



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 03:47 AM UTC

PDB ID : 1MIQ / pdb_00001miq
Title : Crystal structure of proplasmepsin from the human malarial pathogen Plasmodium vivax
Authors : Bernstein, N.K.; Cherney, M.M.; Yowell, C.A.; Dame, J.B.; James, M.N.
Deposited on : 2002-08-23
Resolution : 2.50 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)	:	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

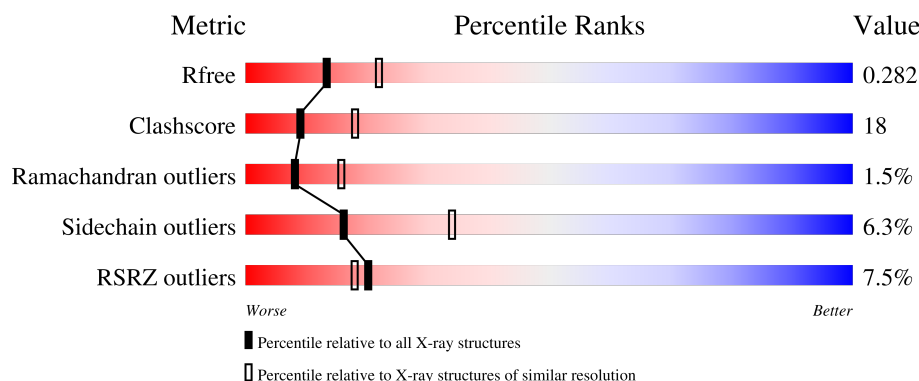
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

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	375	2% 67% 27% • •
1	B	375	13% 66% 29% 5%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 6032 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 plasmepsin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	373	Total	C	N	O	S	0	0	0
			2976	1927	457	579	13			
1	B	375	Total	C	N	O	S	0	0	0
			2993	1935	460	584	14			

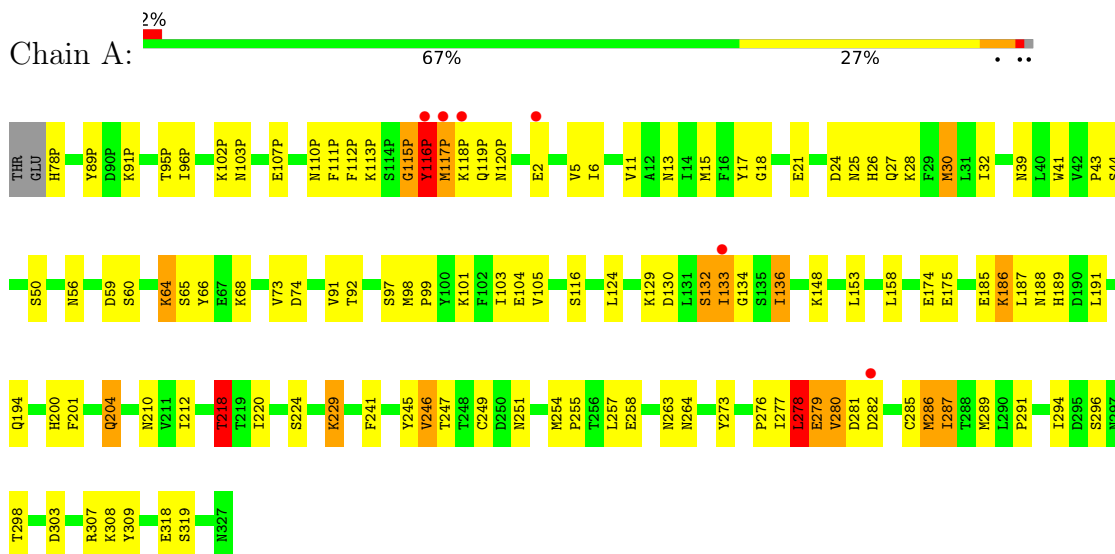
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	49	Total	O	0	0
			49	49		
2	B	14	Total	O	0	0
			14	14		

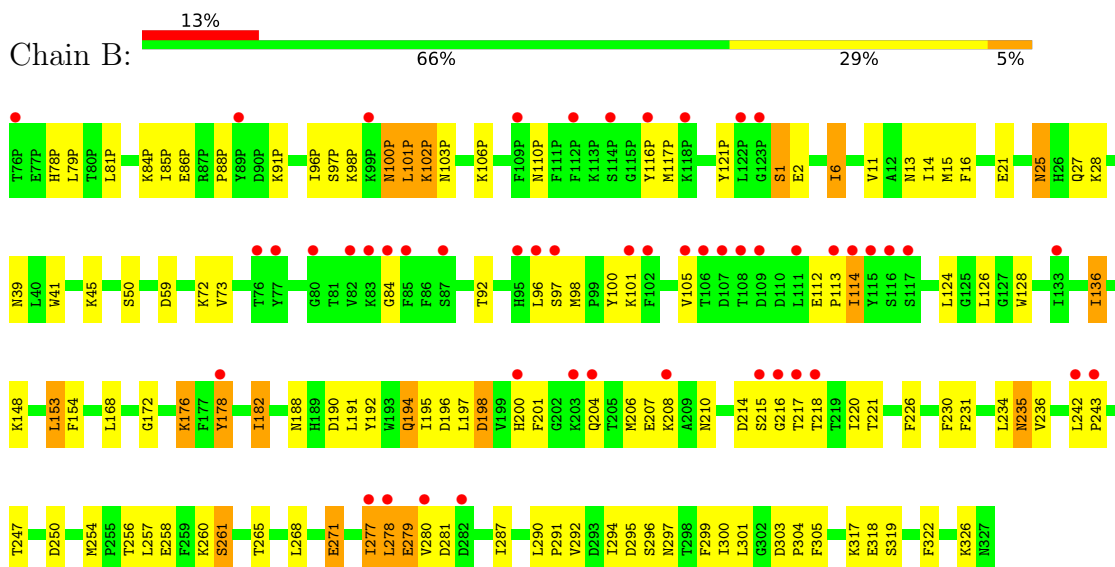
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: plasmepsin



• Molecule 1: plasmepsin



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	149.41Å 92.73Å 99.13Å 90.00° 130.11° 90.00°	Depositor
Resolution (Å)	30.00 – 2.50 30.00 – 2.50	Depositor EDS
% Data completeness (in resolution range)	99.3 (30.00-2.50) 99.3 (30.00-2.50)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.91 (at 2.51Å)	Xtriage
Refinement program	REFMAC 5.0	Depositor
R, R_{free}	0.203 , 0.245 (Not available) , 0.282	Depositor DCC
R_{free} test set	1852 reflections (5.19%)	wwPDB-VP
Wilson B-factor (Å ²)	54.2	Xtriage
Anisotropy	0.100	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 54.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.018 for -h-2*k,l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	6032	wwPDB-VP
Average B, all atoms (Å ²)	18.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.09% 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	0.81	2/3049 (0.1%)	1.11	11/4131 (0.3%)
1	B	0.67	0/3065	1.04	8/4153 (0.2%)
All	All	0.74	2/6114 (0.0%)	1.08	19/8284 (0.2%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	303	ASP	CA-C	5.66	1.58	1.52
1	A	30	MET	SD-CE	-5.25	1.66	1.79

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	134	GLY	N-CA-C	-7.31	102.72	112.81
1	A	294	ILE	N-CA-C	-7.24	105.59	111.81
1	A	39	ASN	N-CA-C	6.71	120.41	110.48
1	B	220	ILE	N-CA-C	-6.16	99.52	108.87
1	A	218	THR	OG1-CB-CG2	-6.10	97.09	109.30
1	B	114	ILE	N-CA-C	6.02	118.58	111.05
1	B	261	SER	CA-C-O	5.98	122.10	118.33
1	A	132	SER	N-CA-C	-5.55	106.27	113.16
1	A	298	THR	N-CA-C	5.53	118.25	109.24
1	A	220	ILE	N-CA-C	-5.41	101.86	109.21
1	B	214	ASP	N-CA-C	5.37	117.37	108.13
1	A	224	SER	N-CA-C	5.34	117.11	111.28
1	B	198	ASP	N-CA-C	-5.22	100.80	109.46
1	A	264	ASN	N-CA-C	5.16	117.04	109.24
1	B	178	TYR	N-CA-C	5.13	116.99	109.24
1	B	39	ASN	N-CA-C	5.13	118.07	110.48
1	B	261	SER	CB-CA-C	-5.06	109.09	116.53
1	A	120(P)	ASN	N-CA-C	-5.03	104.49	111.28
1	A	246	VAL	N-CA-C	5.01	116.93	108.81

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	2976	0	2877	107	0
1	B	2993	0	2897	112	0
2	A	49	0	0	0	0
2	B	14	0	0	0	0
All	All	6032	0	5774	216	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 18.

All (216) 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:194:GLN:NE2	1:A:210:ASN:HB3	1.58	1.16
1:A:194:GLN:HE21	1:A:210:ASN:HB3	1.07	1.02
1:B:278:LEU:H	1:B:278:LEU:CD2	1.72	1.01
1:B:78(P):HIS:CE1	1:B:172:GLY:HA3	1.99	0.98
1:A:189:HIS:HD2	1:A:191:LEU:H	1.05	0.97
1:B:191:LEU:C	1:B:192:TYR:HD2	1.77	0.92
1:A:186:LYS:HD2	1:A:187:LEU:O	1.69	0.91
1:B:278:LEU:H	1:B:278:LEU:HD23	1.35	0.91
1:A:17:TYR:C	1:A:30:MET:HE1	1.94	0.91
1:B:235:ASN:O	1:B:247:THR:HG22	1.71	0.90
1:B:25:ASN:H	1:B:25:ASN:HD22	1.18	0.85
1:B:101:LYS:HD3	1:B:136:ILE:HD11	1.56	0.84
1:A:44:SER:HB2	1:A:104:GLU:HG2	1.58	0.84
1:A:27:GLN:HE22	1:A:59:ASP:H	1.21	0.84
1:B:117(P):MET:HE1	1:B:121(P):TYR:HB2	1.58	0.83
1:A:30:MET:HE3	1:A:30:MET:HA	1.61	0.83
1:A:247:THR:HG21	1:A:254:MET:CE	2.09	0.82
1:A:116(P):TYR:H	1:A:116(P):TYR:HD1	1.28	0.82
1:B:278:LEU:HD23	1:B:278:LEU:N	1.94	0.81

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:189:HIS:CD2	1:A:191:LEU:H	1.96	0.79
1:A:186:LYS:HD3	1:A:187:LEU:N	1.96	0.79
1:B:79(P):LEU:HD22	1:B:96:LEU:HD12	1.64	0.79
1:A:277:ILE:HG22	1:A:286:MET:HE3	1.66	0.78
1:B:277:ILE:CG2	1:B:280:VAL:HG12	2.15	0.77
1:B:191:LEU:C	1:B:192:TYR:CD2	2.61	0.77
1:A:17:TYR:C	1:A:30:MET:CE	2.61	0.73
1:A:247:THR:HG21	1:A:254:MET:HE3	1.69	0.72
1:B:191:LEU:O	1:B:192:TYR:HD2	1.72	0.72
1:A:11:VAL:O	1:A:218:THR:HG22	1.91	0.71
1:A:251:ASN:ND2	1:A:254:MET:HE2	2.06	0.70
1:A:279:GLU:OE1	1:A:281:ASP:O	2.09	0.70
1:B:78(P):HIS:ND1	1:B:172:GLY:HA3	2.05	0.70
1:A:287:ILE:HD12	1:A:287:ILE:N	2.07	0.70
1:B:101:LYS:HD3	1:B:136:ILE:CD1	2.23	0.69
1:A:245:TYR:O	1:A:286:MET:HA	1.95	0.67
1:B:45:LYS:NZ	1:B:59:ASP:OD2	2.26	0.66
1:A:249:CYS:SG	1:A:282:ASP:HB3	2.36	0.66
1:B:277:ILE:HG22	1:B:280:VAL:HG12	1.76	0.65
1:B:206:MET:HE2	1:B:299:PHE:HE2	1.61	0.65
1:A:18:GLY:N	1:A:30:MET:HE1	2.11	0.65
1:B:234:LEU:HB3	1:B:254:MET:HE1	1.78	0.64
1:B:278:LEU:H	1:B:278:LEU:HD22	1.60	0.64
1:A:279:GLU:O	1:A:281:ASP:N	2.31	0.64
1:B:86(P):GLU:HG3	1:B:16:PHE:CE1	2.32	0.64
1:A:129:LYS:HE2	1:A:191:LEU:CD1	2.28	0.64
1:A:117(P):MET:O	1:A:119(P):GLN:N	2.29	0.64
1:A:194:GLN:NE2	1:A:210:ASN:CB	2.49	0.63
1:B:13:ASN:HD21	1:B:218:THR:HG23	1.64	0.63
1:B:206:MET:CE	1:B:299:PHE:HE2	2.13	0.61
1:A:153:LEU:C	1:A:153:LEU:HD12	2.25	0.61
1:B:236:VAL:HA	1:B:247:THR:HG23	1.82	0.60
1:A:247:THR:HG22	1:A:287:ILE:HD11	1.82	0.60
1:A:186:LYS:HD3	1:A:187:LEU:H	1.65	0.60
1:B:11:VAL:HG12	1:B:11:VAL:O	2.01	0.60
1:B:295:ASP:O	1:B:297:ASN:N	2.29	0.60
1:B:153:LEU:HD12	1:B:153:LEU:C	2.27	0.60
1:B:101(P):LEU:O	1:B:103(P):ASN:N	2.35	0.60
1:A:21:GLU:HG2	1:A:28:LYS:HD3	1.84	0.60
1:B:201:PHE:CD1	1:B:257:LEU:HD22	2.36	0.59
1:B:178:TYR:O	1:B:326:LYS:HE3	2.03	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:102(P):LYS:HB2	1:A:278:LEU:HD21	1.83	0.59
1:B:206:MET:HE1	1:B:297:ASN:HA	1.84	0.59
1:B:235:ASN:O	1:B:247:THR:CG2	2.50	0.59
1:A:2:GLU:H	1:A:2:GLU:CD	2.10	0.59
1:A:17:TYR:O	1:A:30:MET:CE	2.51	0.58
1:A:279:GLU:C	1:A:281:ASP:N	2.57	0.58
1:B:301:LEU:HD22	1:B:305:PHE:CD2	2.39	0.58
1:B:278:LEU:CD2	1:B:278:LEU:N	2.47	0.57
1:B:201:PHE:HB2	1:B:204:GLN:HB2	1.86	0.56
1:A:186:LYS:CD	1:A:187:LEU:N	2.68	0.56
1:A:194:GLN:HE21	1:A:210:ASN:CB	1.98	0.56
1:A:279:GLU:C	1:A:281:ASP:H	2.13	0.56
1:A:116(P):TYR:CD1	1:A:116(P):TYR:N	2.63	0.56
1:A:89(P):TYR:OH	1:A:278:LEU:HB3	2.06	0.56
1:B:13:ASN:ND2	1:B:218:THR:HG23	2.20	0.56
1:B:98:MET:HB3	1:B:148:LYS:HE3	1.88	0.56
1:B:128:TRP:HB2	1:B:191:LEU:O	2.06	0.56
1:B:194:GLN:CD	1:B:210:ASN:OD1	2.49	0.55
1:B:201:PHE:CD2	1:B:226:PHE:HE1	2.24	0.55
1:A:251:ASN:CG	1:A:254:MET:HE2	2.32	0.55
1:B:197:LEU:HD23	1:B:261:SER:HB3	1.89	0.55
1:A:112(P):PHE:HB2	1:A:116(P):TYR:OH	2.07	0.55
1:A:110(P):ASN:O	1:A:113(P):LYS:HG2	2.07	0.55
1:B:25:ASN:HD22	1:B:25:ASN:N	1.87	0.54
1:A:15:MET:O	1:A:32:ILE:HA	2.07	0.54
1:B:194:GLN:HE22	1:B:210:ASN:HD21	1.56	0.54
1:B:25:ASN:HD21	1:B:27:GLN:HE21	1.54	0.54
1:B:14:ILE:N	1:B:14:ILE:HD13	2.23	0.54
1:B:277:ILE:HB	1:B:280:VAL:CG1	2.38	0.53
1:B:200:HIS:HB2	1:B:258:GLU:HB2	1.89	0.53
1:A:249:CYS:CB	1:A:282:ASP:HB3	2.38	0.53
1:B:196:ASP:O	1:B:197:LEU:HG	2.08	0.53
1:A:279:GLU:O	1:A:280:VAL:C	2.50	0.53
1:A:18:GLY:HA2	1:A:30:MET:HE3	1.91	0.53
1:B:192:TYR:CD2	1:B:192:TYR:N	2.68	0.53
1:A:111(P):PHE:HD2	1:A:116(P):TYR:CE1	2.27	0.53
1:A:30:MET:HE3	1:A:30:MET:CA	2.36	0.53
1:B:206:MET:HE3	1:B:297:ASN:HB2	1.90	0.53
1:A:11:VAL:C	1:A:218:THR:HG22	2.33	0.53
1:B:86(P):GLU:HG3	1:B:16:PHE:HE1	1.73	0.52
1:A:111(P):PHE:HD2	1:A:116(P):TYR:HE1	1.57	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:41:TRP:CE3	1:B:105:VAL:HG21	2.45	0.52
1:B:81(P):LEU:HD12	1:B:168:LEU:HD23	1.90	0.52
1:B:13:ASN:C	1:B:14:ILE:HD13	2.35	0.52
1:B:25:ASN:H	1:B:25:ASN:ND2	1.98	0.52
1:B:250:ASP:OD1	1:B:250:ASP:C	2.53	0.51
1:A:129:LYS:HE2	1:A:191:LEU:HD13	1.92	0.51
1:B:98(P):LYS:O	1:B:102(P):LYS:HB3	2.10	0.51
1:A:273:TYR:CD1	1:A:289:MET:HE3	2.46	0.51
1:A:308:LYS:HD3	1:A:309:TYR:CE1	2.46	0.51
1:B:124:LEU:C	1:B:124:LEU:HD23	2.36	0.51
1:A:96(P):ILE:HD12	1:A:96(P):ILE:N	2.27	0.50
1:A:187:LEU:HG	1:A:318:GLU:O	2.11	0.50
1:B:11:VAL:O	1:B:11:VAL:CG1	2.59	0.50
1:B:112:GLU:HB3	1:B:113:PRO:HA	1.93	0.50
1:B:114:ILE:HD12	1:B:114:ILE:C	2.36	0.50
1:B:6:ILE:HD12	1:B:291:PRO:HD2	1.94	0.50
1:A:279:GLU:CD	1:A:281:ASP:O	2.55	0.50
1:B:198:ASP:OD2	1:B:208:LYS:HD2	2.11	0.50
1:B:6:ILE:CD1	1:B:290:LEU:HD22	2.42	0.50
1:A:92:THR:HG1	1:A:97:SER:HG	1.60	0.49
1:A:117(P):MET:C	1:A:119(P):GLN:N	2.70	0.49
1:B:231:PHE:O	1:B:234:LEU:N	2.42	0.49
1:A:194:GLN:HG3	1:A:212:ILE:HG13	1.94	0.49
1:A:130:ASP:OD2	1:A:136:ILE:HB	2.13	0.48
1:A:158:LEU:HB3	1:A:307:ARG:CZ	2.43	0.48
1:A:117(P):MET:C	1:A:119(P):GLN:H	2.21	0.48
1:A:78(P):HIS:HB2	1:A:174:GLU:OE1	2.13	0.48
1:A:200:HIS:HB2	1:A:258:GLU:HB2	1.96	0.48
1:B:176:LYS:HZ2	1:B:176:LYS:HB3	1.78	0.48
1:A:21:GLU:OE2	1:A:28:LYS:HE3	2.14	0.48
1:B:235:ASN:C	1:B:247:THR:HG22	2.39	0.48
1:A:291:PRO:O	1:A:291:PRO:HG2	2.13	0.48
1:B:206:MET:HE2	1:B:299:PHE:CE2	2.45	0.48
1:A:251:ASN:HB3	1:A:254:MET:HG2	1.95	0.48
1:A:287:ILE:N	1:A:287:ILE:CD1	2.75	0.48
1:B:88(P):PRO:HD2	1:B:218:THR:HG21	1.96	0.48
1:A:247:THR:CG2	1:A:254:MET:HE3	2.43	0.48
1:A:103(P):ASN:O	1:A:107(P):GLU:HB2	2.14	0.47
1:B:96(P):ILE:O	1:B:96(P):ILE:HG23	2.15	0.47
1:B:84(P):LYS:HD3	1:B:85(P):ILE:N	2.29	0.47
1:B:235:ASN:C	1:B:247:THR:CG2	2.88	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:60:SER:HB2	1:A:66:TYR:CG	2.49	0.47
1:A:73:VAL:HG21	1:A:103:ILE:HD13	1.96	0.47
1:A:278:LEU:HD23	1:A:279:GLU:H	1.79	0.47
1:A:111(P):PHE:O	1:A:115(P):GLY:N	2.42	0.47
1:A:257:LEU:HD11	1:A:289:MET:HE2	1.97	0.47
1:B:221:THR:OG1	1:B:300:ILE:HB	2.15	0.47
1:A:11:VAL:O	1:A:11:VAL:HG12	2.14	0.46
1:A:5:VAL:HG12	1:A:6:ILE:N	2.30	0.46
1:A:204:GLN:OE1	1:A:229:LYS:HG2	2.16	0.46
1:B:101(P):LEU:HG	1:B:102(P):LYS:H	1.81	0.46
1:B:271:GLU:H	1:B:271:GLU:HG3	1.50	0.46
1:A:254:MET:HA	1:A:255:PRO:HD3	1.80	0.46
1:A:194:GLN:HG3	1:A:212:ILE:CG1	2.45	0.45
1:B:182:ILE:HA	1:B:322:PHE:O	2.17	0.45
1:B:257:LEU:HD12	1:B:268:LEU:HD23	1.99	0.45
1:B:91(P):LYS:HE3	1:B:91(P):LYS:HB3	1.87	0.44
1:A:43:PRO:HG2	1:A:56:ASN:O	2.18	0.44
1:B:281:ASP:C	1:B:281:ASP:OD2	2.59	0.44
1:A:25:ASN:O	1:A:26:HIS:HB2	2.17	0.44
1:B:21:GLU:OE1	1:B:28:LYS:NZ	2.51	0.44
1:A:246:VAL:HA	1:A:285:CYS:O	2.17	0.44
1:B:198:ASP:HA	1:B:207:GLU:HA	1.98	0.44
1:A:98:MET:HB3	1:A:148:LYS:HE3	2.00	0.43
1:A:186:LYS:CD	1:A:186:LYS:C	2.91	0.43
1:A:276:PRO:HG3	1:A:282:ASP:OD2	2.18	0.43
1:A:107(P):GLU:HG2	1:B:103(P):ASN:HB3	2.00	0.43
1:B:279:GLU:H	1:B:279:GLU:HG2	1.59	0.43
1:A:188:ASN:OD1	1:A:188:ASN:C	2.62	0.43
1:B:96(P):ILE:O	1:B:96(P):ILE:CG2	2.66	0.43
1:B:97(P):SER:O	1:B:100(P):ASN:OD1	2.36	0.43
1:B:15:MET:HE2	1:B:216:GLY:CA	2.49	0.43
1:A:201:PHE:O	1:A:204:GLN:HB2	2.19	0.43
1:A:41:TRP:CE3	1:A:105:VAL:HG21	2.54	0.43
1:A:185:GLU:O	1:A:319:SER:HB3	2.19	0.43
1:B:101(P):LEU:O	1:B:102(P):LYS:C	2.62	0.43
1:B:260:LYS:HG2	1:B:265:THR:HG23	2.01	0.43
1:B:277:ILE:CG2	1:B:280:VAL:CG1	2.91	0.42
1:B:317:LYS:O	1:B:318:GLU:C	2.61	0.42
1:A:133:ILE:O	1:A:133:ILE:CG1	2.66	0.42
1:B:292:VAL:HG12	1:B:294:ILE:HG13	2.01	0.42
1:A:98:MET:HA	1:A:99:PRO:HD3	1.85	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:72:LYS:HD3	1:B:84:GLY:O	2.19	0.42
1:A:95(P):THR:HB	1:A:96(P):ILE:HD12	2.02	0.42
1:A:132:SER:O	1:A:133:ILE:C	2.62	0.42
1:B:235:ASN:HD22	1:B:235:ASN:HA	1.63	0.42
1:A:11:VAL:O	1:A:11:VAL:CG1	2.68	0.42
1:B:188:ASN:C	1:B:188:ASN:OD1	2.62	0.42
1:B:257:LEU:HD12	1:B:268:LEU:HB3	2.02	0.42
1:B:297:ASN:N	1:B:297:ASN:OD1	2.53	0.41
1:A:96(P):ILE:HD11	1:B:116(P):TYR:HB2	2.02	0.41
1:A:282:ASP:OD1	1:A:282:ASP:N	2.53	0.41
1:A:13:ASN:ND2	1:A:218:THR:HB	2.35	0.41
1:A:25:ASN:O	1:A:26:HIS:CB	2.65	0.41
1:B:92:THR:HG23	1:B:97:SER:HB3	2.02	0.41
1:B:303:ASP:HB3	1:B:304:PRO:HD3	2.03	0.41
1:A:186:LYS:HD3	1:A:186:LYS:C	2.45	0.41
1:B:236:VAL:HG13	1:B:287:ILE:HD13	2.03	0.41
1:A:25:ASN:C	1:A:26:HIS:CG	2.96	0.41
1:A:101:LYS:HB2	1:A:101:LYS:HE2	1.84	0.41
1:B:79(P):LEU:CD2	1:B:96:LEU:HD12	2.43	0.41
1:B:126:LEU:HB3	1:B:154:PHE:CZ	2.55	0.41
1:B:215:SER:C	1:B:217:THR:H	2.29	0.41
1:B:106(P):LYS:O	1:B:110(P):ASN:HB2	2.21	0.41
1:B:1:SER:OG	1:B:2:GLU:N	2.54	0.41
1:B:242:LEU:HA	1:B:243:PRO:HD3	1.87	0.40
1:B:257:LEU:HB2	1:B:268:LEU:HB3	2.03	0.40
1:A:24:ASP:OD2	1:A:64:LYS:HG2	2.22	0.40
1:A:73:VAL:O	1:A:74:ASP:OD2	2.39	0.40
1:A:124:LEU:HD23	1:A:124:LEU:C	2.47	0.40
1:B:231:PHE:CD2	1:B:236:VAL:HG11	2.56	0.40
1:A:241:PHE:CZ	1:B:121(P):TYR:CG	3.09	0.40
1:B:6:ILE:HD13	1:B:290:LEU:HD22	2.03	0.40
1:B:194:GLN:NE2	1:B:210:ASN:HD21	2.17	0.40
1:B:201:PHE:HB3	1:B:230:PHE:CD1	2.57	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	371/375 (99%)	348 (94%)	17 (5%)	6 (2%)	7	14
1	B	225/375 (60%)	210 (93%)	12 (5%)	3 (1%)	9	18
All	All	596/750 (80%)	558 (94%)	29 (5%)	9 (2%)	8	16

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	101(P)	LEU
1	B	102(P)	LYS
1	B	296	SER
1	A	115(P)	GLY
1	A	278	LEU
1	A	117(P)	MET
1	A	118(P)	LYS
1	A	280	VAL
1	A	116(P)	TYR

5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	332/340 (98%)	311 (94%)	21 (6%)	16	34
1	B	335/340 (98%)	314 (94%)	21 (6%)	16	34
All	All	667/680 (98%)	625 (94%)	42 (6%)	16	34

All (42) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	91(P)	LYS
1	A	116(P)	TYR
1	A	50	SER
1	A	64	LYS
1	A	65	SER
1	A	68	LYS
1	A	91	VAL
1	A	116	SER
1	A	133	ILE
1	A	136	ILE
1	A	175	GLU
1	A	186	LYS
1	A	204	GLN
1	A	218	THR
1	A	229	LYS
1	A	263	ASN
1	A	278	LEU
1	A	279	GLU
1	A	286	MET
1	A	287	ILE
1	A	296	SER
1	B	100(P)	ASN
1	B	1	SER
1	B	6	ILE
1	B	25	ASN
1	B	50	SER
1	B	73	VAL
1	B	100	TYR
1	B	136	ILE
1	B	153	LEU
1	B	176	LYS
1	B	182	ILE
1	B	190	ASP
1	B	194	GLN
1	B	195	ILE
1	B	235	ASN
1	B	256	THR
1	B	271	GLU
1	B	277	ILE
1	B	278	LEU
1	B	279	GLU
1	B	319	SER

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	100(P)	ASN
1	A	3	ASN
1	A	13	ASN
1	A	27	GLN
1	A	189	HIS
1	A	194	GLN
1	A	275	ASN
1	B	103(P)	ASN
1	B	110(P)	ASN
1	B	13	ASN
1	B	25	ASN
1	B	26	HIS
1	B	161	HIS
1	B	194	GLN
1	B	228	ASN
1	B	235	ASN
1	B	275	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 ⓘ

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	373/375 (99%)	-0.37	6 (1%) 70 67	2, 11, 28, 53	0
1	B	375/375 (100%)	0.83	50 (13%) 7 6	5, 20, 42, 59	0
All	All	748/750 (99%)	0.23	56 (7%) 20 18	2, 15, 40, 59	0

All (56) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	84	GLY	5.4
1	B	106	THR	4.6
1	B	105	VAL	4.6
1	B	109	ASP	4.6
1	B	133	ILE	4.6
1	B	108	THR	4.4
1	B	111	LEU	4.2
1	B	82	VAL	4.1
1	B	99(P)	LYS	4.0
1	A	116(P)	TYR	3.9
1	B	107	ASP	3.9
1	B	77	TYR	3.8
1	B	115	TYR	3.8
1	B	218	THR	3.7
1	B	76	THR	3.7
1	A	282	ASP	3.6
1	B	83	LYS	3.6
1	A	117(P)	MET	3.5
1	B	97	SER	3.5
1	B	113	PRO	3.4
1	B	76(P)	THR	3.3
1	B	122(P)	LEU	3.1
1	B	123(P)	GLY	3.1
1	B	89(P)	TYR	3.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	280	VAL	2.9
1	B	116(P)	TYR	2.9
1	B	87	SER	2.8
1	B	215	SER	2.8
1	B	243	PRO	2.8
1	B	200	HIS	2.8
1	B	101	LYS	2.7
1	B	114(P)	SER	2.7
1	B	85	PHE	2.7
1	B	112(P)	PHE	2.6
1	B	282	ASP	2.5
1	B	95	HIS	2.4
1	B	118(P)	LYS	2.4
1	B	216	GLY	2.4
1	A	133	ILE	2.4
1	B	117	SER	2.3
1	A	118(P)	LYS	2.3
1	B	116	SER	2.3
1	B	277	ILE	2.3
1	B	208	LYS	2.3
1	B	217	THR	2.2
1	B	204	GLN	2.2
1	B	80	GLY	2.2
1	A	2	GLU	2.1
1	B	242	LEU	2.1
1	B	114	ILE	2.1
1	B	96	LEU	2.1
1	B	278	LEU	2.1
1	B	203	LYS	2.1
1	B	102	PHE	2.0
1	B	109(P)	PHE	2.0
1	B	178	TYR	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.