	HIS	-	expression tag	UNP Q9AR86
B	50	HIS	-	expression tag	UNP Q9AR86

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Chain	Residue	Modelled	Actual	Comment	Reference
B	51	GLY	-	expression tag	UNP Q9AR86
B	52	SER	-	expression tag	UNP Q9AR86
B	59	ASP	ASN	engineered mutation	UNP Q9AR86
B	308	ARG	LYS	engineered mutation	UNP Q9AR86
B	533	TRP	CYS	engineered mutation	UNP Q9AR86

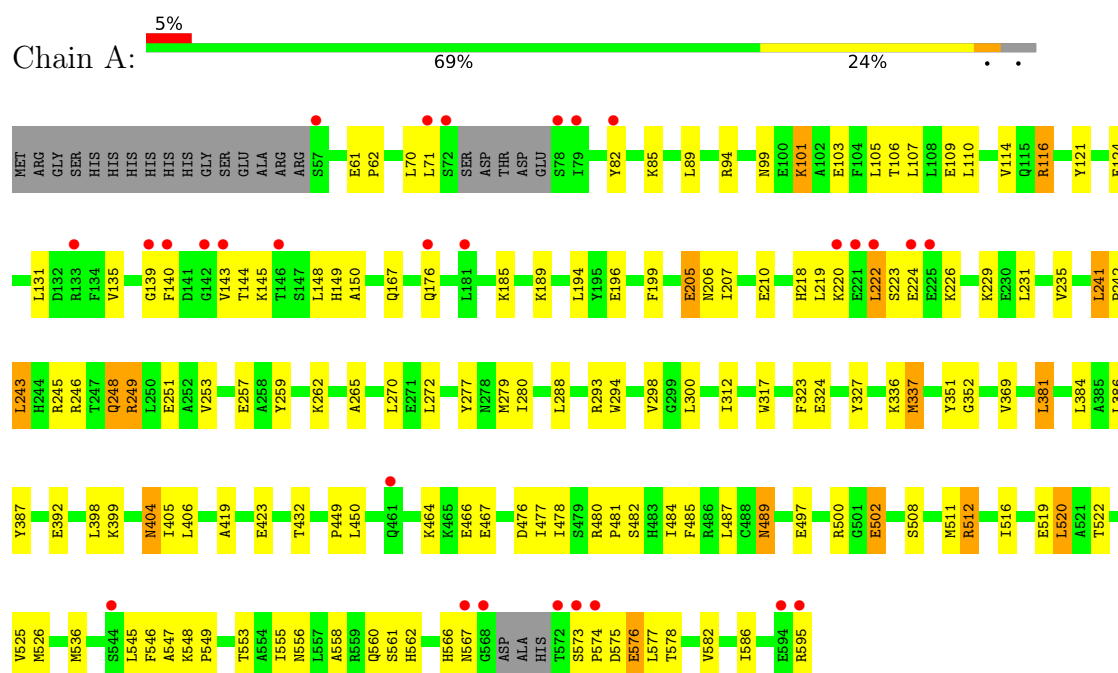
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	160	Total	O	0	0
			160	160		
2	B	164	Total	O	0	0
			164	164		

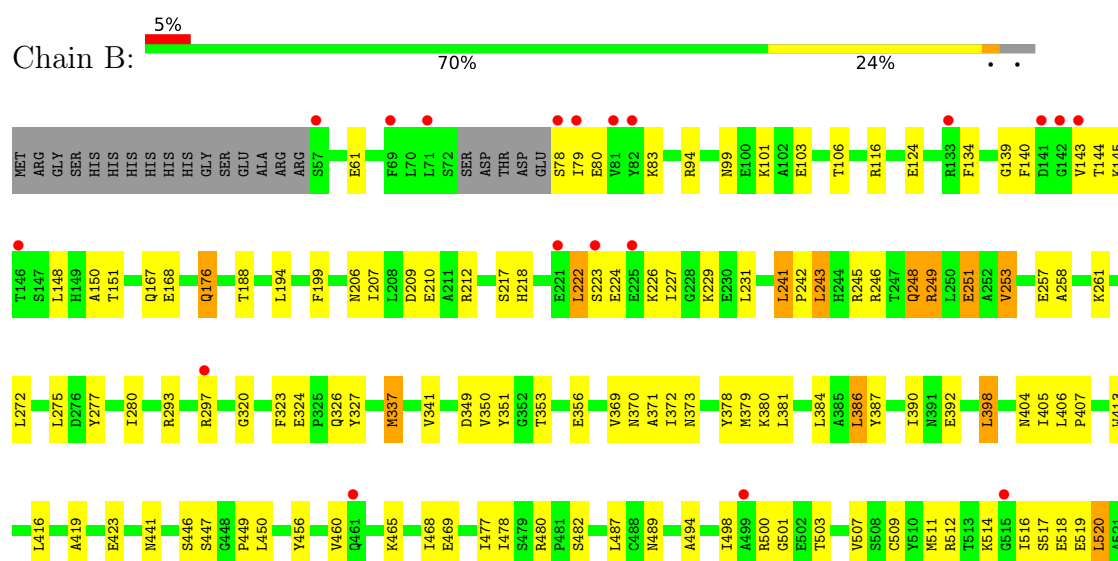
3 Residue-property plots

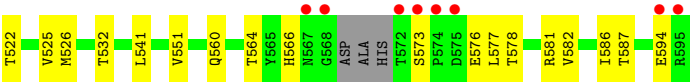
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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



• Molecule 1: Isoprene synthase





4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α , β , γ	155.42Å 155.42Å 142.03Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.10 – 2.70 39.10 – 2.70	Depositor EDS
% Data completeness (in resolution range)	95.1 (39.10-2.70) 95.1 (39.10-2.70)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	0.15	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.96 (at 2.69Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.198 , 0.245 0.198 , 0.244	Depositor DCC
R_{free} test set	4863 reflections (10.09%)	wwPDB-VP
Wilson B-factor (Å ²)	30.4	Xtriage
Anisotropy	0.012	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 54.9	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	0.93	EDS
Total number of atoms	8976	wwPDB-VP
Average B, all atoms (Å ²)	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.42% 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	0.44	0/4415	0.83	3/5966 (0.1%)
1	B	0.45	0/4415	0.83	6/5966 (0.1%)
All	All	0.45	0/8830	0.83	9/11932 (0.1%)

There are no bond length outliers.

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	586	ILE	N-CA-C	7.44	117.96	111.56
1	A	586	ILE	N-CA-C	6.68	117.73	112.12
1	A	351	TYR	N-CA-C	6.39	119.19	111.40
1	B	349	ASP	N-CA-C	5.78	117.65	111.36
1	B	351	TYR	N-CA-C	5.54	118.16	111.40
1	B	586	ILE	CB-CA-C	-5.46	106.25	111.44
1	B	419	ALA	N-CA-C	-5.20	105.69	111.36
1	A	352	GLY	N-CA-C	5.11	119.53	112.37
1	B	350	VAL	N-CA-C	5.06	119.86	109.34

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	4326	0	4241	101	0
1	B	4326	0	4241	100	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	160	0	0	1	0
2	B	164	0	0	7	0
All	All	8976	0	8482	201	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 12.

All (201) 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:A:248:GLN:HE22	1:A:249:ARG:HH21	1.17	0.91
1:B:337:MET:HA	1:B:337:MET:HE3	1.50	0.90
1:B:560:GLN:HE21	1:B:564:THR:HG23	1.39	0.86
1:A:337:MET:HE3	1:A:337:MET:HA	1.55	0.85
1:A:248:GLN:NE2	1:A:249:ARG:HH21	1.75	0.85
1:A:206:ASN:O	1:A:210:GLU:HG3	1.85	0.77
1:B:167:GLN:HG3	1:B:207:ILE:HD12	1.70	0.74
1:A:167:GLN:HG3	1:A:207:ILE:HD12	1.70	0.73
1:A:241:LEU:HD23	1:A:242:PRO:HD2	1.71	0.73
1:A:248:GLN:HE21	1:A:249:ARG:HE	1.36	0.73
1:B:477:ILE:HG23	1:B:478:ILE:HG23	1.70	0.72
1:A:105:LEU:O	1:A:109:GLU:HG3	1.89	0.71
1:A:489:ASN:C	1:A:489:ASN:HD22	1.98	0.71
1:B:516:ILE:HD12	1:B:520:LEU:HB3	1.74	0.70
1:A:246:ARG:HD2	1:A:251:GLU:HG2	1.73	0.70
1:A:477:ILE:HG23	1:A:478:ILE:HG23	1.75	0.69
1:A:71:LEU:HD11	1:A:279:MET:SD	2.34	0.67
1:B:144:THR:HA	1:B:151:THR:OG1	1.96	0.65
1:A:573:SER:HB3	1:A:576:GLU:HB2	1.78	0.65
1:A:248:GLN:HG2	1:A:323:PHE:CE2	2.33	0.64
1:B:223:SER:N	1:B:226:LYS:HZ3	1.95	0.64
1:B:227:ILE:HD12	1:B:231:LEU:HB3	1.79	0.63
1:B:337:MET:HA	1:B:337:MET:CE	2.28	0.63
1:B:78:SER:HB3	2:B:729:HOH:O	1.99	0.62
1:B:212:ARG:HD3	2:B:663:HOH:O	2.00	0.62
1:B:560:GLN:HE21	1:B:564:THR:CG2	2.11	0.62
1:B:176:GLN:NE2	1:B:176:GLN:H	1.97	0.62
1:A:464:LYS:HB2	1:A:467:GLU:HG3	1.82	0.62
1:B:337:MET:HE2	1:B:413:TRP:HZ2	1.63	0.62
1:B:456:TYR:O	1:B:460:VAL:HG22	2.00	0.61
1:A:116:ARG:HD3	1:A:243:LEU:HD11	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:294:TRP:CZ3	1:A:336:LYS:HG2	2.37	0.60
1:A:404:ASN:C	1:A:404:ASN:HD22	2.07	0.60
1:B:337:MET:HE2	1:B:413:TRP:CZ2	2.37	0.59
1:B:337:MET:O	1:B:341:VAL:HG23	2.02	0.58
1:A:522:THR:O	1:A:526:MET:HG2	2.02	0.58
1:A:262:LYS:HB2	1:A:265:ALA:HB2	1.85	0.58
1:B:224:GLU:HG3	1:B:229:LYS:HA	1.84	0.58
1:B:487:LEU:HD22	1:B:525:VAL:HG13	1.85	0.58
1:A:70:LEU:C	1:A:71:LEU:HD12	2.29	0.58
1:B:140:PHE:O	1:B:144:THR:HG23	2.04	0.58
1:A:224:GLU:HG3	1:A:229:LYS:HA	1.85	0.57
1:A:404:ASN:ND2	1:A:406:LEU:H	2.03	0.57
1:B:511:MET:HE3	1:B:518:GLU:N	2.19	0.57
1:A:497:GLU:HB3	1:A:502:GLU:HB2	1.86	0.57
1:B:99:ASN:ND2	1:B:99:ASN:C	2.63	0.56
1:A:467:GLU:HB3	1:A:546:PHE:CE1	2.40	0.56
1:B:99:ASN:C	1:B:99:ASN:HD22	2.14	0.56
1:A:566:HIS:CD2	1:A:577:LEU:HD23	2.40	0.55
1:A:140:PHE:O	1:A:144:THR:HG23	2.07	0.55
1:B:206:ASN:O	1:B:210:GLU:HG3	2.06	0.55
1:A:248:GLN:NE2	1:A:249:ARG:NH2	2.51	0.55
1:A:218:HIS:O	1:A:222:LEU:HD13	2.07	0.55
1:B:522:THR:O	1:B:526:MET:HG2	2.07	0.55
1:B:218:HIS:NE2	1:B:222:LEU:HD11	2.22	0.54
1:B:480:ARG:HG3	1:B:532:THR:HG23	1.89	0.54
1:B:514:LYS:O	1:B:516:ILE:HG23	2.07	0.54
1:A:248:GLN:HG2	1:A:323:PHE:CZ	2.43	0.54
1:B:369:VAL:O	1:B:372:ILE:HG23	2.08	0.54
1:A:567:ASN:O	1:A:574:PRO:HG3	2.07	0.54
1:B:243:LEU:HD13	2:B:621:HOH:O	2.07	0.54
1:B:103:GLU:HB2	1:B:106:THR:OG1	2.10	0.52
1:A:139:GLY:O	1:A:143:VAL:HG23	2.09	0.52
1:A:248:GLN:HG2	1:A:323:PHE:CD2	2.44	0.52
1:B:248:GLN:HG2	1:B:323:PHE:CE2	2.45	0.52
1:A:337:MET:HA	1:A:337:MET:CE	2.32	0.51
1:A:449:PRO:HD3	1:A:482:SER:OG	2.09	0.51
1:B:241:LEU:CD2	1:B:242:PRO:HD2	2.40	0.51
1:B:489:ASN:C	1:B:489:ASN:HD22	2.17	0.51
1:B:253:VAL:HG13	1:B:277:TYR:CZ	2.45	0.51
1:A:249:ARG:O	1:A:253:VAL:HG23	2.11	0.51
1:B:139:GLY:O	1:B:143:VAL:HG23	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:241:LEU:HD23	1:B:242:PRO:HD2	1.91	0.51
1:B:519:GLU:H	1:B:519:GLU:CD	2.20	0.50
1:A:300:LEU:HD12	1:A:381:LEU:HD13	1.94	0.50
1:A:404:ASN:C	1:A:404:ASN:ND2	2.69	0.50
1:B:241:LEU:HD22	1:B:245:ARG:HB2	1.94	0.50
1:B:320:GLY:HA3	1:B:560:GLN:OE1	2.12	0.50
1:B:248:GLN:HG2	1:B:323:PHE:CD2	2.47	0.50
1:B:249:ARG:NE	1:B:249:ARG:HA	2.27	0.49
1:A:196:GLU:OE2	1:A:243:LEU:HB2	2.13	0.49
1:A:476:ASP:HB3	1:A:480:ARG:NH1	2.28	0.49
1:A:317:TRP:HA	1:A:560:GLN:NE2	2.28	0.49
1:B:450:LEU:C	1:B:450:LEU:HD23	2.38	0.49
1:B:78:SER:C	1:B:80:GLU:H	2.20	0.48
1:B:404:ASN:C	1:B:404:ASN:HD22	2.19	0.48
1:A:573:SER:CB	1:A:576:GLU:HB2	2.42	0.48
1:B:168:GLU:HG3	2:B:735:HOH:O	2.12	0.48
1:B:249:ARG:HB2	2:B:654:HOH:O	2.13	0.48
1:B:188:THR:OG1	1:B:222:LEU:HD21	2.13	0.48
1:B:280:ILE:HD12	2:B:3:HOH:O	2.13	0.48
1:B:253:VAL:HG13	1:B:277:TYR:OH	2.13	0.48
1:A:116:ARG:HD3	1:A:243:LEU:HD21	1.96	0.48
1:A:404:ASN:HD22	1:A:405:ILE:N	2.12	0.48
1:A:249:ARG:NH1	2:A:598:HOH:O	2.45	0.47
1:B:218:HIS:CE1	1:B:222:LEU:HD11	2.49	0.47
1:B:465:LYS:HA	1:B:468:ILE:HD11	1.95	0.47
1:A:404:ASN:HD22	1:A:406:LEU:H	1.62	0.47
1:A:536:MET:HG2	1:A:555:ILE:HG12	1.95	0.47
1:A:103:GLU:HB2	1:A:106:THR:OG1	2.14	0.47
1:B:578:THR:O	1:B:582:VAL:HG23	2.15	0.47
1:B:449:PRO:HD3	1:B:482:SER:OG	2.14	0.47
1:B:143:VAL:C	1:B:145:LYS:H	2.22	0.47
1:A:199:PHE:CE2	1:A:242:PRO:HB3	2.50	0.47
1:A:484:ILE:HD12	1:A:536:MET:HE1	1.96	0.47
1:A:558:ALA:O	1:A:561:SER:HB2	2.15	0.47
1:B:143:VAL:HG13	1:B:150:ALA:HB3	1.97	0.47
1:B:222:LEU:HD23	1:B:227:ILE:HD13	1.97	0.47
1:B:258:ALA:HA	1:B:261:LYS:HE2	1.97	0.46
1:B:398:LEU:HD22	1:B:398:LEU:O	2.16	0.46
1:B:353:THR:OG1	1:B:356:GLU:HG3	2.15	0.46
1:A:149:HIS:NE2	1:A:189:LYS:HE3	2.31	0.46
1:A:241:LEU:HD22	1:A:245:ARG:HB2	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:519:GLU:H	1:A:519:GLU:CD	2.22	0.46
1:A:185:LYS:HE2	1:A:218:HIS:HB2	1.98	0.46
1:A:547:ALA:HB1	1:A:549:PRO:HD2	1.98	0.46
1:B:324:GLU:HB3	1:B:326:GLN:OE1	2.16	0.46
1:A:167:GLN:NE2	1:A:205:GLU:HA	2.30	0.46
1:A:219:LEU:HA	1:A:222:LEU:HD22	1.98	0.46
1:A:222:LEU:HD23	1:A:235:VAL:HG21	1.97	0.46
1:A:324:GLU:HB2	1:A:327:TYR:CD2	2.51	0.45
1:B:573:SER:HB3	1:B:576:GLU:HB2	1.98	0.45
1:B:560:GLN:NE2	1:B:564:THR:HG23	2.21	0.45
1:A:294:TRP:O	1:A:298:VAL:HG23	2.17	0.45
1:A:288:LEU:HD21	1:A:312:ILE:HD12	1.99	0.45
1:B:199:PHE:CE1	1:B:242:PRO:HG3	2.52	0.45
1:B:199:PHE:CD1	1:B:242:PRO:HG3	2.53	0.44
1:A:404:ASN:HD21	1:A:406:LEU:CB	2.30	0.44
1:A:131:LEU:O	1:A:135:VAL:HG23	2.18	0.44
1:A:369:VAL:HB	1:A:387:TYR:CE2	2.53	0.44
1:B:324:GLU:HB2	1:B:327:TYR:CD2	2.53	0.44
1:B:477:ILE:CD1	1:B:551:VAL:HG22	2.46	0.44
1:B:511:MET:HE3	1:B:517:SER:C	2.43	0.44
1:A:548:LYS:N	1:A:549:PRO:CD	2.81	0.44
1:A:241:LEU:HD11	1:A:562:HIS:HB3	1.99	0.44
1:A:553:THR:HA	1:A:556:ASN:HD22	1.83	0.44
1:B:449:PRO:HG2	2:B:597:HOH:O	2.16	0.44
1:B:489:ASN:C	1:B:489:ASN:ND2	2.76	0.44
1:A:223:SER:N	1:A:226:LYS:HZ3	2.16	0.44
1:A:485:PHE:HA	1:A:561:SER:OG	2.18	0.44
1:B:248:GLN:HG2	1:B:323:PHE:CZ	2.52	0.44
1:A:143:VAL:C	1:A:145:LYS:H	2.26	0.43
1:A:466:GLU:HG2	1:A:545:LEU:HD21	2.00	0.43
1:B:406:LEU:HB3	1:B:407:PRO:HD3	2.00	0.43
1:A:61:GLU:HG3	1:A:62:PRO:HD2	1.99	0.43
1:A:450:LEU:C	1:A:450:LEU:HD23	2.42	0.43
1:B:373:ASN:HA	1:B:380:LYS:HE2	1.99	0.43
1:B:566:HIS:CD2	1:B:577:LEU:HD23	2.53	0.43
1:B:509:CYS:HA	1:B:512:ARG:HH12	1.83	0.43
1:B:404:ASN:C	1:B:404:ASN:ND2	2.76	0.43
1:A:419:ALA:O	1:A:423:GLU:HG3	2.18	0.43
1:A:219:LEU:O	1:A:222:LEU:HB2	2.18	0.43
1:A:497:GLU:HG2	1:A:500:ARG:NH2	2.34	0.43
1:B:498:ILE:C	1:B:500:ARG:H	2.27	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:143:VAL:HG13	1:A:150:ALA:CB	2.49	0.43
1:A:480:ARG:N	1:A:481:PRO:HD2	2.34	0.43
1:B:378:TYR:OH	1:B:379:MET:HE3	2.19	0.43
1:B:494:ALA:O	1:B:498:ILE:HG13	2.19	0.43
1:A:248:GLN:HG3	1:A:249:ARG:N	2.34	0.42
1:B:423:GLU:HG3	1:B:441:ASN:ND2	2.34	0.42
1:A:71:LEU:HD12	1:A:71:LEU:N	2.34	0.42
1:A:85:LYS:O	1:A:89:LEU:HG	2.19	0.42
1:A:489:ASN:C	1:A:489:ASN:ND2	2.68	0.42
1:B:275:LEU:C	1:B:275:LEU:HD23	2.44	0.42
1:A:259:TYR:HD2	1:A:270:LEU:HD23	1.85	0.42
1:B:80:GLU:HG3	1:B:83:LYS:HE2	2.01	0.42
1:B:416:LEU:HD22	1:B:450:LEU:HD13	2.01	0.42
1:A:508:SER:O	1:A:511:MET:HB2	2.20	0.42
1:B:386:LEU:HD22	1:B:390:ILE:HG12	2.00	0.42
1:A:253:VAL:HG22	1:A:277:TYR:OH	2.20	0.42
1:A:167:GLN:HE22	1:A:205:GLU:HA	1.84	0.42
1:A:432:THR:O	1:A:512:ARG:NH2	2.52	0.42
1:B:369:VAL:HG13	1:B:370:ASN:N	2.33	0.42
1:A:399:LYS:HB3	1:A:399:LYS:HE2	1.90	0.42
1:A:99:ASN:HD21	1:A:101:LYS:HG2	1.85	0.41
1:A:110:LEU:O	1:A:114:VAL:HG23	2.20	0.41
1:A:220:LYS:C	1:A:222:LEU:H	2.28	0.41
1:B:246:ARG:HD2	1:B:251:GLU:HG2	2.01	0.41
1:B:293:ARG:O	1:B:297:ARG:HB2	2.20	0.41
1:A:241:LEU:CD2	1:A:242:PRO:HD2	2.47	0.41
1:B:477:ILE:HD11	1:B:551:VAL:HG22	2.01	0.41
1:A:121:TYR:OH	1:A:280:ILE:HD11	2.20	0.41
1:A:578:THR:O	1:A:582:VAL:HG23	2.21	0.41
1:B:446:SER:O	1:B:447:SER:OG	2.36	0.41
1:B:369:VAL:HB	1:B:387:TYR:CE2	2.56	0.41
1:B:507:VAL:O	1:B:511:MET:HG3	2.21	0.41
1:A:487:LEU:HD22	1:A:525:VAL:HG13	2.02	0.41
1:A:516:ILE:HD12	1:A:520:LEU:HB3	2.02	0.41
1:B:134:PHE:CE1	1:B:140:PHE:HB2	2.56	0.41
1:B:507:VAL:HG22	1:B:525:VAL:HG21	2.02	0.41
1:A:185:LYS:CE	1:A:218:HIS:HB2	2.51	0.41
1:A:259:TYR:CE2	1:A:265:ALA:HB1	2.55	0.41
1:B:324:GLU:HB3	1:B:326:GLN:CD	2.46	0.41
1:B:577:LEU:O	1:B:581:ARG:HG3	2.21	0.41
1:B:404:ASN:ND2	1:B:406:LEU:H	2.19	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:249:ARG:HE	1:A:249:ARG:HA	1.85	0.40
1:A:294:TRP:CD2	1:A:336:LYS:HE2	2.57	0.40
1:B:404:ASN:HD22	1:B:405:ILE:N	2.19	0.40
1:B:248:GLN:HG2	1:B:323:PHE:CG	2.56	0.40
1:B:369:VAL:C	1:B:371:ALA:H	2.28	0.40
1:B:501:GLY:O	1:B:503:THR:HG23	2.22	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	525/555 (95%)	506 (96%)	18 (3%)	1 (0%)	43 68
1	B	525/555 (95%)	504 (96%)	19 (4%)	2 (0%)	30 54
All	All	1050/1110 (95%)	1010 (96%)	37 (4%)	3 (0%)	36 60

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	205	GLU
1	B	79	ILE
1	B	222	LEU

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	466/486 (96%)	434 (93%)	32 (7%)	14	34
1	B	466/486 (96%)	437 (94%)	29 (6%)	16	39
All	All	932/972 (96%)	871 (94%)	61 (6%)	15	37

All (61) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	82	TYR
1	A	94	ARG
1	A	101	LYS
1	A	107	LEU
1	A	116	ARG
1	A	124	GLU
1	A	148	LEU
1	A	176	GLN
1	A	194	LEU
1	A	222	LEU
1	A	231	LEU
1	A	241	LEU
1	A	243	LEU
1	A	248	GLN
1	A	249	ARG
1	A	257	GLU
1	A	272	LEU
1	A	293	ARG
1	A	337	MET
1	A	381	LEU
1	A	384	LEU
1	A	386	LEU
1	A	392	GLU
1	A	398	LEU
1	A	404	ASN
1	A	489	ASN
1	A	502	GLU
1	A	512	ARG
1	A	520	LEU
1	A	575	ASP
1	A	576	GLU
1	A	595	ARG
1	B	61	GLU
1	B	94	ARG
1	B	101	LYS

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Mol	Chain	Res	Type
1	B	116	ARG
1	B	124	GLU
1	B	148	LEU
1	B	176	GLN
1	B	194	LEU
1	B	209	ASP
1	B	217	SER
1	B	241	LEU
1	B	243	LEU
1	B	248	GLN
1	B	249	ARG
1	B	251	GLU
1	B	253	VAL
1	B	257	GLU
1	B	272	LEU
1	B	337	MET
1	B	381	LEU
1	B	384	LEU
1	B	386	LEU
1	B	392	GLU
1	B	398	LEU
1	B	469	GLU
1	B	520	LEU
1	B	541	LEU
1	B	587	THR
1	B	594	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	63	ASN
1	A	99	ASN
1	A	115	GLN
1	A	160	GLN
1	A	176	GLN
1	A	179	ASN
1	A	218	HIS
1	A	237	HIS
1	A	248	GLN
1	A	373	ASN
1	A	388	ASN
1	A	404	ASN

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Mol	Chain	Res	Type
1	A	422	GLN
1	A	472	GLN
1	A	483	HIS
1	A	489	ASN
1	A	527	ASN
1	A	556	ASN
1	B	99	ASN
1	B	176	GLN
1	B	179	ASN
1	B	248	GLN
1	B	370	ASN
1	B	404	ASN
1	B	422	GLN
1	B	483	HIS
1	B	489	ASN
1	B	560	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	531/555 (95%)	0.11	28 (5%)	32 28	13, 31, 69, 83	5 (0%)
1	B	531/555 (95%)	0.02	27 (5%)	33 29	9, 28, 65, 82	5 (0%)
All	All	1062/1110 (95%)	0.06	55 (5%)	33 29	9, 30, 67, 83	10 (0%)

All (55) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	572	THR	12.8
1	B	568	GLY	12.6
1	B	572	THR	12.1
1	A	568	GLY	11.4
1	A	567	ASN	9.7
1	A	595	ARG	9.5
1	A	594	GLU	8.1
1	B	594	GLU	7.2
1	B	595	ARG	7.0
1	B	567	ASN	6.9
1	B	79	ILE	4.9
1	A	78	SER	4.2
1	B	78	SER	4.1
1	A	79	ILE	4.0
1	A	143	VAL	3.9
1	B	143	VAL	3.8
1	B	573	SER	3.4
1	A	72	SER	3.4
1	A	57	SER	3.1
1	B	221	GLU	3.0
1	A	461	GLN	3.0
1	A	71	LEU	2.9
1	A	140	PHE	2.8
1	A	574	PRO	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	133	ARG	2.7
1	A	146	THR	2.7
1	A	82	TYR	2.6
1	A	222	LEU	2.6
1	A	142	GLY	2.6
1	A	544	SER	2.6
1	B	574	PRO	2.6
1	A	176	GLN	2.6
1	B	82	TYR	2.5
1	B	142	GLY	2.5
1	A	573	SER	2.4
1	B	225	GLU	2.4
1	B	141	ASP	2.3
1	A	220	LYS	2.3
1	B	499	ALA	2.2
1	A	221	GLU	2.2
1	B	461	GLN	2.2
1	A	181	LEU	2.2
1	B	71	LEU	2.2
1	B	146	THR	2.1
1	B	81	VAL	2.1
1	B	297	ARG	2.1
1	A	139	GLY	2.1
1	B	69	PHE	2.1
1	A	224	GLU	2.0
1	A	225	GLU	2.0
1	B	133	ARG	2.0
1	B	515	GLY	2.0
1	B	575	ASP	2.0
1	B	57	SER	2.0
1	B	223	SER	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.