Full wwPDB X-ray Structure Validation Report ⓘ

Oct 15, 2023 – 10:46 AM EDT

PDB ID	:	7UCQ
Title	:	Pfs230 D1 domain in complex with 230AS-18
Authors	:	Tang, W.K.; Tolia, N.H.
Deposited on	:	2022-03-17
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:

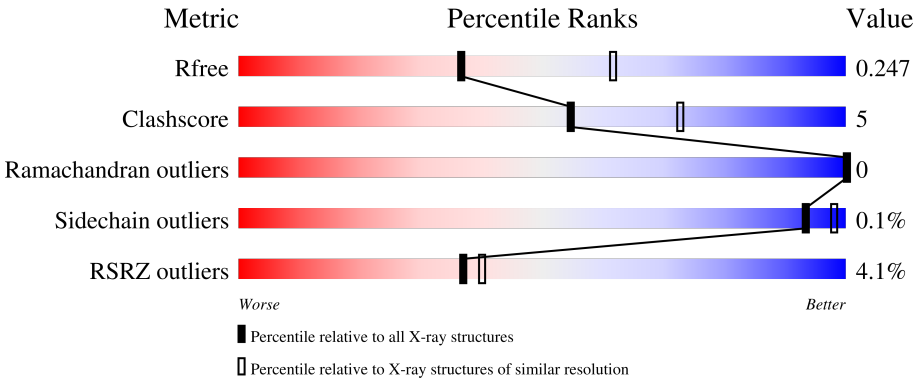
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

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}	130704	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (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 <=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	191	6% 83% 9% 8%
1	B	191	16% 83% 9% 8%
1	C	191	5% 75% 17% 8%
1	D	191	4% 83% 9% 8%
2	H	261	83% 6% 11%

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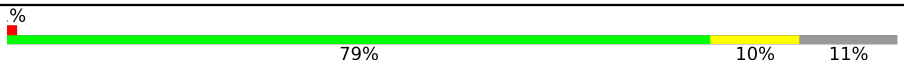
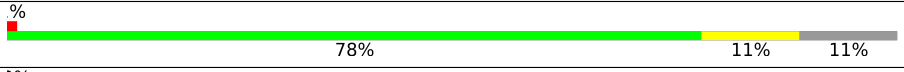
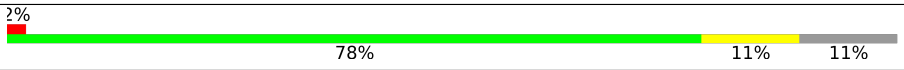
Mol	Chain	Length	Quality of chain
2	I	261	
2	J	261	
2	K	261	

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 25470 atoms, of which 12580 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 Gametocyte surface protein P230.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	176	Total	C	H	N	O	S	0	0	0
			2825	901	1418	219	283	4			
1	B	176	Total	C	H	N	O	S	0	0	0
			2825	901	1418	219	283	4			
1	C	176	Total	C	H	N	O	S	0	0	0
			2825	901	1418	219	283	4			
1	D	176	Total	C	H	N	O	S	0	0	0
			2825	901	1418	219	283	4			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	585	GLN	ASN	engineered mutation	UNP P68874
B	585	GLN	ASN	engineered mutation	UNP P68874
C	585	GLN	ASN	engineered mutation	UNP P68874
D	585	GLN	ASN	engineered mutation	UNP P68874

- Molecule 2 is a protein called 230AS-18.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	H	233	Total	C	H	N	O	S	0	0	0
			3514	1130	1727	306	345	6			
2	I	233	Total	C	H	N	O	S	0	0	0
			3514	1130	1727	306	345	6			
2	J	233	Total	C	H	N	O	S	0	0	0
			3514	1130	1727	306	345	6			
2	K	233	Total	C	H	N	O	S	0	0	0
			3514	1130	1727	306	345	6			

- Molecule 3 is water.

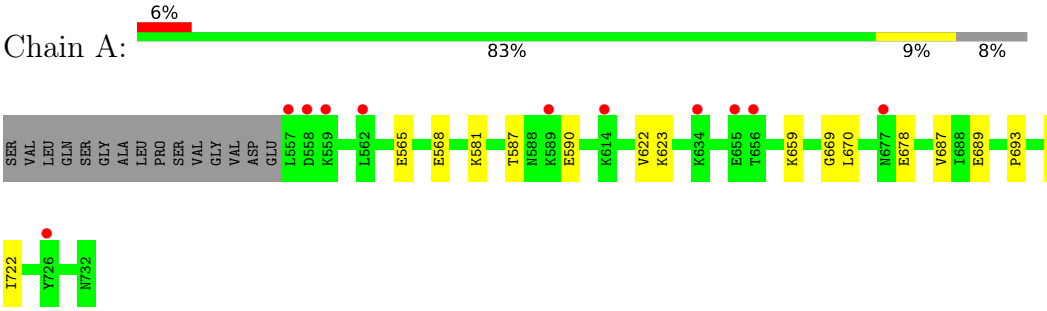
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	10	Total O 10 10	0	0
3	H	23	Total O 23 23	0	0
3	B	6	Total O 6 6	0	0
3	I	19	Total O 19 19	0	0
3	C	10	Total O 10 10	0	0
3	J	12	Total O 12 12	0	0
3	D	10	Total O 10 10	0	0
3	K	24	Total O 24 24	0	0

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.

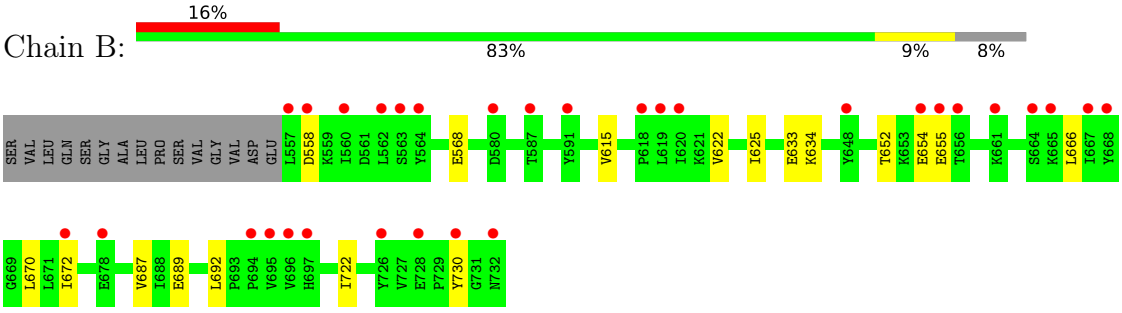
• Molecule 1: Gametocyte surface protein P230

Chain A:



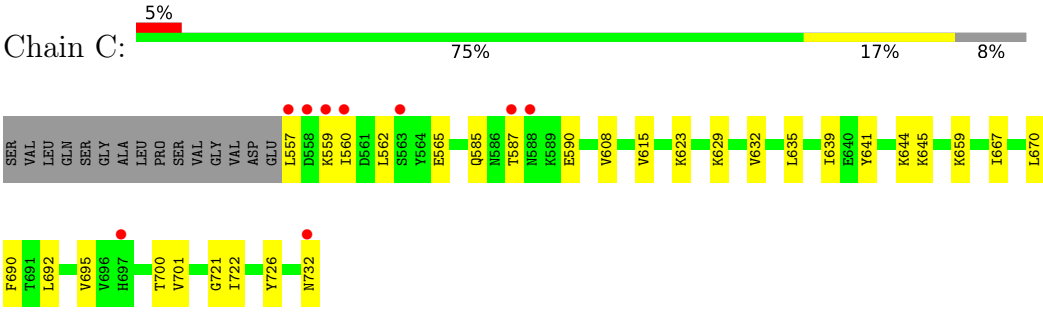
• Molecule 1: Gametocyte surface protein P230

Chain B:



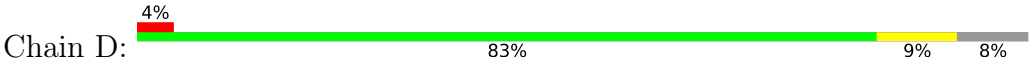
• Molecule 1: Gametocyte surface protein P230

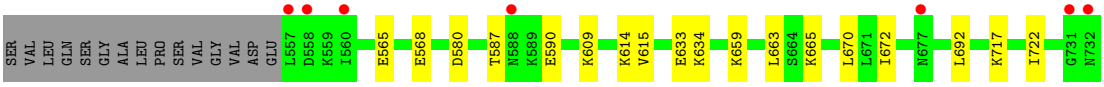
Chain C:



• Molecule 1: Gametocyte surface protein P230

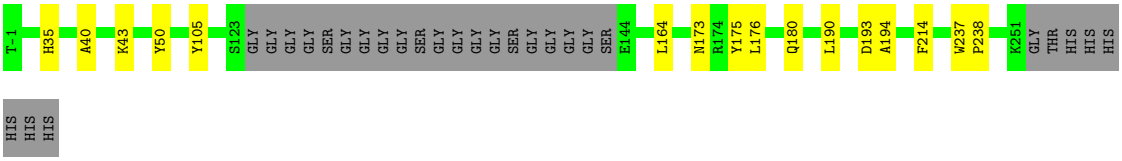
Chain D:





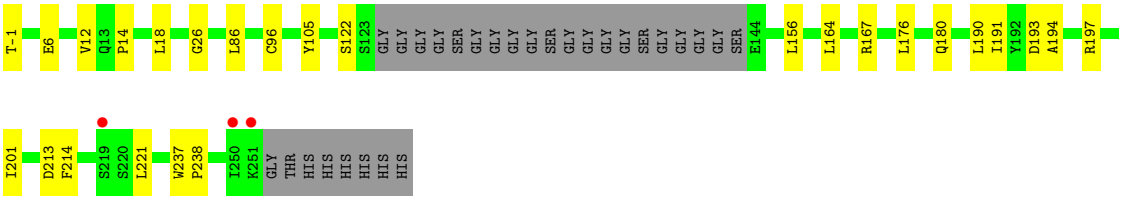
• Molecule 2: 230AS-18

Chain H:



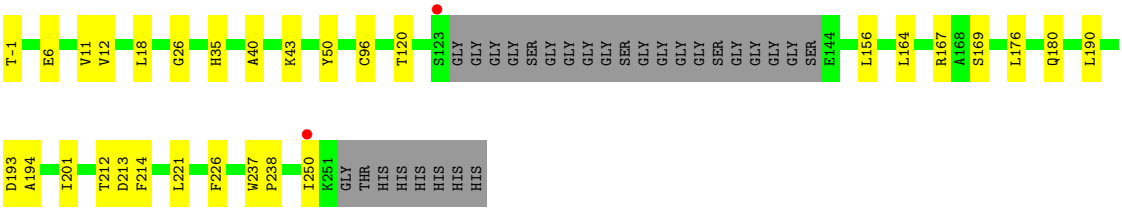
• Molecule 2: 230AS-18

Chain I:



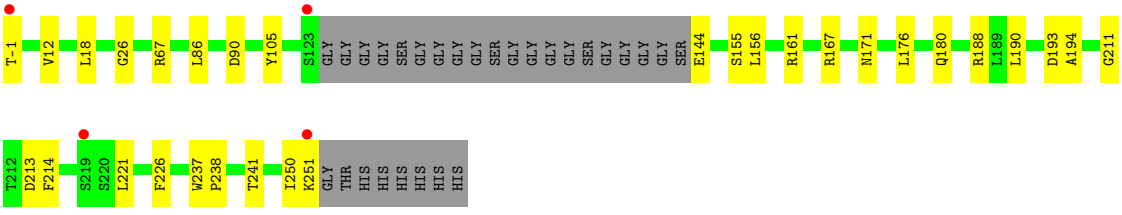
• Molecule 2: 230AS-18

Chain J:



• Molecule 2: 230AS-18

Chain K:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	75.22Å 145.73Å 78.27Å 90.00° 90.92° 90.00°	Depositor
Resolution (Å)	41.27 – 2.50 41.27 – 2.50	Depositor EDS
% Data completeness (in resolution range)	97.7 (41.27-2.50) 97.7 (41.27-2.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.01 (at 2.48Å)	Xtriage
Refinement program	PHENIX 1.19.2_4158	Depositor
R, R_{free}	0.204 , 0.248 0.203 , 0.247	Depositor DCC
R_{free} test set	2863 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	47.3	Xtriage
Anisotropy	0.249	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 23.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.003 for l,k,-h 0.117 for h,-k,-l 0.023 for l,-k,h	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	25470	wwPDB-VP
Average B, all atoms (Å^2)	68.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.67% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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	0.32	0/1433	0.55	0/1938
1	B	0.29	0/1433	0.53	0/1938
1	C	0.32	0/1433	0.54	0/1938
1	D	0.30	0/1433	0.52	0/1938
2	H	0.32	0/1829	0.58	0/2480
2	I	0.31	0/1829	0.57	0/2480
2	J	0.34	0/1829	0.59	0/2480
2	K	0.33	0/1829	0.59	0/2480
All	All	0.32	0/13048	0.56	0/17672

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

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	1407	1418	1418	15	0
1	B	1407	1418	1418	13	0
1	C	1407	1418	1418	30	0
1	D	1407	1418	1418	13	0
2	H	1787	1727	1727	9	0
2	I	1787	1727	1727	16	0
2	J	1787	1727	1727	22	0
2	K	1787	1727	1727	22	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	10	0	0	0	0
3	B	6	0	0	0	0
3	C	10	0	0	0	0
3	D	10	0	0	1	0
3	H	23	0	0	0	0
3	I	19	0	0	0	0
3	J	12	0	0	0	0
3	K	24	0	0	0	0
All	All	12890	12580	12580	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:105:TYR:OH	2:H:193:ASP:OD2	1.96	0.82
2:I:105:TYR:OH	2:I:193:ASP:OD2	1.97	0.81
2:J:167:ARG:NH1	2:J:213:ASP:HB2	1.99	0.77
2:J:12:VAL:HG11	2:J:18:LEU:HG	1.72	0.71
1:C:557:LEU:N	1:C:645:LYS:HZ3	1.89	0.70
1:A:568:GLU:O	1:A:722:ILE:HD11	1.91	0.70
2:I:167:ARG:NH1	2:I:213:ASP:OD1	2.24	0.69
1:B:568:GLU:O	1:B:722:ILE:HD11	1.92	0.69
2:K:167:ARG:NH1	2:K:213:ASP:OD1	2.25	0.68
1:B:655:GLU:OE2	1:C:732:ASN:N	2.26	0.68
2:K:12:VAL:HG11	2:K:18:LEU:HD13	1.72	0.68
2:I:190:LEU:HD23	2:I:201:ILE:HD12	1.76	0.66
1:A:581:LYS:O	1:C:585:GLN:NE2	2.29	0.65
1:C:560:ILE:HG13	1:C:562:LEU:HD11	1.77	0.65
2:J:11:VAL:HG22	2:J:120:THR:HB	1.79	0.65
2:K:12:VAL:CG1	2:K:18:LEU:HD13	2.30	0.61
2:K:167:ARG:HG2	2:K:213:ASP:OD1	2.01	0.60
1:B:652:THR:HG21	1:B:666:LEU:HD11	1.81	0.60
1:C:608:VAL:HG13	1:C:722:ILE:HD13	1.82	0.60
1:B:625:ILE:HG12	1:B:687:VAL:HG22	1.84	0.59
2:J:167:ARG:HA	2:J:212:THR:O	2.03	0.59
2:J:40:ALA:HB3	2:J:43:LYS:HD2	1.83	0.58
2:K:105:TYR:OH	2:K:193:ASP:OD2	2.11	0.57
1:A:670:LEU:C	2:K:161:ARG:HH22	2.08	0.57
1:C:629:LYS:H	1:C:629:LYS:HD2	1.70	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:641:TYR:CD1	1:C:644:LYS:HD3	2.39	0.57
1:B:670:LEU:CD2	1:B:672:ILE:HG13	2.34	0.57
2:I:237:TRP:HB2	2:I:238:PRO:HA	1.87	0.57
1:C:615:VAL:HG11	1:C:692:LEU:HD12	1.85	0.56
1:C:560:ILE:HG13	1:C:562:LEU:CD1	2.35	0.56
2:K:180:GLN:OE1	2:K:188:ARG:NH2	2.39	0.56
2:J:11:VAL:HA	2:J:120:THR:O	2.06	0.55
1:C:641:TYR:CE1	1:C:644:LYS:HD3	2.44	0.53
2:K:12:VAL:HG21	2:K:86:LEU:HD13	1.90	0.53
2:J:156:LEU:HD12	2:J:221:LEU:HD11	1.91	0.53
1:B:652:THR:HG21	1:B:666:LEU:CD1	2.39	0.53
1:A:565:GLU:HG2	1:A:659:LYS:HD3	1.91	0.53
2:H:164:LEU:HD12	2:H:164:LEU:N	2.24	0.53
1:C:667:ILE:HD11	1:C:700:THR:HG21	1.91	0.52
2:K:155:SER:HB3	2:K:251:LYS:HB3	1.89	0.52
2:J:167:ARG:HD2	2:J:213:ASP:OD1	2.09	0.52
1:C:670:LEU:HD21	1:C:690:PHE:HB2	1.92	0.52
2:H:180:GLN:HB2	2:H:190:LEU:HD11	1.92	0.51
2:H:237:TRP:HB2	2:H:238:PRO:HA	1.93	0.51
2:J:237:TRP:HB2	2:J:238:PRO:HA	1.93	0.51
2:I:156:LEU:HD12	2:I:221:LEU:HD11	1.93	0.51
1:C:721:GLY:C	1:C:722:ILE:HD12	2.31	0.50
1:D:565:GLU:HG2	1:D:659:LYS:HD3	1.93	0.50
1:C:565:GLU:HG2	1:C:659:LYS:HD3	1.94	0.50
2:K:180:GLN:HB2	2:K:190:LEU:HD11	1.93	0.50
1:C:632:VAL:HG11	1:C:635:LEU:HD12	1.93	0.50
2:I:176:LEU:HD22	2:I:214:PHE:CG	2.46	0.50
1:C:615:VAL:HG11	1:C:692:LEU:CD1	2.41	0.50
2:J:180:GLN:HB2	2:J:190:LEU:HD11	1.93	0.49
1:B:615:VAL:HG11	1:B:692:LEU:HD12	1.94	0.49
2:J:164:LEU:HD12	2:J:164:LEU:N	2.28	0.49
2:K:237:TRP:HB2	2:K:238:PRO:HA	1.95	0.49
2:I:12:VAL:HG21	2:I:86:LEU:HD13	1.95	0.48
1:A:623:LYS:HE3	1:A:687:VAL:HG21	1.94	0.48
1:C:641:TYR:CE1	1:C:644:LYS:CD	2.96	0.48
1:C:629:LYS:HE3	1:C:639:ILE:O	2.14	0.48
2:J:226:PHE:CZ	2:J:250:ILE:HG12	2.49	0.48
1:B:622:VAL:O	1:B:689:GLU:HA	2.15	0.47
2:H:40:ALA:HB3	2:H:43:LYS:HD2	1.95	0.47
1:C:722:ILE:HD12	1:C:722:ILE:N	2.30	0.47
2:K:144:GLU:CG	2:K:241:THR:HG21	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:568:GLU:O	1:D:722:ILE:HD11	2.14	0.47
2:K:67:ARG:NH2	2:K:90:ASP:OD2	2.46	0.47
1:C:587:THR:HG22	1:C:590:GLU:HB3	1.95	0.47
2:I:197:ARG:HG2	2:I:201:ILE:HB	1.96	0.47
2:I:12:VAL:HG11	2:I:18:LEU:HG	1.97	0.46
1:A:669:GLY:C	1:A:693:PRO:HB3	2.35	0.46
1:D:587:THR:O	1:D:587:THR:HG23	2.15	0.46
1:B:655:GLU:HG3	1:C:695:VAL:CG1	2.45	0.46
2:J:169:SER:HA	1:D:665:LYS:HE3	1.96	0.46
1:D:663:LEU:HG	1:D:670:LEU:HD13	1.97	0.46
1:B:730:TYR:CD1	1:B:730:TYR:O	2.69	0.45
1:C:623:LYS:HE2	1:C:689:GLU:OE2	2.16	0.45
1:C:629:LYS:HG3	1:C:639:ILE:HG22	1.98	0.45
1:A:670:LEU:O	2:K:161:ARG:NH2	2.34	0.45
1:A:678:GLU:CG	1:A:678:GLU:O	2.64	0.45
1:A:678:GLU:O	1:A:678:GLU:HG2	2.16	0.45
2:H:193:ASP:O	2:H:194:ALA:HB3	2.17	0.45
2:I:193:ASP:O	2:I:194:ALA:HB3	2.17	0.45
1:D:587:THR:HG22	1:D:590:GLU:HB3	1.98	0.45
1:D:633:GLU:HG2	1:D:634:LYS:HG3	1.99	0.45
1:A:713:ASP:HB3	1:A:716:LYS:HE3	1.99	0.45
1:A:565:GLU:HG2	1:A:659:LYS:CD	2.48	0.44
2:J:193:ASP:O	2:J:194:ALA:HB3	2.18	0.44
1:C:587:THR:O	1:C:587:THR:HG23	2.17	0.44
2:J:167:ARG:HG2	2:J:213:ASP:HA	1.99	0.44
1:D:615:VAL:HG11	1:D:692:LEU:HD12	1.99	0.44
2:J:-1:THR:OG1	2:J:26:GLY:O	2.25	0.44
1:C:670:LEU:CD2	1:C:672:ILE:HG13	2.48	0.44
2:J:167:ARG:CG	2:J:213:ASP:OD1	2.66	0.44
1:A:670:LEU:C	2:K:161:ARG:NH2	2.72	0.44
2:J:176:LEU:HD22	2:J:214:PHE:CG	2.53	0.43
2:H:176:LEU:HD22	2:H:214:PHE:CG	2.53	0.43
1:A:587:THR:HG22	1:A:590:GLU:HB3	1.99	0.43
2:K:156:LEU:HD12	2:K:221:LEU:HD11	2.01	0.43
1:A:622:VAL:O	1:A:689:GLU:HA	2.18	0.43
1:B:654:GLU:O	1:B:655:GLU:HB2	2.19	0.43
1:B:633:GLU:O	1:B:634:LYS:HB2	2.19	0.43
1:C:565:GLU:HG2	1:C:659:LYS:CD	2.49	0.43
2:I:6:GLU:HG3	2:I:96:CYS:SG	2.58	0.42
1:C:559:LYS:HD3	1:C:560:ILE:O	2.18	0.42
2:K:144:GLU:HG3	2:K:241:THR:HG21	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:180:GLN:HB2	2:I:190:LEU:HD11	2.00	0.42
1:C:701:VAL:HG22	1:C:726:TYR:CD1	2.55	0.42
2:I:191:ILE:HD13	2:I:197:ARG:HA	2.02	0.42
2:J:190:LEU:HD23	2:J:201:ILE:HD12	2.02	0.42
2:K:226:PHE:CD2	2:K:250:ILE:HD11	2.55	0.42
2:H:173:ASN:HB2	2:H:175:TYR:CD2	2.54	0.41
2:J:35:HIS:CE1	2:J:50:TYR:HD2	2.38	0.41
2:K:171:ASN:OD1	2:K:211:GLY:HA2	2.19	0.41
1:C:560:ILE:O	1:C:562:LEU:HD12	2.20	0.41
1:A:587:THR:HG23	1:A:587:THR:O	2.20	0.41
1:D:670:LEU:CD2	1:D:672:ILE:HG13	2.51	0.41
2:J:6:GLU:HG3	2:J:96:CYS:SG	2.61	0.41
1:D:717:LYS:NZ	3:D:804:HOH:O	2.53	0.41
2:I:14:PRO:HD3	2:I:122:SER:O	2.21	0.41
1:D:580:ASP:HB2	1:D:609:LYS:HD3	2.02	0.41
1:D:633:GLU:O	1:D:634:LYS:HB2	2.20	0.41
2:K:176:LEU:HD22	2:K:214:PHE:CG	2.55	0.41
2:K:193:ASP:O	2:K:194:ALA:HB3	2.20	0.41
2:I:-1:THR:OG1	2:I:26:GLY:O	2.31	0.41
1:C:629:LYS:H	1:C:629:LYS:CD	2.34	0.41
2:H:35:HIS:CE1	2:H:50:TYR:HD2	2.39	0.41
2:I:164:LEU:HD12	2:I:164:LEU:N	2.36	0.41
2:J:169:SER:CA	1:D:665:LYS:HE3	2.52	0.40
2:K:-1:THR:OG1	2:K:26:GLY:O	2.31	0.40
1:B:558:ASP:CG	1:B:558:ASP:O	2.60	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	174/191 (91%)	169 (97%)	5 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	174/191 (91%)	169 (97%)	5 (3%)	0	100	100
1	C	174/191 (91%)	168 (97%)	6 (3%)	0	100	100
1	D	174/191 (91%)	166 (95%)	8 (5%)	0	100	100
2	H	229/261 (88%)	221 (96%)	8 (4%)	0	100	100
2	I	229/261 (88%)	222 (97%)	7 (3%)	0	100	100
2	J	229/261 (88%)	221 (96%)	8 (4%)	0	100	100
2	K	229/261 (88%)	222 (97%)	7 (3%)	0	100	100
All	All	1612/1808 (89%)	1558 (97%)	54 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	165/177 (93%)	165 (100%)	0	100	100
1	B	165/177 (93%)	165 (100%)	0	100	100
1	C	165/177 (93%)	165 (100%)	0	100	100
1	D	165/177 (93%)	164 (99%)	1 (1%)	86	95
2	H	187/198 (94%)	187 (100%)	0	100	100
2	I	187/198 (94%)	187 (100%)	0	100	100
2	J	187/198 (94%)	187 (100%)	0	100	100
2	K	187/198 (94%)	187 (100%)	0	100	100
All	All	1408/1500 (94%)	1407 (100%)	1 (0%)	93	98

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	614	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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

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, 95^{th} 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	176/191 (92%)	0.20	11 (6%) 20 21	37, 63, 101, 157	0
1	B	176/191 (92%)	0.84	31 (17%) 1 1	42, 89, 131, 148	0
1	C	176/191 (92%)	0.35	9 (5%) 28 29	40, 64, 105, 143	0
1	D	176/191 (92%)	0.15	7 (3%) 38 41	41, 59, 101, 119	0
2	H	233/261 (89%)	-0.25	0 100 100	35, 46, 68, 84	0
2	I	233/261 (89%)	-0.21	3 (1%) 77 79	35, 47, 82, 118	0
2	J	233/261 (89%)	-0.22	2 (0%) 84 86	36, 53, 91, 109	0
2	K	233/261 (89%)	-0.12	4 (1%) 70 72	37, 52, 91, 139	0
All	All	1636/1808 (90%)	0.05	67 (4%) 37 40	35, 56, 107, 157	0

All (67) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	557	LEU	11.5
1	B	562	LEU	8.8
1	C	732	ASN	7.6
1	B	696	VAL	6.1
1	B	619	LEU	6.1
1	A	557	LEU	6.0
1	D	588	ASN	5.9
2	K	123	SER	5.8
1	D	557	LEU	5.6
2	I	250	ILE	5.4
1	B	726	TYR	5.4
1	C	560	ILE	4.9
1	B	655	GLU	4.6
1	D	732	ASN	4.6
1	B	557	LEU	4.5
2	J	123	SER	4.3

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Mol	Chain	Res	Type	RSRZ
1	B	620	ILE	4.2
1	C	587	THR	4.0
2	K	219	SER	4.0
1	B	665	LYS	3.9
1	C	588	ASN	3.6
1	A	559	LYS	3.5
1	B	587	THR	3.4
1	B	730	TYR	3.4
1	C	558	ASP	3.3
1	B	618	PRO	3.3
1	B	591	TYR	3.3
1	B	558	ASP	3.3
1	A	562	LEU	3.2
1	C	559	LYS	3.1
1	B	654	GLU	3.1
1	B	564	TYR	3.0
1	B	656	THR	3.0
1	B	694	PRO	2.9
1	D	560	ILE	2.9
1	D	558	ASP	2.8
2	I	251	LYS	2.8
1	A	677	ASN	2.7
2	J	250	ILE	2.6
2	K	-1	THR	2.6
1	B	695	VAL	2.6
1	B	678	GLU	2.5
1	B	668	TYR	2.5
2	K	251	LYS	2.5
2	I	219	SER	2.4
1	A	614	LYS	2.4
1	B	661	LYS	2.4
1	B	672	ILE	2.3
1	A	655	GLU	2.3
1	D	677	ASN	2.3
1	A	558	ASP	2.3
1	B	697	HIS	2.3
1	C	697	HIS	2.3
1	B	648	TYR	2.3
1	B	580	ASP	2.2
1	B	560	ILE	2.2
1	B	728	GLU	2.2
1	A	634	LYS	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	664	SER	2.2
1	C	563	SER	2.2
1	B	732	ASN	2.1
1	A	656	THR	2.1
1	B	563	SER	2.1
1	B	667	ILE	2.1
1	D	731	GLY	2.1
1	A	726	TYR	2.0
1	A	589	LYS	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 monosaccharides 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.