



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 26, 2026 – 03:04 AM EDT

PDB ID : 8UKH / pdb_00008ukh
Title : Crystal structure of Plasmodium falciparum CelTOS in complex with antibody 4h12
Authors : Tang, W.K.; Tolia, N.H.; Urusova, D.
Deposited on : 2023-10-13
Resolution : 3.52 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

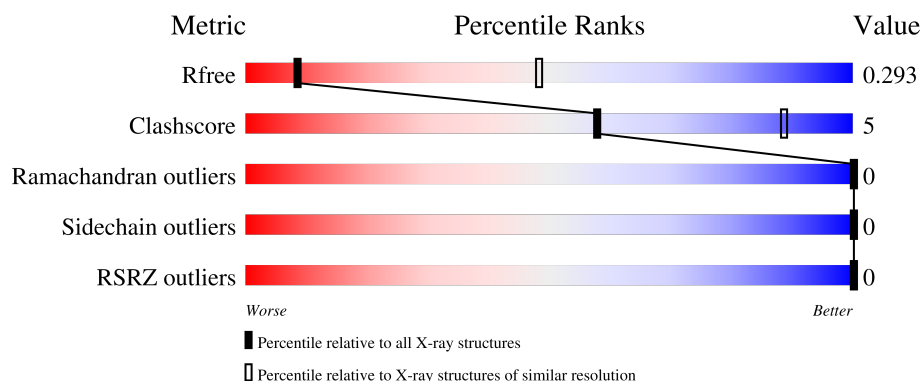
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.52 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.



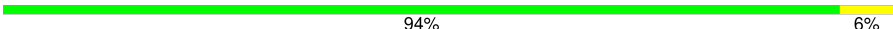
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1025 (3.56-3.48)
Clashscore	190562	1079 (3.56-3.48)
Ramachandran outliers	187476	1052 (3.56-3.48)
Sidechain outliers	187428	1053 (3.56-3.48)
RSRZ outliers	180081	1024 (3.56-3.48)

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	168	
1	B	168	
1	C	168	
1	D	168	
2	H	218	

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Mol	Chain	Length	Quality of chain
2	I	218	 90%9%
2	J	218	 94%6%
2	K	218	 89%11%
3	L	210	 91%9%
3	M	210	 93%7%
3	N	210	 89%11%
3	O	210	 85%15%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 29232 atoms, of which 14469 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 Cell traversal protein for ookinetes and sporozoites.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	57	Total	C	H	N	O	S	0	0	0
			899	277	461	71	88	2			
1	B	56	Total	C	H	N	O	S	0	0	0
			888	274	456	70	86	2			
1	C	58	Total	C	H	N	O	S	0	0	0
			915	282	468	73	90	2			
1	D	58	Total	C	H	N	O	S	0	0	0
			915	282	468	73	90	2			

There are 40 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	23	MET	-	initiating methionine	UNP Q8I5P1
A	24	GLY	-	expression tag	UNP Q8I5P1
A	183	LEU	-	expression tag	UNP Q8I5P1
A	184	GLU	-	expression tag	UNP Q8I5P1
A	185	HIS	-	expression tag	UNP Q8I5P1
A	186	HIS	-	expression tag	UNP Q8I5P1
A	187	HIS	-	expression tag	UNP Q8I5P1
A	188	HIS	-	expression tag	UNP Q8I5P1
A	189	HIS	-	expression tag	UNP Q8I5P1
A	190	HIS	-	expression tag	UNP Q8I5P1
B	23	MET	-	initiating methionine	UNP Q8I5P1
B	24	GLY	-	expression tag	UNP Q8I5P1
B	183	LEU	-	expression tag	UNP Q8I5P1
B	184	GLU	-	expression tag	UNP Q8I5P1
B	185	HIS	-	expression tag	UNP Q8I5P1
B	186	HIS	-	expression tag	UNP Q8I5P1
B	187	HIS	-	expression tag	UNP Q8I5P1
B	188	HIS	-	expression tag	UNP Q8I5P1
B	189	HIS	-	expression tag	UNP Q8I5P1
B	190	HIS	-	expression tag	UNP Q8I5P1
C	23	MET	-	initiating methionine	UNP Q8I5P1

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Chain	Residue	Modelled	Actual	Comment	Reference
C	24	GLY	-	expression tag	UNP Q8I5P1
C	183	LEU	-	expression tag	UNP Q8I5P1
C	184	GLU	-	expression tag	UNP Q8I5P1
C	185	HIS	-	expression tag	UNP Q8I5P1
C	186	HIS	-	expression tag	UNP Q8I5P1
C	187	HIS	-	expression tag	UNP Q8I5P1
C	188	HIS	-	expression tag	UNP Q8I5P1
C	189	HIS	-	expression tag	UNP Q8I5P1
C	190	HIS	-	expression tag	UNP Q8I5P1
D	23	MET	-	initiating methionine	UNP Q8I5P1
D	24	GLY	-	expression tag	UNP Q8I5P1
D	183	LEU	-	expression tag	UNP Q8I5P1
D	184	GLU	-	expression tag	UNP Q8I5P1
D	185	HIS	-	expression tag	UNP Q8I5P1
D	186	HIS	-	expression tag	UNP Q8I5P1
D	187	HIS	-	expression tag	UNP Q8I5P1
D	188	HIS	-	expression tag	UNP Q8I5P1
D	189	HIS	-	expression tag	UNP Q8I5P1
D	190	HIS	-	expression tag	UNP Q8I5P1

- Molecule 2 is a protein called 4h12 heavy chain.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	H	217	Total	C	H	N	O	S	0	0	0
			3209	1023	1596	268	317	5			
2	I	217	Total	C	H	N	O	S	0	0	0
			3209	1023	1596	268	317	5			
2	J	217	Total	C	H	N	O	S	0	0	0
			3209	1023	1596	268	317	5			
2	K	218	Total	C	H	N	O	S	0	0	0
			3221	1027	1600	269	320	5			

- Molecule 3 is a protein called 4h12 light chain.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
3	L	210	Total	C	H	N	O	S	0	0	0
			3189	1014	1557	279	332	7			
3	M	210	Total	C	H	N	O	S	0	0	0
			3189	1014	1557	279	332	7			
3	N	210	Total	C	H	N	O	S	0	0	0
			3189	1014	1557	279	332	7			

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Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
3	O	210	Total	C	H	N	O	S	0	0	0
			3189	1014	1557	279	332	7			

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	C	1	Total	O	0	0
			1	1		
4	H	1	Total	O	0	0
			1	1		
4	J	3	Total	O	0	0
			3	3		
4	K	1	Total	O	0	0
			1	1		
4	N	3	Total	O	0	0
			3	3		
4	O	2	Total	O	0	0
			2	2		

- Molecule 1: Cell traversal protein for ookinetes and sporozoites



ALA GLU ASN VAL LYS PRO PRO LYS VAL ASP PRO ALA THR TYR GLY ILE VAL PRO VAL LEU THR SER LEU PHE ASN VAL GLU THR ALA VAL GLY ALA LYS VAL SER ASP GLU ILE TRP TYR ASN SER ASP VAL SER GLU GLU SER LEU SER ASP PHE

ASP LEU GLU HIS HIS HIS HIS HIS

• Molecule 2: 4h12 heavy chain

Chain H:  89% 11%

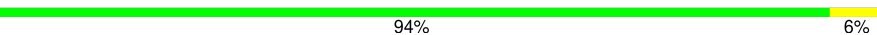
Q1 L4 V12 K13 A16 S17 V18 A24 V37 L45 E46 R50 L86 R98 Q99 G100 T101 V102 T155 L163 V185 W192 P193 T198 A202 D211 K212 R217 ASP

• Molecule 2: 4h12 heavy chain

Chain I:  90% 9%

Q1 L4 Q5 Q6 L11 V12 K13 P14 G15 A16 C22 K23 A24 L34 W47 C96 T114 V115 S116 V140 C144 W158 W192 C199 I214 R217 ASP

• Molecule 2: 4h12 heavy chain

Chain J:  94% 6%

Q1 V12 K13 V102 P130 V140 W158 L163 V185 T191 W192 E195 C199 R217 ASP

• Molecule 2: 4h12 heavy chain

Chain K:  89% 11%

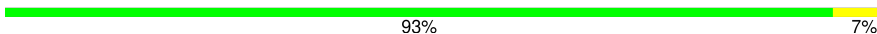
Q1 Q6 L11 V12 K13 K19 V33 K36 R50 Y80 L81 Q82 F95 R98 V102 V103 F104 D105 Y106 K119 N137 E152 P153 V154 W158 L181 S189 C199 D218

• Molecule 3: 4h12 light chain

Chain L:  91% 9%

D1 M4 F10 C23 A32 V33 L83 Q89 Q90 Y91 F97 T102 L105 E122 D169 S170 T171 K182 Y185 E186 Y191 R210

• Molecule 3: 4h12 light chain

Chain M:  93% 7%

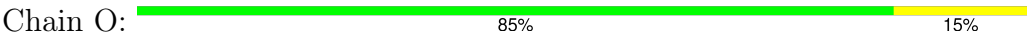
D1 M4 F10 C23 V33 L83 Q89 Q90 S94 L95 T102 L105 K146 E153 D169 S170 T171 R210

• Molecule 3: 4h12 light chain

Chain N:  89% 11%



● Molecule 3: 4h12 light chain



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	59.69Å 59.73Å 153.44Å 82.07° 82.20° 72.27°	Depositor
Resolution (Å)	19.86 – 3.52 19.86 – 3.52	Depositor EDS
% Data completeness (in resolution range)	97.1 (19.86-3.52) 97.7 (19.86-3.52)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.68 (at 3.52Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.268 , 0.293 0.266 , 0.293	Depositor DCC
R_{free} test set	1215 reflections (2.23%)	wwPDB-VP
Wilson B-factor (Å ²)	37.0	Xtriage
Anisotropy	1.391	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 19.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.398 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	29232	wwPDB-VP
Average B, all atoms (Å ²)	54.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 44.32 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.5516e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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 [i](#)

5.1 Standard geometry [i](#)

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	0.11	0/442	0.39	0/591
1	B	0.11	0/436	0.33	0/583
1	C	0.14	0/451	0.38	0/603
1	D	0.11	0/451	0.33	0/603
2	H	0.13	0/1655	0.38	0/2264
2	I	0.14	0/1655	0.36	0/2264
2	J	0.13	0/1655	0.38	0/2264
2	K	0.16	0/1663	0.39	0/2275
3	L	0.10	0/1668	0.31	0/2264
3	M	0.10	0/1668	0.33	0/2264
3	N	0.11	0/1668	0.35	0/2264
3	O	0.11	0/1668	0.36	0/2264
All	All	0.12	0/15080	0.36	0/20503

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 [i](#)

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	438	461	460	1	0
1	B	432	456	455	1	0
1	C	447	468	468	7	0
1	D	447	468	468	11	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	H	1613	1596	1596	24	0
2	I	1613	1596	1596	14	0
2	J	1613	1596	1596	9	0
2	K	1621	1600	1600	20	0
3	L	1632	1557	1557	14	0
3	M	1632	1557	1557	11	0
3	N	1632	1557	1557	16	0
3	O	1632	1557	1557	20	0
4	C	1	0	0	0	0
4	H	1	0	0	0	0
4	J	3	0	0	0	0
4	K	1	0	0	0	0
4	N	3	0	0	0	0
4	O	2	0	0	0	0
All	All	14763	14469	14467	132	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 5.

All (132) 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)
2:H:12:VAL:HG11	2:H:86:LEU:HD12	1.43	1.00
2:H:12:VAL:HG21	2:H:18:VAL:HG13	1.61	0.82
3:N:107:ARG:NH1	3:N:108:ALA:O	2.15	0.80
2:H:12:VAL:CG1	2:H:16:ALA:HB3	2.12	0.79
2:H:198:THR:HG21	2:H:211:ASP:OD1	1.85	0.75
2:H:12:VAL:HG13	2:H:16:ALA:HB3	1.68	0.75
3:N:109:ASP:HB3	3:N:199:THR:HG21	1.70	0.72
2:H:12:VAL:CG1	2:H:86:LEU:HD12	2.19	0.71
2:I:140:VAL:HG21	2:I:192:TRP:CZ3	2.26	0.71
3:N:85:ASP:OD1	3:N:102:THR:HG22	1.92	0.70
2:K:154:VAL:CG2	2:K:181:LEU:HD21	2.22	0.68
3:M:89:GLN:HE21	3:M:95:LEU:HD22	1.58	0.68
2:H:102:VAL:HG11	3:L:91:TYR:CG	2.29	0.68
1:A:114:LEU:O	1:A:114:LEU:HD12	1.94	0.67
2:H:12:VAL:HG21	2:H:18:VAL:CG1	2.26	0.65
3:O:145:VAL:HG21	3:O:174:MET:HE2	1.80	0.64
3:O:29:VAL:HG11	3:O:90:GLN:HG3	1.78	0.64
3:N:169:ASP:O	3:N:171:THR:N	2.32	0.63
2:K:33:TRP:CZ3	2:K:50:ARG:HG3	2.34	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:O:24:LYS:NZ	3:O:70:ASP:OD1	2.33	0.61
3:O:83:LEU:HD11	3:O:105:LEU:HD21	1.82	0.61
1:C:72:ILE:CD1	1:D:72:ILE:HD11	2.30	0.61
2:I:47:TRP:CG	3:M:95:LEU:HD12	2.36	0.60
2:H:198:THR:HG23	2:H:212:LYS:O	2.01	0.60
2:K:19:LYS:HG3	2:K:82:GLN:HG2	1.84	0.60
2:H:12:VAL:HG12	2:H:13:LYS:O	2.02	0.60
3:M:89:GLN:NE2	3:M:95:LEU:HD22	2.17	0.59
3:O:36:TYR:CE1	3:O:46:LEU:HD12	2.38	0.59
2:I:22:CYS:SG	2:I:34:LEU:HD11	2.43	0.58
2:K:154:VAL:HG23	2:K:181:LEU:HD21	1.83	0.58
2:I:199:CYS:SG	2:I:214:ILE:HD11	2.44	0.58
2:I:11:LEU:HD23	2:I:114:THR:HB	1.86	0.57
2:H:45:LEU:HD23	3:L:97:PHE:CD1	2.38	0.57
1:C:72:ILE:HD12	1:D:72:ILE:HD11	1.87	0.57
3:L:83:LEU:HD11	3:L:105:LEU:HD21	1.86	0.56
2:H:4:LEU:HD23	2:H:24:ALA:HA	1.88	0.56
2:J:12:VAL:HG12	2:J:13:LYS:N	2.20	0.56
1:C:68:LEU:O	1:C:72:ILE:HG12	2.05	0.55
3:O:11:MET:HE2	3:O:20:ASN:O	2.07	0.55
3:N:29:VAL:HG11	3:N:90:GLN:HG3	1.89	0.55
3:O:90:GLN:OE1	3:O:92:SER:N	2.39	0.54
2:J:130:PRO:HD2	2:J:192:TRP:HH2	1.73	0.53
3:L:32:ALA:HB1	3:L:91:TYR:CD2	2.44	0.53
2:H:198:THR:HG23	2:H:212:LYS:C	2.34	0.52
3:M:169:ASP:O	3:M:171:THR:N	2.42	0.52
3:L:4:MET:HE3	3:L:23:CYS:SG	2.50	0.52
2:K:13:LYS:HE3	2:K:119:LYS:NZ	2.25	0.51
1:C:80:LEU:HD22	1:D:114:LEU:HD21	1.93	0.51
2:H:102:VAL:HG11	3:L:91:TYR:CD2	2.45	0.51
3:O:85:ASP:OD1	3:O:102:THR:HG22	2.11	0.51
3:L:169:ASP:O	3:L:171:THR:N	2.44	0.50
3:L:10:PHE:CD2	3:L:102:THR:OG1	2.62	0.50
2:K:12:VAL:HG12	2:K:13:LYS:N	2.25	0.50
3:N:10:PHE:CD2	3:N:102:THR:OG1	2.66	0.49
2:I:144:CYS:SG	2:I:158:TRP:CH2	3.05	0.49
2:I:140:VAL:HG21	2:I:192:TRP:CE3	2.47	0.49
3:M:146:LYS:HE3	3:M:153:GLU:HG3	1.94	0.49
3:M:10:PHE:CD2	3:M:102:THR:OG1	2.62	0.48
3:M:33:VAL:HA	3:M:89:GLN:O	2.14	0.48
1:C:72:ILE:HD13	1:D:68:LEU:HD11	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:107:ARG:HH12	3:N:110:ALA:HB2	1.78	0.48
2:H:212:LYS:NZ	3:L:122:GLU:OE1	2.46	0.47
3:N:166:ASP:HB3	3:N:169:ASP:O	2.14	0.47
3:O:4:MET:SD	3:O:90:GLN:HB2	2.54	0.47
3:O:46:LEU:HD23	3:O:55:HIS:CG	2.50	0.47
2:H:50:ARG:CZ	2:H:101:THR:HG23	2.45	0.47
2:J:130:PRO:HD2	2:J:192:TRP:CH2	2.49	0.47
2:I:4:LEU:HD23	2:I:24:ALA:HA	1.97	0.46
3:M:90:GLN:NE2	3:M:94:SER:O	2.48	0.46
2:K:11:LEU:C	2:K:12:VAL:HG23	2.40	0.46
2:K:152:GLU:HB3	2:K:153:PRO:HA	1.98	0.46
2:H:98:ARG:HG2	2:H:99:GLY:N	2.30	0.46
2:I:12:VAL:CG1	2:I:16:ALA:HB3	2.45	0.46
2:K:105:ASP:O	2:K:106:TYR:CD1	2.69	0.46
3:O:180:LEU:HD22	3:O:184:GLU:OE1	2.16	0.46
3:L:33:VAL:HA	3:L:89:GLN:O	2.16	0.46
2:K:154:VAL:HG21	2:K:181:LEU:HD21	1.95	0.46
3:L:182:LYS:NZ	3:L:186:GLU:OE2	2.37	0.46
1:D:84:SER:HB3	1:D:88:LEU:HD11	1.98	0.45
2:J:12:VAL:CG1	2:J:13:LYS:N	2.79	0.45
2:K:19:LYS:HE3	2:K:80:TYR:CD1	2.51	0.45
2:H:12:VAL:CG2	2:H:18:VAL:CG1	2.94	0.45
2:H:192:TRP:CG	2:H:193:PRO:HA	2.51	0.45
2:K:6:GLN:HE22	2:K:95:PHE:HA	1.82	0.45
3:O:18:ARG:HG2	3:O:76:SER:O	2.17	0.45
3:N:154:ARG:NH2	3:N:180:LEU:CD2	2.80	0.45
2:K:13:LYS:HE2	2:K:119:LYS:HE2	1.99	0.45
3:O:4:MET:HE3	3:O:23:CYS:SG	2.55	0.45
2:K:98:ARG:O	2:K:104:PHE:HA	2.17	0.45
2:H:45:LEU:HD23	3:L:97:PHE:CE1	2.51	0.44
3:N:180:LEU:HD22	3:N:184:GLU:OE1	2.17	0.44
2:J:163:LEU:CD2	2:J:185:VAL:HG21	2.47	0.44
2:I:11:LEU:CD2	2:I:114:THR:HB	2.47	0.44
3:O:2:ILE:O	3:O:96:THR:HG21	2.18	0.43
1:C:72:ILE:HD12	1:D:68:LEU:HG	2.01	0.43
2:J:191:THR:O	2:J:195:GLU:HB2	2.18	0.43
3:M:4:MET:HE3	3:M:23:CYS:SG	2.59	0.43
2:H:163:LEU:HD21	2:H:185:VAL:HG21	2.00	0.43
1:B:111:LYS:O	1:B:114:LEU:HG	2.18	0.43
3:N:124:LEU:O	3:N:182:LYS:HD2	2.19	0.42
2:I:14:PRO:HD3	2:I:116:SER:C	2.45	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:47:TRP:CD2	3:M:95:LEU:HD12	2.55	0.42
3:M:83:LEU:HD11	3:M:105:LEU:HD21	2.02	0.42
3:L:185:TYR:HA	3:L:191:TYR:OH	2.20	0.42
3:O:107:ARG:HG2	3:O:108:ALA:N	2.34	0.42
2:H:102:VAL:CG1	3:L:91:TYR:CG	3.01	0.42
1:D:114:LEU:N	1:D:115:PRO:CD	2.82	0.42
2:K:12:VAL:CG1	2:K:13:LYS:N	2.82	0.42
2:K:13:LYS:HE3	2:K:119:LYS:HZ3	1.85	0.42
2:K:158:TRP:CZ3	2:K:199:CYS:HB3	2.54	0.42
3:O:10:PHE:CD1	3:O:102:THR:OG1	2.72	0.42
2:I:6:GLN:OE1	2:I:96:CYS:SG	2.77	0.42
2:I:23:LYS:HB2	2:I:23:LYS:HE3	1.89	0.42
2:K:102:VAL:HA	3:O:95:LEU:HD21	2.01	0.42
1:D:114:LEU:N	1:D:115:PRO:HD2	2.34	0.41
3:N:148:LYS:HE2	3:N:153:GLU:HG2	2.02	0.41
3:N:85:ASP:CG	3:N:102:THR:HG22	2.45	0.41
2:H:37:VAL:HG13	2:H:46:GLU:O	2.21	0.41
1:C:113:GLY:HA3	1:D:80:LEU:HD13	2.03	0.41
2:J:158:TRP:CZ3	2:J:199:CYS:HB3	2.55	0.41
3:O:33:VAL:HA	3:O:89:GLN:O	2.19	0.41
1:D:87:PHE:O	1:D:88:LEU:HB2	2.21	0.41
2:K:36:TRP:HA	2:K:95:PHE:O	2.21	0.41
2:K:137:ASN:O	2:K:189:SER:HB3	2.21	0.41
3:N:169:ASP:OD1	3:N:169:ASP:C	2.63	0.41
2:J:140:VAL:O	2:J:140:VAL:HG13	2.21	0.41
3:O:33:VAL:HG21	3:O:71:PHE:CE2	2.56	0.40
2:J:102:VAL:HG12	3:N:95:LEU:HD11	2.03	0.40
2:H:155:THR:HB	2:H:202:ALA:HB3	2.02	0.40
1:D:73:SER:OG	1:D:95:LYS:HG3	2.21	0.40
3:N:39:ARG:HB3	3:N:40:PRO:CD	2.51	0.40
3:O:95:LEU:HD12	3:O:95:LEU:N	2.37	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	55/168 (33%)	52 (94%)	3 (6%)	0	100	100
1	B	54/168 (32%)	53 (98%)	1 (2%)	0	100	100
1	C	56/168 (33%)	53 (95%)	3 (5%)	0	100	100
1	D	56/168 (33%)	53 (95%)	3 (5%)	0	100	100
2	H	215/218 (99%)	206 (96%)	9 (4%)	0	100	100
2	I	215/218 (99%)	213 (99%)	2 (1%)	0	100	100
2	J	215/218 (99%)	207 (96%)	8 (4%)	0	100	100
2	K	216/218 (99%)	204 (94%)	12 (6%)	0	100	100
3	L	208/210 (99%)	200 (96%)	8 (4%)	0	100	100
3	M	208/210 (99%)	202 (97%)	6 (3%)	0	100	100
3	N	208/210 (99%)	200 (96%)	8 (4%)	0	100	100
3	O	208/210 (99%)	196 (94%)	12 (6%)	0	100	100
All	All	1914/2384 (80%)	1839 (96%)	75 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	53/153 (35%)	53 (100%)	0	100	100
1	B	52/153 (34%)	52 (100%)	0	100	100
1	C	54/153 (35%)	54 (100%)	0	100	100
1	D	54/153 (35%)	54 (100%)	0	100	100
2	H	183/184 (100%)	183 (100%)	0	100	100
2	I	183/184 (100%)	183 (100%)	0	100	100
2	J	183/184 (100%)	183 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	K	184/184 (100%)	184 (100%)	0	100	100
3	L	185/185 (100%)	185 (100%)	0	100	100
3	M	185/185 (100%)	185 (100%)	0	100	100
3	N	185/185 (100%)	185 (100%)	0	100	100
3	O	185/185 (100%)	185 (100%)	0	100	100
All	All	1686/2088 (81%)	1686 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

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	62	ASN
1	B	74	ASN
1	B	101	HIS
2	I	200	ASN
2	J	39	GLN
3	L	144	ASN
3	M	188	HIS
3	N	8	HIS
3	N	20	ASN
3	O	144	ASN
3	O	189	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

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 [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	57/168 (33%)	-0.88	0 100 100	61, 69, 84, 86	0
1	B	56/168 (33%)	-0.94	0 100 100	64, 71, 85, 94	0
1	C	58/168 (34%)	-0.91	0 100 100	28, 41, 71, 80	0
1	D	58/168 (34%)	-1.03	0 100 100	26, 40, 68, 74	0
2	H	217/218 (99%)	-0.84	0 100 100	63, 66, 78, 85	0
2	I	217/218 (99%)	-0.82	0 100 100	56, 63, 72, 84	0
2	J	217/218 (99%)	-1.02	0 100 100	29, 34, 53, 72	0
2	K	218/218 (100%)	-1.01	0 100 100	29, 37, 53, 76	0
3	L	210/210 (100%)	-0.79	0 100 100	62, 72, 81, 86	0
3	M	210/210 (100%)	-0.87	0 100 100	58, 67, 76, 82	0
3	N	210/210 (100%)	-1.01	0 100 100	27, 38, 56, 65	0
3	O	210/210 (100%)	-1.00	0 100 100	30, 42, 61, 67	0
All	All	1938/2384 (81%)	-0.92	0 100 100	26, 60, 77, 94	0

There are no RSRZ outliers to report.

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.