



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 04:16 AM UTC

PDB ID : 1HH2 / pdb_00001hh2
Title : Crystal structure of NusA from *Thermotoga maritima*
Authors : Worbs, M.; Bourenkov, G.P.; Bartunik, H.D.; Huber, R.; Wahl, M.C.
Deposited on : 2000-12-18
Resolution : 2.10 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) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

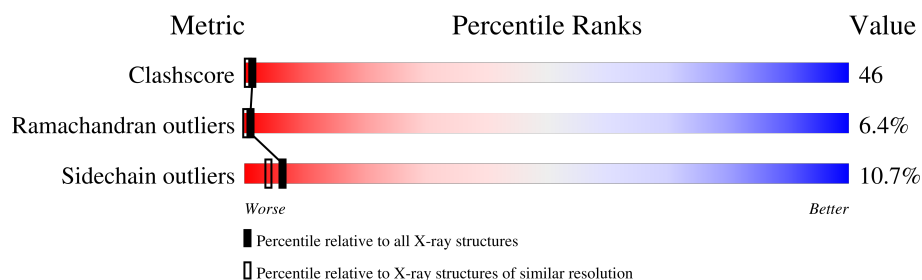
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 Å.

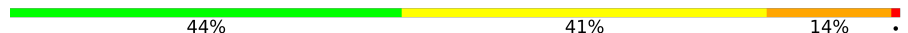
Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)

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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	P	344	 44% 41% 14% .

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 3024 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 N UTILIZATION SUBSTANCE PROTEIN A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	P	344	Total	C	N	O	S	0	0	0
			2667	1702	456	504	5			

- Molecule 2 is water.

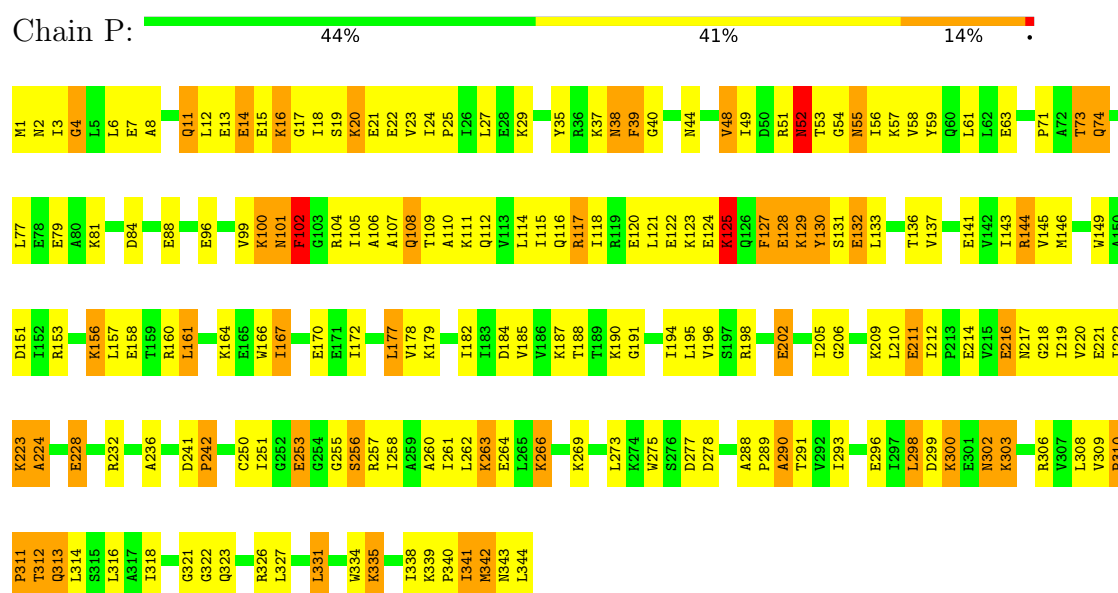
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	P	357	Total	O	0	0
			357	357		

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: N UTILIZATION SUBSTANCE PROTEIN A



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α , β , γ	115.53Å 115.53Å 63.81Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	15.00 – 2.10	Depositor
% Data completeness (in resolution range)	99.0 (15.00-2.10)	Depositor
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.244 , 0.319	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	3024	wwPDB-VP
Average B, all atoms (Å ²)	66.0	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	P	0.67	1/2698 (0.0%)	1.14	22/3640 (0.6%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	P	312	THR	CA-CB	5.49	1.60	1.54

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	P	311	PRO	N-CA-C	-8.76	98.27	111.41
1	P	256	SER	N-CA-C	-8.73	99.27	110.53
1	P	167	ILE	N-CA-C	-7.91	101.20	108.95
1	P	73	THR	N-CA-C	-7.15	95.56	110.80
1	P	218	GLY	N-CA-C	-7.10	105.42	114.37
1	P	310	PRO	CA-C-N	-6.93	113.17	120.03
1	P	310	PRO	C-N-CA	-6.93	113.17	120.03
1	P	84	ASP	CA-C-N	6.78	128.31	119.84
1	P	84	ASP	C-N-CA	6.78	128.31	119.84
1	P	216	GLU	CA-C-N	6.74	129.31	120.28
1	P	216	GLU	C-N-CA	6.74	129.31	120.28
1	P	335	LYS	N-CA-C	-6.12	99.68	109.96
1	P	288	ALA	N-CA-C	-5.71	102.38	109.64
1	P	151	ASP	N-CA-C	-5.42	100.45	109.46
1	P	198	ARG	N-CA-C	-5.37	105.56	113.61
1	P	323	GLN	N-CA-C	5.33	117.09	111.28
1	P	228	GLU	CA-C-N	5.31	126.48	119.84
1	P	228	GLU	C-N-CA	5.31	126.48	119.84
1	P	255	GLY	N-CA-C	-5.15	108.14	115.30
1	P	312	THR	N-CA-C	-5.13	105.71	113.51
1	P	52	ASN	CB-CA-C	-5.10	110.71	116.63
1	P	177	LEU	N-CA-C	-5.07	100.91	109.07

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	P	2667	0	2844	256	1
2	P	357	0	0	38	0
All	All	3024	0	2844	256	1

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 46.

All (256) 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:P:263:LYS:HE2	1:P:263:LYS:HA	1.36	1.07
1:P:124:GLU:HG3	1:P:129:LYS:HA	1.40	1.02
1:P:143:ILE:O	1:P:144:ARG:HG2	1.72	0.89
1:P:224:ALA:N	2:P:2263:HOH:O	2.12	0.83
1:P:1:MET:HE1	1:P:38:ASN:HB3	1.58	0.83
1:P:111:LYS:HZ1	1:P:112:GLN:HB2	1.45	0.81
1:P:8:ALA:O	1:P:11:GLN:HB3	1.80	0.80
1:P:341:ILE:HG22	1:P:342:MET:H	1.46	0.79
1:P:24:ILE:HG13	1:P:25:PRO:HD3	1.66	0.77
1:P:12:LEU:HD11	1:P:18:ILE:HB	1.66	0.77
1:P:3:ILE:HG12	1:P:56:ILE:O	1.85	0.77
1:P:2:ASN:ND2	1:P:105:ILE:HG13	2.01	0.76
1:P:12:LEU:HD21	1:P:18:ILE:H	1.50	0.76
1:P:291:THR:H	1:P:313:GLN:NE2	1.83	0.76
1:P:4:GLY:O	1:P:6:LEU:HG	1.86	0.75
1:P:52:ASN:N	1:P:52:ASN:HD22	1.85	0.74
1:P:187:LYS:HZ1	1:P:191:GLY:HA2	1.52	0.74
1:P:256:SER:O	1:P:257:ARG:HB2	1.87	0.74
1:P:308:LEU:HB3	1:P:341:ILE:CD1	2.18	0.73
1:P:124:GLU:HG3	1:P:129:LYS:CA	2.17	0.73
1:P:13:GLU:O	1:P:14:GLU:HB2	1.89	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:251:ILE:O	1:P:256:SER:O	2.07	0.73
1:P:311:PRO:HA	2:P:2337:HOH:O	1.88	0.72
1:P:338:ILE:O	1:P:339:LYS:HD2	1.90	0.72
1:P:310:PRO:HG2	1:P:313:GLN:HG3	1.71	0.72
1:P:331:LEU:HD13	1:P:331:LEU:O	1.90	0.72
1:P:40:GLY:HA3	2:P:2067:HOH:O	1.90	0.72
1:P:263:LYS:HA	1:P:263:LYS:CE	2.14	0.71
1:P:223:LYS:C	2:P:2263:HOH:O	2.32	0.71
1:P:308:LEU:HB3	1:P:341:ILE:HD12	1.73	0.71
1:P:71:PRO:HG2	2:P:2106:HOH:O	1.91	0.70
1:P:300:LYS:HB2	1:P:300:LYS:NZ	2.07	0.69
1:P:128:GLU:HA	1:P:187:LYS:HB2	1.74	0.69
1:P:117:ARG:O	1:P:121:LEU:HD23	1.92	0.69
1:P:228:GLU:HG3	1:P:327:LEU:HD21	1.74	0.69
1:P:128:GLU:O	1:P:129:LYS:HB2	1.93	0.68
1:P:161:LEU:HD22	1:P:166:TRP:CD1	2.28	0.68
1:P:24:ILE:CG1	1:P:25:PRO:HD3	2.23	0.68
1:P:110:ALA:O	1:P:114:LEU:HG	1.92	0.68
1:P:344:LEU:HD23	1:P:344:LEU:H	1.57	0.68
1:P:24:ILE:HD11	1:P:51:ARG:CZ	2.23	0.68
1:P:1:MET:HE1	1:P:38:ASN:HD22	1.58	0.68
1:P:24:ILE:HG13	1:P:25:PRO:CD	2.24	0.67
1:P:311:PRO:O	2:P:2336:HOH:O	2.12	0.67
1:P:18:ILE:HD11	1:P:118:ILE:HD11	1.76	0.67
1:P:228:GLU:OE2	1:P:326:ARG:HD2	1.95	0.67
1:P:104:ARG:HG2	1:P:105:ILE:H	1.60	0.67
1:P:130:TYR:HD1	1:P:131:SER:N	1.93	0.67
1:P:190:LYS:O	1:P:190:LYS:HG2	1.94	0.66
1:P:74:GLN:N	2:P:2110:HOH:O	1.95	0.66
1:P:115:ILE:O	1:P:118:ILE:HB	1.95	0.66
1:P:290:ALA:HA	1:P:313:GLN:NE2	2.11	0.66
1:P:190:LYS:HB3	2:P:2238:HOH:O	1.95	0.65
1:P:253:GLU:HG3	2:P:2131:HOH:O	1.94	0.65
1:P:108:GLN:HE21	1:P:108:GLN:C	2.04	0.65
1:P:149:TRP:CD1	1:P:160:ARG:HG3	2.32	0.65
1:P:290:ALA:HA	1:P:313:GLN:HE22	1.61	0.65
1:P:312:THR:N	2:P:2337:HOH:O	1.95	0.65
1:P:223:LYS:O	1:P:224:ALA:HB3	1.96	0.65
1:P:12:LEU:HD21	1:P:17:GLY:HA2	1.79	0.64
1:P:12:LEU:HD11	1:P:18:ILE:CB	2.28	0.64
1:P:331:LEU:HD13	1:P:331:LEU:C	2.23	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:16:LYS:HE3	1:P:118:ILE:HD12	1.78	0.63
1:P:1:MET:HE2	2:P:2060:HOH:O	1.99	0.63
1:P:105:ILE:HD11	1:P:107:ALA:HB3	1.81	0.63
1:P:108:GLN:C	1:P:108:GLN:NE2	2.57	0.63
1:P:299:ASP:CG	1:P:302:ASN:HB2	2.24	0.63
1:P:132:GLU:HG2	1:P:185:VAL:HB	1.80	0.62
1:P:161:LEU:HD22	1:P:166:TRP:HD1	1.64	0.62
1:P:11:GLN:OE1	1:P:12:LEU:HD13	1.99	0.62
1:P:127:PHE:HB3	1:P:128:GLU:OE1	2.00	0.62
1:P:123:LYS:C	1:P:125:LYS:H	2.08	0.61
1:P:61:LEU:N	1:P:61:LEU:HD12	2.15	0.61
1:P:219:ILE:HD12	2:P:2255:HOH:O	2.00	0.61
1:P:275:TRP:CZ3	1:P:277:ASP:OD1	2.54	0.61
1:P:179:LYS:HB2	1:P:264:GLU:CD	2.26	0.60
1:P:172:ILE:HD13	1:P:266:LYS:HZ2	1.67	0.60
1:P:275:TRP:NE1	2:P:2307:HOH:O	2.20	0.60
1:P:303:LYS:NZ	1:P:303:LYS:HB3	2.16	0.60
1:P:311:PRO:CA	2:P:2337:HOH:O	2.47	0.60
1:P:172:ILE:HD13	1:P:266:LYS:NZ	2.17	0.59
1:P:221:GLU:OE2	2:P:2257:HOH:O	2.17	0.59
1:P:2:ASN:HD22	1:P:105:ILE:HG13	1.66	0.58
1:P:22:GLU:C	1:P:25:PRO:HD2	2.28	0.58
1:P:22:GLU:O	1:P:25:PRO:HD2	2.02	0.58
1:P:128:GLU:HG2	1:P:132:GLU:HG3	1.86	0.58
1:P:232:ARG:HD3	1:P:269:LYS:HE2	1.84	0.58
1:P:293:ILE:HG13	1:P:341:ILE:HG13	1.85	0.58
1:P:130:TYR:CD1	1:P:130:TYR:C	2.81	0.58
1:P:120:GLU:O	1:P:125:LYS:HG3	2.04	0.58
1:P:289:PRO:O	1:P:290:ALA:HB2	2.04	0.58
1:P:59:TYR:CE1	1:P:96:GLU:HB2	2.38	0.58
1:P:27:LEU:CD2	1:P:110:ALA:HA	2.34	0.57
1:P:187:LYS:HZ1	1:P:191:GLY:CA	2.15	0.57
1:P:11:GLN:CD	1:P:12:LEU:HD13	2.30	0.57
1:P:309:VAL:N	1:P:341:ILE:HD11	2.20	0.57
1:P:63:GLU:O	1:P:74:GLN:HA	2.05	0.56
1:P:129:LYS:HG2	1:P:131:SER:HB3	1.87	0.56
1:P:331:LEU:C	1:P:331:LEU:CD1	2.78	0.56
1:P:51:ARG:HD2	1:P:51:ARG:N	2.21	0.56
1:P:3:ILE:HG13	1:P:99:VAL:HG11	1.87	0.56
1:P:124:GLU:HG2	1:P:129:LYS:HD2	1.88	0.56
1:P:128:GLU:HA	1:P:187:LYS:CD	2.36	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:1:MET:CE	1:P:38:ASN:HD22	2.18	0.55
1:P:1:MET:SD	1:P:38:ASN:ND2	2.79	0.55
1:P:73:THR:HB	2:P:2110:HOH:O	2.05	0.55
1:P:289:PRO:O	1:P:290:ALA:CB	2.55	0.55
1:P:52:ASN:N	1:P:52:ASN:ND2	2.51	0.55
1:P:3:ILE:HG13	1:P:99:VAL:CG1	2.37	0.55
1:P:302:ASN:C	1:P:303:LYS:HG2	2.32	0.55
1:P:217:ASN:HB3	1:P:219:ILE:HG13	1.87	0.55
1:P:308:LEU:C	1:P:341:ILE:HD11	2.32	0.55
1:P:300:LYS:HB2	1:P:300:LYS:HZ3	1.71	0.54
1:P:179:LYS:HB2	1:P:264:GLU:OE2	2.08	0.54
1:P:130:TYR:HD1	1:P:130:TYR:C	2.16	0.53
1:P:124:GLU:O	1:P:125:LYS:O	2.27	0.53
1:P:12:LEU:HB2	2:P:2017:HOH:O	2.08	0.53
1:P:14:GLU:O	1:P:15:GLU:HB2	2.09	0.52
1:P:182:ILE:HD12	1:P:194:ILE:CG2	2.38	0.52
1:P:223:LYS:NZ	1:P:223:LYS:HB3	2.25	0.52
1:P:156:LYS:HD3	1:P:156:LYS:H	1.75	0.52
1:P:11:GLN:HG2	1:P:20:LYS:NZ	2.24	0.52
1:P:275:TRP:CH2	1:P:277:ASP:OD1	2.63	0.51
1:P:101:ASN:O	1:P:102:PHE:HB2	2.09	0.51
1:P:130:TYR:C	1:P:132:GLU:H	2.17	0.51
1:P:12:LEU:HD21	1:P:18:ILE:N	2.21	0.51
1:P:182:ILE:HD12	1:P:194:ILE:HG21	1.91	0.51
1:P:49:ILE:HG23	1:P:54:GLY:CA	2.41	0.51
1:P:79:GLU:HG3	2:P:2118:HOH:O	2.10	0.51
1:P:303:LYS:HB2	1:P:334:TRP:CD2	2.46	0.51
1:P:73:THR:O	1:P:74:GLN:O	2.29	0.51
1:P:27:LEU:HD21	1:P:110:ALA:HA	1.92	0.51
1:P:128:GLU:O	1:P:129:LYS:CB	2.59	0.50
1:P:19:SER:C	1:P:21:GLU:H	2.18	0.50
1:P:57:LYS:HD2	1:P:96:GLU:OE2	2.11	0.50
1:P:223:LYS:O	1:P:236:ALA:HB3	2.11	0.50
1:P:123:LYS:HD2	1:P:191:GLY:HA2	1.92	0.50
1:P:16:LYS:CE	1:P:118:ILE:HD12	2.42	0.50
1:P:123:LYS:C	1:P:124:GLU:HG2	2.37	0.50
1:P:18:ILE:CD1	1:P:118:ILE:HD11	2.41	0.49
1:P:302:ASN:O	1:P:303:LYS:HG2	2.13	0.49
1:P:2:ASN:O	1:P:56:ILE:HD12	2.12	0.49
1:P:205:ILE:HG23	1:P:222:ILE:HD12	1.95	0.49
1:P:11:GLN:CD	1:P:20:LYS:HE2	2.37	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:49:ILE:HG23	1:P:54:GLY:HA2	1.95	0.49
1:P:170:GLU:HB2	1:P:266:LYS:HD2	1.94	0.49
1:P:202:GLU:CD	1:P:202:GLU:H	2.21	0.49
1:P:124:GLU:HG3	1:P:129:LYS:CB	2.43	0.49
1:P:1:MET:CE	1:P:38:ASN:HB3	2.36	0.48
1:P:128:GLU:N	1:P:128:GLU:CD	2.71	0.48
1:P:177:LEU:HG	2:P:2226:HOH:O	2.13	0.48
1:P:124:GLU:CG	1:P:129:LYS:HA	2.27	0.48
1:P:77:LEU:C	1:P:77:LEU:HD13	2.39	0.48
1:P:57:LYS:HE3	1:P:59:TYR:OH	2.13	0.48
1:P:184:ASP:OD1	1:P:185:VAL:N	2.45	0.48
1:P:216:GLU:HA	1:P:216:GLU:OE1	2.13	0.48
1:P:133:LEU:HD13	1:P:136:THR:OG1	2.14	0.47
1:P:123:LYS:O	1:P:125:LYS:N	2.45	0.47
1:P:232:ARG:CD	1:P:269:LYS:HE2	2.44	0.47
1:P:59:TYR:HE1	1:P:96:GLU:HB2	1.80	0.47
1:P:111:LYS:NZ	1:P:112:GLN:HB2	2.24	0.47
1:P:37:LYS:O	1:P:38:ASN:HB2	2.13	0.47
1:P:53:THR:HG21	1:P:55:ASN:HD21	1.80	0.47
1:P:124:GLU:CG	1:P:129:LYS:HD2	2.44	0.47
1:P:121:LEU:HD22	1:P:125:LYS:HE3	1.96	0.47
1:P:1:MET:HE3	1:P:35:TYR:HA	1.97	0.46
1:P:158:GLU:HB2	2:P:2205:HOH:O	2.15	0.46
1:P:223:LYS:O	1:P:224:ALA:CB	2.58	0.46
1:P:209:LYS:HB3	1:P:216:GLU:OE1	2.15	0.46
1:P:258:ILE:O	1:P:262:LEU:HG	2.16	0.46
1:P:111:LYS:O	1:P:112:GLN:C	2.57	0.46
1:P:39:PHE:HB2	2:P:2060:HOH:O	2.15	0.46
1:P:129:LYS:HG2	1:P:131:SER:CB	2.46	0.45
1:P:156:LYS:HD3	2:P:2202:HOH:O	2.15	0.45
1:P:257:ARG:O	1:P:261:ILE:HG12	2.15	0.45
1:P:318:ILE:HG22	1:P:322:GLY:HA2	1.97	0.45
1:P:99:VAL:O	1:P:100:LYS:HB3	2.16	0.45
1:P:19:SER:N	2:P:2040:HOH:O	2.45	0.45
1:P:88:GLU:HG3	2:P:2135:HOH:O	2.16	0.45
1:P:153:ARG:HH11	1:P:153:ARG:HG2	1.81	0.45
1:P:241:ASP:HA	1:P:242:PRO:HD2	1.80	0.45
1:P:296:GLU:OE1	1:P:306:ARG:NH2	2.49	0.45
1:P:299:ASP:OD2	1:P:302:ASN:HB2	2.15	0.45
1:P:309:VAL:O	1:P:340:PRO:HA	2.16	0.45
1:P:182:ILE:HD13	1:P:196:VAL:HG12	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:104:ARG:HB3	2:P:2158:HOH:O	2.18	0.44
1:P:137:VAL:HG23	1:P:206:GLY:HA3	2.00	0.44
1:P:53:THR:HB	1:P:55:ASN:ND2	2.33	0.44
1:P:209:LYS:CE	2:P:2248:HOH:O	2.65	0.44
1:P:303:LYS:C	1:P:334:TRP:CE3	2.95	0.44
1:P:127:PHE:O	1:P:187:LYS:CB	2.65	0.44
1:P:211:GLU:HG2	1:P:260:ALA:HB3	1.98	0.44
1:P:44:ASN:ND2	1:P:61:LEU:HD22	2.32	0.44
1:P:122:GLU:O	1:P:122:GLU:HG3	2.18	0.44
1:P:303:LYS:HB3	1:P:303:LYS:HZ3	1.80	0.44
1:P:309:VAL:O	1:P:341:ILE:HG12	2.17	0.44
1:P:51:ARG:N	1:P:51:ARG:CD	2.81	0.44
1:P:275:TRP:HZ3	1:P:277:ASP:OD1	1.97	0.44
1:P:223:LYS:CA	2:P:2263:HOH:O	2.64	0.44
1:P:157:LEU:HD13	2:P:2186:HOH:O	2.17	0.44
1:P:170:GLU:OE1	1:P:266:LYS:HD2	2.18	0.44
1:P:335:LYS:HD3	2:P:2176:HOH:O	2.18	0.44
1:P:146:MET:HE3	1:P:146:MET:HB3	1.91	0.43
1:P:321:GLY:O	1:P:326:ARG:NH2	2.50	0.43
1:P:48:VAL:C	1:P:49:ILE:HG13	2.42	0.43
1:P:111:LYS:HZ1	1:P:112:GLN:CB	2.22	0.43
1:P:132:GLU:HA	1:P:185:VAL:HG21	1.99	0.43
1:P:164:LYS:O	1:P:164:LYS:HG2	2.19	0.43
1:P:172:ILE:HD12	1:P:178:VAL:HG11	2.00	0.43
1:P:256:SER:O	1:P:257:ARG:CB	2.58	0.43
1:P:263:LYS:HE3	2:P:2289:HOH:O	2.18	0.43
1:P:313:GLN:HE21	1:P:313:GLN:HB3	1.64	0.43
1:P:124:GLU:OE2	1:P:129:LYS:HE3	2.19	0.43
1:P:212:ILE:HD13	1:P:250:CYS:HA	2.00	0.43
1:P:232:ARG:HB2	1:P:269:LYS:HB2	2.01	0.43
1:P:108:GLN:O	1:P:111:LYS:HB3	2.19	0.43
1:P:153:ARG:HG3	1:P:157:LEU:O	2.19	0.42
1:P:303:LYS:HG3	2:P:2351:HOH:O	2.20	0.42
1:P:1:MET:HE1	1:P:38:ASN:ND2	2.29	0.42
1:P:128:GLU:OE1	1:P:128:GLU:N	2.51	0.42
1:P:179:LYS:NZ	1:P:210:LEU:HD13	2.34	0.42
1:P:188:THR:C	1:P:190:LYS:H	2.26	0.42
1:P:12:LEU:CD2	1:P:17:GLY:HA2	2.48	0.42
1:P:104:ARG:HG2	1:P:105:ILE:N	2.32	0.42
1:P:11:GLN:O	1:P:11:GLN:HG3	2.20	0.42
1:P:109:THR:C	1:P:111:LYS:N	2.78	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:128:GLU:HA	1:P:187:LYS:HD2	2.02	0.42
1:P:112:GLN:HG2	2:P:2168:HOH:O	2.19	0.42
1:P:167:ILE:O	1:P:170:GLU:HG2	2.19	0.42
1:P:214:GLU:HA	1:P:217:ASN:HB2	2.01	0.42
1:P:209:LYS:HE3	2:P:2248:HOH:O	2.20	0.42
1:P:1:MET:HE1	1:P:38:ASN:CB	2.39	0.41
1:P:12:LEU:HD11	1:P:18:ILE:H	1.85	0.41
1:P:81:LYS:HE2	2:P:2130:HOH:O	2.20	0.41
1:P:278:ASP:OD1	1:P:278:ASP:C	2.64	0.41
1:P:344:LEU:H	1:P:344:LEU:CD2	2.30	0.41
1:P:12:LEU:HD22	2:P:2017:HOH:O	2.21	0.41
1:P:73:THR:CA	2:P:2110:HOH:O	2.68	0.41
1:P:338:ILE:C	1:P:339:LYS:HD2	2.44	0.41
1:P:29:LYS:HE2	2:P:2050:HOH:O	2.20	0.41
1:P:293:ILE:HD11	1:P:310:PRO:HD3	2.02	0.41
1:P:106:ALA:O	1:P:109:THR:HG23	2.21	0.41
1:P:116:GLN:HE21	1:P:116:GLN:HB2	1.65	0.41
1:P:20:LYS:HA	1:P:23:VAL:HG23	2.02	0.41
1:P:115:ILE:O	1:P:118:ILE:N	2.44	0.41
1:P:275:TRP:CZ2	2:P:2307:HOH:O	2.72	0.41
1:P:59:TYR:CD1	1:P:96:GLU:HA	2.56	0.41
1:P:111:LYS:O	1:P:114:LEU:N	2.54	0.41
1:P:223:LYS:HB2	1:P:275:TRP:CD1	2.56	0.40
1:P:24:ILE:HG13	1:P:25:PRO:N	2.36	0.40
1:P:54:GLY:O	1:P:55:ASN:O	2.39	0.40
1:P:61:LEU:N	1:P:61:LEU:CD1	2.82	0.40
1:P:12:LEU:CD1	1:P:18:ILE:HB	2.44	0.40
1:P:214:GLU:HB3	1:P:220:VAL:HG23	2.02	0.40
1:P:298:LEU:HD11	1:P:306:ARG:HB2	2.04	0.40
1:P:339:LYS:HD2	1:P:339:LYS:HA	1.84	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:15:GLU:OE1	1:P:15:GLU:OE1[7_465]	1.56	0.64

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	P	342/344 (99%)	281 (82%)	39 (11%)	22 (6%)	1 0

All (22) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	P	38	ASN
1	P	55	ASN
1	P	74	GLN
1	P	125	LYS
1	P	129	LYS
1	P	290	ALA
1	P	302	ASN
1	P	39	PHE
1	P	100	LYS
1	P	253	GLU
1	P	7	GLU
1	P	16	LYS
1	P	102	PHE
1	P	144	ARG
1	P	224	ALA
1	P	266	LYS
1	P	14	GLU
1	P	101	ASN
1	P	4	GLY
1	P	20	LYS
1	P	341	ILE
1	P	242	PRO

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	P	291/291 (100%)	260 (89%)	31 (11%)	6 4

All (31) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	P	11	GLN
1	P	48	VAL
1	P	52	ASN
1	P	58	VAL
1	P	102	PHE
1	P	108	GLN
1	P	117	ARG
1	P	125	LYS
1	P	127	PHE
1	P	128	GLU
1	P	130	TYR
1	P	132	GLU
1	P	141	GLU
1	P	145	VAL
1	P	156	LYS
1	P	161	LEU
1	P	195	LEU
1	P	202	GLU
1	P	211	GLU
1	P	223	LYS
1	P	263	LYS
1	P	273	LEU
1	P	298	LEU
1	P	300	LYS
1	P	303	LYS
1	P	313	GLN
1	P	314	LEU
1	P	316	LEU
1	P	331	LEU
1	P	342	MET
1	P	343	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	P	11	GLN
1	P	38	ASN
1	P	44	ASN
1	P	52	ASN
1	P	55	ASN
1	P	60	GLN
1	P	108	GLN
1	P	116	GLN
1	P	126	GLN
1	P	240	ASN
1	P	302	ASN
1	P	313	GLN
1	P	343	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 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

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.