Full wwPDB X-ray Structure Validation Report (i)

Aug 3, 2023 – 04:58 AM EDT

PDB ID	:	1HM7
Title	:	N219L PENTALENENE SYNTHASE
Authors	:	Seemann, M.; Paschall, C.M.; Christianson, D.W.; Cane, D.E.
Deposited on	:	2000-12-05
Resolution	:	2.90 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 (i) 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 (i)) were used in the production of this report:

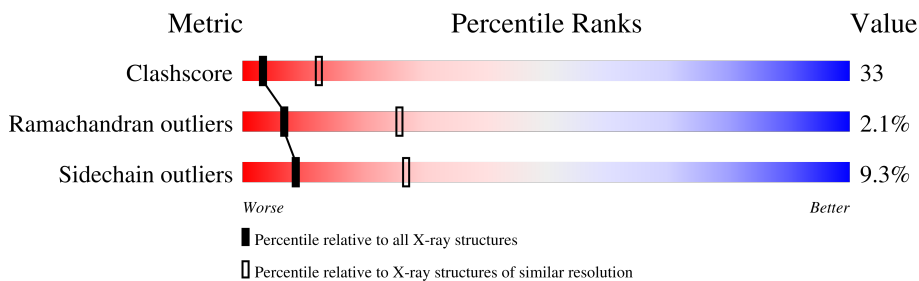|		
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.34

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 2.90 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	Percentile Ranks	Value
Clashscore		33
Ramachandran outliers		2.1%
Sidechain outliers		9.3%

Worse   *Better*

■ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)

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%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	336	44% 36% • 15%
1	B	336	42% 41% 8% 9%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 4736 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	284	Total	C	N	O	S	0	0	0
			2268	1421	416	420	11			
1	B	305	Total	C	N	O	S	0	0	0
			2442	1527	450	453	12			

There are 2 discrepancies between the modelled and reference sequences:

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

- Molecule 2 is water.

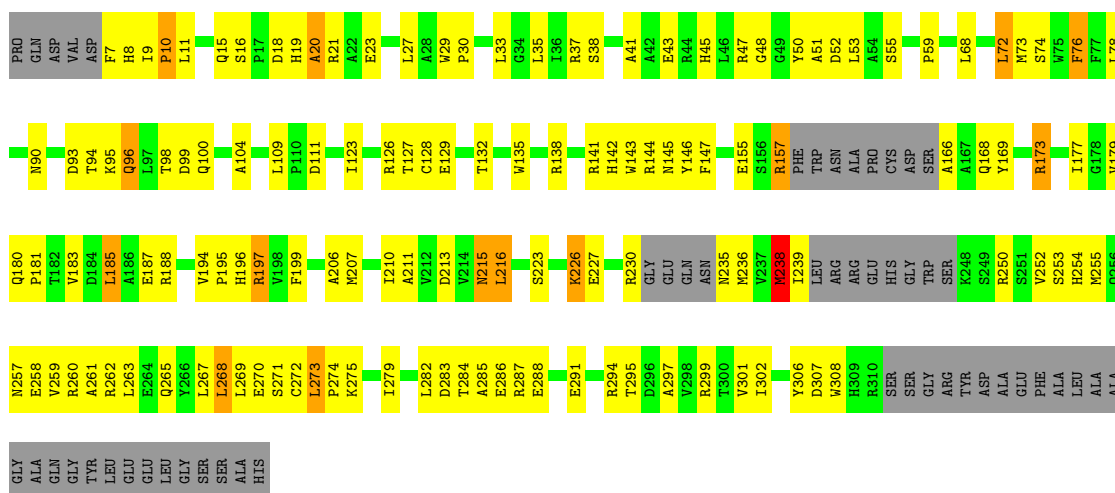| Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	15	Total	O	0	0
			15	15		
2	B	11	Total	O	0	0
			11	11		

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. 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.
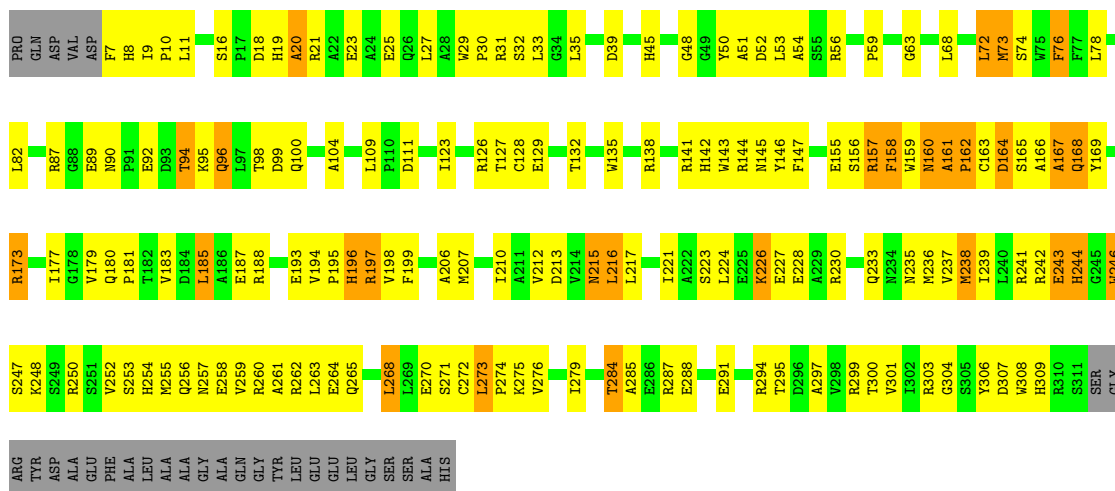
Note EDS was not executed.

• 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, α, β, γ	181.40Å 181.40Å 56.40Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	20.00 – 2.90	Depositor
% Data completeness (in resolution range)	93.3 (20.00-2.90)	Depositor
R_{merge}	0.08	Depositor
R_{sym}	0.08	Depositor
Refinement program	CNS	Depositor
R, R_{free}	0.263 , 0.308	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	4736	wwPDB-VP
Average B, all atoms (Å^2)	45.0	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	0.45	0/2320	0.60	0/3144
1	B	0.42	0/2504	0.64	2/3399 (0.1%)
All	All	0.44	0/4824	0.62	2/6543 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	166	ALA	N-CA-C	-7.00	92.10	111.00
1	B	156	SER	N-CA-C	-6.66	93.03	111.00

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	2268	0	2186	135	0
1	B	2442	0	2336	172	0
2	A	15	0	0	2	0
2	B	11	0	0	1	0
All	All	4736	0	4522	302	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 33.

All (302) 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:183:VAL:HG22	1:B:301:VAL:HG21	1.32	1.08
1:A:282:LEU:HD22	1:A:286:GLU:HB3	1.46	0.97
1:A:157:ARG:HE	1:A:157:ARG:C	1.67	0.96
1:B:157:ARG:HD3	1:B:158:PHE:N	1.83	0.93
1:B:158:PHE:HB3	1:B:160:ASN:HD22	1.37	0.86
1:A:183:VAL:HG22	1:A:301:VAL:HG21	1.58	0.85
1:B:7:PHE:N	1:B:306:TYR:HH	1.78	0.82
1:B:226:LYS:H	1:B:226:LYS:HD2	1.45	0.81
1:A:123:ILE:O	1:A:127:THR:HG23	1.80	0.80
1:A:226:LYS:H	1:A:226:LYS:HD2	1.45	0.79
1:A:10:PRO:HG3	1:A:267:LEU:HD11	1.64	0.79
1:B:123:ILE:O	1:B:127:THR:HG23	1.84	0.78
1:B:158:PHE:CB	1:B:160:ASN:HD22	1.97	0.76
1:B:9:ILE:HD13	1:B:263:LEU:HD11	1.66	0.76
1:B:183:VAL:CG2	1:B:301:VAL:HG21	2.15	0.74
1:B:294:ARG:O	1:B:299:ARG:HG3	1.87	0.73
1:A:168:GLN:HG3	1:A:169:TYR:N	2.03	0.73
1:B:241:ARG:HD2	1:B:248:LYS:HA	1.67	0.73
1:B:89:GLU:O	1:B:157:ARG:HB2	1.88	0.73
1:B:90:ASN:O	1:B:94:THR:HG22	1.88	0.72
1:A:284:THR:HG22	1:A:287:ARG:NH2	2.04	0.72
1:B:169:TYR:HB2	1:B:239:ILE:HD13	1.72	0.70
1:B:144:ARG:HG3	1:B:144:ARG:HH11	1.55	0.69
1:A:15:GLN:NE2	1:A:19:HIS:CG	2.60	0.69
1:B:284:THR:HG23	1:B:287:ARG:NH2	2.08	0.69
1:B:165:SER:HA	1:B:168:GLN:HB2	1.73	0.69
1:B:226:LYS:HD2	1:B:226:LYS:N	2.07	0.69
1:A:9:ILE:HG13	1:A:263:LEU:HD11	1.73	0.69
1:A:72:LEU:HD22	1:A:76:PHE:CE1	2.28	0.69
1:B:72:LEU:HD22	1:B:76:PHE:CE1	2.29	0.68
1:A:226:LYS:HD2	1:A:226:LYS:N	2.08	0.68
1:B:291:GLU:OE2	1:B:294:ARG:HD3	1.94	0.67
1:B:270:GLU:HA	1:B:273:LEU:HD22	1.76	0.67
1:B:226:LYS:O	1:B:230:ARG:HG3	1.94	0.67
1:B:56:ARG:O	1:B:59:PRO:HD3	1.93	0.67
1:A:144:ARG:HG3	1:A:144:ARG:HH11	1.59	0.67
1:A:109:LEU:HD12	1:A:109:LEU:N	2.11	0.66
1:A:223:SER:O	1:A:227:GLU:HG3	1.95	0.66
1:A:270:GLU:HA	1:A:273:LEU:HD22	1.78	0.66
1:B:165:SER:HB2	1:B:169:TYR:H	1.60	0.65
1:B:7:PHE:HE2	1:B:256:GLN:HA	1.60	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:223:SER:O	1:B:227:GLU:HG3	1.96	0.65
1:A:291:GLU:OE2	1:A:294:ARG:HD3	1.98	0.64
1:B:109:LEU:N	1:B:109:LEU:HD12	2.12	0.64
1:A:9:ILE:HD12	1:A:9:ILE:N	2.12	0.64
1:A:226:LYS:H	1:A:226:LYS:CD	2.12	0.63
1:A:207:MET:HE1	1:A:270:GLU:HG3	1.81	0.63
1:A:294:ARG:O	1:A:299:ARG:HG3	1.98	0.63
1:B:226:LYS:H	1:B:226:LYS:CD	2.12	0.63
1:A:127:THR:O	1:A:188:ARG:HD3	2.00	0.62
1:A:35:LEU:HD12	1:A:35:LEU:N	2.15	0.61
1:A:9:ILE:HG13	1:A:263:LEU:CD1	2.30	0.61
1:A:272:CYS:SG	1:B:268:LEU:HD22	2.41	0.61
1:B:21:ARG:NH2	1:B:63:GLY:HA2	2.16	0.61
1:A:21:ARG:CZ	1:A:21:ARG:HB3	2.31	0.61
1:B:138:ARG:O	1:B:141:ARG:HB3	2.01	0.61
1:B:142:HIS:HA	1:B:145:ASN:HD22	1.66	0.60
1:B:144:ARG:HG3	1:B:144:ARG:NH1	2.16	0.60
1:A:169:TYR:CZ	1:A:173:ARG:HG3	2.36	0.60
1:A:142:HIS:HA	1:A:145:ASN:HD22	1.67	0.60
1:A:16:SER:C	1:A:18:ASP:H	2.04	0.60
1:B:53:LEU:HD13	1:B:308:TRP:CD2	2.36	0.60
1:A:90:ASN:OD1	1:A:93:ASP:N	2.33	0.59
1:B:284:THR:HG23	1:B:287:ARG:HH22	1.65	0.59
1:A:35:LEU:HB3	1:A:78:LEU:HD13	1.84	0.59
1:A:185:LEU:HD13	1:A:185:LEU:O	2.01	0.59
1:A:157:ARG:C	1:A:157:ARG:NE	2.49	0.59
1:B:180:GLN:HB3	1:B:181:PRO:HD3	1.84	0.58
1:A:68:LEU:HD21	1:A:127:THR:HG22	1.85	0.58
1:B:82:LEU:O	1:B:87:ARG:HD2	2.03	0.58
1:A:96:GLN:O	1:A:100:GLN:HG3	2.03	0.58
1:A:271:SER:O	1:A:274:PRO:HD2	2.03	0.58
1:B:21:ARG:HH21	1:B:63:GLY:HA2	1.68	0.58
1:B:215:ASN:HD22	1:B:215:ASN:N	2.01	0.58
1:A:8:HIS:CE1	1:A:260:ARG:HE	2.22	0.57
1:A:284:THR:HG22	1:A:287:ARG:HH22	1.67	0.57
1:B:165:SER:HB3	1:B:239:ILE:HG21	1.86	0.57
1:B:169:TYR:CZ	1:B:173:ARG:HG3	2.39	0.57
1:A:33:LEU:HB3	1:A:35:LEU:CD1	2.35	0.57
1:A:180:GLN:HB3	1:A:181:PRO:HD3	1.87	0.57
1:B:96:GLN:O	1:B:100:GLN:HG3	2.05	0.57
1:A:138:ARG:O	1:A:141:ARG:HB3	2.05	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:273:LEU:N	1:A:274:PRO:HD2	2.19	0.57
1:A:226:LYS:O	1:A:230:ARG:HG2	2.05	0.57
1:B:135:TRP:HZ3	1:B:187:GLU:OE1	1.86	0.56
1:B:161:ALA:HB3	1:B:162:PRO:CD	2.35	0.56
1:B:8:HIS:O	1:B:10:PRO:HD3	2.04	0.56
1:A:197:ARG:CD	1:A:197:ARG:H	2.17	0.56
1:B:135:TRP:CZ3	1:B:187:GLU:OE1	2.58	0.56
1:B:196:HIS:N	1:B:196:HIS:ND1	2.52	0.56
1:B:9:ILE:HD13	1:B:263:LEU:CD1	2.34	0.56
1:B:273:LEU:N	1:B:274:PRO:HD2	2.21	0.55
1:B:271:SER:O	1:B:274:PRO:HD2	2.05	0.55
1:A:132:THR:O	1:A:135:TRP:HB3	2.06	0.55
1:A:21:ARG:HB3	1:A:21:ARG:NH1	2.22	0.55
1:B:275:LYS:O	1:B:279:ILE:HG13	2.06	0.55
1:A:268:LEU:HD22	1:B:272:CYS:SG	2.46	0.55
1:A:275:LYS:HB2	1:B:268:LEU:HD11	1.87	0.55
1:A:282:LEU:HD22	1:A:286:GLU:CB	2.27	0.55
1:A:196:HIS:H	1:A:196:HIS:CD2	2.24	0.54
1:A:199:PHE:C	1:A:199:PHE:CD2	2.80	0.54
1:A:10:PRO:CG	1:A:267:LEU:HD11	2.35	0.54
1:A:33:LEU:HB3	1:A:35:LEU:HD11	1.90	0.54
1:B:132:THR:O	1:B:135:TRP:HB3	2.08	0.54
1:A:215:ASN:N	1:A:215:ASN:HD22	2.04	0.54
1:B:165:SER:C	1:B:167:ALA:N	2.57	0.54
1:B:163:CYS:HB2	1:B:239:ILE:HD11	1.90	0.54
1:B:284:THR:HA	1:B:287:ARG:NH2	2.23	0.54
1:B:241:ARG:HA	1:B:246:TRP:HB2	1.91	0.53
1:B:16:SER:O	1:B:19:HIS:HB3	2.08	0.53
1:B:51:ALA:O	1:B:54:ALA:HB3	2.09	0.53
1:A:135:TRP:HZ3	1:A:187:GLU:CD	2.12	0.53
1:B:235:ASN:HB3	1:B:238:MET:CG	2.39	0.53
1:B:53:LEU:HD13	1:B:308:TRP:CG	2.44	0.53
1:B:241:ARG:HD2	1:B:248:LYS:CA	2.37	0.53
1:A:144:ARG:HG3	1:A:144:ARG:NH1	2.20	0.53
1:A:252:VAL:HA	1:A:255:MET:HG3	1.90	0.53
1:B:10:PRO:O	1:B:11:LEU:HD12	2.08	0.53
1:A:166:ALA:O	1:A:169:TYR:N	2.40	0.53
1:B:23:GLU:HA	1:B:51:ALA:CB	2.39	0.53
1:A:29:TRP:HB3	1:A:30:PRO:CD	2.39	0.52
1:A:98:THR:HG23	1:A:147:PHE:HB3	1.92	0.52
1:B:206:ALA:O	1:B:210:ILE:HG13	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:207:MET:HE1	1:B:270:GLU:HG3	1.90	0.52
1:A:197:ARG:H	1:A:197:ARG:NE	2.07	0.52
1:B:237:VAL:HG23	1:B:255:MET:HE1	1.92	0.52
1:A:273:LEU:HD23	1:A:294:ARG:HD2	1.92	0.52
1:B:8:HIS:CG	1:B:260:ARG:HG3	2.45	0.52
1:A:9:ILE:O	1:A:11:LEU:N	2.33	0.51
1:B:98:THR:HG23	1:B:147:PHE:HB3	1.92	0.51
1:B:162:PRO:HD3	1:B:233:GLN:NE2	2.26	0.51
1:A:141:ARG:O	1:A:145:ASN:ND2	2.43	0.51
1:A:283:ASP:OD1	1:A:283:ASP:C	2.49	0.51
1:B:53:LEU:HD23	1:B:73:MET:HG3	1.92	0.51
1:B:7:PHE:CE2	1:B:256:GLN:HA	2.44	0.51
1:B:207:MET:CE	1:B:270:GLU:HG3	2.41	0.51
1:A:15:GLN:NE2	1:A:19:HIS:CD2	2.79	0.51
1:B:246:TRP:HA	1:B:246:TRP:CE3	2.46	0.50
1:B:52:ASP:OD1	1:B:52:ASP:C	2.49	0.50
1:B:185:LEU:HD13	1:B:185:LEU:O	2.11	0.50
1:B:285:ALA:O	1:B:288:GLU:HB2	2.11	0.50
1:A:72:LEU:HD22	1:A:76:PHE:CD1	2.45	0.50
1:B:90:ASN:OD1	1:B:92:GLU:HB3	2.12	0.50
1:B:143:TRP:O	1:B:146:TYR:HB3	2.11	0.50
1:A:173:ARG:HB3	1:A:216:LEU:HD21	1.94	0.50
1:B:72:LEU:HA	1:B:123:ILE:HD13	1.93	0.50
1:A:135:TRP:CZ3	1:A:187:GLU:CD	2.85	0.50
1:B:187:GLU:OE2	1:B:194:VAL:HG12	2.11	0.50
1:A:38:SER:O	1:A:41:ALA:HB3	2.12	0.50
1:A:45:HIS:HE1	1:A:74:SER:OG	1.94	0.49
1:B:29:TRP:HB3	1:B:30:PRO:CD	2.43	0.49
1:B:135:TRP:CZ3	1:B:187:GLU:CD	2.86	0.49
1:B:221:ILE:HG13	1:B:255:MET:CE	2.43	0.49
1:B:221:ILE:HG13	1:B:255:MET:HE3	1.94	0.49
1:A:72:LEU:HD12	1:A:185:LEU:HG	1.94	0.49
1:A:135:TRP:CH2	1:A:187:GLU:HB2	2.48	0.49
1:A:37:ARG:NH1	2:A:1026:HOH:O	2.45	0.49
1:B:197:ARG:HG3	2:B:1005:HOH:O	2.13	0.48
1:B:270:GLU:O	1:B:273:LEU:HD22	2.13	0.48
1:A:284:THR:HA	1:A:287:ARG:NH2	2.28	0.48
1:A:279:ILE:HD13	1:B:264:GLU:HB3	1.95	0.48
1:B:31:ARG:C	1:B:33:LEU:H	2.16	0.48
1:B:159:TRP:O	1:B:162:PRO:HD2	2.12	0.48
1:B:161:ALA:HB3	1:B:162:PRO:HD2	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:7:PHE:C	1:A:9:ILE:HD12	2.34	0.48
1:A:183:VAL:CG2	1:A:301:VAL:HG21	2.39	0.48
1:B:135:TRP:HZ3	1:B:187:GLU:CD	2.17	0.48
1:B:241:ARG:O	1:B:244:HIS:O	2.32	0.48
1:B:246:TRP:HA	1:B:246:TRP:HE3	1.76	0.48
1:A:23:GLU:HA	1:A:51:ALA:CB	2.43	0.48
1:A:35:LEU:N	1:A:35:LEU:CD1	2.76	0.48
1:B:7:PHE:CE2	1:B:256:GLN:HG2	2.49	0.48
1:A:43:GLU:O	1:A:47:ARG:HG3	2.14	0.47
1:A:52:ASP:O	1:A:55:SER:OG	2.26	0.47
1:A:9:ILE:C	1:A:11:LEU:H	2.13	0.47
1:B:161:ALA:O	1:B:162:PRO:C	2.52	0.47
1:B:195:PRO:O	1:B:198:VAL:HG22	2.15	0.47
1:B:247:SER:H	1:B:250:ARG:HD2	1.79	0.47
1:A:199:PHE:CD2	1:A:199:PHE:O	2.67	0.47
1:A:213:ASP:O	1:A:216:LEU:HB3	2.15	0.47
1:A:250:ARG:O	1:A:253:SER:HB3	2.14	0.47
1:A:252:VAL:O	1:A:255:MET:HB2	2.14	0.47
1:B:21:ARG:NH1	1:B:25:GLU:OE1	2.44	0.47
1:B:177:ILE:HG13	1:B:179:VAL:HG23	1.96	0.47
1:A:284:THR:CG2	1:A:287:ARG:NH2	2.76	0.47
1:B:243:GLU:HG2	1:B:244:HIS:ND1	2.30	0.47
1:A:306:TYR:O	1:A:307:ASP:C	2.53	0.47
1:B:250:ARG:O	1:B:253:SER:HB3	2.14	0.47
1:B:252:VAL:HA	1:B:255:MET:HG3	1.97	0.47
1:B:165:SER:HB2	1:B:169:TYR:CB	2.45	0.47
1:B:165:SER:HB3	1:B:239:ILE:CG2	2.45	0.47
1:A:18:ASP:OD2	1:A:21:ARG:NH1	2.44	0.46
1:B:262:ARG:HG3	1:B:262:ARG:HH11	1.80	0.46
1:B:291:GLU:O	1:B:295:THR:HG23	2.15	0.46
1:A:285:ALA:O	1:A:288:GLU:HB2	2.14	0.46
1:A:11:LEU:HG	1:A:299:ARG:HD3	1.97	0.46
1:B:104:ALA:HA	1:B:109:LEU:HD11	1.96	0.46
1:A:206:ALA:O	1:A:210:ILE:HG13	2.15	0.46
1:A:135:TRP:HH2	1:A:187:GLU:HB2	1.80	0.46
1:B:48:GLY:HA3	1:B:50:TYR:CZ	2.50	0.46
1:B:252:VAL:O	1:B:255:MET:HB2	2.16	0.46
1:A:95:LYS:HE2	1:A:99:ASP:OD2	2.16	0.46
1:A:177:ILE:HG13	1:A:179:VAL:HG23	1.98	0.46
1:B:141:ARG:O	1:B:145:ASN:ND2	2.49	0.46
1:B:157:ARG:HD3	1:B:157:ARG:C	2.34	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:160:ASN:O	1:B:161:ALA:C	2.55	0.46
1:B:161:ALA:O	1:B:163:CYS:N	2.48	0.46
1:B:126:ARG:HA	1:B:129:GLU:OE2	2.15	0.46
1:A:238:MET:O	1:A:239:ILE:C	2.55	0.45
1:A:294:ARG:NH1	1:A:295:THR:HG22	2.32	0.45
1:A:16:SER:C	1:A:18:ASP:N	2.69	0.45
1:A:236:MET:HG3	1:A:255:MET:SD	2.57	0.45
1:B:7:PHE:HB3	1:B:8:HIS:H	1.48	0.45
1:B:90:ASN:OD1	1:B:92:GLU:N	2.49	0.45
1:A:143:TRP:O	1:A:146:TYR:HB3	2.17	0.45
1:A:261:ALA:O	1:A:265:GLN:HG3	2.16	0.45
1:B:29:TRP:O	1:B:33:LEU:HD23	2.17	0.45
1:B:164:ASP:HB2	1:B:168:GLN:NE2	2.31	0.45
1:A:196:HIS:CD2	1:A:196:HIS:N	2.85	0.45
1:B:255:MET:O	1:B:259:VAL:HG23	2.17	0.45
1:A:258:GLU:O	1:A:262:ARG:HG2	2.16	0.45
1:B:72:LEU:HD22	1:B:76:PHE:CD1	2.51	0.45
1:B:53:LEU:HB2	1:B:308:TRP:CD1	2.52	0.45
1:B:35:LEU:HD13	1:B:78:LEU:HD13	1.99	0.45
1:B:261:ALA:O	1:B:265:GLN:HG3	2.16	0.44
1:A:8:HIS:O	1:A:263:LEU:HD13	2.17	0.44
1:B:109:LEU:N	1:B:109:LEU:CD1	2.80	0.44
1:B:297:ALA:O	1:B:301:VAL:HG23	2.17	0.44
1:A:53:LEU:HD13	1:A:308:TRP:CG	2.53	0.44
1:A:16:SER:O	1:A:18:ASP:N	2.48	0.44
1:A:104:ALA:HA	1:A:109:LEU:HD11	1.99	0.44
1:A:169:TYR:OH	1:A:173:ARG:HG3	2.17	0.44
1:B:273:LEU:O	1:B:276:VAL:HB	2.17	0.44
1:B:294:ARG:NH1	1:B:295:THR:HG22	2.32	0.44
1:A:109:LEU:N	1:A:109:LEU:CD1	2.79	0.44
1:B:306:TYR:O	1:B:307:ASP:C	2.56	0.44
1:B:244:HIS:ND1	1:B:244:HIS:N	2.65	0.44
1:A:20:ALA:HB2	2:A:1015:HOH:O	2.18	0.44
1:A:270:GLU:O	1:A:273:LEU:HD22	2.17	0.44
1:A:255:MET:O	1:A:259:VAL:HG23	2.18	0.44
1:A:207:MET:CE	1:A:270:GLU:HG3	2.45	0.44
1:B:9:ILE:CG2	1:B:303:ARG:HH11	2.31	0.44
1:B:68:LEU:HD13	1:B:126:ARG:CZ	2.48	0.43
1:B:179:VAL:HG13	1:B:301:VAL:HG11	1.99	0.43
1:B:258:GLU:O	1:B:262:ARG:HG2	2.18	0.43
1:A:48:GLY:HA3	1:A:50:TYR:CZ	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:235:ASN:HB3	1:B:238:MET:HG3	2.00	0.43
1:B:300:THR:O	1:B:304:GLY:N	2.47	0.43
1:A:262:ARG:HG3	1:A:262:ARG:HH11	1.83	0.43
1:A:270:GLU:HG2	1:A:294:ARG:HE	1.83	0.43
1:B:8:HIS:CD2	1:B:260:ARG:HE	2.36	0.43
1:B:95:LYS:HA	1:B:98:THR:HB	2.00	0.43
1:B:165:SER:HB2	1:B:169:TYR:HB3	2.01	0.43
1:A:254:HIS:HA	1:A:257:ASN:HB2	2.00	0.43
1:B:213:ASP:O	1:B:217:LEU:HG	2.19	0.43
1:A:294:ARG:NH1	1:A:295:THR:CG2	2.82	0.43
1:B:235:ASN:O	1:B:236:MET:C	2.56	0.43
1:B:95:LYS:HE2	1:B:99:ASP:OD2	2.18	0.43
1:B:45:HIS:HE1	1:B:74:SER:OG	2.02	0.42
1:B:272:CYS:O	1:B:276:VAL:HG23	2.19	0.42
1:A:291:GLU:O	1:A:295:THR:HG23	2.19	0.42
1:B:163:CYS:O	1:B:242:ARG:NH1	2.36	0.42
1:B:213:ASP:O	1:B:216:LEU:HB3	2.19	0.42
1:B:53:LEU:HB2	1:B:308:TRP:NE1	2.34	0.42
1:B:177:ILE:HG21	1:B:212:VAL:HG13	2.01	0.42
1:B:127:THR:O	1:B:188:ARG:HD3	2.20	0.42
1:B:228:GLU:C	1:B:230:ARG:H	2.22	0.42
1:B:162:PRO:HD3	1:B:233:GLN:HE22	1.84	0.42
1:A:95:LYS:HA	1:A:98:THR:HB	2.01	0.42
1:A:16:SER:N	1:A:59:PRO:HA	2.35	0.42
1:B:238:MET:H	1:B:238:MET:HG2	1.37	0.42
1:B:18:ASP:C	1:B:20:ALA:N	2.73	0.42
1:B:236:MET:HB3	1:B:255:MET:SD	2.60	0.42
1:B:160:ASN:O	1:B:162:PRO:CD	2.67	0.42
1:A:211:ALA:HA	1:A:302:ILE:HG12	2.02	0.41
1:B:159:TRP:O	1:B:160:ASN:C	2.59	0.41
1:B:173:ARG:HB3	1:B:216:LEU:HD21	2.01	0.41
1:B:224:LEU:HD11	1:B:238:MET:CE	2.51	0.41
1:A:72:LEU:CD2	1:A:76:PHE:CE1	3.01	0.41
1:A:135:TRP:CH2	1:A:187:GLU:CB	3.03	0.41
1:A:169:TYR:CZ	1:A:173:ARG:CG	3.03	0.41
1:A:194:VAL:O	1:A:195:PRO:C	2.58	0.41
1:B:132:THR:HG23	1:B:193:GLU:OE2	2.20	0.41
1:B:254:HIS:HA	1:B:257:ASN:HB2	2.02	0.41
1:A:126:ARG:HA	1:A:129:GLU:OE2	2.20	0.41
1:A:272:CYS:SG	1:B:268:LEU:CD2	3.09	0.41
1:A:297:ALA:O	1:A:301:VAL:HG23	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:269:LEU:O	1:A:272:CYS:N	2.51	0.41
1:B:161:ALA:CB	1:B:162:PRO:CD	2.99	0.41
1:B:169:TYR:OH	1:B:173:ARG:HG3	2.21	0.41
1:B:197:ARG:CD	1:B:197:ARG:H	2.34	0.41
1:B:198:VAL:CG2	1:B:199:PHE:N	2.84	0.41
1:B:294:ARG:NH1	1:B:295:THR:CG2	2.84	0.41
1:A:235:ASN:OD1	1:A:236:MET:N	2.54	0.41
1:B:167:ALA:O	1:B:169:TYR:N	2.54	0.41
1:A:9:ILE:N	1:A:9:ILE:CD1	2.82	0.40
1:B:247:SER:OG	1:B:250:ARG:HG3	2.21	0.40
1:B:270:GLU:CA	1:B:273:LEU:HD22	2.47	0.40
1:A:18:ASP:C	1:A:20:ALA:N	2.74	0.40
1:A:272:CYS:C	1:A:274:PRO:HD2	2.42	0.40
1:B:56:ARG:H	1:B:56:ARG:HG2	1.73	0.40
1:B:224:LEU:HD11	1:B:238:MET:HE1	2.02	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	276/336 (82%)	248 (90%)	25 (9%)	3 (1%)	14	42
1	B	303/336 (90%)	260 (86%)	34 (11%)	9 (3%)	4	17
All	All	579/672 (86%)	508 (88%)	59 (10%)	12 (2%)	7	26

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	160	ASN
1	B	161	ALA
1	B	168	GLN

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Mol	Chain	Res	Type
1	A	20	ALA
1	A	238	MET
1	B	309	HIS
1	B	20	ALA
1	B	32	SER
1	B	162	PRO
1	B	167	ALA
1	B	243	GLU
1	A	10	PRO

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	233/272 (86%)	214 (92%)	19 (8%)	11	32
1	B	251/272 (92%)	225 (90%)	26 (10%)	7	21
All	All	484/544 (89%)	439 (91%)	45 (9%)	9	27

All (45) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	27	LEU
1	A	72	LEU
1	A	73	MET
1	A	76	PHE
1	A	94	THR
1	A	96	GLN
1	A	111	ASP
1	A	128	CYS
1	A	155	GLU
1	A	157	ARG
1	A	173	ARG
1	A	185	LEU
1	A	197	ARG
1	A	215	ASN

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Mol	Chain	Res	Type
1	A	216	LEU
1	A	226	LYS
1	A	238	MET
1	A	268	LEU
1	A	273	LEU
1	B	27	LEU
1	B	39	ASP
1	B	72	LEU
1	B	73	MET
1	B	76	PHE
1	B	94	THR
1	B	96	GLN
1	B	111	ASP
1	B	128	CYS
1	B	155	GLU
1	B	157	ARG
1	B	158	PHE
1	B	164	ASP
1	B	173	ARG
1	B	185	LEU
1	B	196	HIS
1	B	197	ARG
1	B	215	ASN
1	B	216	LEU
1	B	226	LYS
1	B	238	MET
1	B	244	HIS
1	B	246	TRP
1	B	268	LEU
1	B	273	LEU
1	B	284	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) 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	100	GLN
1	A	145	ASN
1	A	196	HIS

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Mol	Chain	Res	Type
1	A	215	ASN
1	B	15	GLN
1	B	26	GLN
1	B	45	HIS
1	B	96	GLN
1	B	100	GLN
1	B	145	ASN
1	B	160	ASN
1	B	215	ASN
1	B	233	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 monosaccharides 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 ⓘ

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.