



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 05:27 PM UTC

PDB ID : 1Y7E / pdb_00001y7e
Title : The Crystal Structure of Aminopeptidase I from *Borrelia burgdorferi* B31
Authors : Min, T.; Gorman, J.; Shapiro, L.; Burley, S.K.; New York SGX Research Center for Structural Genomics (NYSGXRC)
Deposited on : 2004-12-08
Resolution : 3.20 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
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

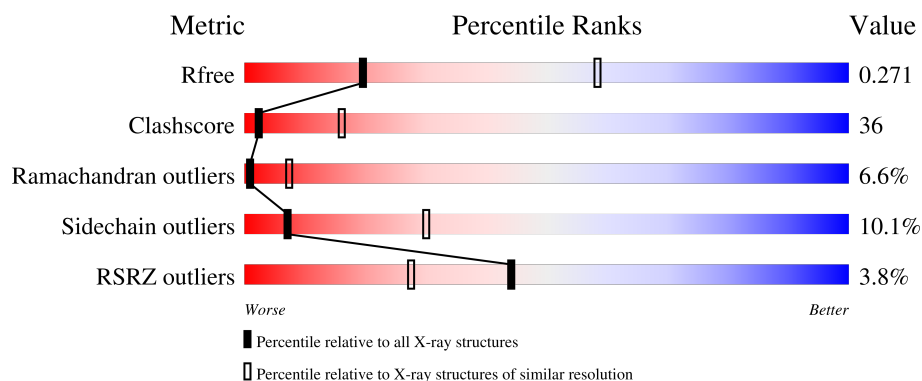
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.20 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1466 (3.20-3.20)
Clashscore	190562	1573 (3.20-3.20)
Ramachandran outliers	187476	1548 (3.20-3.20)
Sidechain outliers	187428	1547 (3.20-3.20)
RSRZ outliers	180081	1466 (3.20-3.20)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	458	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 3296 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 Probable M18-family aminopeptidase 1.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	404	Total	C	N	O	S	Se	0	0	0
			3232	2088	517	616	4	7			

There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	61	MSE	MET	modified residue	UNP Q45055
A	89	MSE	MET	modified residue	UNP Q45055
A	308	MSE	MET	modified residue	UNP Q45055
A	363	MSE	MET	modified residue	UNP Q45055
A	426	MSE	MET	modified residue	UNP Q45055
A	433	MSE	MET	modified residue	UNP Q45055
A	437	MSE	MET	modified residue	UNP Q45055

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	64	Total	O	0	0
			64	64		

- Molecule 1: Probable M18-family aminopeptidase 1



4 Data and refinement statistics

Property	Value	Source
Space group	F 4 3 2	Depositor
Cell constants a, b, c, α , β , γ	244.27Å 244.27Å 244.27Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.81 – 3.20 19.81 – 3.20	Depositor EDS
% Data completeness (in resolution range)	95.2 (19.81-3.20) 97.3 (19.81-3.20)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.42 (at 2.69Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.202 , 0.258 0.209 , 0.271	Depositor DCC
R_{free} test set	870 reflections (2.70%)	wwPDB-VP
Wilson B-factor (Å ²)	31.0	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 57.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	3296	wwPDB-VP
Average B, all atoms (Å ²)	23.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.46% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.48	0/3287	1.08	29/4418 (0.7%)

There are no bond length outliers.

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	452	TYR	N-CA-C	-9.67	98.20	110.19
1	A	225	ASP	N-CA-C	-8.94	101.47	112.38
1	A	275	ASN	N-CA-C	-7.66	97.58	109.76
1	A	58	LYS	N-CA-C	-7.65	103.97	113.38
1	A	321	HIS	N-CA-C	-6.86	96.20	110.80
1	A	101	LEU	N-CA-C	6.84	122.17	113.55
1	A	48	LYS	N-CA-C	-6.69	99.36	109.79
1	A	270	LEU	N-CA-C	-6.59	102.44	110.88
1	A	271	GLU	N-CA-C	6.44	115.89	108.49
1	A	50	GLY	N-CA-C	6.37	124.94	115.64
1	A	227	VAL	N-CA-C	-6.33	96.18	109.34
1	A	413	ALA	N-CA-C	-6.29	104.34	111.07
1	A	8	ILE	N-CA-C	6.08	117.55	110.62
1	A	260	VAL	N-CA-C	-6.01	104.64	110.42
1	A	194	ILE	CB-CA-C	-5.94	105.83	111.06
1	A	47	LYS	N-CA-C	-5.88	104.87	111.28
1	A	155	ASP	N-CA-C	-5.78	101.10	109.31
1	A	108	ILE	N-CA-C	5.73	116.40	108.84
1	A	430	VAL	N-CA-C	5.69	117.62	108.85
1	A	195	GLY	N-CA-C	5.48	118.49	110.38
1	A	93	VAL	N-CA-C	5.41	120.59	109.34
1	A	5	ASN	CA-C-N	5.28	126.44	119.84
1	A	5	ASN	C-N-CA	5.28	126.44	119.84
1	A	414	LYS	N-CA-C	-5.25	101.56	109.60
1	A	223	GLU	N-CA-C	-5.15	102.76	110.23
1	A	82	LYS	N-CA-C	5.14	116.56	111.07
1	A	197	LEU	CA-C-N	5.09	126.20	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	197	LEU	C-N-CA	5.09	126.20	119.84
1	A	286	GLU	N-CA-C	-5.01	105.82	111.28

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	3232	0	3254	231	0
2	A	64	0	0	5	1
All	All	3296	0	3254	231	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 36.

All (231) 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:117:ILE:HG13	1:A:194:ILE:HD11	1.23	1.15
1:A:68:TYR:H	1:A:76:ALA:HB3	1.24	0.98
1:A:336:VAL:HG21	1:A:430:VAL:HG23	1.48	0.94
1:A:259:CYS:HB3	1:A:334:ALA:HB1	1.55	0.88
1:A:350:GLU:HG3	1:A:352:ASN:H	1.39	0.87
1:A:68:TYR:HB2	1:A:76:ALA:HB2	1.57	0.86
1:A:341:ASN:HB3	1:A:342:PRO:C	2.04	0.83
1:A:89:MSE:HE2	1:A:279:ILE:HD11	1.62	0.82
1:A:362:ILE:HG23	1:A:424:ILE:HD11	1.64	0.79
1:A:203:GLU:HG2	1:A:209:LEU:HD11	1.64	0.76
1:A:265:GLU:O	1:A:270:LEU:HD12	1.85	0.76
1:A:118:LYS:O	1:A:119:THR:HB	1.87	0.75
1:A:313:LYS:HB2	1:A:316:GLU:HG3	1.67	0.75
1:A:336:VAL:CG2	1:A:430:VAL:HG23	2.15	0.75
1:A:26:LYS:HA	1:A:29:ILE:HD11	1.69	0.75
1:A:101:LEU:HB2	1:A:233:ILE:HB	1.68	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:337:CYS:HB3	1:A:363:MSE:HE3	1.68	0.74
1:A:60:LEU:HD22	1:A:80:ILE:HG12	1.70	0.73
1:A:335:ASP:HB2	2:A:476:HOH:O	1.89	0.73
1:A:48:LYS:C	1:A:50:GLY:H	1.97	0.72
1:A:259:CYS:CB	1:A:334:ALA:HB1	2.19	0.72
1:A:141:VAL:HG22	1:A:229:SER:HB2	1.71	0.71
1:A:117:ILE:HG13	1:A:194:ILE:CD1	2.13	0.71
1:A:321:HIS:O	1:A:323:GLN:N	2.24	0.71
1:A:247:ALA:HB3	2:A:475:HOH:O	1.90	0.70
1:A:336:VAL:HG21	1:A:430:VAL:CG2	2.22	0.69
1:A:36:ARG:HH22	1:A:230:GLU:CD	2.01	0.69
1:A:268:PHE:O	1:A:270:LEU:N	2.25	0.69
1:A:363:MSE:HE3	1:A:401:LEU:HD21	1.75	0.68
1:A:341:ASN:HB3	1:A:342:PRO:CA	2.24	0.68
1:A:155:ASP:O	1:A:156:ASN:HB2	1.92	0.68
1:A:336:VAL:HG23	1:A:428:PRO:C	2.21	0.66
1:A:29:ILE:HD12	1:A:30:SER:N	2.09	0.66
1:A:441:SER:HB3	1:A:444:ASP:OD2	1.95	0.66
1:A:85:ILE:HD11	1:A:89:MSE:HE3	1.78	0.66
1:A:68:TYR:N	1:A:76:ALA:HB3	2.05	0.65
1:A:68:TYR:HB2	1:A:76:ALA:CB	2.25	0.65
1:A:104:LYS:HG2	1:A:120:ASN:HD21	1.61	0.65
1:A:309:ILE:HD13	1:A:322:VAL:HA	1.79	0.65
1:A:270:LEU:HD13	1:A:449:TYR:OH	1.96	0.63
1:A:414:LYS:O	1:A:416:LEU:N	2.31	0.62
1:A:336:VAL:HG23	1:A:428:PRO:O	2.00	0.62
1:A:223:GLU:O	1:A:224:GLU:HB3	2.00	0.61
1:A:314:LYS:CD	1:A:314:LYS:H	2.13	0.61
1:A:258:ILE:HG13	1:A:445:LEU:HD23	1.82	0.61
1:A:336:VAL:HG22	1:A:337:CYS:H	1.65	0.61
1:A:245:ASP:HB3	2:A:517:HOH:O	2.00	0.61
1:A:104:LYS:HG2	1:A:120:ASN:ND2	2.16	0.61
1:A:48:LYS:O	1:A:50:GLY:N	2.34	0.60
1:A:38:VAL:HG21	1:A:257:LYS:HE3	1.83	0.60
1:A:95:HIS:HA	1:A:283:VAL:O	2.01	0.60
1:A:43:LEU:O	1:A:47:LYS:HG2	2.02	0.59
1:A:92:ILE:O	1:A:332:ILE:O	2.21	0.59
1:A:55:GLU:C	1:A:57:LYS:H	2.10	0.59
1:A:388:LEU:HD11	1:A:455:PHE:HA	1.84	0.59
1:A:55:GLU:O	1:A:56:GLU:HB2	2.03	0.59
1:A:341:ASN:CB	1:A:342:PRO:CA	2.80	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:138:ARG:NH2	1:A:155:ASP:OD2	2.35	0.59
1:A:385:ILE:HD11	1:A:424:ILE:HG21	1.85	0.58
1:A:452:TYR:O	1:A:453:LYS:HB3	2.02	0.58
1:A:29:ILE:HD12	1:A:30:SER:H	1.66	0.58
1:A:94:SER:O	1:A:282:LEU:HA	2.03	0.58
1:A:48:LYS:C	1:A:50:GLY:N	2.62	0.58
1:A:95:HIS:HE2	1:A:335:ASP:CG	2.12	0.57
1:A:256:ASP:OD1	1:A:335:ASP:HA	2.03	0.57
1:A:196:SER:O	1:A:197:LEU:HD12	2.05	0.57
1:A:336:VAL:HG22	1:A:337:CYS:N	2.19	0.57
1:A:103:ALA:HA	1:A:119:THR:HA	1.85	0.57
1:A:334:ALA:O	1:A:335:ASP:C	2.46	0.57
1:A:125:ILE:HG22	1:A:127:LYS:H	1.71	0.56
1:A:192:ILE:HD12	1:A:192:ILE:N	2.21	0.56
1:A:68:TYR:HB3	1:A:300:TYR:OH	2.07	0.55
1:A:76:ALA:O	1:A:77:PHE:HB2	2.06	0.55
1:A:228:SER:O	1:A:229:SER:O	2.25	0.55
1:A:73:LYS:O	1:A:96:THR:HG21	2.05	0.55
1:A:431:ILE:HB	1:A:439:ILE:HB	1.87	0.55
1:A:126:LYS:HD2	1:A:128:TYR:CE1	2.42	0.55
1:A:254:GLN:HG3	1:A:438:GLU:HB2	1.88	0.55
1:A:452:TYR:O	1:A:454:ALA:N	2.40	0.55
1:A:313:LYS:HG3	1:A:317:TYR:HA	1.89	0.55
1:A:92:ILE:HG22	1:A:93:VAL:N	2.22	0.54
1:A:92:ILE:HG21	1:A:263:SER:HB2	1.89	0.54
1:A:4:GLN:C	1:A:4:GLN:HE21	2.15	0.54
1:A:35:GLU:HG2	1:A:36:ARG:N	2.21	0.54
1:A:281:PHE:O	1:A:282:LEU:HB2	2.08	0.54
1:A:317:TYR:CG	1:A:318:ASN:N	2.75	0.54
1:A:70:CYS:O	1:A:71:ARG:HG3	2.07	0.53
1:A:228:SER:OG	1:A:229:SER:N	2.41	0.53
1:A:242:VAL:HB	1:A:248:LEU:HB2	1.90	0.53
1:A:189:ASN:CG	1:A:190:LEU:H	2.15	0.53
1:A:125:ILE:HG22	1:A:127:LYS:N	2.24	0.53
1:A:104:LYS:O	1:A:107:PRO:HD3	2.09	0.53
1:A:223:GLU:O	1:A:224:GLU:CB	2.55	0.53
1:A:337:CYS:HB3	1:A:363:MSE:CE	2.36	0.53
1:A:203:GLU:CG	1:A:209:LEU:HD11	2.35	0.53
1:A:362:ILE:CG2	1:A:424:ILE:HD11	2.34	0.53
1:A:25:TYR:O	1:A:29:ILE:HG13	2.08	0.52
1:A:115:THR:HG22	1:A:194:ILE:HB	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:234:VAL:HG13	1:A:235:PRO:HD2	1.90	0.52
1:A:95:HIS:NE2	1:A:335:ASP:OD1	2.38	0.52
1:A:118:LYS:O	1:A:190:LEU:O	2.27	0.52
1:A:39:THR:HG23	1:A:75:VAL:HG22	1.92	0.52
1:A:55:GLU:C	1:A:57:LYS:N	2.66	0.52
1:A:126:LYS:HB3	1:A:129:GLN:HG3	1.91	0.51
1:A:219:TYR:O	1:A:220:LYS:HB2	2.11	0.51
1:A:11:ASN:HD21	1:A:13:GLU:HB3	1.76	0.51
1:A:253:GLY:O	1:A:257:LYS:HB2	2.10	0.51
1:A:227:VAL:O	1:A:228:SER:C	2.52	0.51
1:A:26:LYS:C	1:A:28:PHE:N	2.68	0.51
1:A:281:PHE:O	1:A:282:LEU:CB	2.58	0.51
1:A:412:VAL:O	1:A:414:LYS:O	2.29	0.51
1:A:168:LEU:C	1:A:168:LEU:HD13	2.36	0.51
1:A:143:LEU:HA	1:A:225:ASP:OD1	2.11	0.50
1:A:49:LEU:O	1:A:65:LYS:HE3	2.12	0.50
1:A:135:LEU:HB2	1:A:162:PHE:O	2.12	0.50
1:A:226:PHE:C	1:A:227:VAL:O	2.48	0.50
1:A:360:ILE:H	1:A:447:ASN:HD21	1.59	0.49
1:A:21:PHE:CD2	1:A:445:LEU:HD13	2.46	0.49
1:A:26:LYS:O	1:A:29:ILE:HD12	2.12	0.49
1:A:46:ALA:O	1:A:51:PHE:HB2	2.12	0.49
1:A:29:ILE:HD13	1:A:239:ALA:HB2	1.93	0.49
1:A:196:SER:O	1:A:197:LEU:O	2.30	0.49
1:A:314:LYS:H	1:A:314:LYS:HD3	1.78	0.49
1:A:213:GLN:O	1:A:217:GLU:HG3	2.13	0.49
1:A:320:LEU:C	1:A:321:HIS:O	2.48	0.49
1:A:62:PRO:HA	1:A:80:ILE:HG22	1.95	0.49
1:A:331:SER:HB3	1:A:421:ILE:HG21	1.94	0.49
1:A:287:GLU:HB2	1:A:297:ASP:OD2	2.13	0.49
1:A:100:ARG:O	1:A:125:ILE:HD11	2.13	0.49
1:A:413:ALA:C	1:A:414:LYS:O	2.54	0.49
1:A:341:ASN:CB	1:A:342:PRO:HA	2.43	0.48
1:A:61:MSE:O	1:A:64:ASP:HB2	2.13	0.48
1:A:254:GLN:HB2	1:A:438:GLU:HB2	1.94	0.48
1:A:271:GLU:HB3	1:A:457:ARG:CZ	2.44	0.48
1:A:313:LYS:HE2	1:A:313:LYS:HB3	1.76	0.48
1:A:453:LYS:O	1:A:454:ALA:C	2.56	0.48
1:A:86:GLU:OE2	1:A:321:HIS:HB3	2.13	0.48
1:A:92:ILE:CG2	1:A:93:VAL:N	2.76	0.48
1:A:44:ASP:O	1:A:48:LYS:HG3	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:272:GLU:O	1:A:273:THR:C	2.57	0.48
1:A:265:GLU:O	1:A:266:SER:C	2.56	0.48
1:A:266:SER:CB	1:A:453:LYS:HB2	2.43	0.48
1:A:101:LEU:O	1:A:120:ASN:O	2.32	0.47
1:A:198:PRO:HB3	1:A:206:LYS:HB2	1.96	0.47
1:A:361:PRO:HD2	1:A:427:GLY:O	2.14	0.47
1:A:198:PRO:HB3	1:A:206:LYS:CB	2.44	0.47
1:A:288:ILE:HG13	1:A:411:THR:HG21	1.95	0.47
1:A:35:GLU:HA	1:A:96:THR:OG1	2.15	0.47
1:A:309:ILE:HD13	1:A:322:VAL:HG22	1.97	0.47
1:A:314:LYS:CD	1:A:314:LYS:N	2.78	0.47
1:A:51:PHE:CE1	1:A:65:LYS:HD2	2.50	0.47
1:A:424:ILE:CG2	1:A:426:MSE:HE2	2.45	0.47
1:A:4:GLN:C	1:A:4:GLN:NE2	2.73	0.47
1:A:452:TYR:O	1:A:453:LYS:CB	2.63	0.46
1:A:266:SER:HB2	1:A:453:LYS:HB2	1.97	0.46
1:A:388:LEU:HD23	1:A:388:LEU:O	2.16	0.46
1:A:224:GLU:C	1:A:226:PHE:N	2.68	0.46
1:A:233:ILE:N	1:A:233:ILE:HD12	2.30	0.46
1:A:254:GLN:HB2	1:A:438:GLU:OE1	2.15	0.46
1:A:256:ASP:OD1	1:A:335:ASP:N	2.49	0.46
1:A:57:LYS:NZ	1:A:59:ASN:HB2	2.31	0.46
1:A:360:ILE:H	1:A:447:ASN:ND2	2.14	0.46
1:A:198:PRO:HG3	1:A:207:VAL:HG22	1.97	0.46
1:A:301:LEU:HA	1:A:304:PHE:CE2	2.51	0.45
1:A:189:ASN:ND2	1:A:190:LEU:H	2.14	0.45
1:A:433:MSE:HE3	1:A:434:HIS:NE2	2.31	0.45
1:A:201:THR:HG21	1:A:209:LEU:HD12	1.98	0.45
1:A:110:GLU:OE1	1:A:205:ASN:HB3	2.17	0.45
1:A:238:THR:HG22	2:A:496:HOH:O	2.16	0.45
1:A:309:ILE:HD13	1:A:322:VAL:CA	2.45	0.44
1:A:362:ILE:CD1	1:A:396:TRP:HB2	2.47	0.44
1:A:254:GLN:N	1:A:438:GLU:OE1	2.50	0.44
1:A:271:GLU:HA	1:A:457:ARG:NH2	2.33	0.44
1:A:85:ILE:HD11	1:A:89:MSE:HG2	1.98	0.44
1:A:227:VAL:HG12	1:A:228:SER:N	2.33	0.44
1:A:259:CYS:HB3	1:A:334:ALA:CB	2.36	0.44
1:A:309:ILE:CD1	1:A:322:VAL:HA	2.46	0.44
1:A:256:ASP:OD1	1:A:259:CYS:HB2	2.17	0.44
1:A:297:ASP:N	2:A:461:HOH:O	2.51	0.44
1:A:304:PHE:CD1	1:A:304:PHE:C	2.95	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:401:LEU:HD12	1:A:401:LEU:N	2.33	0.44
1:A:52:ILE:HG22	1:A:53:ASN:O	2.18	0.43
1:A:67:PHE:CD1	1:A:67:PHE:C	2.96	0.43
1:A:141:VAL:HA	1:A:229:SER:HB2	1.99	0.43
1:A:267:ILE:HG23	1:A:268:PHE:N	2.32	0.43
1:A:385:ILE:O	1:A:389:LEU:HG	2.19	0.43
1:A:451:ALA:C	1:A:452:TYR:O	2.55	0.43
1:A:387:GLN:O	1:A:391:LYS:HB2	2.19	0.43
1:A:248:LEU:HD23	1:A:441:SER:HA	2.01	0.43
1:A:227:VAL:HG12	1:A:228:SER:H	1.83	0.43
1:A:341:ASN:HB2	1:A:342:PRO:HA	1.99	0.42
1:A:68:TYR:CD2	1:A:304:PHE:HB2	2.53	0.42
1:A:196:SER:HB2	1:A:197:LEU:H	1.72	0.42
1:A:26:LYS:O	1:A:27:LYS:C	2.61	0.42
1:A:133:THR:O	1:A:135:LEU:HD13	2.20	0.42
1:A:89:MSE:HE1	1:A:308:MSE:SE	2.69	0.42
1:A:130:TRP:CH2	1:A:235:PRO:HD3	2.55	0.42
1:A:19:LEU:O	1:A:23:GLU:HG2	2.20	0.42
1:A:33:LYS:HD3	1:A:234:VAL:HG11	2.01	0.42
1:A:209:LEU:O	1:A:210:ALA:C	2.62	0.42
1:A:360:ILE:N	1:A:447:ASN:ND2	2.68	0.42
1:A:110:GLU:HA	1:A:114:LEU:O	2.19	0.42
1:A:199:ILE:HG23	1:A:201:THR:HG22	2.01	0.42
1:A:361:PRO:HB3	1:A:397:GLN:HB2	2.02	0.42
1:A:430:VAL:CG1	1:A:438:GLU:HB3	2.50	0.42
1:A:76:ALA:O	1:A:77:PHE:CB	2.68	0.42
1:A:48:LYS:O	1:A:49:LEU:HB2	2.20	0.41
1:A:155:ASP:O	1:A:159:ASP:CB	2.69	0.41
1:A:221:ILE:HG23	1:A:225:ASP:HB2	2.01	0.41
1:A:71:ARG:C	1:A:72:GLU:HG2	2.45	0.41
1:A:85:ILE:CD1	1:A:89:MSE:HG2	2.50	0.41
1:A:89:MSE:CE	1:A:279:ILE:HD11	2.43	0.41
1:A:264:LEU:HD23	1:A:280:CYS:SG	2.60	0.41
1:A:336:VAL:HG11	1:A:430:VAL:HG21	2.02	0.41
1:A:80:ILE:HD11	1:A:308:MSE:HE3	2.01	0.41
1:A:118:LYS:O	1:A:119:THR:CB	2.58	0.41
1:A:267:ILE:HB	1:A:456:TYR:CE1	2.56	0.41
1:A:305:VAL:O	1:A:309:ILE:HD12	2.20	0.41
1:A:203:GLU:CB	1:A:209:LEU:HD11	2.50	0.41
1:A:75:VAL:O	1:A:281:PHE:O	2.37	0.41
1:A:197:LEU:HA	1:A:198:PRO:HD3	1.73	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:450:LEU:O	1:A:454:ALA:HB2	2.21	0.41
1:A:25:TYR:OH	1:A:254:GLN:OE1	2.21	0.41
1:A:264:LEU:HD21	1:A:282:LEU:HD11	2.03	0.41
1:A:268:PHE:O	1:A:269:ASP:C	2.65	0.40
1:A:21:PHE:HD2	1:A:445:LEU:HD13	1.86	0.40
1:A:11:ASN:ND2	1:A:13:GLU:HB3	2.35	0.40
1:A:336:VAL:CG2	1:A:428:PRO:O	2.68	0.40
1:A:125:ILE:HG22	1:A:126:LYS:N	2.37	0.40
1:A:383:SER:O	1:A:387:GLN:HG3	2.21	0.40
1:A:260:VAL:O	1:A:264:LEU:HG	2.22	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)
2:A:465:HOH:O	2:A:465:HOH:O[74_555]	1.88	0.32

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	392/458 (86%)	319 (81%)	47 (12%)	26 (7%)	 

All (26) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	127	LYS
1	A	197	LEU
1	A	204	LYS
1	A	229	SER
1	A	269	ASP
1	A	281	PHE

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Mol	Chain	Res	Type
1	A	314	LYS
1	A	329	SER
1	A	341	ASN
1	A	93	VAL
1	A	102	ASP
1	A	224	GLU
1	A	335	ASP
1	A	13	GLU
1	A	72	GLU
1	A	167	ILE
1	A	282	LEU
1	A	318	ASN
1	A	5	ASN
1	A	49	LEU
1	A	255	ASP
1	A	428	PRO
1	A	414	LYS
1	A	322	VAL
1	A	336	VAL
1	A	107	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	355/391 (91%)	319 (90%)	36 (10%)	7	30

All (36) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	GLN
1	A	29	ILE
1	A	56	GLU
1	A	59	ASN
1	A	75	VAL
1	A	92	ILE

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Mol	Chain	Res	Type
1	A	93	VAL
1	A	98	SER
1	A	100	ARG
1	A	117	ILE
1	A	119	THR
1	A	121	TYR
1	A	135	LEU
1	A	153	ILE
1	A	159	ASP
1	A	167	ILE
1	A	196	SER
1	A	214	LEU
1	A	220	LYS
1	A	229	SER
1	A	232	GLU
1	A	271	GLU
1	A	274	PRO
1	A	309	ILE
1	A	313	LYS
1	A	314	LYS
1	A	318	ASN
1	A	323	GLN
1	A	327	TRP
1	A	380	GLU
1	A	381	LEU
1	A	386	ARG
1	A	388	LEU
1	A	415	PHE
1	A	437	MSE
1	A	445	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	4	GLN
1	A	11	ASN
1	A	16	ASN
1	A	17	GLN
1	A	120	ASN
1	A	156	ASN
1	A	189	ASN
1	A	319	ASN

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Mol	Chain	Res	Type
1	A	341	ASN
1	A	387	GLN
1	A	447	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 [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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	397/458 (86%)	-0.01	15 (3%) 44 27	1, 16, 62, 104	0

All (15) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	286	GLU	4.5
1	A	121	TYR	4.3
1	A	402	GLY	3.2
1	A	269	ASP	2.9
1	A	270	LEU	2.7
1	A	298	SER	2.6
1	A	256	ASP	2.4
1	A	55	GLU	2.4
1	A	167	ILE	2.2
1	A	168	LEU	2.2
1	A	327	TRP	2.2
1	A	56	GLU	2.1
1	A	315	SER	2.1
1	A	342	PRO	2.1
1	A	189	ASN	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.