



# Full wwPDB X-ray Structure Validation Report i

Feb 19, 2024 – 03:54 PM JST

PDB ID : 8IJT  
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](mailto: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 i symbol.

The types of validation reports are described at  
<http://www.wwpdb.org/validation/2017/FAQs#types>.

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The following versions of software and data (see [references](#) ①) were used in the production of this report:

MolProbity : 4.02b-467  
Xtriage (Phenix) : 1.13  
EDS : 2.36  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.36

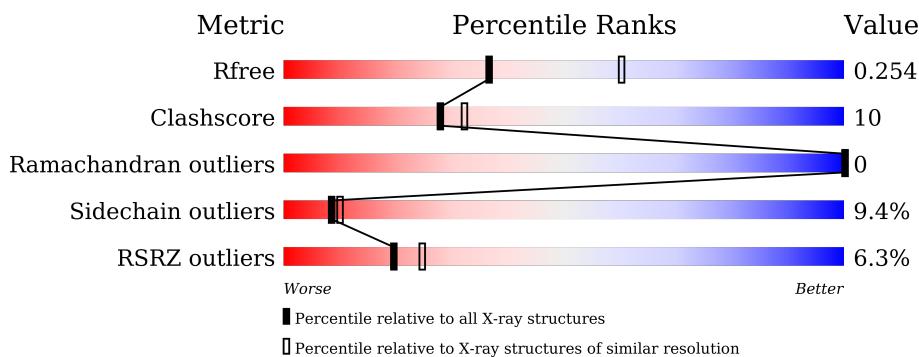
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

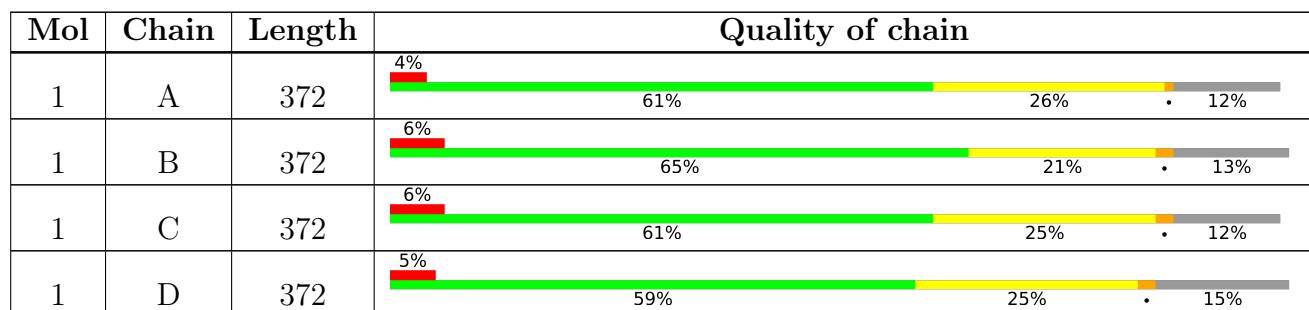
The reported resolution of this entry is 2.56 Å.

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))
$R_{free}$	130704	1279 (2.58-2.54)
Clashscore	141614	1327 (2.58-2.54)
Ramachandran outliers	138981	1312 (2.58-2.54)
Sidechain outliers	138945	1312 (2.58-2.54)
RSRZ outliers	127900	1269 (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 <=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.



## 2 Entry composition (i)

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 2607	N 1664	O 444	S 482	17	0	0
1	B	325	Total	C 2576	N 1642	O 437	S 480	17	0	0
1	C	328	Total	C 2577	N 1649	O 431	S 480	17	0	0
1	D	318	Total	C 2469	N 1583	O 403	S 467	16	0	0

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

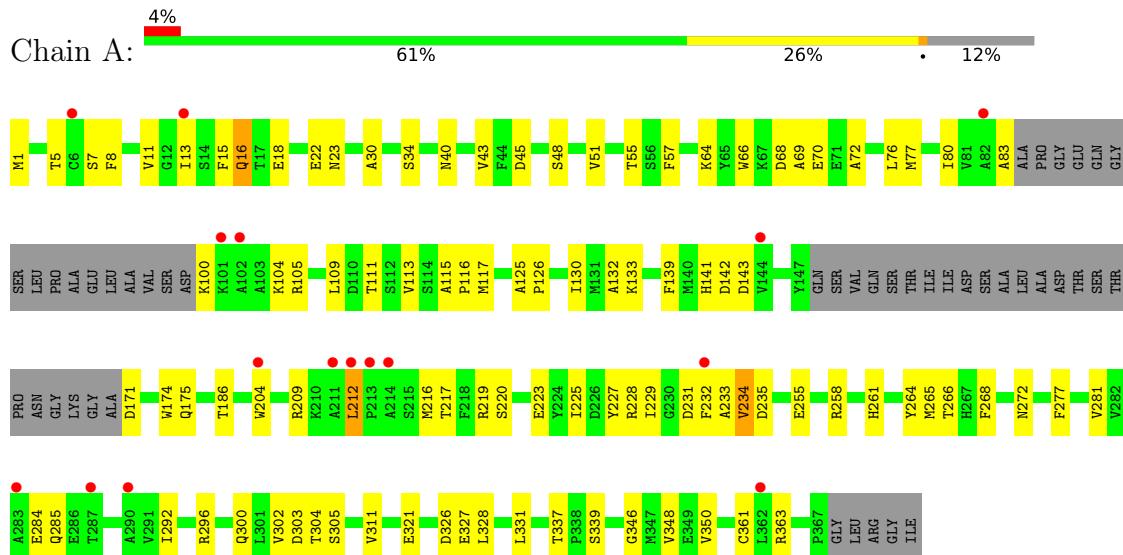
- Molecule 2 is water.

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

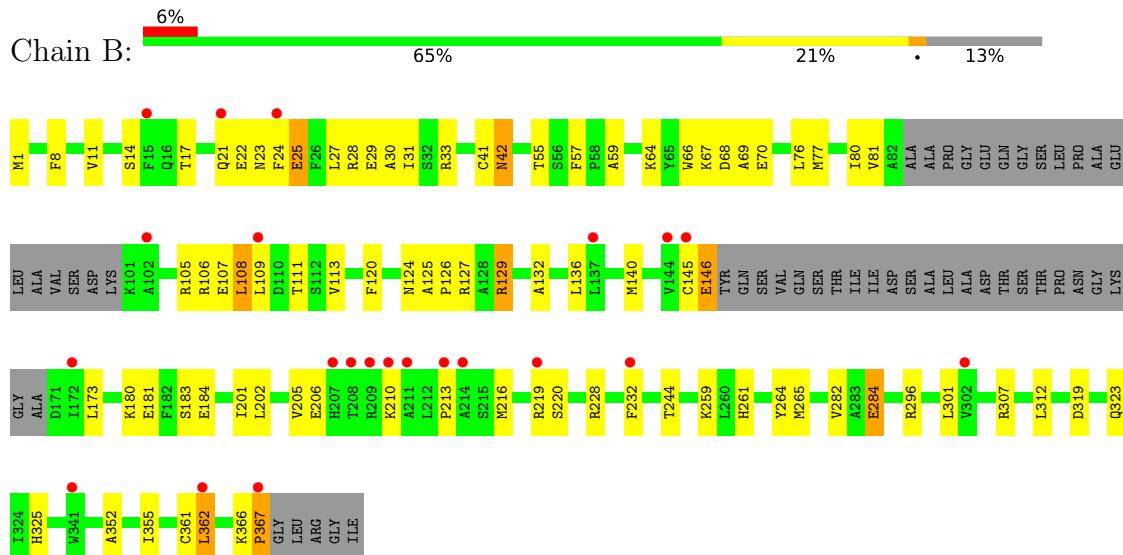
### 3 Residue-property plots [i](#)

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.

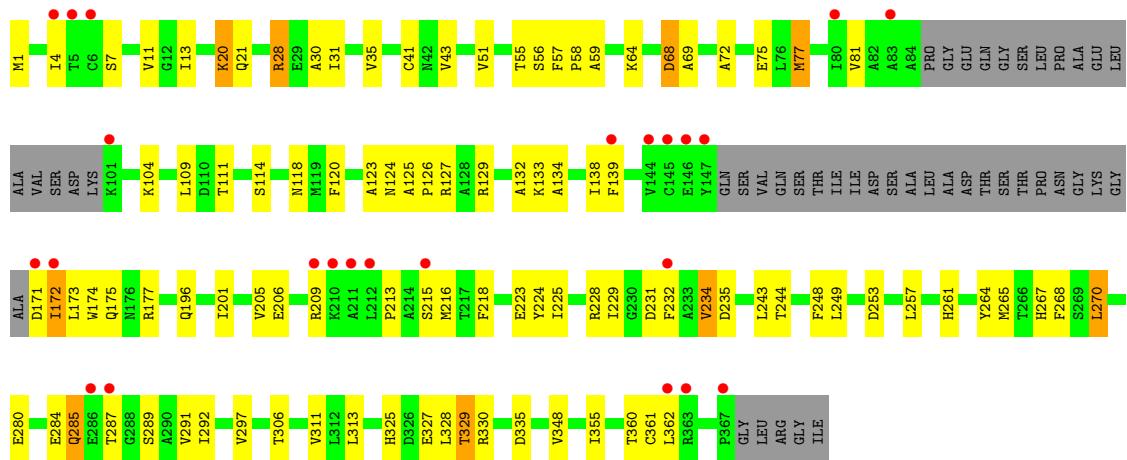
- Molecule 1: Terpene synthase



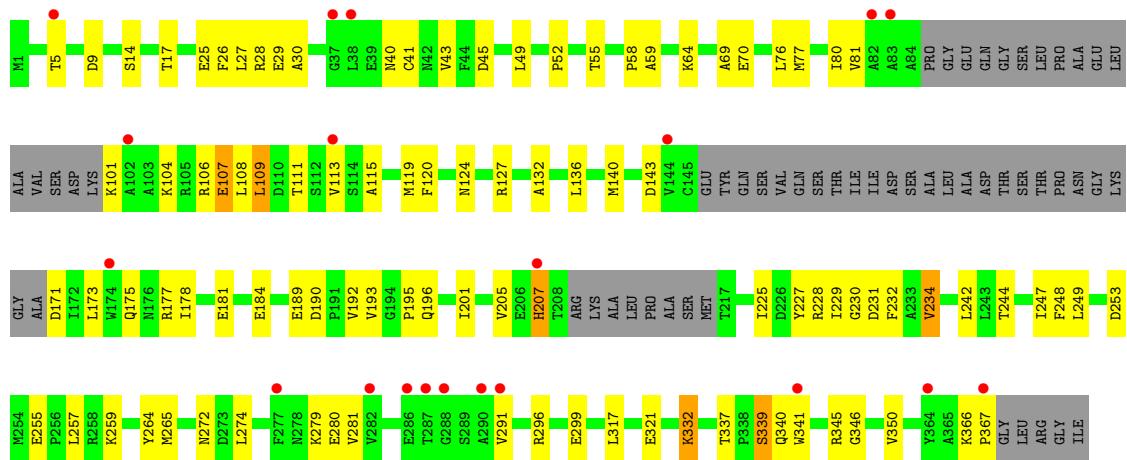
- Molecule 1: Terpene synthase



- Molecule 1: Terpene synthase



- Molecule 1: Terpene synthase



## 4 Data and refinement statistics i

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	45.87 Å    86.23 Å    102.35 Å 77.50°    85.91°    87.69°	Depositor
Resolution (Å)	31.37 – 2.56 47.60 – 2.56	Depositor EDS
% Data completeness (in resolution range)	97.6 (31.37-2.56) 88.0 (47.60-2.56)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$< I/\sigma(I) >$ <sup>1</sup>	1.49 (at 2.54 Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
$R$ , $R_{free}$	0.201 , 0.252 0.210 , 0.254	Depositor DCC
$R_{free}$ test set	2311 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	47.8	Xtriage
Anisotropy	0.418	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 55.7	EDS
L-test for twinning <sup>2</sup>	$<  L  > = 0.49$ , $< L^2 > = 0.32$	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 <sup>2</sup> )	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.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $< |L| >$ ,  $< L^2 >$  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	0.33	0/2667	0.55	0/3618
1	B	0.36	0/2635	0.58	0/3579
1	C	0.38	0/2637	0.59	0/3584
1	D	0.39	0/2526	0.62	0/3439
All	All	0.36	0/10465	0.59	0/14220

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [\(i\)](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2607	0	2551	54	0
1	B	2576	0	2504	49	0
1	C	2577	0	2502	51	0
1	D	2469	0	2361	48	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	199	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 10.

All (199) 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: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: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
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:H	1:D:173:LEU:HD12	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:109:LEU:O	1:D:113:VAL:HG23	2.05	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: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
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:213:PRO:C	1:C:215:SER:H	2.14	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: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: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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:234:VAL:HB	1:C:265:MET:HE3	1.95	0.48
1:D:70:GLU:HG2	1:D:113:VAL:HG11	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: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: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:D:107:GLU:O	1:D:111:THR:HG22	2.15	0.46
1:C:335:ASP:C	1:C:335:ASP:OD2	2.54	0.46
1:A:115:ALA:HB3	1:A:116:PRO:HD3	1.97	0.46
1:B:366:LYS:O	1:B:367:PRO:C	2.53	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:A:142:ASP:C	1:A:142:ASP:OD2	2.54	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:A:40:ASN:O	1:A:64:LYS:HG2	2.16	0.45
1:A:83:ALA:HB1	1:A:175:GLN:OE1	2.16	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:HA	1:D:228:ARG:HD2	1.81	0.45
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:D:366:LYS:O	1:D:367:PRO:C	2.56	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: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:HA	1:C:285:GLN:OE1	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:D:234:VAL:HB	1:D:265:MET:HE3	2.01	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:145:CYS:O	1:B:146:GLU:C	2.58	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
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:C:291:VAL:C	1:C:292:ILE:HD13	2.41	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: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:230:GLY:C	1:D:232:PHE:H	2.24	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:B:22:GLU:HG2	1:B:23:ASN:N	2.36	0.40
1:C:267:HIS:CE1	1:C:355:ILE:HD11	2.57	0.40
1:C:330:ARG:HH11	1:C:330:ARG:HG2	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 [\(i\)](#)

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	278/315 (88%)	257 (92%)	21 (8%)	13 17
1	B	275/315 (87%)	252 (92%)	23 (8%)	11 13
1	C	273/315 (87%)	245 (90%)	28 (10%)	7 8
1	D	260/315 (82%)	230 (88%)	30 (12%)	5 5
All	All	1086/1260 (86%)	984 (91%)	102 (9%)	8 10

All (102) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	8	PHE

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Mol	Chain	Res	Type
1	A	15	PHE
1	A	16	GLN
1	A	18	GLU
1	A	22	GLU
1	A	23	ASN
1	A	34	SER
1	A	68	ASP
1	A	100	LYS
1	A	104	LYS
1	A	143	ASP
1	A	212	LEU
1	A	216	MET
1	A	217	THR
1	A	219	ARG
1	A	220	SER
1	A	231	ASP
1	A	234	VAL
1	A	235	ASP
1	A	264	TYR
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	67	LYS
1	B	105	ARG
1	B	106	ARG
1	B	108	LEU
1	B	129	ARG
1	B	146	GLU
1	B	183	SER
1	B	210	LYS
1	B	219	ARG
1	B	259	LYS
1	B	264	TYR
1	B	284	GLU
1	B	307	ARG
1	B	312	LEU
1	B	361	CYS
1	B	362	LEU
1	B	367	PRO

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Mol	Chain	Res	Type
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	64	LYS
1	C	68	ASP
1	C	77	MET
1	C	104	LYS
1	C	171	ASP
1	C	172	ILE
1	C	173	LEU
1	C	175	GLN
1	C	216	MET
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
1	C	306	THR
1	C	329	THR
1	C	361	CYS
1	C	362	LEU
1	D	5	THR
1	D	14	SER
1	D	17	THR
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	143	ASP
1	D	184	GLU

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Mol	Chain	Res	Type
1	D	193	VAL
1	D	196	GLN
1	D	207	HIS
1	D	227	TYR
1	D	231	ASP
1	D	234	VAL
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	332	LYS
1	D	339	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	141	HIS
1	C	203	ASN
1	C	261	HIS
1	D	16	GLN
1	D	300	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 monosaccharides 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 i

### 6.1 Protein, DNA and RNA chains i

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	328/372 (88%)	0.54	16 (4%) 29 37	37, 57, 95, 116	0
1	B	325/372 (87%)	0.48	22 (6%) 17 22	38, 58, 96, 116	0
1	C	328/372 (88%)	0.72	24 (7%) 15 19	40, 61, 98, 125	0
1	D	318/372 (85%)	0.59	20 (6%) 20 25	43, 69, 96, 109	0
All	All	1299/1488 (87%)	0.58	82 (6%) 20 25	37, 61, 97, 125	0

All (82) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	211	ALA	7.4
1	C	367	PRO	5.5
1	C	5	THR	4.9
1	C	210	LYS	4.7
1	B	209	ARG	4.6
1	A	232	PHE	4.5
1	B	367	PRO	4.5
1	A	212	LEU	4.4
1	B	144	VAL	4.2
1	D	82	ALA	4.2
1	C	363	ARG	4.0
1	C	212	LEU	4.0
1	A	101	LYS	3.9
1	D	286	GLU	3.8
1	B	219	ARG	3.7
1	C	286	GLU	3.7
1	C	232	PHE	3.6
1	B	210	LYS	3.6
1	D	282	VAL	3.4
1	D	290	ALA	3.4
1	C	144	VAL	3.3

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Mol	Chain	Res	Type	RSRZ
1	D	367	PRO	3.2
1	C	83	ALA	3.2
1	A	211	ALA	3.2
1	A	13	ILE	3.2
1	A	144	VAL	3.1
1	A	102	ALA	3.1
1	C	147	TYR	3.1
1	D	287	THR	3.0
1	D	38	LEU	2.9
1	B	172	ILE	2.9
1	C	80	ILE	2.9
1	B	362	LEU	2.9
1	B	145	CYS	2.9
1	C	146	GLU	2.8
1	A	283	ALA	2.8
1	C	171	ASP	2.8
1	A	290	ALA	2.8
1	D	102	ALA	2.8
1	B	24	PHE	2.7
1	A	214	ALA	2.7
1	C	145	CYS	2.7
1	D	288	GLY	2.7
1	B	109	LEU	2.7
1	D	5	THR	2.6
1	B	341	TRP	2.6
1	C	6	CYS	2.6
1	B	302	VAL	2.6
1	D	113	VAL	2.5
1	A	362	LEU	2.5
1	D	144	VAL	2.5
1	B	208	THR	2.5
1	C	362	LEU	2.4
1	B	207	HIS	2.4
1	A	82	ALA	2.4
1	A	204	TRP	2.4
1	D	341	TRP	2.4
1	B	213	PRO	2.4
1	D	277	PHE	2.4
1	C	4	ILE	2.3
1	B	21	GLN	2.3
1	C	172	ILE	2.3
1	D	83	ALA	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	211	ALA	2.2
1	D	207	HIS	2.2
1	A	213	PRO	2.2
1	C	215	SER	2.2
1	D	174	TRP	2.2
1	C	139	PHE	2.2
1	C	101	LYS	2.1
1	B	102	ALA	2.1
1	D	291	VAL	2.1
1	A	287	THR	2.1
1	C	287	THR	2.1
1	B	15	PHE	2.1
1	B	232	PHE	2.1
1	D	364	TYR	2.1
1	C	209	ARG	2.1
1	D	37	GLY	2.0
1	B	214	ALA	2.0
1	A	6	CYS	2.0
1	B	137	LEU	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 monosaccharides 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.