Full wwPDB X-ray Structure Validation Report ⓘ

Oct 15, 2023 – 06:36 AM EDT

PDB ID	:	7UBS
Title	:	Pfs230 D1 domain in complex with 230AS-26
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Deposited on	:	2022-03-15
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:

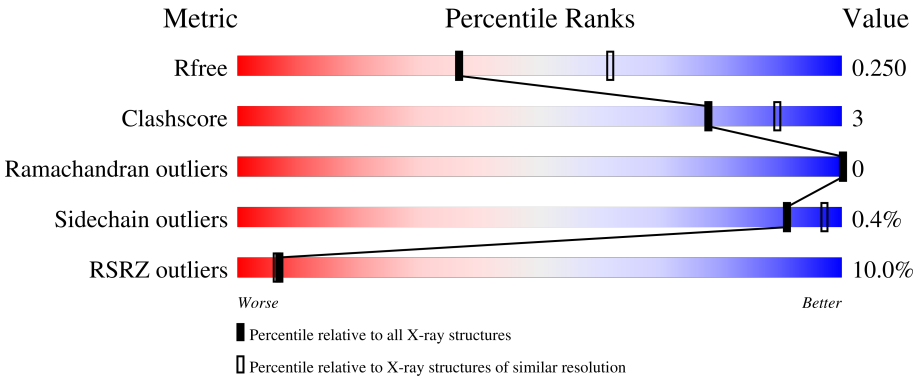
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation 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	19% 82% 8% 10%
1	B	191	15% 83% 8% 9%
1	C	191	16% 73% · 24%
1	D	191	12% 73% · 23%
2	H	264	5% 79% 9% 12%

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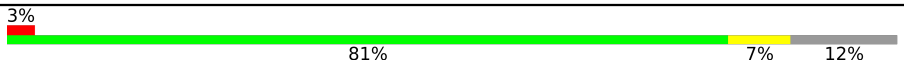
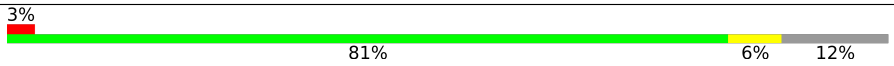
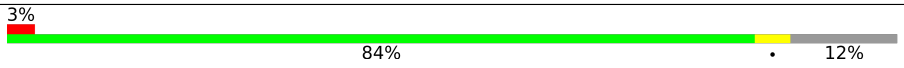
Mol	Chain	Length	Quality of chain
2	I	264	
2	J	264	
2	K	264	

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 24542 atoms, of which 12159 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	172	Total	C	H	N	O	S	0	0	0
			2745	877	1375	213	276	4			
1	B	173	Total	C	H	N	O	S	0	0	0
			2764	883	1386	214	277	4			
1	C	145	Total	C	H	N	O	S	0	0	0
			2371	756	1205	184	222	4			
1	D	147	Total	C	H	N	O	S	0	0	0
			2399	764	1218	187	226	4			

There are 4 discrepancies between the modelled and reference sequences:

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

- Molecule 2 is a protein called 230AS-26.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	H	232	Total	C	H	N	O	S	0	0	0
			3532	1135	1734	299	356	8			
2	I	233	Total	C	H	N	O	S	0	0	0
			3554	1141	1747	301	357	8			
2	J	233	Total	C	H	N	O	S	0	0	0
			3554	1141	1747	301	357	8			
2	K	233	Total	C	H	N	O	S	0	0	0
			3554	1141	1747	301	357	8			

- Molecule 3 is water.

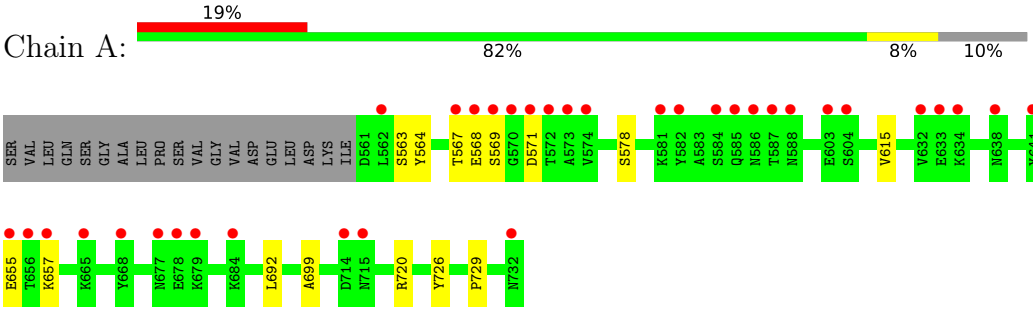
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	4	Total O 4 4	0	0
3	B	3	Total O 3 3	0	0
3	C	3	Total O 3 3	0	0
3	H	12	Total O 12 12	0	0
3	I	13	Total O 13 13	0	0
3	J	19	Total O 19 19	0	0
3	K	15	Total O 15 15	0	0

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.

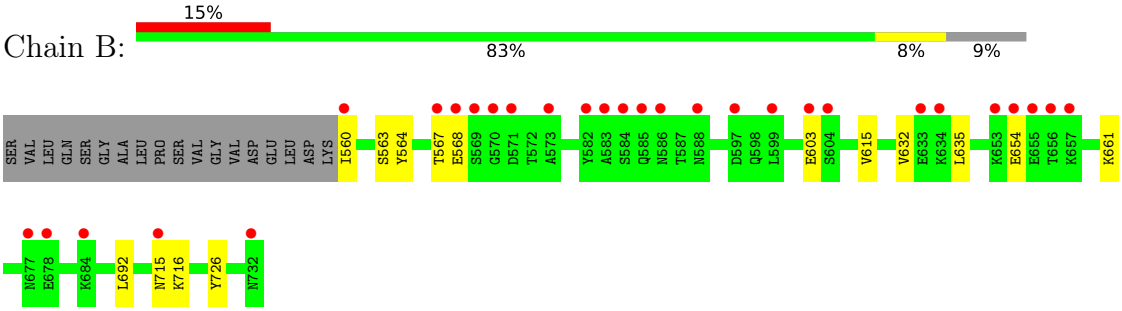
• Molecule 1: Gametocyte surface protein P230

Chain A:



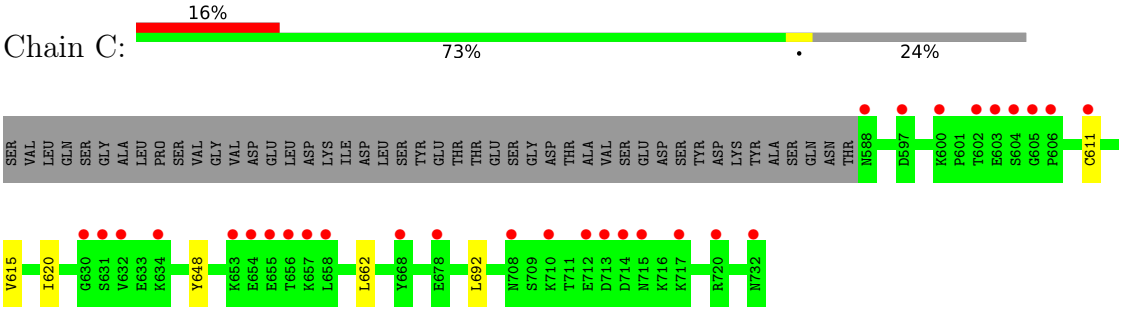
• Molecule 1: Gametocyte surface protein P230

Chain B:



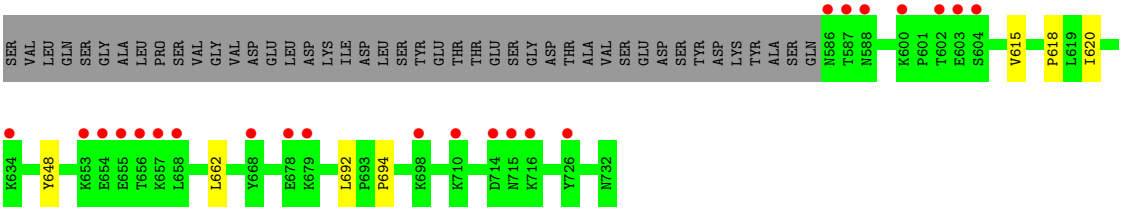
• Molecule 1: Gametocyte surface protein P230

Chain C:

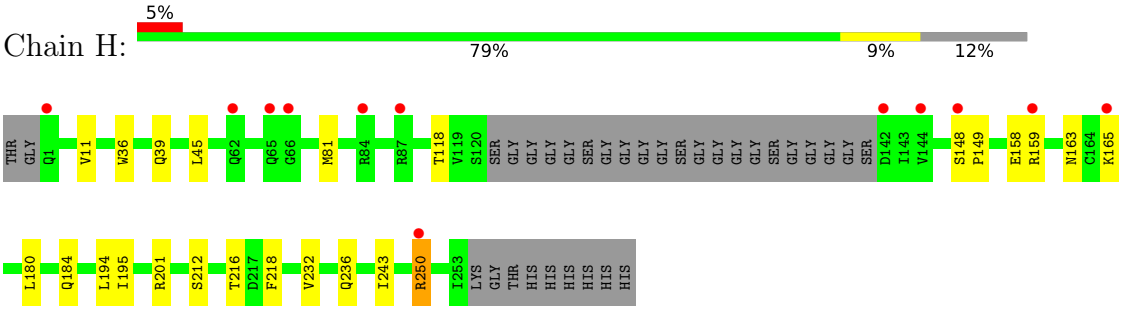


• Molecule 1: Gametocyte surface protein P230

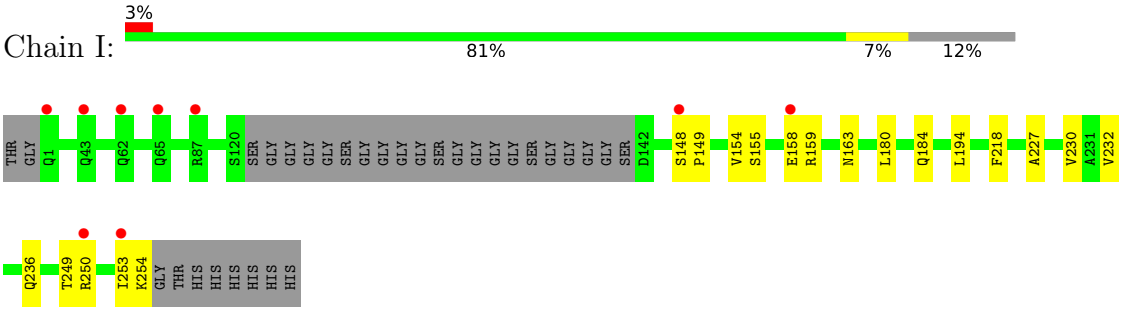
Chain D:



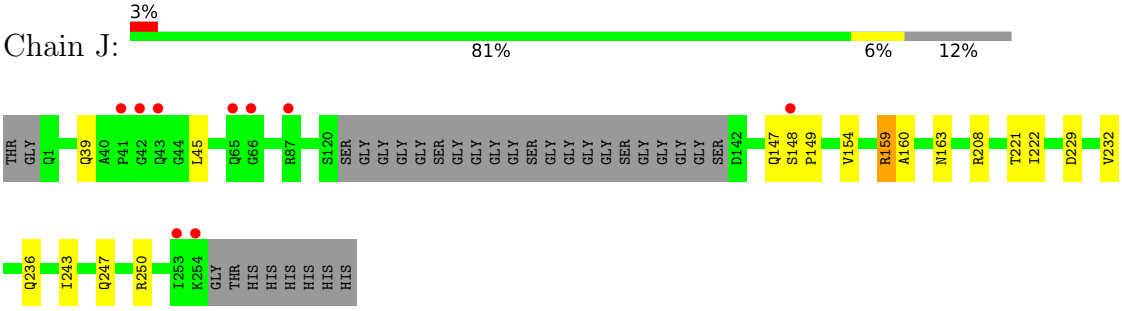
• Molecule 2: 230AS-26



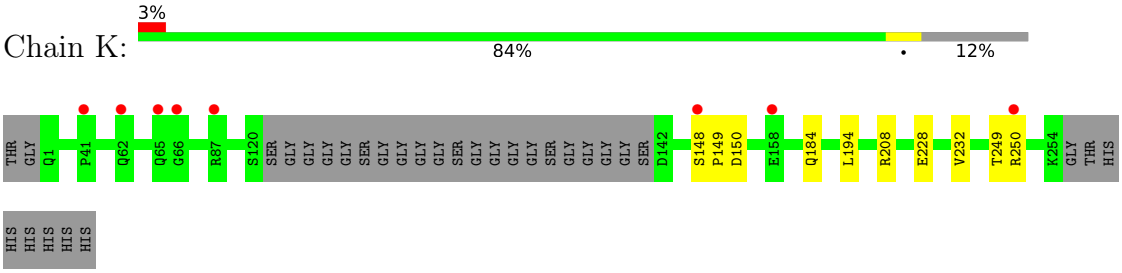
• Molecule 2: 230AS-26



• Molecule 2: 230AS-26



• Molecule 2: 230AS-26



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	46.88Å 205.51Å 93.86Å 90.00° 103.01° 90.00°	Depositor
Resolution (Å)	19.98 – 2.50 19.98 – 2.50	Depositor EDS
% Data completeness (in resolution range)	93.5 (19.98-2.50) 93.5 (19.98-2.50)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.64 (at 2.50Å)	Xtriage
Refinement program	PHENIX 1.19.2_4158	Depositor
R, R_{free}	0.209 , 0.250 0.210 , 0.250	Depositor DCC
R_{free} test set	2782 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	22.3	Xtriage
Anisotropy	0.019	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.42 , 42.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.031 for h,-k,-h-l	Xtriage
F_o,F_c correlation	0.90	EDS
Total number of atoms	24542	wwPDB-VP
Average B, all atoms (Å^2)	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.31% 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	0.31	0/1396	0.55	0/1889
1	B	0.35	0/1404	0.55	0/1900
1	C	0.30	0/1189	0.51	0/1606
1	D	0.31	0/1204	0.49	0/1627
2	H	0.32	0/1840	0.55	1/2502 (0.0%)
2	I	0.32	0/1849	0.55	0/2513
2	J	0.37	0/1849	0.57	0/2513
2	K	0.33	0/1849	0.57	0/2513
All	All	0.33	0/12580	0.55	1/17063 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	H	250	ARG	CG-CD-NE	-5.17	100.94	111.80

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	1370	1375	1373	8	0
1	B	1378	1386	1384	11	0
1	C	1166	1205	1205	5	0
1	D	1181	1218	1218	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	H	1798	1734	1736	17	0
2	I	1807	1747	1749	14	0
2	J	1807	1747	1749	10	0
2	K	1807	1747	1749	5	0
3	A	4	0	0	0	0
3	B	3	0	0	0	0
3	C	3	0	0	0	0
3	H	12	0	0	0	0
3	I	13	0	0	0	0
3	J	19	0	0	0	0
3	K	15	0	0	0	0
All	All	12383	12159	12163	71	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 3.

All (71) 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:J:148:SER:OG	2:J:149:PRO:HD3	1.71	0.91
1:A:578:SER:OG	1:C:611:CYS:SG	2.34	0.86
2:I:148:SER:OG	2:I:149:PRO:HD3	1.83	0.78
1:D:615:VAL:HG13	1:D:620:ILE:HD12	1.66	0.77
2:H:148:SER:OG	2:H:149:PRO:HD3	1.86	0.75
2:I:232:VAL:HG22	2:I:250:ARG:HG2	1.72	0.71
2:J:232:VAL:HG22	2:J:250:ARG:HG2	1.73	0.70
2:H:180:LEU:HD22	2:H:218:PHE:CD2	2.28	0.68
1:A:567:THR:HG1	1:B:560:ILE:N	1.95	0.65
1:C:615:VAL:HG11	1:C:692:LEU:HD12	1.79	0.65
1:D:615:VAL:HG11	1:D:692:LEU:CD1	2.28	0.63
1:B:615:VAL:HG11	1:B:692:LEU:CD1	2.30	0.62
2:K:148:SER:HB3	2:K:149:PRO:HD3	1.82	0.60
1:D:615:VAL:HG11	1:D:692:LEU:HD12	1.82	0.60
1:C:615:VAL:HG11	1:C:692:LEU:CD1	2.33	0.58
1:B:615:VAL:HG11	1:B:692:LEU:HD13	1.87	0.57
2:I:148:SER:OG	2:I:163:ASN:HB2	2.04	0.56
2:I:227:ALA:HA	2:I:253:ILE:HD11	1.87	0.56
2:H:180:LEU:HD22	2:H:218:PHE:CG	2.40	0.56
2:H:158:GLU:HG3	2:H:159:ARG:N	2.20	0.55
2:I:180:LEU:HD12	2:I:236:GLN:O	2.06	0.55
2:H:158:GLU:HG3	2:H:159:ARG:H	1.71	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:180:LEU:HD22	2:I:218:PHE:CG	2.41	0.55
2:H:195:ILE:HD13	2:H:201:ARG:HA	1.88	0.54
2:K:232:VAL:HG22	2:K:250:ARG:HG2	1.90	0.54
1:D:648:TYR:CE2	1:D:662:LEU:HD22	2.42	0.53
2:K:184:GLN:HB2	2:K:194:LEU:HD11	1.90	0.53
2:H:158:GLU:CG	2:H:159:ARG:H	2.21	0.53
2:J:154:VAL:HG21	2:J:160:ALA:HB2	1.92	0.51
1:B:632:VAL:HG11	1:B:635:LEU:HD12	1.95	0.49
2:I:180:LEU:HD22	2:I:218:PHE:CD1	2.49	0.48
2:J:159:ARG:HA	2:J:222:ILE:O	2.13	0.48
2:H:232:VAL:HG22	2:H:250:ARG:HG2	1.95	0.48
2:H:158:GLU:CG	2:H:159:ARG:N	2.77	0.47
2:J:148:SER:OG	2:J:163:ASN:HB3	2.15	0.47
2:H:11:VAL:HG12	2:H:118:THR:HB	1.97	0.46
1:A:563:SER:HB2	1:B:563:SER:HB2	1.97	0.46
2:H:148:SER:OG	2:H:163:ASN:HB2	2.15	0.46
2:I:158:GLU:HG3	2:I:159:ARG:N	2.30	0.46
1:C:648:TYR:CE2	1:C:662:LEU:HD22	2.50	0.46
1:B:603:GLU:N	1:B:716:LYS:HG2	2.31	0.46
2:I:227:ALA:HA	2:I:253:ILE:CD1	2.45	0.45
2:J:159:ARG:HD3	2:J:221:THR:HG23	1.96	0.45
2:H:236:GLN:HE21	2:H:243:ILE:HG23	1.82	0.45
2:I:154:VAL:O	2:I:254:LYS:N	2.49	0.45
2:K:208:ARG:NH2	2:K:228:GLU:OE2	2.50	0.45
1:D:618:PRO:HB3	1:D:694:PRO:HA	1.99	0.44
2:J:147:GLN:O	2:J:247:GLN:NE2	2.46	0.44
1:B:654:GLU:OE2	1:B:661:LYS:HE3	2.17	0.44
2:J:236:GLN:HE21	2:J:243:ILE:HG23	1.82	0.44
1:A:615:VAL:HG11	1:A:692:LEU:HD13	1.99	0.44
1:A:699:ALA:HB2	1:A:729:PRO:HD3	1.98	0.44
2:H:36:TRP:CE2	2:H:81:MET:HB2	2.53	0.44
2:I:184:GLN:HB2	2:I:194:LEU:HD11	1.99	0.44
1:C:615:VAL:HG13	1:C:620:ILE:HG13	1.99	0.44
1:A:569:SER:HA	1:A:720:ARG:HH12	1.82	0.43
1:B:615:VAL:HG11	1:B:692:LEU:HD12	2.00	0.43
2:I:230:VAL:CG2	2:I:253:ILE:HG13	2.48	0.43
1:B:715:ASN:OD1	2:H:212:SER:HB3	2.18	0.43
2:H:165:LYS:HD2	2:H:216:THR:O	2.19	0.42
2:H:39:GLN:HB2	2:H:45:LEU:HD23	2.02	0.42
2:J:208:ARG:NH1	2:J:229:ASP:OD2	2.52	0.42
2:J:39:GLN:HB2	2:J:45:LEU:HD23	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:568:GLU:OE1	1:A:571:ASP:HB3	2.21	0.41
1:B:567:THR:O	1:B:568:GLU:HB2	2.21	0.41
1:B:603:GLU:HG3	1:B:716:LYS:HZ3	1.86	0.41
1:A:655:GLU:HG3	1:A:657:LYS:HE2	2.01	0.41
2:I:154:VAL:HG12	2:I:155:SER:N	2.36	0.41
2:H:184:GLN:HB2	2:H:194:LEU:HD11	2.02	0.40
2:K:149:PRO:O	2:K:249:THR:HG23	2.22	0.40
2:I:149:PRO:O	2:I:249:THR:HG23	2.22	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	170/191 (89%)	162 (95%)	8 (5%)	0	100	100
1	B	171/191 (90%)	163 (95%)	8 (5%)	0	100	100
1	C	143/191 (75%)	141 (99%)	2 (1%)	0	100	100
1	D	145/191 (76%)	141 (97%)	4 (3%)	0	100	100
2	H	228/264 (86%)	219 (96%)	9 (4%)	0	100	100
2	I	229/264 (87%)	221 (96%)	8 (4%)	0	100	100
2	J	229/264 (87%)	222 (97%)	7 (3%)	0	100	100
2	K	229/264 (87%)	221 (96%)	8 (4%)	0	100	100
All	All	1544/1820 (85%)	1490 (96%)	54 (4%)	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	160/177 (90%)	158 (99%)	2 (1%)	69 87
1	B	161/177 (91%)	159 (99%)	2 (1%)	71 88
1	C	137/177 (77%)	137 (100%)	0	100 100
1	D	139/177 (78%)	139 (100%)	0	100 100
2	H	196/210 (93%)	196 (100%)	0	100 100
2	I	197/210 (94%)	197 (100%)	0	100 100
2	J	197/210 (94%)	196 (100%)	1 (0%)	88 96
2	K	197/210 (94%)	196 (100%)	1 (0%)	88 96
All	All	1384/1548 (89%)	1378 (100%)	6 (0%)	91 97

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	564	TYR
1	A	726	TYR
1	B	564	TYR
1	B	726	TYR
2	J	159	ARG
2	K	150	ASP

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

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 monosaccharides 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

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	172/191 (90%)	1.03	37 (21%)	0	0	18, 34, 65, 87	0
1	B	173/191 (90%)	1.00	29 (16%)	1	1	12, 30, 66, 84	0
1	C	145/191 (75%)	1.02	30 (20%)	1	0	14, 32, 69, 96	0
1	D	147/191 (76%)	0.78	23 (15%)	2	1	12, 29, 63, 76	0
2	H	232/264 (87%)	0.38	12 (5%)	27	29	12, 27, 50, 64	0
2	I	233/264 (88%)	0.25	9 (3%)	39	42	11, 22, 48, 66	0
2	J	233/264 (88%)	0.18	9 (3%)	39	42	8, 18, 41, 53	0
2	K	233/264 (88%)	0.19	8 (3%)	45	48	8, 18, 36, 51	0
All	All	1568/1820 (86%)	0.54	157 (10%)	7	6	8, 25, 59, 96	0

All (157) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	570	GLY	12.1
1	B	585	GLN	11.3
1	C	656	THR	10.4
1	A	585	GLN	8.8
1	A	570	GLY	8.2
1	B	584	SER	7.2
1	B	571	ASP	7.1
1	C	714	ASP	7.1
1	D	656	THR	6.6
1	A	584	SER	6.5
1	A	582	TYR	6.0
1	B	582	TYR	5.8
2	H	66	GLY	5.7
1	B	656	THR	5.6
1	C	603	GLU	5.4
1	A	571	ASP	5.4

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Mol	Chain	Res	Type	RSRZ
2	J	65	GLN	5.3
1	B	677	ASN	5.2
1	D	715	ASN	5.0
1	D	714	ASP	4.9
2	H	148	SER	4.8
1	C	713	ASP	4.7
1	A	572	THR	4.6
2	I	87	ARG	4.5
1	B	603	GLU	4.5
1	D	603	GLU	4.3
1	A	588	ASN	4.3
1	C	634	LYS	4.3
1	A	715	ASN	4.2
1	A	656	THR	4.2
2	J	148	SER	4.2
1	D	655	GLU	4.1
1	B	655	GLU	4.0
1	C	655	GLU	4.0
1	B	678	GLU	3.9
2	K	66	GLY	3.9
1	A	684	LYS	3.8
1	B	586	ASN	3.8
1	A	632	VAL	3.8
1	D	653	LYS	3.7
2	J	42	GLY	3.7
1	D	586	ASN	3.7
1	B	567	THR	3.6
2	I	253	ILE	3.5
1	A	677	ASN	3.5
2	H	87	ARG	3.4
1	C	632	VAL	3.4
1	D	587	THR	3.4
1	A	603	GLU	3.4
1	C	657	LYS	3.4
1	A	568	GLU	3.4
1	B	653	LYS	3.4
1	A	665	LYS	3.4
1	A	732	ASN	3.3
2	I	148	SER	3.3
1	B	568	GLU	3.2
1	D	657	LYS	3.2
1	C	717	LYS	3.2

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Mol	Chain	Res	Type	RSRZ
1	C	732	ASN	3.1
1	D	634	LYS	3.1
1	A	657	LYS	3.1
2	K	65	GLN	3.1
2	H	250	ARG	3.1
1	A	634	LYS	3.0
2	J	253	ILE	2.9
1	D	600	LYS	2.9
1	C	605	GLY	2.9
1	C	600	LYS	2.9
1	B	588	ASN	2.9
1	B	715	ASN	2.9
1	A	668	TYR	2.9
1	C	597	ASP	2.9
2	I	250	ARG	2.9
1	B	573	ALA	2.8
1	B	583	ALA	2.8
1	A	641	TYR	2.8
2	J	66	GLY	2.8
1	A	633	GLU	2.8
2	I	65	GLN	2.8
2	K	250	ARG	2.8
2	H	62	GLN	2.7
1	A	574	VAL	2.7
1	C	668	TYR	2.7
1	B	634	LYS	2.7
1	A	638	ASN	2.7
2	J	87	ARG	2.7
2	K	158	GLU	2.7
1	B	684	LYS	2.7
2	H	159	ARG	2.6
1	A	587	THR	2.6
1	A	645	LYS	2.6
1	D	658	LEU	2.6
1	B	633	GLU	2.6
2	K	62	GLN	2.6
1	C	604	SER	2.6
2	J	43	GLN	2.6
2	K	87	ARG	2.6
2	J	41	PRO	2.6
1	B	657	LYS	2.6
1	C	710	LYS	2.6

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Mol	Chain	Res	Type	RSRZ
2	H	142	ASP	2.6
1	C	606	PRO	2.6
1	A	714	ASP	2.6
1	B	569	SER	2.6
2	H	84	ARG	2.5
2	H	1	GLN	2.5
1	A	678	GLU	2.5
1	D	698	LYS	2.5
1	D	678	GLU	2.5
2	H	165	LYS	2.4
1	C	658	LEU	2.4
1	B	604	SER	2.4
1	D	716	LYS	2.4
1	C	654	GLU	2.4
1	B	560	ILE	2.4
1	C	630	GLY	2.4
2	K	41	PRO	2.4
2	J	254	LYS	2.4
1	D	588	ASN	2.4
1	C	588	ASN	2.3
1	A	567	THR	2.3
2	I	1	GLN	2.3
1	C	712	GLU	2.3
1	D	668	TYR	2.3
1	A	562	LEU	2.3
1	A	573	ALA	2.3
2	K	148	SER	2.3
1	B	599	LEU	2.3
1	C	653	LYS	2.3
1	C	715	ASN	2.3
1	B	597	ASP	2.3
1	A	654	GLU	2.3
1	D	726	TYR	2.3
1	D	602	THR	2.2
1	C	611	CYS	2.2
2	I	43	GLN	2.2
1	A	655	GLU	2.2
1	D	710	LYS	2.2
1	A	581	LYS	2.2
1	B	732	ASN	2.2
1	D	654	GLU	2.2
2	H	144	VAL	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	586	ASN	2.1
1	B	654	GLU	2.1
1	C	720	ARG	2.1
2	I	62	GLN	2.1
1	D	679	LYS	2.1
1	D	604	SER	2.1
1	C	678	GLU	2.1
2	H	65	GLN	2.1
1	C	631	SER	2.0
1	A	679	LYS	2.0
1	C	602	THR	2.0
1	A	604	SER	2.0
2	I	158	GLU	2.0
1	A	569	SER	2.0
1	C	708	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 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.