



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 26, 2018 – 12:17 AM EDT

PDB ID : 1HM4  
Title : N219L PENTALENENE SYNTHASE  
Authors : Seemann, M.; Paschall, C.M.; Christianson, D.W.; Cane, D.E.  
Deposited on : 2000-12-04  
Resolution : 3.47 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 ⓘ symbol.

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

MolProbity : 4.02b-467  
Xtriage (Phenix) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : rb-20031021

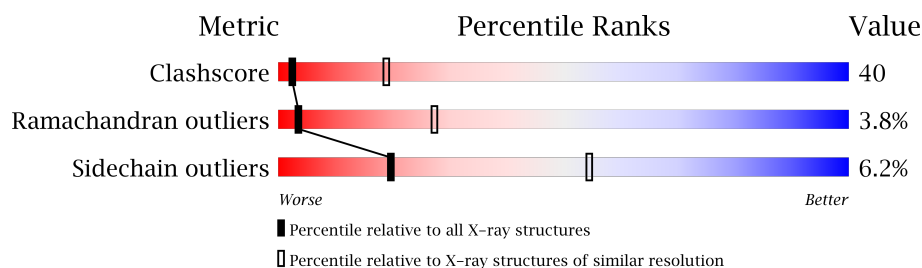
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.47 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))
Clashscore	122126	1235 (3.56-3.40)
Ramachandran outliers	120053	1202 (3.56-3.40)
Sidechain outliers	120020	1203 (3.56-3.40)

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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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  $\leq 5\%$ .

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	336	
1	B	336	

## 2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 4683 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 PENTALENENE SYNTHASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	289	Total	C	N	O	S	0	0	0
			2293	1433	418	431	11			
1	B	300	Total	C	N	O	S	0	0	0
			2390	1496	436	446	12			

There are 2 discrepancies between the modelled and reference sequences:

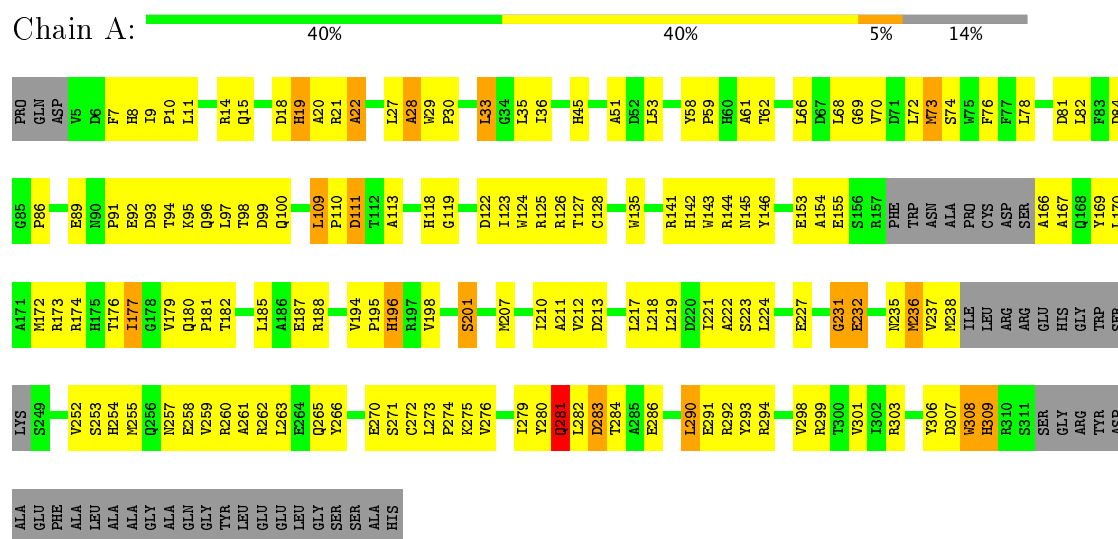
Chain	Residue	Modelled	Actual	Comment	Reference
A	219	LEU	ASN	ENGINEERED	UNP Q55012
B	219	LEU	ASN	ENGINEERED	UNP Q55012

### 3 Residue-property plots

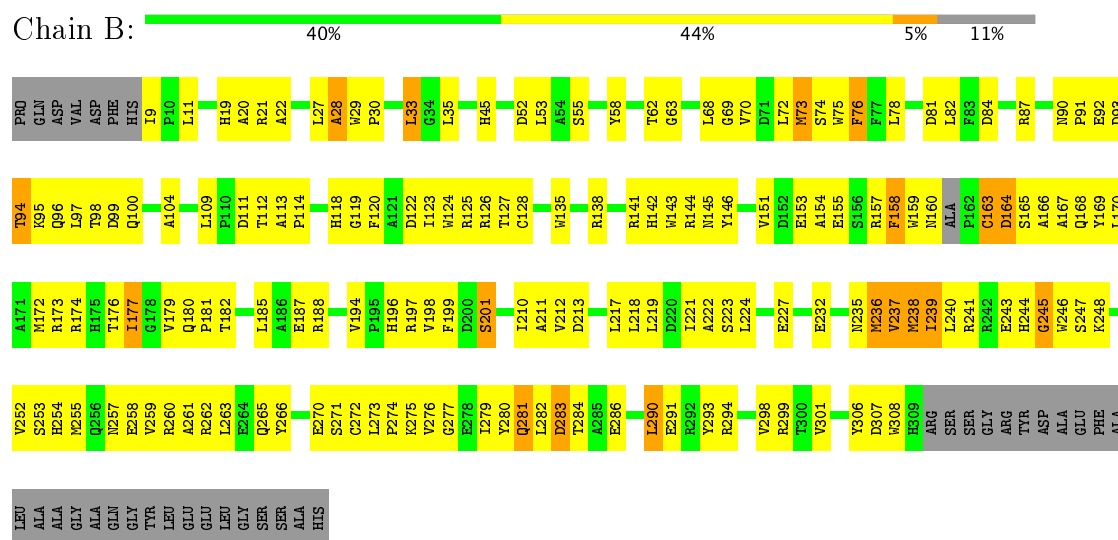
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according 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. 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.

Note EDS was not executed.

#### • Molecule 1: PENTALENENE SYNTHASE



#### • Molecule 1: PENTALENENE SYNTHASE



## 4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 63	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	182.00 Å   182.00 Å   56.40 Å 90.00°   90.00°   120.00°	Depositor
Resolution (Å)	20.00 – 3.47	Depositor
% Data completeness (in resolution range)	(Not available) (20.00-3.47)	Depositor
$R_{merge}$	0.16	Depositor
$R_{sym}$	0.16	Depositor
Refinement program	CNS	Depositor
R, $R_{free}$	0.225 , 0.299	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	4683	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	39.0	wwPDB-VP

## 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	0.41	0/2346	0.62	0/3183
1	B	0.39	0/2449	0.61	0/3324
All	All	0.40	0/4795	0.61	0/6507

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

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	2293	0	2189	159	0
1	B	2390	0	2282	203	0
All	All	4683	0	4471	362	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 40.

All (362) 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:69:GLY:HA2	1:A:185:LEU:HD21	1.40	1.02
1:B:127:THR:HB	1:B:188:ARG:HD3	1.43	1.01

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:127:THR:HB	1:A:188:ARG:HD3	1.44	0.96
1:A:9:ILE:HA	1:A:263:LEU:HD13	1.59	0.82
1:A:109:LEU:N	1:A:109:LEU:HD12	1.95	0.82
1:B:160:ASN:HA	1:B:163:CYS:SG	2.21	0.81
1:B:69:GLY:HA2	1:B:185:LEU:HD21	1.59	0.81
1:A:109:LEU:H	1:A:109:LEU:HD12	1.46	0.81
1:B:277:GLY:HA2	1:B:282:LEU:HD23	1.61	0.80
1:B:244:HIS:HB2	1:B:246:TRP:CD1	2.17	0.79
1:A:258:GLU:O	1:A:262:ARG:HG2	1.84	0.78
1:A:283:ASP:HB3	1:A:286:GLU:HG3	1.65	0.77
1:B:53:LEU:HB2	1:B:308:TRP:HZ2	1.48	0.77
1:A:185:LEU:HD13	1:A:188:ARG:HD2	1.65	0.77
1:A:45:HIS:HE1	1:A:74:SER:OG	1.66	0.77
1:B:258:GLU:O	1:B:262:ARG:HG2	1.85	0.76
1:A:235:ASN:HD21	1:A:237:VAL:HG23	1.49	0.76
1:B:198:VAL:O	1:B:201:SER:HB3	1.87	0.75
1:B:35:LEU:HD13	1:B:78:LEU:HD13	1.68	0.75
1:B:185:LEU:HD13	1:B:188:ARG:HD2	1.68	0.75
1:B:223:SER:O	1:B:227:GLU:HG3	1.86	0.74
1:A:123:ILE:O	1:A:127:THR:HG23	1.88	0.74
1:A:194:VAL:HG12	1:A:195:PRO:HD2	1.66	0.74
1:A:33:LEU:HB3	1:A:35:LEU:HD13	1.68	0.74
1:B:194:VAL:HG21	1:B:293:TYR:CG	2.22	0.73
1:A:33:LEU:HD12	1:A:119:GLY:HA2	1.69	0.73
1:B:283:ASP:HB3	1:B:286:GLU:HG3	1.71	0.73
1:A:95:LYS:HA	1:A:98:THR:HB	1.71	0.72
1:A:223:SER:O	1:A:227:GLU:HG3	1.89	0.72
1:B:270:GLU:O	1:B:273:LEU:HB2	1.90	0.72
1:A:185:LEU:HD12	1:A:188:ARG:HB2	1.69	0.72
1:A:170:LEU:O	1:A:174:ARG:HB2	1.89	0.72
1:B:170:LEU:O	1:B:174:ARG:HB2	1.87	0.72
1:B:185:LEU:HD12	1:B:188:ARG:HB2	1.72	0.71
1:B:123:ILE:O	1:B:127:THR:HG23	1.90	0.71
1:A:270:GLU:O	1:A:273:LEU:HB2	1.90	0.71
1:B:157:ARG:HG3	1:B:158:PHE:N	2.06	0.71
1:B:95:LYS:HA	1:B:98:THR:HB	1.71	0.71
1:B:104:ALA:CB	1:B:109:LEU:HD21	2.20	0.71
1:A:33:LEU:HB3	1:A:35:LEU:CD1	2.21	0.70
1:B:261:ALA:O	1:B:265:GLN:HG3	1.91	0.70
1:B:213:ASP:O	1:B:217:LEU:HG	1.92	0.69
1:B:160:ASN:C	1:B:163:CYS:H	1.95	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:237:VAL:HG22	1:B:255:MET:HE1	1.73	0.69
1:B:280:TYR:HB2	1:B:282:LEU:HD21	1.74	0.69
1:A:45:HIS:CE1	1:A:74:SER:OG	2.46	0.68
1:A:144:ARG:HH11	1:A:144:ARG:HG3	1.57	0.68
1:B:141:ARG:O	1:B:144:ARG:HB2	1.93	0.68
1:B:235:ASN:O	1:B:238:MET:HG2	1.93	0.68
1:B:144:ARG:HH11	1:B:144:ARG:HG3	1.57	0.67
1:B:87:ARG:O	1:B:94:THR:HG22	1.95	0.67
1:A:213:ASP:O	1:A:217:LEU:HG	1.95	0.67
1:A:221:ILE:HD12	1:A:221:ILE:C	2.14	0.67
1:A:33:LEU:CB	1:A:35:LEU:HD13	2.24	0.67
1:B:235:ASN:O	1:B:237:VAL:N	2.28	0.67
1:B:122:ASP:O	1:B:126:ARG:HD3	1.95	0.66
1:A:298:VAL:O	1:A:301:VAL:HG12	1.95	0.66
1:B:104:ALA:HB2	1:B:109:LEU:HD21	1.78	0.66
1:A:218:LEU:O	1:A:221:ILE:HG13	1.96	0.66
1:A:261:ALA:O	1:A:265:GLN:HG3	1.95	0.65
1:A:141:ARG:O	1:A:144:ARG:HB2	1.96	0.65
1:A:271:SER:O	1:A:274:PRO:HD2	1.97	0.65
1:B:271:SER:O	1:B:274:PRO:HD2	1.97	0.64
1:B:158:PHE:H	1:B:158:PHE:HD2	1.45	0.64
1:B:235:ASN:HD22	1:B:237:VAL:HG23	1.63	0.64
1:B:255:MET:O	1:B:259:VAL:HG23	1.97	0.64
1:B:72:LEU:HA	1:B:123:ILE:HD13	1.80	0.64
1:A:185:LEU:CD1	1:A:188:ARG:HD2	2.27	0.64
1:A:122:ASP:O	1:A:126:ARG:HD3	1.98	0.64
1:A:53:LEU:HD23	1:A:73:MET:HG3	1.80	0.64
1:A:235:ASN:ND2	1:A:237:VAL:HG23	2.13	0.64
1:B:167:ALA:HA	1:B:170:LEU:HD13	1.79	0.63
1:B:81:ASP:HA	1:B:84:ASP:OD2	1.98	0.63
1:A:255:MET:O	1:A:259:VAL:HG23	1.97	0.63
1:B:277:GLY:O	1:B:282:LEU:HD23	1.97	0.63
1:B:163:CYS:O	1:B:164:ASP:HB2	1.98	0.63
1:A:135:TRP:HH2	1:A:187:GLU:HB2	1.64	0.63
1:A:273:LEU:HD23	1:A:294:ARG:HD3	1.79	0.63
1:B:58:TYR:OH	1:B:185:LEU:HD23	1.99	0.63
1:A:135:TRP:CH2	1:A:187:GLU:HB2	2.34	0.62
1:B:280:TYR:HB2	1:B:282:LEU:CD2	2.29	0.62
1:B:21:ARG:NH1	1:B:63:GLY:HA2	2.14	0.62
1:A:81:ASP:HA	1:A:84:ASP:OD2	1.98	0.62
1:B:218:LEU:O	1:B:221:ILE:HG13	1.99	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:254:HIS:HA	1:B:257:ASN:HB2	1.81	0.62
1:B:185:LEU:CD1	1:B:188:ARG:HD2	2.29	0.62
1:B:221:ILE:C	1:B:221:ILE:HD12	2.20	0.62
1:B:53:LEU:HB2	1:B:308:TRP:CZ2	2.32	0.62
1:B:53:LEU:HD23	1:B:73:MET:HG3	1.82	0.62
1:B:235:ASN:ND2	1:B:237:VAL:HG23	2.14	0.61
1:B:19:HIS:CG	1:B:20:ALA:N	2.67	0.61
1:B:298:VAL:O	1:B:301:VAL:HG12	1.99	0.61
1:B:306:TYR:O	1:B:308:TRP:N	2.31	0.61
1:B:237:VAL:HG22	1:B:255:MET:CE	2.29	0.60
1:A:290:LEU:HD23	1:A:290:LEU:C	2.21	0.60
1:A:198:VAL:O	1:A:201:SER:HB3	2.01	0.60
1:A:19:HIS:HA	1:A:22:ALA:HB3	1.82	0.60
1:A:290:LEU:HD23	1:A:291:GLU:N	2.16	0.60
1:B:224:LEU:HD22	1:B:237:VAL:HG21	1.82	0.60
1:A:167:ALA:HA	1:A:170:LEU:HD13	1.84	0.59
1:A:68:LEU:HD21	1:A:127:THR:HG22	1.84	0.59
1:B:277:GLY:CA	1:B:282:LEU:HD23	2.31	0.59
1:B:198:VAL:HG11	1:B:290:LEU:HD12	1.84	0.59
1:B:35:LEU:CD1	1:B:78:LEU:HD13	2.30	0.59
1:B:290:LEU:HD23	1:B:291:GLU:N	2.18	0.59
1:A:254:HIS:HA	1:A:257:ASN:HB2	1.83	0.59
1:A:91:PRO:HD3	1:A:154:ALA:O	2.03	0.59
1:B:104:ALA:HA	1:B:109:LEU:HD21	1.85	0.59
1:B:170:LEU:N	1:B:170:LEU:HD12	2.18	0.59
1:B:33:LEU:HD12	1:B:119:GLY:HA2	1.85	0.58
1:A:221:ILE:HD12	1:A:222:ALA:N	2.19	0.58
1:A:8:HIS:HD1	1:A:10:PRO:HD3	1.68	0.58
1:A:9:ILE:CD1	1:A:303:ARG:HA	2.34	0.58
1:B:104:ALA:CA	1:B:109:LEU:HD21	2.33	0.58
1:B:194:VAL:HG22	1:B:293:TYR:HB2	1.85	0.58
1:A:283:ASP:HB3	1:A:286:GLU:CG	2.33	0.57
1:B:280:TYR:O	1:B:281:GLN:C	2.42	0.57
1:B:290:LEU:HD23	1:B:290:LEU:C	2.25	0.57
1:A:18:ASP:O	1:A:20:ALA:N	2.37	0.57
1:A:180:GLN:HB3	1:A:181:PRO:HD3	1.85	0.57
1:B:275:LYS:O	1:B:279:ILE:HG13	2.05	0.57
1:B:165:SER:HB2	1:B:168:GLN:HE21	1.70	0.56
1:B:160:ASN:HA	1:B:163:CYS:HG	1.68	0.56
1:B:227:GLU:HB3	1:B:232:GLU:HB3	1.87	0.56
1:A:185:LEU:HA	1:A:188:ARG:CG	2.36	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:180:GLN:HB3	1:B:181:PRO:HD3	1.88	0.56
1:B:244:HIS:HB2	1:B:246:TRP:NE1	2.21	0.56
1:A:9:ILE:HG23	1:A:9:ILE:O	2.06	0.56
1:A:185:LEU:HA	1:A:188:ARG:HG3	1.87	0.55
1:B:235:ASN:O	1:B:236:MET:C	2.45	0.55
1:A:29:TRP:HB3	1:A:30:PRO:CD	2.36	0.55
1:B:33:LEU:CD1	1:B:119:GLY:HA2	2.36	0.55
1:B:185:LEU:HA	1:B:188:ARG:CG	2.36	0.55
1:B:96:GLN:O	1:B:100:GLN:HG3	2.07	0.55
1:B:164:ASP:OD1	1:B:172:MET:SD	2.65	0.54
1:A:170:LEU:HD12	1:A:170:LEU:N	2.22	0.54
1:B:194:VAL:HG21	1:B:293:TYR:CD1	2.43	0.54
1:B:283:ASP:HB3	1:B:286:GLU:CG	2.38	0.54
1:A:15:GLN:NE2	1:A:19:HIS:CD2	2.75	0.54
1:B:177:ILE:HD13	1:B:177:ILE:O	2.07	0.54
1:B:185:LEU:HA	1:B:188:ARG:HG3	1.90	0.54
1:B:236:MET:HG3	1:B:240:LEU:CD1	2.37	0.54
1:B:29:TRP:HB3	1:B:30:PRO:CD	2.38	0.54
1:A:283:ASP:CB	1:A:286:GLU:HG3	2.37	0.53
1:A:10:PRO:O	1:A:11:LEU:HD23	2.08	0.53
1:A:96:GLN:O	1:A:100:GLN:HG3	2.07	0.53
1:B:185:LEU:HA	1:B:188:ARG:CD	2.37	0.53
1:A:109:LEU:CD1	1:A:109:LEU:N	2.68	0.53
1:A:9:ILE:HD13	1:A:303:ARG:HA	1.91	0.53
1:B:53:LEU:HD23	1:B:73:MET:CG	2.38	0.53
1:B:221:ILE:HD12	1:B:222:ALA:N	2.23	0.53
1:B:33:LEU:HD12	1:B:119:GLY:CA	2.38	0.53
1:A:135:TRP:CH2	1:A:187:GLU:CB	2.91	0.53
1:A:166:ALA:O	1:A:169:TYR:HB3	2.09	0.53
1:A:185:LEU:HA	1:A:188:ARG:CD	2.39	0.53
1:A:35:LEU:HD23	1:A:78:LEU:HD13	1.90	0.53
1:B:157:ARG:CG	1:B:158:PHE:N	2.72	0.53
1:B:237:VAL:O	1:B:241:ARG:HG3	2.09	0.53
1:A:231:GLY:O	1:A:232:GLU:C	2.47	0.52
1:B:241:ARG:HG2	1:B:247:SER:O	2.09	0.52
1:B:45:HIS:HE1	1:B:74:SER:OG	1.92	0.52
1:A:82:LEU:HD23	1:A:97:LEU:HD21	1.90	0.52
1:A:51:ALA:HA	1:A:70:VAL:HG13	1.91	0.52
1:A:280:TYR:O	1:A:282:LEU:N	2.43	0.52
1:B:236:MET:HG3	1:B:240:LEU:HD11	1.91	0.52
1:A:113:ALA:HB3	1:A:118:HIS:NE2	2.25	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:275:LYS:O	1:A:279:ILE:HG13	2.10	0.52
1:A:15:GLN:NE2	1:A:19:HIS:NE2	2.58	0.52
1:B:166:ALA:O	1:B:169:TYR:HB3	2.10	0.52
1:A:135:TRP:CZ3	1:A:187:GLU:CD	2.83	0.51
1:B:144:ARG:NH1	1:B:144:ARG:HG3	2.24	0.51
1:A:196:HIS:N	1:A:196:HIS:ND1	2.59	0.51
1:B:11:LEU:HD22	1:B:299:ARG:CZ	2.41	0.51
1:B:273:LEU:N	1:B:274:PRO:HD2	2.26	0.51
1:A:153:GLU:C	1:A:155:GLU:H	2.13	0.51
1:B:243:GLU:OE1	1:B:244:HIS:NE2	2.44	0.51
1:A:177:ILE:HD13	1:A:177:ILE:O	2.09	0.51
1:A:7:PHE:HD2	1:A:306:TYR:CE1	2.28	0.51
1:B:160:ASN:O	1:B:163:CYS:N	2.32	0.51
1:B:45:HIS:CE1	1:B:74:SER:OG	2.64	0.51
1:B:163:CYS:O	1:B:164:ASP:CB	2.59	0.50
1:B:177:ILE:HG23	1:B:179:VAL:HG23	1.93	0.50
1:B:9:ILE:HG22	1:B:11:LEU:H	1.76	0.50
1:B:170:LEU:HB3	1:B:174:ARG:HD3	1.92	0.50
1:B:68:LEU:HD21	1:B:127:THR:HG22	1.92	0.50
1:A:187:GLU:OE2	1:A:194:VAL:HG23	2.12	0.50
1:A:273:LEU:N	1:A:274:PRO:HD2	2.26	0.50
1:A:53:LEU:HD23	1:A:73:MET:CG	2.40	0.50
1:B:124:TRP:O	1:B:125:ARG:C	2.48	0.50
1:A:254:HIS:O	1:A:258:GLU:HB2	2.11	0.49
1:B:170:LEU:HD12	1:B:170:LEU:H	1.77	0.49
1:B:219:LEU:C	1:B:219:LEU:HD13	2.32	0.49
1:B:273:LEU:HD23	1:B:294:ARG:HD3	1.94	0.49
1:B:254:HIS:O	1:B:258:GLU:HB2	2.12	0.49
1:A:124:TRP:O	1:A:125:ARG:C	2.51	0.49
1:B:142:HIS:HA	1:B:145:ASN:HD22	1.77	0.49
1:B:170:LEU:H	1:B:170:LEU:CD1	2.25	0.49
1:B:166:ALA:HB3	1:B:243:GLU:OE2	2.12	0.49
1:A:306:TYR:C	1:A:308:TRP:H	2.16	0.49
1:B:153:GLU:C	1:B:155:GLU:H	2.15	0.49
1:B:166:ALA:HB2	1:B:243:GLU:CD	2.33	0.49
1:B:52:ASP:O	1:B:55:SER:OG	2.31	0.49
1:B:262:ARG:HH11	1:B:262:ARG:HG3	1.77	0.49
1:B:244:HIS:O	1:B:245:GLY:C	2.51	0.49
1:A:272:CYS:O	1:A:276:VAL:HG23	2.13	0.49
1:B:272:CYS:O	1:B:276:VAL:HG23	2.12	0.49
1:A:69:GLY:CA	1:A:185:LEU:HD21	2.29	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:19:HIS:O	1:A:20:ALA:C	2.52	0.48
1:A:11:LEU:HD22	1:A:299:ARG:CZ	2.42	0.48
1:A:177:ILE:HG23	1:A:179:VAL:HG23	1.96	0.48
1:A:144:ARG:HG3	1:A:144:ARG:NH1	2.26	0.48
1:A:282:LEU:HD12	1:A:286:GLU:OE1	2.13	0.48
1:A:252:VAL:O	1:A:255:MET:HB2	2.14	0.48
1:A:219:LEU:HD13	1:A:219:LEU:C	2.34	0.48
1:A:170:LEU:CD1	1:A:170:LEU:H	2.26	0.47
1:A:169:TYR:O	1:A:172:MET:HB2	2.13	0.47
1:A:170:LEU:HB3	1:A:174:ARG:HD3	1.96	0.47
1:A:135:TRP:CH2	1:A:187:GLU:CD	2.88	0.47
1:A:194:VAL:CG1	1:A:195:PRO:HD2	2.41	0.47
1:A:173:ARG:NH2	1:A:232:GLU:OE1	2.48	0.47
1:B:163:CYS:SG	1:B:164:ASP:N	2.88	0.47
1:B:169:TYR:O	1:B:172:MET:HB2	2.15	0.47
1:B:68:LEU:HA	1:B:126:ARG:NH2	2.30	0.47
1:A:170:LEU:HD12	1:A:170:LEU:H	1.80	0.47
1:A:14:ARG:HB3	1:A:59:PRO:HB3	1.96	0.47
1:B:238:MET:O	1:B:239:ILE:C	2.52	0.47
1:B:169:TYR:CD2	1:B:239:ILE:HD12	2.50	0.47
1:A:58:TYR:OH	1:A:185:LEU:HD23	2.15	0.47
1:B:221:ILE:HG22	1:B:255:MET:HE1	1.97	0.47
1:B:213:ASP:HB3	1:B:262:ARG:NH1	2.30	0.47
1:A:142:HIS:HA	1:A:145:ASN:HD22	1.80	0.46
1:B:138:ARG:HH21	1:B:196:HIS:HD2	1.63	0.46
1:B:252:VAL:O	1:B:255:MET:HB2	2.15	0.46
1:B:19:HIS:O	1:B:22:ALA:HB3	2.15	0.46
1:B:263:LEU:O	1:B:266:TYR:HB3	2.15	0.46
1:B:138:ARG:HH21	1:B:196:HIS:CD2	2.33	0.46
1:B:127:THR:HG21	1:B:188:ARG:NH1	2.30	0.46
1:B:283:ASP:CB	1:B:286:GLU:HG3	2.43	0.46
1:A:273:LEU:CD2	1:A:294:ARG:HD3	2.46	0.46
1:A:281:GLN:HB3	1:A:281:GLN:HE21	1.58	0.46
1:B:238:MET:O	1:B:241:ARG:N	2.49	0.46
1:A:257:ASN:O	1:A:260:ARG:HB3	2.16	0.45
1:A:93:ASP:O	1:A:96:GLN:HB2	2.17	0.45
1:A:292:ARG:HG3	1:A:292:ARG:HH11	1.82	0.45
1:B:70:VAL:O	1:B:74:SER:HB2	2.16	0.45
1:A:9:ILE:CA	1:A:263:LEU:HD13	2.38	0.45
1:A:9:ILE:O	1:A:11:LEU:N	2.46	0.45
1:A:70:VAL:O	1:A:74:SER:HB2	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:210:ILE:O	1:B:211:ALA:C	2.54	0.45
1:B:273:LEU:O	1:B:276:VAL:HB	2.16	0.45
1:B:169:TYR:CD2	1:B:236:MET:HE1	2.52	0.45
1:B:166:ALA:HB2	1:B:243:GLU:OE1	2.16	0.45
1:B:27:LEU:O	1:B:28:ALA:C	2.55	0.45
1:B:151:VAL:O	1:B:154:ALA:N	2.50	0.45
1:B:166:ALA:H	1:B:239:ILE:HG22	1.81	0.45
1:A:8:HIS:ND1	1:A:10:PRO:HD3	2.32	0.45
1:A:93:ASP:HA	1:A:96:GLN:HE21	1.81	0.45
1:A:18:ASP:O	1:A:21:ARG:N	2.49	0.44
1:A:8:HIS:O	1:A:263:LEU:HD13	2.17	0.44
1:B:158:PHE:CD2	1:B:158:PHE:N	2.80	0.44
1:A:143:TRP:O	1:A:146:TYR:HB3	2.18	0.44
1:A:170:LEU:HD11	1:A:236:MET:CE	2.47	0.44
1:A:173:ARG:HA	1:A:176:THR:OG1	2.17	0.44
1:B:160:ASN:CA	1:B:163:CYS:H	2.30	0.44
1:B:93:ASP:O	1:B:96:GLN:HB2	2.17	0.44
1:A:210:ILE:O	1:A:211:ALA:C	2.55	0.44
1:A:262:ARG:HH11	1:A:262:ARG:HG3	1.82	0.44
1:B:135:TRP:CH2	1:B:187:GLU:HB2	2.52	0.44
1:B:90:ASN:HA	1:B:91:PRO:HD2	1.86	0.44
1:A:153:GLU:C	1:A:155:GLU:N	2.70	0.44
1:A:182:THR:O	1:A:185:LEU:HB3	2.17	0.44
1:A:280:TYR:O	1:A:281:GLN:C	2.56	0.44
1:B:170:LEU:N	1:B:170:LEU:CD1	2.79	0.44
1:B:75:TRP:CZ2	1:B:120:PHE:HB2	2.52	0.44
1:B:153:GLU:C	1:B:155:GLU:N	2.71	0.44
1:B:227:GLU:O	1:B:232:GLU:HB3	2.18	0.43
1:B:91:PRO:O	1:B:92:GLU:C	2.55	0.43
1:A:253:SER:C	1:A:255:MET:H	2.22	0.43
1:A:110:PRO:O	1:A:111:ASP:C	2.55	0.43
1:A:27:LEU:O	1:A:28:ALA:C	2.55	0.43
1:B:185:LEU:HA	1:B:188:ARG:HD2	2.01	0.43
1:A:27:LEU:O	1:A:30:PRO:HG2	2.19	0.43
1:A:91:PRO:O	1:A:92:GLU:C	2.56	0.43
1:B:143:TRP:O	1:B:146:TYR:HB3	2.17	0.43
1:B:283:ASP:CG	1:B:284:THR:N	2.72	0.43
1:A:135:TRP:HH2	1:A:187:GLU:CB	2.30	0.43
1:A:86:PRO:O	1:A:89:GLU:HB2	2.19	0.43
1:B:127:THR:HB	1:B:188:ARG:CD	2.31	0.43
1:B:213:ASP:HB3	1:B:262:ARG:HH12	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:221:ILE:HG22	1:B:255:MET:CE	2.48	0.43
1:B:194:VAL:CG2	1:B:293:TYR:HB2	2.49	0.43
1:A:207:MET:HB3	1:A:207:MET:HE2	1.83	0.43
1:B:111:ASP:HA	1:B:118:HIS:CE1	2.53	0.43
1:A:35:LEU:N	1:A:35:LEU:CD1	2.82	0.43
1:B:253:SER:C	1:B:255:MET:H	2.22	0.43
1:B:21:ARG:HH12	1:B:63:GLY:HA2	1.84	0.42
1:B:93:ASP:HA	1:B:96:GLN:HE21	1.84	0.42
1:A:135:TRP:HZ3	1:A:187:GLU:OE2	2.01	0.42
1:B:69:GLY:CA	1:B:185:LEU:HD21	2.38	0.42
1:B:169:TYR:HD2	1:B:236:MET:HE1	1.84	0.42
1:B:266:TYR:CE2	1:B:270:GLU:OE1	2.72	0.42
1:B:127:THR:CG2	1:B:188:ARG:HH11	2.32	0.42
1:B:276:VAL:HA	1:B:279:ILE:HD12	2.01	0.42
1:B:62:THR:O	1:B:62:THR:HG23	2.19	0.42
1:A:170:LEU:CD1	1:A:170:LEU:N	2.82	0.42
1:A:276:VAL:HA	1:A:279:ILE:HD12	2.01	0.42
1:A:179:VAL:O	1:A:182:THR:HB	2.20	0.42
1:A:8:HIS:O	1:A:263:LEU:CD1	2.67	0.42
1:B:165:SER:CB	1:B:168:GLN:HE21	2.33	0.42
1:B:173:ARG:HA	1:B:176:THR:OG1	2.19	0.42
1:B:273:LEU:HD12	1:B:273:LEU:HA	1.87	0.42
1:A:263:LEU:O	1:A:266:TYR:HB3	2.19	0.42
1:A:306:TYR:O	1:A:308:TRP:N	2.52	0.42
1:B:198:VAL:O	1:B:199:PHE:C	2.58	0.42
1:B:244:HIS:O	1:B:246:TRP:N	2.52	0.42
1:A:266:TYR:CE2	1:A:270:GLU:OE1	2.72	0.42
1:A:273:LEU:O	1:A:276:VAL:HB	2.19	0.42
1:A:14:ARG:HB2	1:A:59:PRO:HG2	2.02	0.42
1:B:160:ASN:HA	1:B:163:CYS:CB	2.49	0.42
1:B:238:MET:H	1:B:238:MET:HG2	1.44	0.42
1:A:194:VAL:HG22	1:A:293:TYR:CG	2.55	0.42
1:A:33:LEU:HD12	1:A:119:GLY:CA	2.46	0.42
1:A:35:LEU:N	1:A:35:LEU:HD12	2.35	0.42
1:B:135:TRP:CZ3	1:B:187:GLU:OE1	2.73	0.42
1:B:235:ASN:HD22	1:B:237:VAL:CG2	2.31	0.42
1:B:194:VAL:CG2	1:B:293:TYR:CG	2.99	0.42
1:B:82:LEU:HD23	1:B:97:LEU:HD21	2.01	0.42
1:A:224:LEU:HD22	1:A:237:VAL:HG21	2.02	0.42
1:A:30:PRO:HB2	1:A:36:ILE:HG12	2.00	0.42
1:B:146:TYR:HE1	1:B:176:THR:O	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:69:GLY:HA2	1:B:185:LEU:CD2	2.41	0.41
1:A:111:ASP:O	1:A:113:ALA:N	2.53	0.41
1:A:72:LEU:HA	1:A:123:ILE:HD13	2.00	0.41
1:B:113:ALA:HB1	1:B:114:PRO:HD2	2.03	0.41
1:B:27:LEU:O	1:B:30:PRO:HG2	2.19	0.41
1:B:169:TYR:OH	1:B:173:ARG:HD2	2.20	0.41
1:B:11:LEU:HD22	1:B:299:ARG:NE	2.35	0.41
1:A:282:LEU:HD11	1:A:286:GLU:HB3	2.01	0.41
1:A:62:THR:O	1:A:62:THR:HG23	2.20	0.41
1:B:72:LEU:HD11	1:B:76:PHE:CE1	2.56	0.41
1:B:165:SER:N	1:B:168:GLN:NE2	2.68	0.41
1:B:58:TYR:CZ	1:B:185:LEU:HD23	2.55	0.41
1:B:127:THR:HG21	1:B:188:ARG:HH11	1.84	0.41
1:B:257:ASN:O	1:B:260:ARG:HB3	2.20	0.41
1:A:61:ALA:O	1:A:66:LEU:HB2	2.21	0.41
1:B:236:MET:O	1:B:237:VAL:C	2.58	0.41
1:B:283:ASP:CG	1:B:284:THR:H	2.24	0.41
1:A:308:TRP:O	1:A:309:HIS:O	2.39	0.41
1:B:277:GLY:O	1:B:282:LEU:CD2	2.67	0.41
1:B:9:ILE:HG13	1:B:263:LEU:CD1	2.50	0.41
1:A:33:LEU:CD1	1:A:119:GLY:HA2	2.47	0.41
1:A:135:TRP:CZ3	1:A:187:GLU:OE2	2.74	0.41
1:B:182:THR:O	1:B:185:LEU:HB3	2.21	0.41
1:A:169:TYR:OH	1:A:173:ARG:HD2	2.20	0.40
1:B:165:SER:HB2	1:B:168:GLN:NE2	2.34	0.40
1:B:9:ILE:HG13	1:B:263:LEU:HD13	2.04	0.40
1:B:75:TRP:HB2	1:B:123:ILE:HD11	2.04	0.40
1:B:179:VAL:O	1:B:182:THR:HB	2.22	0.40
1:B:236:MET:HB2	1:B:236:MET:HE2	1.84	0.40
1:A:283:ASP:CG	1:A:284:THR:N	2.75	0.40
1:B:141:ARG:HG2	1:B:145:ASN:HD21	1.87	0.40
1:B:238:MET:O	1:B:240:LEU:N	2.54	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	283/336 (84%)	228 (81%)	44 (16%)	11 (4%)	3	27
1	B	296/336 (88%)	236 (80%)	49 (17%)	11 (4%)	4	28
All	All	579/672 (86%)	464 (80%)	93 (16%)	22 (4%)	3	27

All (22) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	281	GLN
1	A	309	HIS
1	B	164	ASP
1	B	236	MET
1	B	307	ASP
1	A	19	HIS
1	A	232	GLU
1	B	159	TRP
1	B	283	ASP
1	A	283	ASP
1	A	307	ASP
1	A	22	ALA
1	A	236	MET
1	B	237	VAL
1	B	239	ILE
1	B	281	GLN
1	A	28	ALA
1	A	231	GLY
1	B	28	ALA
1	B	245	GLY
1	B	212	VAL
1	A	212	VAL

### 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	235/272 (86%)	220 (94%)	15 (6%)	19	53
1	B	245/272 (90%)	230 (94%)	15 (6%)	20	55
All	All	480/544 (88%)	450 (94%)	30 (6%)	20	54

All (30) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	33	LEU
1	A	73	MET
1	A	76	PHE
1	A	94	THR
1	A	99	ASP
1	A	109	LEU
1	A	111	ASP
1	A	128	CYS
1	A	177	ILE
1	A	196	HIS
1	A	201	SER
1	A	238	MET
1	A	281	GLN
1	A	290	LEU
1	A	308	TRP
1	B	33	LEU
1	B	73	MET
1	B	76	PHE
1	B	94	THR
1	B	99	ASP
1	B	112	THR
1	B	128	CYS
1	B	158	PHE
1	B	163	CYS
1	B	177	ILE
1	B	197	ARG
1	B	201	SER
1	B	238	MET
1	B	248	LYS
1	B	290	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	15	GLN
1	A	26	GLN
1	A	45	HIS
1	A	96	GLN
1	A	145	ASN
1	A	168	GLN
1	A	215	ASN
1	A	234	ASN
1	A	235	ASN
1	A	281	GLN
1	B	15	GLN
1	B	26	GLN
1	B	45	HIS
1	B	96	GLN
1	B	145	ASN
1	B	160	ASN
1	B	168	GLN
1	B	209	GLN
1	B	215	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

## 5.5 Carbohydrates [i](#)

There are no carbohydrates 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 ⓘ

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

### 6.3 Carbohydrates ⓘ

EDS was not executed - this section is therefore empty.

### 6.4 Ligands ⓘ

EDS was not executed - this section is therefore empty.

### 6.5 Other polymers ⓘ

EDS was not executed - this section is therefore empty.