



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 12:14 AM UTC

PDB ID : 8IJT / pdb_00008ijt
Title : crystal structure of Hyp N135A mutant from Hypoxylon sp. E7406B
Authors : Gao, J.; Su, L.Q.; Li, Q.; Han, X.; Wei, H.L.; Dai, Z.J.; Liu, W.D.
Deposited on : 2023-02-28
Resolution : 2.56 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

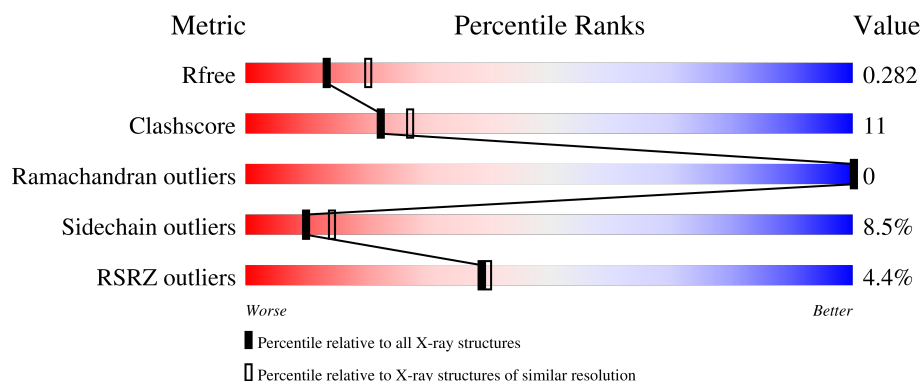
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.56 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	1853 (2.58-2.54)
Clashscore	190562	1897 (2.58-2.54)
Ramachandran outliers	187476	1875 (2.58-2.54)
Sidechain outliers	187428	1875 (2.58-2.54)
RSRZ outliers	180081	1853 (2.58-2.54)

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	372	0% 62% 24% • 12%
1	B	372	4% 66% 19% • 13%
1	C	372	5% 60% 25% • 12%
1	D	372	5% 56% 27% • 15%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 10300 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 Terpene synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	328	Total	C	N	O	S	0	0	0
			2607	1664	444	482	17			
1	B	325	Total	C	N	O	S	0	0	0
			2576	1642	437	480	17			
1	C	328	Total	C	N	O	S	0	0	0
			2577	1649	431	480	17			
1	D	318	Total	C	N	O	S	0	0	0
			2469	1583	403	467	16			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	135	ALA	ASN	engineered mutation	UNP A0A023W2U8
B	135	ALA	ASN	engineered mutation	UNP A0A023W2U8
C	135	ALA	ASN	engineered mutation	UNP A0A023W2U8
D	135	ALA	ASN	engineered mutation	UNP A0A023W2U8

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	30	Total	O	0	0
			30	30		
2	B	20	Total	O	0	0
			20	20		
2	C	10	Total	O	0	0
			10	10		
2	D	11	Total	O	0	0
			11	11		

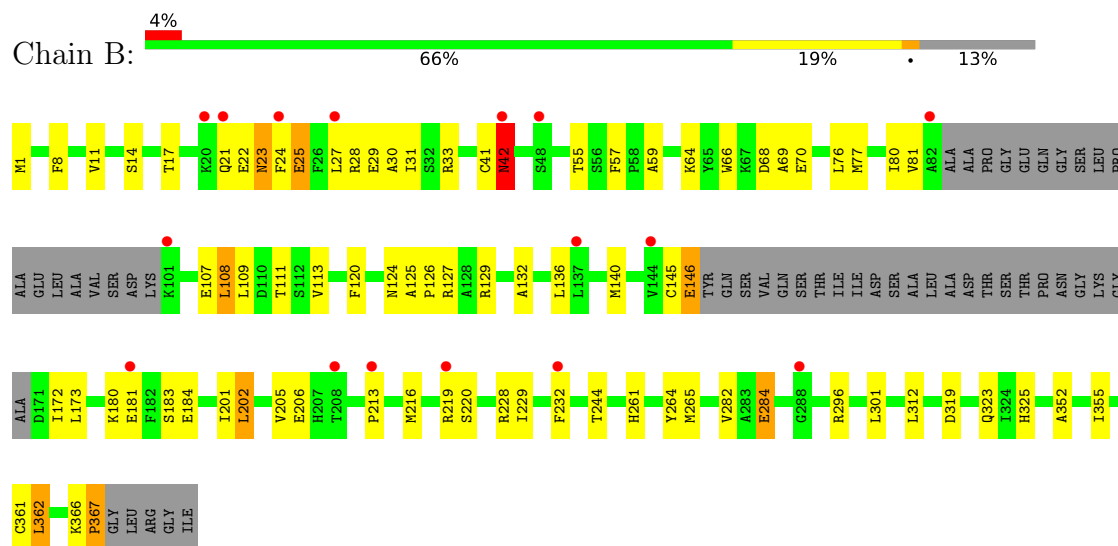
3 Residue-property plots [i](#)

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: Terpene synthase

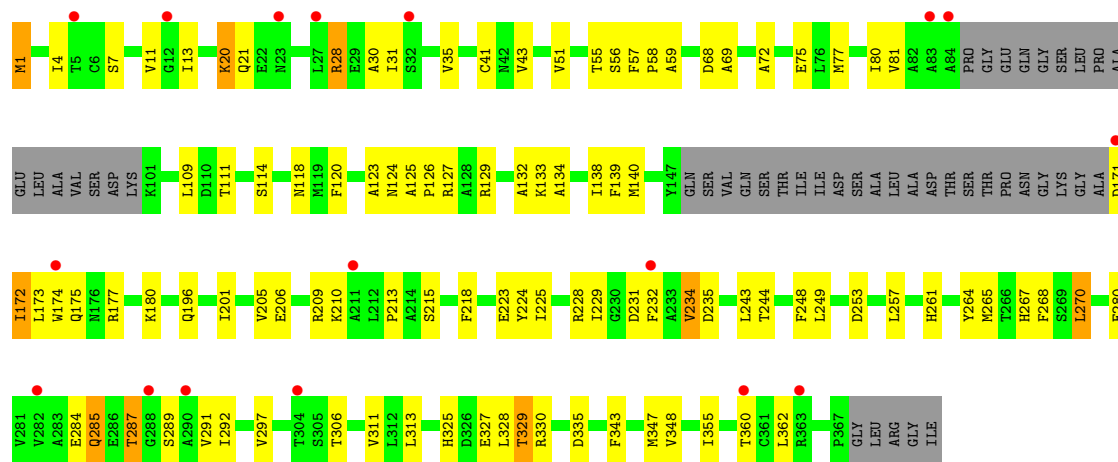


• Molecule 1: Terpene synthase

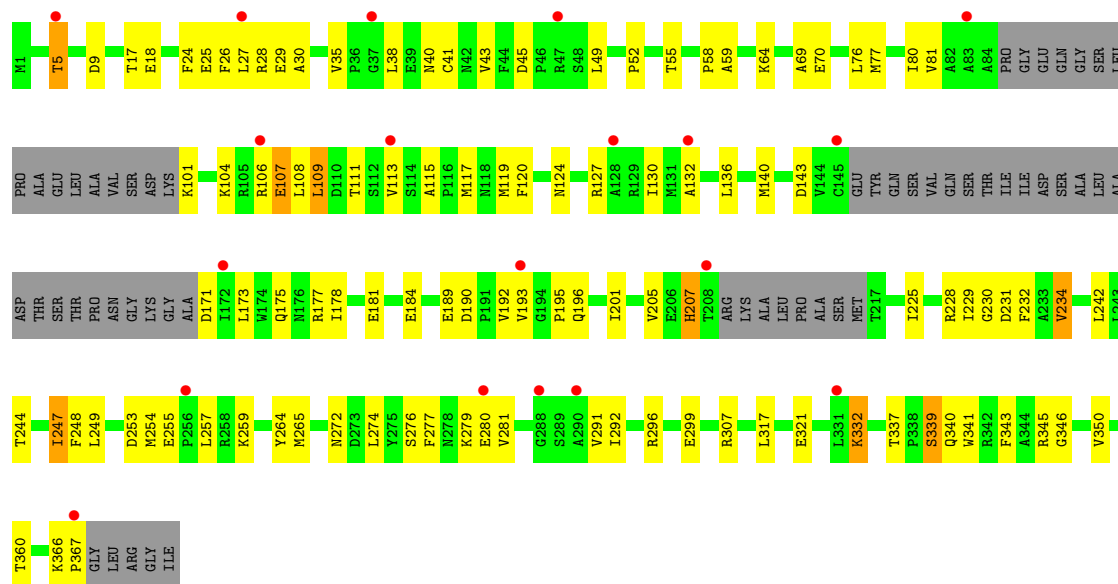


• Molecule 1: Terpene synthase





• Molecule 1: Terpene synthase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	45.87Å 86.23Å 102.35Å 77.50° 85.91° 87.69°	Depositor
Resolution (Å)	31.37 – 2.56 31.37 – 2.56	Depositor EDS
% Data completeness (in resolution range)	97.6 (31.37-2.56) 75.9 (31.37-2.56)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.49 (at 2.54Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.201 , 0.252 (Not available) , 0.282	Depositor DCC
R_{free} test set	2398 reflections (4.86%)	wwPDB-VP
Wilson B-factor (Å ²)	47.8	Xtriage
Anisotropy	0.418	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 54.1	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	10300	wwPDB-VP
Average B, all atoms (Å ²)	64.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.94% 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

5.1 Standard geometry

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	0.29	0/2667	0.56	4/3618 (0.1%)
1	B	0.34	0/2635	0.62	3/3579 (0.1%)
1	C	0.42	0/2637	0.66	1/3584 (0.0%)
1	D	0.47	0/2526	0.79	5/3439 (0.1%)
All	All	0.39	0/10465	0.66	13/14220 (0.1%)

There are no bond length outliers.

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	307	ARG	N-CA-CB	5.96	118.89	110.12
1	A	223	GLU	N-CA-C	-5.92	104.90	111.36
1	C	287	THR	OG1-CB-CG2	5.85	121.01	109.30
1	D	5	THR	OG1-CB-CG2	5.48	120.26	109.30
1	B	42	ASN	CA-C-N	5.38	129.71	122.93
1	B	42	ASN	C-N-CA	5.38	129.71	122.93
1	D	18	GLU	N-CA-C	-5.33	106.56	113.16
1	A	232	PHE	CA-C-O	-5.20	115.03	120.55
1	D	24	PHE	CA-C-N	-5.20	111.45	121.58
1	D	24	PHE	C-N-CA	-5.20	111.45	121.58
1	A	291	VAL	CA-C-N	5.19	128.69	122.26
1	A	291	VAL	C-N-CA	5.19	128.69	122.26
1	B	23	ASN	CA-C-O	-5.02	115.89	121.81

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	2607	0	2551	59	0
1	B	2576	0	2504	51	0
1	C	2577	0	2502	55	0
1	D	2469	0	2361	51	0
2	A	30	0	0	3	0
2	B	20	0	0	2	0
2	C	10	0	0	0	0
2	D	11	0	0	2	0
All	All	10300	0	9918	213	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 (213) 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:213:PRO:HB2	1:B:216:MET:HB2	1.61	0.82
1:C:80:ILE:HG21	1:C:140:MET:HE1	1.61	0.81
1:A:72:ALA:HB1	1:A:133:LYS:HE2	1.72	0.71
1:A:296:ARG:O	1:A:300:GLN:HG3	1.90	0.70
1:B:108:LEU:HD21	1:B:140:MET:HG2	1.75	0.68
1:B:1:MET:N	2:B:402:HOH:O	2.22	0.67
1:D:175:GLN:HA	1:D:178:ILE:HD12	1.77	0.67
1:D:26:PHE:HA	1:D:29:GLU:HG3	1.78	0.66
1:D:27:LEU:HB2	1:D:58:PRO:HG2	1.76	0.66
1:D:76:LEU:O	1:D:80:ILE:HG13	1.95	0.66
1:A:255:GLU:OE2	1:A:258:ARG:NH2	2.30	0.64
1:C:55:THR:HG22	1:C:57:PHE:H	1.62	0.64
1:A:77:MET:HG2	1:A:109:LEU:HD21	1.78	0.64
1:A:232:PHE:HE1	1:A:268:PHE:HB3	1.63	0.64
1:D:136:LEU:O	1:D:140:MET:HG3	1.99	0.63
1:B:55:THR:HG22	1:B:57:PHE:H	1.63	0.63
1:B:180:LYS:O	1:B:181:GLU:HG2	1.99	0.62
1:D:115:ALA:O	1:D:119:MET:HG3	1.99	0.62
1:C:21:GLN:HB3	1:C:325:HIS:CD2	2.34	0.62
1:D:117:MET:HA	1:D:117:MET:HE2	1.82	0.62
1:D:101:LYS:NZ	2:D:402:HOH:O	2.33	0.61
1:C:327:GLU:OE2	1:C:330:ARG:NH2	2.33	0.61
1:B:136:LEU:O	1:B:140:MET:HG3	2.01	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:7:SER:HB2	1:A:51:VAL:HG13	1.82	0.60
1:D:225:ILE:O	1:D:229:ILE:HG12	2.01	0.60
1:D:127:ARG:NH2	1:D:190:ASP:OD1	2.34	0.60
1:B:23:ASN:HB2	1:B:325:HIS:CD2	2.37	0.60
1:A:55:THR:HG22	1:A:57:PHE:H	1.66	0.60
1:C:225:ILE:O	1:C:229:ILE:HG13	2.02	0.60
1:D:173:LEU:HD12	1:D:173:LEU:H	1.67	0.59
1:A:229:ILE:HD11	1:A:266:THR:HA	1.85	0.58
1:A:228:ARG:NH2	1:A:272:ASN:OD1	2.36	0.58
1:A:69:ALA:HB1	1:A:132:ALA:HB2	1.86	0.58
1:C:7:SER:HB2	1:C:51:VAL:HG13	1.85	0.58
1:A:83:ALA:HB2	1:A:174:TRP:CD1	2.39	0.58
1:A:284:GLU:OE2	1:A:285:GLN:HG2	2.04	0.57
1:C:249:LEU:HD22	1:C:253:ASP:HB3	1.85	0.57
1:B:107:GLU:O	1:B:111:THR:HG22	2.04	0.57
1:D:207:HIS:O	1:D:207:HIS:ND1	2.34	0.57
1:D:69:ALA:HB1	1:D:132:ALA:HB2	1.86	0.56
1:D:249:LEU:HD21	1:D:340:GLN:HA	1.87	0.56
1:A:212:LEU:HG	1:A:227:TYR:CE1	2.40	0.56
1:D:109:LEU:O	1:D:113:VAL:HG23	2.05	0.56
1:C:213:PRO:C	1:C:215:SER:H	2.14	0.56
1:A:76:LEU:O	1:A:80:ILE:HG13	2.07	0.55
1:B:173:LEU:HD12	1:B:173:LEU:H	1.71	0.55
1:D:77:MET:O	1:D:81:VAL:HG22	2.06	0.55
1:C:196:GLN:NE2	1:C:248:PHE:HE1	2.03	0.55
1:D:337:THR:OG1	1:D:340:GLN:HB2	2.06	0.55
1:D:346:GLY:O	1:D:350:VAL:HG23	2.07	0.54
1:A:260:LEU:HD23	1:A:347:MET:HE3	1.88	0.54
1:C:261:HIS:O	1:C:265:MET:HG3	2.08	0.54
1:C:111:THR:HG22	1:C:139:PHE:CE2	2.43	0.54
1:C:72:ALA:HB1	1:C:133:LYS:HE2	1.89	0.53
1:C:328:LEU:HD11	1:C:348:VAL:HG21	1.90	0.53
1:A:232:PHE:HD2	1:A:234:VAL:HB	1.74	0.53
1:C:206:GLU:O	1:C:209:ARG:HG2	2.09	0.53
1:C:232:PHE:HE1	1:C:268:PHE:HB3	1.74	0.53
1:A:229:ILE:O	1:A:232:PHE:HB2	2.08	0.53
1:A:125:ALA:HB3	1:A:126:PRO:HD3	1.90	0.52
1:C:30:ALA:HB1	1:C:43:VAL:HG21	1.92	0.52
1:D:177:ARG:NH1	1:D:181:GLU:OE1	2.42	0.52
1:B:77:MET:O	1:B:81:VAL:HG22	2.10	0.52
1:A:105:ARG:O	1:A:109:LEU:HD23	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:325:HIS:O	1:C:329:THR:OG1	2.28	0.51
1:C:28:ARG:HE	1:C:58:PRO:HB2	1.75	0.51
1:C:335:ASP:OD2	1:C:335:ASP:C	2.54	0.51
1:A:11:VAL:HG12	1:A:13:ILE:HD13	1.92	0.51
1:A:303:ASP:OD2	1:B:220:SER:OG	2.21	0.51
1:C:196:GLN:HE22	1:C:248:PHE:HE1	1.58	0.51
1:A:142:ASP:OD2	1:A:142:ASP:C	2.54	0.50
1:A:361:CYS:SG	1:A:363:ARG:HG3	2.51	0.50
1:B:68:ASP:OD2	2:B:401:HOH:O	2.20	0.50
1:D:234:VAL:HB	1:D:265:MET:HE3	1.94	0.50
1:A:232:PHE:HB3	1:A:234:VAL:HG12	1.93	0.50
1:C:75:GLU:OE1	1:C:129:ARG:NH2	2.43	0.50
1:C:218:PHE:HD2	1:C:223:GLU:HG2	1.76	0.50
1:B:366:LYS:O	1:B:367:PRO:C	2.53	0.50
1:B:125:ALA:O	1:B:129:ARG:HG3	2.12	0.50
1:D:120:PHE:HB3	1:D:244:THR:HG21	1.94	0.49
1:C:224:TYR:CE1	1:C:228:ARG:HG3	2.47	0.49
1:C:4:ILE:HG23	1:C:360:THR:HG23	1.92	0.49
1:D:249:LEU:HG	1:D:253:ASP:HB3	1.95	0.49
1:B:261:HIS:O	1:B:265:MET:HG3	2.12	0.49
1:A:141:HIS:HE1	1:A:209:ARG:HH12	1.60	0.49
1:A:66:TRP:HB3	1:A:117:MET:HG3	1.95	0.49
1:D:254:MET:HE1	1:D:343:PHE:CZ	2.47	0.49
1:D:366:LYS:O	1:D:367:PRO:C	2.56	0.48
1:A:327:GLU:OE2	1:A:331:LEU:HG	2.14	0.48
1:D:177:ARG:O	1:D:181:GLU:HG2	2.13	0.48
1:B:42:ASN:ND2	1:B:64:LYS:HD3	2.28	0.48
1:C:69:ALA:HB1	1:C:132:ALA:HB2	1.96	0.48
1:C:20:LYS:HB3	1:C:20:LYS:HE3	1.60	0.48
1:C:114:SER:O	1:C:118:ASN:ND2	2.46	0.48
1:D:296:ARG:O	1:D:299:GLU:HG2	2.13	0.48
1:C:134:ALA:O	1:C:138:ILE:HG13	2.14	0.48
1:D:201:ILE:O	1:D:205:VAL:HG23	2.12	0.48
1:A:292:ILE:O	1:A:292:ILE:HG22	2.13	0.48
1:D:70:GLU:HG2	1:D:113:VAL:HG11	1.96	0.48
1:C:234:VAL:HB	1:C:265:MET:HE3	1.96	0.48
1:C:280:GLU:O	1:C:284:GLU:N	2.47	0.47
1:C:124:ASN:OD1	1:C:127:ARG:HG3	2.13	0.47
1:A:5:THR:OG1	2:A:401:HOH:O	2.20	0.47
1:A:11:VAL:HG13	1:A:311:VAL:HG22	1.96	0.47
1:C:1:MET:HE2	1:C:1:MET:HB3	1.69	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:212:LEU:HG	1:A:227:TYR:HE1	1.80	0.47
1:B:181:GLU:H	1:B:184:GLU:HG3	1.80	0.47
1:B:362:LEU:H	1:B:362:LEU:HG	1.47	0.47
1:C:224:TYR:CD2	1:C:297:VAL:HG21	2.50	0.47
1:C:270:LEU:HG	1:C:313:LEU:HD11	1.97	0.47
1:A:261:HIS:O	1:A:265:MET:HG3	2.14	0.47
1:B:29:GLU:O	1:B:33:ARG:HG2	2.14	0.47
1:A:171:ASP:O	1:A:175:GLN:HG2	2.15	0.47
1:A:337:THR:HG22	1:A:339:SER:N	2.30	0.47
1:B:69:ALA:HB1	1:B:132:ALA:HB2	1.96	0.47
1:A:16:GLN:HB3	1:B:14:SER:HB2	1.96	0.47
1:C:343:PHE:CD1	1:C:347:MET:HE2	2.50	0.47
1:A:55:THR:HG23	1:A:321:GLU:OE2	2.15	0.46
1:A:328:LEU:HD11	1:A:348:VAL:HG21	1.97	0.46
1:B:21:GLN:HG3	1:B:325:HIS:CG	2.51	0.46
1:B:140:MET:HE2	1:B:140:MET:HB3	1.76	0.46
1:D:107:GLU:O	1:D:111:THR:HG22	2.15	0.46
1:A:115:ALA:HB3	1:A:116:PRO:HD3	1.97	0.46
1:C:31:ILE:HD11	1:C:59:ALA:HB2	1.97	0.46
1:C:270:LEU:HD12	1:C:270:LEU:HA	1.79	0.46
1:B:145:CYS:O	1:B:146:GLU:C	2.58	0.46
1:A:337:THR:HG22	1:A:339:SER:H	1.81	0.46
1:B:284:GLU:OE1	1:B:296:ARG:NH2	2.49	0.46
1:C:291:VAL:C	1:C:292:ILE:HD13	2.41	0.45
1:D:230:GLY:C	1:D:232:PHE:H	2.24	0.45
1:A:40:ASN:O	1:A:64:LYS:HG2	2.16	0.45
1:A:77:MET:HE3	1:A:81:VAL:CG1	2.47	0.45
1:A:83:ALA:HB1	1:A:175:GLN:OE1	2.16	0.45
1:A:261:HIS:CE1	1:A:265:MET:HE2	2.52	0.45
1:B:125:ALA:HB3	1:B:126:PRO:HD3	1.97	0.45
1:C:174:TRP:HE1	1:C:177:ARG:NH2	2.15	0.45
1:A:204:TRP:CD1	1:A:233:ALA:HB2	2.51	0.45
1:B:232:PHE:O	1:B:232:PHE:CG	2.70	0.45
1:B:55:THR:HG21	1:B:57:PHE:CD2	2.52	0.45
1:B:66:TRP:O	1:B:70:GLU:HG3	2.17	0.45
1:B:76:LEU:HG	1:B:80:ILE:HD12	1.98	0.45
1:C:127:ARG:HD3	1:C:243:LEU:HG	1.98	0.45
1:C:172:ILE:H	1:C:172:ILE:HG13	1.39	0.45
1:D:127:ARG:NH1	1:D:189:GLU:OE2	2.49	0.45
1:B:202:LEU:O	1:B:206:GLU:HG2	2.16	0.45
1:D:228:ARG:HD2	1:D:228:ARG:HA	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:70:GLU:HG2	1:B:113:VAL:HG11	1.99	0.44
1:C:11:VAL:HG13	1:C:311:VAL:HG22	1.99	0.44
1:A:111:THR:HG22	1:A:139:PHE:CE2	2.52	0.44
1:C:123:ALA:HB2	1:C:244:THR:HG22	1.98	0.44
1:C:124:ASN:OD1	1:C:126:PRO:HD2	2.17	0.44
1:B:22:GLU:O	1:B:25:GLU:HB2	2.18	0.44
1:C:125:ALA:HB3	1:C:126:PRO:HD3	1.98	0.44
1:A:77:MET:HE3	1:A:81:VAL:HG13	1.99	0.44
1:D:30:ALA:HB3	1:D:43:VAL:HG11	1.99	0.44
1:D:247:ILE:HD13	1:D:339:SER:HB2	1.99	0.44
1:D:332:LYS:HD3	1:D:332:LYS:HA	1.87	0.44
1:D:173:LEU:HD12	1:D:173:LEU:N	2.32	0.43
1:B:201:ILE:O	1:B:205:VAL:HG23	2.19	0.43
1:D:276:SER:O	1:D:277:PHE:C	2.61	0.43
1:D:232:PHE:CD1	1:D:265:MET:HG2	2.52	0.43
1:B:352:ALA:HA	1:B:355:ILE:HD12	2.00	0.43
1:A:130:ILE:HD13	1:A:186:THR:HA	1.99	0.43
1:C:68:ASP:OD2	1:C:68:ASP:N	2.52	0.43
1:B:23:ASN:O	1:B:24:PHE:HB2	2.18	0.43
1:D:280:GLU:HB3	1:D:291:VAL:HG22	2.01	0.43
1:A:302:VAL:HA	1:B:301:LEU:HD13	2.01	0.43
1:C:285:GLN:OE1	1:C:285:GLN:HA	2.18	0.43
1:A:141:HIS:HE1	1:A:209:ARG:NH1	2.17	0.42
1:A:45:ASP:O	1:A:48:SER:OG	2.36	0.42
1:B:120:PHE:HB3	1:B:244:THR:HG21	2.00	0.42
1:D:9:ASP:HB2	1:D:52:PRO:HB2	2.01	0.42
1:B:319:ASP:O	1:B:323:GLN:HG3	2.19	0.42
1:A:304:THR:HG23	1:A:305:SER:O	2.20	0.42
1:C:120:PHE:HB3	1:C:244:THR:HG21	2.00	0.42
1:D:27:LEU:HB3	1:D:59:ALA:HB3	2.02	0.42
1:D:124:ASN:OD1	1:D:127:ARG:HB2	2.19	0.42
1:B:228:ARG:HD2	1:B:228:ARG:HA	1.89	0.42
1:A:223:GLU:CB	2:A:429:HOH:O	2.67	0.42
1:C:11:VAL:O	1:C:13:ILE:HG13	2.20	0.42
1:A:30:ALA:HB1	1:A:43:VAL:HG21	2.00	0.42
1:A:346:GLY:O	1:A:350:VAL:HG23	2.20	0.42
1:B:124:ASN:OD1	1:B:127:ARG:HG2	2.20	0.42
1:A:70:GLU:HA	1:A:113:VAL:HG21	2.02	0.41
1:C:77:MET:HG2	1:C:109:LEU:HD11	2.02	0.41
1:C:77:MET:O	1:C:81:VAL:HG13	2.19	0.41
1:D:317:LEU:O	1:D:321:GLU:HG3	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:326:ASP:OD1	2:A:402:HOH:O	2.22	0.41
1:B:28:ARG:HH11	1:B:28:ARG:HD3	1.64	0.41
1:B:22:GLU:HG2	1:B:23:ASN:H	1.85	0.41
1:B:30:ALA:HA	1:B:33:ARG:O	2.20	0.41
1:B:27:LEU:HB3	1:B:59:ALA:HB3	2.01	0.41
1:B:28:ARG:O	1:B:31:ILE:HG13	2.21	0.41
1:B:282:VAL:HG11	1:B:367:PRO:HB3	2.01	0.41
1:C:229:ILE:HG23	1:C:265:MET:HE2	2.02	0.41
1:D:101:LYS:HE3	1:D:101:LYS:HB3	1.94	0.41
1:D:171:ASP:OD2	2:D:401:HOH:O	2.22	0.41
1:A:225:ILE:HG23	1:A:229:ILE:HD13	2.03	0.41
1:D:30:ALA:HB1	1:D:43:VAL:HG21	2.03	0.40
1:D:25:GLU:O	1:D:28:ARG:N	2.55	0.40
1:D:242:LEU:HD22	1:D:248:PHE:HA	2.03	0.40
1:D:341:TRP:HE1	1:D:345:ARG:HE	1.69	0.40
1:A:261:HIS:ND1	1:A:265:MET:HE2	2.37	0.40
1:B:22:GLU:HG2	1:B:23:ASN:N	2.36	0.40
1:B:124:ASN:CG	1:B:126:PRO:HD2	2.46	0.40
1:C:267:HIS:CE1	1:C:355:ILE:HD11	2.57	0.40
1:C:330:ARG:HG2	1:C:330:ARG:HH11	1.85	0.40
1:A:277:PHE:O	1:A:281:VAL:HG23	2.21	0.40
1:B:109:LEU:O	1:B:113:VAL:HG23	2.22	0.40
1:B:206:GLU:HG2	1:B:206:GLU:H	1.64	0.40
1:C:201:ILE:O	1:C:205:VAL:HG23	2.21	0.40
1:D:192:VAL:O	1:D:195:PRO:HD2	2.21	0.40
1:D:40:ASN:O	1:D:64:LYS:HG3	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	322/372 (87%)	314 (98%)	8 (2%)	0	100	100
1	B	319/372 (86%)	315 (99%)	4 (1%)	0	100	100
1	C	322/372 (87%)	313 (97%)	9 (3%)	0	100	100
1	D	310/372 (83%)	303 (98%)	7 (2%)	0	100	100
All	All	1273/1488 (86%)	1245 (98%)	28 (2%)	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	278/315 (88%)	263 (95%)	15 (5%)	20	30
1	B	275/315 (87%)	256 (93%)	19 (7%)	14	20
1	C	273/315 (87%)	249 (91%)	24 (9%)	9	13
1	D	260/315 (82%)	226 (87%)	34 (13%)	4	4
All	All	1086/1260 (86%)	994 (92%)	92 (8%)	10	14

All (92) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	18	GLU
1	A	20	LYS
1	A	100	LYS
1	A	104	LYS
1	A	108	LEU
1	A	188	ARG
1	A	212	LEU
1	A	217	THR
1	A	231	ASP
1	A	234	VAL
1	A	235	ASP
1	A	258	ARG
1	A	284	GLU

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Mol	Chain	Res	Type
1	A	302	VAL
1	A	362	LEU
1	B	8	PHE
1	B	11	VAL
1	B	17	THR
1	B	25	GLU
1	B	41	CYS
1	B	42	ASN
1	B	108	LEU
1	B	146	GLU
1	B	172	ILE
1	B	183	SER
1	B	202	LEU
1	B	219	ARG
1	B	229	ILE
1	B	264	TYR
1	B	284	GLU
1	B	312	LEU
1	B	361	CYS
1	B	362	LEU
1	B	367	PRO
1	C	1	MET
1	C	20	LYS
1	C	28	ARG
1	C	35	VAL
1	C	41	CYS
1	C	56	SER
1	C	171	ASP
1	C	172	ILE
1	C	173	LEU
1	C	175	GLN
1	C	180	LYS
1	C	210	LYS
1	C	231	ASP
1	C	234	VAL
1	C	235	ASP
1	C	257	LEU
1	C	264	TYR
1	C	270	LEU
1	C	285	GLN
1	C	287	THR
1	C	289	SER

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Mol	Chain	Res	Type
1	C	306	THR
1	C	329	THR
1	C	362	LEU
1	D	5	THR
1	D	17	THR
1	D	35	VAL
1	D	38	LEU
1	D	41	CYS
1	D	45	ASP
1	D	49	LEU
1	D	55	THR
1	D	104	LYS
1	D	106	ARG
1	D	107	GLU
1	D	108	LEU
1	D	109	LEU
1	D	130	ILE
1	D	143	ASP
1	D	184	GLU
1	D	193	VAL
1	D	196	GLN
1	D	207	HIS
1	D	231	ASP
1	D	234	VAL
1	D	247	ILE
1	D	255	GLU
1	D	257	LEU
1	D	259	LYS
1	D	264	TYR
1	D	272	ASN
1	D	274	LEU
1	D	279	LYS
1	D	281	VAL
1	D	292	ILE
1	D	332	LYS
1	D	339	SER
1	D	360	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	40	ASN

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Mol	Chain	Res	Type
1	A	42	ASN
1	A	141	HIS
1	A	207	HIS
1	A	222	ASN
1	A	323	GLN
1	B	199	GLN
1	C	16	GLN
1	C	21	GLN
1	C	42	ASN
1	C	187	ASN
1	C	199	GLN
1	D	16	GLN
1	D	187	ASN
1	D	300	GLN
1	D	323	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](#)

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	328/372 (88%)	0.31	5 (1%) 72 73	37, 57, 95, 116	0
1	B	325/372 (87%)	0.49	16 (4%) 35 35	38, 58, 96, 116	0
1	C	328/372 (88%)	0.49	17 (5%) 33 33	40, 61, 98, 125	0
1	D	318/372 (85%)	0.75	19 (5%) 27 27	43, 69, 96, 109	0
All	All	1299/1488 (87%)	0.51	57 (4%) 39 40	37, 61, 97, 125	0

All (57) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	290	ALA	4.4
1	D	288	GLY	4.1
1	C	23	ASN	3.6
1	C	363	ARG	3.5
1	B	137	LEU	3.5
1	B	288	GLY	3.3
1	C	171	ASP	3.3
1	D	37	GLY	3.1
1	B	48	SER	3.1
1	D	128	ALA	3.0
1	D	208	THR	3.0
1	B	82	ALA	3.0
1	A	290	ALA	2.9
1	D	367	PRO	2.9
1	C	83	ALA	2.9
1	A	232	PHE	2.9
1	C	32	SER	2.9
1	D	47	ARG	2.8
1	C	84	ALA	2.8
1	D	113	VAL	2.7
1	C	232	PHE	2.7

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Mol	Chain	Res	Type	RSRZ
1	C	304	THR	2.6
1	C	211	ALA	2.6
1	C	5	THR	2.6
1	D	5	THR	2.5
1	A	291	VAL	2.5
1	C	282	VAL	2.5
1	C	27	LEU	2.5
1	D	145	CYS	2.4
1	C	288	GLY	2.4
1	D	106	ARG	2.4
1	B	42	ASN	2.4
1	B	21	GLN	2.4
1	B	232	PHE	2.4
1	B	208	THR	2.4
1	B	219	ARG	2.4
1	B	144	VAL	2.3
1	D	132	ALA	2.3
1	D	27	LEU	2.3
1	D	331	LEU	2.2
1	B	181	GLU	2.2
1	D	193	VAL	2.2
1	C	174	TRP	2.2
1	D	280	GLU	2.2
1	B	213	PRO	2.2
1	A	211	ALA	2.1
1	B	27	LEU	2.1
1	B	24	PHE	2.1
1	C	360	THR	2.1
1	D	172	ILE	2.1
1	A	23	ASN	2.1
1	C	12	GLY	2.1
1	D	256	PRO	2.1
1	D	83	ALA	2.0
1	D	290	ALA	2.0
1	B	20	LYS	2.0
1	B	101	LYS	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](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.