

Full wwPDB X-ray Structure Validation Report (i)

Feb 21, 2023 – 12:30 pm GMT

PDB ID	:	7ZMK
Title	:	Structure of human MFAP4 in complex with the Fab fragment of the AS0326
		monoclonal antibody
Authors	:	Laursen, N.S.; Andersen, G.R.
Deposited on	:	2022-04-19
Resolution	:	3.40 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 (i) 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 (1)) were used in the production of this report:

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.32.1
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)	:	2.32.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure: $X\text{-}RAY\;DIFFRACTION$

The reported resolution of this entry is 3.40 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	$egin{array}{c} { m Whole \ archive} \ (\#{ m Entries}) \end{array}$	${f Similar\ resolution}\ (\#{ m Entries,\ resolution\ range(Å)})$				
R _{free}	130704	1026 (3.48-3.32)				
Clashscore	141614	1055 (3.48-3.32)				
Ramachandran outliers	138981	1038 (3.48-3.32)				
Sidechain outliers	138945	1038 (3.48-3.32)				
RSRZ outliers	127900	2173 (3.50-3.30)				

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	А	255	78% 8%	•	13%
1	D	255	77% 8%	•	14%
1	Ι	255	79% 7%		14%
1	L	255	76% 11%		13%
1	О	255	.% 	ó •	13%



Mol	Chain	Length	Quality of chain		
1	R	255	% • 78%	8%	14%
1	U	255	3% 77%	9% •	13%
1	Х	255	77%	9%	14%
2	В	222	<u>6%</u> 96%		•
2	Е	222	2% 94%		5%
2	G	222	<u>6%</u> 96%		
2	J	222	2% 94%		6%
2	М	222	92%		7%
2	Р	222	93%		7%
2	S	222	94%		6%
2	V	222	93%		6%
3	С	214	3% 91%		8% •
3	F	214	91%		8% •
3	Н	214	% • 94%		•••
3	K	214	3% 		7% •
3	Ν	214	91%		8% •
3	Q	214	<u>6%</u> 91%		8% •
3	Т	214	90%		9% •
3	W	214	91%		8% •

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2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 80000 atoms, of which 38984 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.

Mol	Chain	Residues			Atoms	5			ZeroOcc	AltConf	Trace
1	Δ	001	Total	С	Η	Ν	0	S	0	0	0
	A	221	3412	1140	1636	294	335	7	0	0	0
1	1 D	220	Total	С	Н	Ν	0	S	0	0	0
1		220	3394	1134	1626	293	334	7	0	0	0
1	1 I	210	Total	С	Η	Ν	0	S	0	0	0
1		219	3377	1129	1618	291	332	7	0	0	0
1	т	221	Total	С	Η	Ν	0	S	0	0	0
1			3412	1140	1636	294	335	7	0	0	0
1	0	001	Total	С	Η	Ν	Ο	\mathbf{S}	0	0	0
1	0	221	3412	1140	1636	294	335	7	0		
1	В	210	Total	С	Η	Ν	Ο	\mathbf{S}	0	0	0
1	п	219	3377	1129	1618	291	332	7	0	0	0
1	II	991	Total	С	Η	Ν	0	\mathbf{S}	0	0	0
	1 0	221	3412	1140	1636	294	335	7	0	0	0
1	1 V	220	Total	С	Н	Ν	0	S	0	0	0
			3394	1134	1626	293	334	7			U

• Molecule 1 is a protein called Microfibril-associated glycoprotein 4.

• Molecule 2 is a protein called heavy chain of antibody AS0326.

Mol	Chain	Residues			Atoms	5			ZeroOcc	AltConf	Trace
9	В	222	Total	С	Н	Ν	0	S	0	0	0
			3361	1076	1654	291	331	9	0	0	0
9	F	<u> </u>	Total	С	Н	Ν	0	S	0	0	0
	Ľ		3361	1076	1654	291	331	9	0	0	0
9	С	222	Total	С	Η	Ν	0	S	0	0	0
	G		3361	1076	1654	291	331	9		0	
9	т	000	Total	\mathbf{C}	Η	Ν	0	\mathbf{S}	0	0	0
	J		3361	1076	1654	291	331	9	0	0	0
9	М	221	Total	С	Η	Ν	0	\mathbf{S}	0	0	0
	2 101	221	3354	1071	1654	290	330	9	0	0	0
2	9 D	222	Total	Ċ	H	N	0	S	0	0	0
	1		3361	1076	1654	291	331	9			0



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2 S	000	Total	С	Η	Ν	0	S	0	0	0	
	G		3361	1076	1654	291	331	9	0	0	0
2 V	001	Total	С	Η	Ν	0	S	0	0	0	
	v	221	3354	1071	1654	290	330	9	0	0	0

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• Molecule 3 is a protein called Light chain of AS0326.

Mol	Chain	Residues			Atoms	s			ZeroOcc	AltConf	Trace
3	С	214	Total	С	Н	Ν	0	S	0	0	0
0	U	217	3239	1033	1590	275	335	6	0	0	0
3	3 F	914	Total	С	Η	Ν	Ο	\mathbf{S}	0	0	0
5		214	3239	1033	1590	275	335	6	0	0	0
3	н	914	Total	С	Η	Ν	Ο	\mathbf{S}	0	0	0
0	о п	214	3239	1033	1590	275	335	6	0	0	
3	K	214	Total	С	Η	Ν	Ο	S	0	0	0
0	Γ		3239	1033	1590	275	335	6	0	0	
3	N	914	Total	С	Η	Ν	Ο	\mathbf{S}	0	0	0
0	11	214	3239	1033	1590	275	335	6	0		
3	0	214	Total	С	Η	Ν	0	\mathbf{S}	0	0	0
0	Q	214	3239	1033	1590	275	335	6	0	0	0
3	т	214	Total	С	Η	Ν	0	\mathbf{S}	0	0	0
0	0 I	214	3239	1033	1590	275	335	6	0	0	0
3	2 W	214	Total	С	Н	Ν	0	S	0	0	0
J	vv		3239	1033	1590	275	335	6	0	U	U

• Molecule 4 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	А	1	Total Ca 1 1	0	0
4	D	1	Total Ca 1 1	0	0
4	Ι	1	Total Ca 1 1	0	0
4	L	1	Total Ca 1 1	0	0
4	О	1	Total Ca 1 1	0	0
4	R	1	Total Ca 1 1	0	0
4	U	1	Total Ca 1 1	0	0



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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	Х	1	Total Ca 1 1	0	0

• Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	А	2	Total O 2 2	0	0
5	D	2	Total O 2 2	0	0
5	Ι	2	Total O 2 2	0	0
5	L	2	Total O 2 2	0	0
5	Ο	2	Total O 2 2	0	0
5	R	2	$\begin{array}{cc} \text{Total} & \text{O} \\ 2 & 2 \end{array}$	0	0
5	U	2	Total O 2 2	0	0
5	Х	2	Total O 2 2	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: Microfibril-associated glycoprotein 4





L98 113 113 138 147 138 138 147 166 1166 1166	R189 L201 N210 N210 N222 R233 R233 R233 R233 R233	
• Molecule 1: Microfi	bril-associated glycoprotein 4	
Chain O:	81%	5%• 13%
MET LYS ALA ALA LEU LEU LEU LEU LEU LEU LEU LEU LEU CAPA	PRO CYS CYS CYS CYS CYS CYS CYS CIA CIA CIA CIA CIA CIA CIA CIA CIA CIA	K63 R64 R65 R65 867 870 870 888 888 888 888 113 113 113
1196 1209 1210 1232 1233 1233 1234		
• Molecule 1: Microfi	bril-associated glycoprotein 4	
Chain R:	78%	8% 14%
MET LYS ALA ALA LEU LEU LEU LEU LEU LEU LEU LEU LEU SER SER PB0	PRO CYS CYS CYS CYS CYS CYS CYS CI CYS CI CI CI CI CI CI CI CI CI CI CI CI CI	020 021 47 47 47 47 46 46 786 46 786 66 766 667 667 191
94 198 113 113 113 113 113 113 113 113 113 11	R233 R233 A234	
• Molecule 1: Microfi	bril-associated glycoprotein 4	
Chain U:	77%	9% • 13%
		· · · · ·
MET MET ALA ALA LEU LEU PRO LEU LEU LEU LEU LEU SER THR	PRO PRO CVS CVS CVS CVS CVS CVS CVS CVS	44 / 44 / 44 / 44 / 44 / 44 / 44 / 44
984 1110 1110 1113 1113 1113 1145 1145 1145 1145 1145	1158 F1366 F1366 F1366 F1366 M1296 M210 M210 M2333 M2333 M2333	
• Molecule 1: Microfi	bril-associated glycoprotein 4	
Chain X:	77%	9% 14%
MET LYS ALA ALA LEU LEU LEU LEU LEU LEU LEU LEU LEU RAR	PRO CYS CYS CYS CYS CYS CYS CYS CYS CYS CYS	V47 V47 C56 C56 C67 C63 C67 C63 C67 C63 C67 C63 C63 C63 C63 C63 C63 C63 C63 C63 C63
L98 D113 F147 F147 F164 F164 R189 R189 R189 R189 I212	K218 R232 A234	
• Molecule 2: heavy of	chain of antibody AS0326	
Chain B:	96%	· ·





• Molecule 2: heavy chain of antibody AS0326

Chain V:	93%	6%
01 148 162 183 183 183 183 183 183 183 183 183 183	V101 V101 V105 V107 C115 C115 V120 V120 V120 V120 V151 V151 V151 V151 V151 V151 V155 V155 V155	V193 T202 Y203 Y203 Y204 Y204 Y204 Y204 Y215 K214 Y217 K218
084		
• Molecule 3: Light ch	ain of AS0326	
Chain C:	91%	8% •
01 12 12 12 12 129 129 129 129 129 129 12	989 990 995 995 995 995 995 995 995 995 99	
• Molecule 3: Light ch	ain of AS0326	
Chain F:	91%	8% •
D1 M4 A25 Y36 Y36 C88 C88 C88 C89 C89 C89 C89 C89 C89 C89	689 E1 05 11 24 11 26 11 24 11 26 11 26 110 110 110 110 110 110 110 110 110 11	
• Molecule 3: Light ch	ain of AS0326	
Chain H:	94%	
01 129 129 129 129 129 129 129 129 100 100	E1 05 F1 18 N1 38 S1 68 S2 02 C2 14 C2 14	
• Molecule 3: Light ch	ain of AS0326	
Chain K:	92%	7% •
D1 12 12 03 04 121 129 129 129 039 039	H91 H92 F94 F94 F94 F94 F94 F94 F104 F104 F105 F105 F105 F105 F105 F105 F105 F105	
• Molecule 3: Light ch	ain of AS0326	
Chain N:	91%	8% •



• Molecule 3: Light chain of AS0326





4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants	317.32Å 126.60Å 187.55Å	Depositor
a, b, c, α , β , γ	90.00° 98.86° 90.00°	Depositor
Bosolution(A)	48.85 - 3.40	Depositor
Resolution (A)	49.25 - 3.40	EDS
% Data completeness	99.7 (48.85-3.40)	Depositor
(in resolution range)	99.8 (49.25-3.40)	EDS
R_{merge}	0.23	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	$1.15 (at 3.40 \text{\AA})$	Xtriage
Refinement program	PHENIX 1.16_3549	Depositor
D D .	0.239 , 0.277	Depositor
n, n_{free}	0.239 , 0.278	DCC
R_{free} test set	2000 reflections $(1.98%)$	wwPDB-VP
Wilson B-factor $(Å^2)$	100.8	Xtriage
Anisotropy	0.651	Xtriage
Bulk solvent $k_{sol}(e/A^3), B_{sol}(A^2)$	0.32 , 72.2	EDS
L-test for $twinning^2$	$ < L >=0.44, < L^2>=0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	80000	wwPDB-VP
Average B, all atoms $(Å^2)$	145.0	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.

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.



¹Intensities estimated from amplitudes.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: CA

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).

Mal	Chain	Bond	Bond lengths		Bond angles	
	Unam	RMSZ	# Z > 5	RMSZ	# Z > 5	
1	А	0.37	0/1830	0.67	1/2475~(0.0%)	
1	D	0.37	0/1822	0.65	0/2464	
1	Ι	0.33	0/1813	0.63	0/2452	
1	L	0.37	0/1830	0.67	0/2475	
1	0	0.34	0/1830	0.65	1/2475~(0.0%)	
1	R	0.34	0/1813	0.64	0/2452	
1	U	0.36	0/1830	0.65	1/2475~(0.0%)	
1	Х	0.36	0/1822	0.65	0/2464	
2	В	0.31	0/1753	0.61	0/2389	
2	Е	0.31	0/1753	0.61	0/2389	
2	G	0.30	0/1753	0.59	0/2389	
2	J	0.31	0/1753	0.59	0/2389	
2	М	0.30	0/1745	0.59	0/2377	
2	Р	0.30	0/1753	0.59	0/2389	
2	S	0.29	0/1753	0.59	0/2389	
2	V	0.30	0/1745	0.59	0/2377	
3	С	0.33	0/1684	0.58	0/2282	
3	F	0.36	0/1684	0.58	0/2282	
3	Н	0.31	0/1684	0.56	0/2282	
3	K	0.31	0/1684	0.57	0/2282	
3	N	0.31	0/1684	0.57	0/2282	
3	Q	0.32	0/1684	0.57	0/2282	
3	Т	0.31	0/1684	0.57	0/2282	
3	W	0.31	0/1684	0.56	0/2282	
All	All	0.33	0/42070	0.61	3/57076~(0.0%)	

There are no bond length outliers.

All (3) bond angle outliers are listed below:



Mol	Chain	Res	Type	Atoms	Z	$\mathbf{Observed}(^{o})$	$Ideal(^{o})$
	<u> </u>	D	-		-		
Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	А	98	LEU	CA-CB-CG	6.07	129.25	115.30
1	0	98	LEU	CA-CB-CG	5.42	127.76	115.30
1	U	98	LEU	CA-CB-CG	5.14	127.13	115.30

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	А	1776	1636	1637	9	0
1	D	1768	1626	1626	11	0
1	Ι	1759	1618	1618	9	0
1	L	1776	1636	1637	13	0
1	0	1776	1636	1637	7	0
1	R	1759	1618	1618	9	0
1	U	1776	1636	1637	11	0
1	Х	1768	1626	1626	10	0
2	В	1707	1654	1661	4	0
2	Е	1707	1654	1661	8	0
2	G	1707	1654	1661	4	0
2	J	1707	1654	1661	5	0
2	М	1700	1654	1654	7	1
2	Р	1707	1654	1661	6	0
2	S	1707	1654	1661	6	0
2	V	1700	1654	1654	6	0
3	С	1649	1590	1603	13	0
3	F	1649	1590	1603	11	0
3	Н	1649	1590	1603	5	0
3	K	1649	1590	1603	11	0
3	N	1649	1590	1603	12	0
3	Q	1649	1590	1603	9	1
3	Т	1649	1590	1603	10	0
3	W	1649	1590	1603	13	0



Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	А	1	0	0	0	0
4	D	1	0	0	0	0
4	Ι	1	0	0	0	0
4	L	1	0	0	0	0
4	0	1	0	0	0	0
4	R	1	0	0	0	0
4	U	1	0	0	0	0
4	Х	1	0	0	0	0
5	А	2	0	0	0	0
5	D	2	0	0	0	0
5	Ι	2	0	0	0	0
5	L	2	0	0	0	0
5	0	2	0	0	0	0
5	R	2	0	0	0	0
5	U	2	0	0	0	0
5	Х	2	0	0	0	0
All	All	41016	38984	39134	201	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 3.

All (201) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom 1	Atom 2	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:A:113:ASP:OD2	1:A:218:LYS:NZ	2.01	0.93
1:D:113:ASP:OD2	1:D:218:LYS:NZ	2.01	0.93
3:K:4:MET:HA	3:K:4:MET:HE2	1.54	0.88
3:K:4:MET:CE	3:K:25:ALA:HA	2.06	0.86
1:I:113:ASP:OD2	1:I:218:LYS:NZ	2.08	0.86
1:X:113:ASP:OD2	1:X:218:LYS:NZ	2.09	0.85
3:N:4:MET:HA	3:N:4:MET:HE2	1.58	0.85
3:W:4:MET:HA	3:W:4:MET:HE2	1.56	0.85
1:U:113:ASP:OD2	1:U:218:LYS:NZ	2.09	0.85
1:0:113:ASP:OD2	1:O:218:LYS:NZ	2.09	0.83
1:R:113:ASP:OD2	1:R:218:LYS:NZ	2.12	0.83
3:T:189:HIS:O	3:T:211:ARG:NH1	2.13	0.82
1:L:113:ASP:OD2	1:L:218:LYS:NZ	2.14	0.81
3:Q:105:GLU:OE1	3:Q:173:TYR:OH	2.00	0.77
3:N:4:MET:CE	3:N:25:ALA:HA	2.15	0.77
1:I:67:GLY:N	1:I:88:GLU:OE2	2.17	0.77
3:N:105:GLU:OE1	3:N:173:TYR:OH	2.03	0.75



	A L O	Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
2:S:82:GLU:OE2	2:S:84:ARG:NH1	2.21	0.73
1:L:201:LEU:HD11	1:L:210:ASN:HD21	1.53	0.73
3:N:4:MET:HE1	3:N:25:ALA:HA	1.71	0.73
3:K:4:MET:HE1	3:K:25:ALA:HA	1.70	0.73
2:P:82:GLU:OE2	2:P:84:ARG:NH1	2.21	0.73
3:W:105:GLU:OE1	3:W:173:TYR:OH	2.06	0.72
3:K:105:GLU:OE1	3:K:173:TYR:OH	2.06	0.72
3:W:4:MET:HE1	3:W:25:ALA:HA	1.71	0.72
3:W:4:MET:CE	3:W:25:ALA:HA	2.19	0.72
2:B:82:GLU:OE2	2:B:84:ARG:NH1	2.24	0.71
3:H:105:GLU:OE1	3:H:173:TYR:OH	2.08	0.70
2:J:82:GLU:OE2	2:J:84:ARG:NH1	2.25	0.70
3:T:105:GLU:OE1	3:T:173:TYR:OH	2.10	0.70
3:F:105:GLU:OE1	3:F:173:TYR:OH	2.09	0.69
1:L:67:GLY:N	1:L:88:GLU:OE2	2.25	0.69
2:M:82:GLU:OE2	2:M:84:ARG:NH1	2.26	0.69
3:N:88:CYS:O	3:N:99:GLY:N	2.26	0.69
3:Q:88:CYS:O	3:Q:99:GLY:N	2.26	0.69
1:O:67:GLY:N	1:O:88:GLU:OE2	2.26	0.68
3:F:88:CYS:O	3:F:99:GLY:N	2.27	0.68
2:G:82:GLU:OE2	2:G:84:ARG:NH1	2.26	0.67
3:T:88:CYS:O	3:T:99:GLY:N	2.27	0.67
1:O:14:LEU:HD23	1:0:14:LEU:O	1.95	0.67
1:U:54:GLU:O	1:U:232:ARG:NH2	2.28	0.66
1:0:70:SER:O	1:O:73:ARG:NH1	2.29	0.66
1:U:207:SER:OG	1:U:210:ASN:ND2	2.29	0.65
1:A:70:SER:O	1:A:73:ARG:NH1	2.30	0.64
1:R:67:GLY:N	1:R:88:GLU:OE2	2.30	0.64
3:C:167:ASP:OD1	3:C:168:SER:N	2.31	0.64
2:V:82:GLU:OE2	2:V:84:ARG:NH1	2.31	0.63
3:K:167:ASP:OD1	3:K:168:SER:N	2.31	0.63
2:E:82:GLU:OE2	2:E:84:ARG:NH1	2.32	0.63
3:W:88:CYS:O	3:W:99:GLY:N	2.31	0.62
3:C:36:TYR:OH	3:C:89:GLN:OE1	2.07	0.62
3:C:105:GLU:OE1	3:C:173:TYR:OH	2.11	0.62
3:F:167:ASP:OD1	3:F:168:SER:N	2.34	0.61
3:H:88:CYS:O	3:H:99:GLY:N	2.33	0.61
3:K:4:MET:HE1	3:K:25:ALA:CA	2.30	0.61
2:S:197:SER:OG	2:S:203:TYR:OH	2.13	0.61
1:L:201:LEU:HD11	1:L:210:ASN:ND2	2.15	0.60
3:F:90:GLN:OE1	3:F:92:ASN:N	2.34	0.60



	A h o	Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
3:K:186:TYR:O	3:K:192:TYR:OH	2.19	0.60
3:F:4:MET:HE2	3:F:25:ALA:HA	1.84	0.59
3:Q:186:TYR:O	3:Q:192:TYR:OH	2.19	0.59
2:B:114:GLN:N	2:B:114:GLN:OE1	2.35	0.59
3:H:167:ASP:OD1	3:H:168:SER:N	2.35	0.59
1:D:207:SER:OG	1:D:210:ASN:ND2	2.36	0.59
1:I:158:TYR:O	1:I:189:ARG:NH1	2.36	0.59
2:P:212:SER:OG	2:P:214:THR:OG1	2.20	0.59
2:B:67:ARG:NH2	2:B:90:ASP:OD2	2.35	0.59
3:N:29:ILE:HD11	3:N:90:GLN:HG2	1.84	0.59
3:W:167:ASP:OD1	3:W:168:SER:N	2.36	0.58
3:Q:167:ASP:OD1	3:Q:168:SER:N	2.36	0.58
3:N:167:ASP:OD1	3:N:168:SER:N	2.37	0.58
1:R:54:GLU:O	1:R:232:ARG:NH2	2.33	0.58
2:J:67:ARG:NH2	2:J:90:ASP:OD2	2.37	0.58
1:X:67:GLY:N	1:X:88:GLU:OE2	2.37	0.57
3:F:36:TYR:OH	3:F:89:GLN:OE1	2.06	0.57
1:D:158:TYR:O	1:D:189:ARG:NH1	2.37	0.56
2:S:67:ARG:NH2	2:S:90:ASP:OD2	2.39	0.56
1:X:47:VAL:HG12	1:X:91:LEU:HD13	1.88	0.56
2:P:44:ARG:HG3	3:Q:100:GLN:HA	1.89	0.55
1:D:19:ASP:OD2	1:D:233:ARG:NH1	2.38	0.55
2:E:138:LYS:NZ	3:F:208:SER:O	2.36	0.55
3:C:2:ILE:HD11	3:C:93:GLU:OE1	2.07	0.54
3:T:124:GLN:OE1	3:T:131:SER:N	2.40	0.54
3:C:2:ILE:HG22	3:C:2:ILE:O	2.07	0.54
3:W:4:MET:HE1	3:W:25:ALA:CA	2.36	0.54
1:U:67:GLY:N	1:U:88:GLU:OE2	2.41	0.54
1:A:158:TYR:O	1:A:189:ARG:NH1	2.40	0.54
1:D:56:GLY:O	1:D:232:ARG:NH2	2.41	0.54
2:J:212:SER:OG	2:J:214:THR:OG1	2.26	0.54
3:N:4:MET:HE1	3:N:25:ALA:CA	2.36	0.54
2:V:106:SER:OG	2:V:107:TRP:N	2.40	0.54
1:A:19:ASP:OD2	1:A:233:ARG:NH1	2.38	0.53
1:O:14:LEU:O	1:O:14:LEU:CD2	2.57	0.53
3:C:2:ILE:HG21	3:C:90:GLN:CG	2.39	0.53
3:C:88:CYS:O	3:C:99:GLY:N	2.42	0.52
2:M:212:SER:OG	2:M:214:THR:OG1	2.27	0.52
3:W:33:LEU:O	3:W:50:SER:N	2.42	0.52
1:R:21:ASP:OD1	1:R:57:LYS:O	2.28	0.52
1:U:158:TYR:O	1:U:189:ARG:NH1	2.41	0.52



	A L O	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
3:F:124:GLN:OE1	3:F:131:SER:N	2.42	0.52
2:S:114:GLN:OE1	2:S:114:GLN:N	2.42	0.52
1:D:84:ARG:NH2	1:L:138:ASP:OD1	2.40	0.52
3:K:88:CYS:O	3:K:99:GLY:N	2.41	0.51
1:D:94:GLN:O	1:D:98:LEU:HD22	2.10	0.51
1:X:158:TYR:O	1:X:189:ARG:NH1	2.42	0.51
3:Q:29:ILE:HD11	3:Q:90:GLN:O	2.11	0.51
1:U:70:SER:O	1:U:73:ARG:NH1	2.44	0.51
2:V:6:GLN:OE1	2:V:115:GLY:N	2.42	0.51
2:M:98:ARG:HB3	2:M:111:VAL:HG12	1.92	0.51
3:W:124:GLN:OE1	3:W:131:SER:N	2.44	0.51
2:M:114:GLN:N	2:M:114:GLN:OE1	2.45	0.50
3:C:4:MET:CE	3:C:25:ALA:HA	2.42	0.50
2:V:67:ARG:NH2	2:V:90:ASP:OD2	2.43	0.50
3:F:4:MET:CE	3:F:25:ALA:HA	2.41	0.50
1:I:50:ASP:OD2	1:I:53:THR:OG1	2.16	0.50
1:L:93:LEU:HD11	1:L:164:PHE:CD2	2.46	0.50
1:I:47:VAL:HG12	1:I:91:LEU:HD13	1.94	0.50
1:A:213:ASN:ND2	1:A:222:TYR:O	2.45	0.50
3:C:29:ILE:HD11	3:C:90:GLN:O	2.12	0.50
3:T:167:ASP:OD1	3:T:168:SER:N	2.45	0.50
1:I:56:GLY:O	1:I:232:ARG:NH2	2.43	0.49
1:O:56:GLY:O	1:O:232:ARG:NH2	2.45	0.49
2:G:6:GLN:OE1	2:G:115:GLY:N	2.45	0.49
1:L:94:GLN:O	1:L:98:LEU:HD22	2.13	0.49
2:S:6:GLN:OE1	2:S:115:GLY:N	2.44	0.49
1:R:47:VAL:HG12	1:R:91:LEU:HD13	1.95	0.49
2:P:6:GLN:OE1	2:P:115:GLY:N	2.43	0.49
1:R:138:ASP:OD2	1:U:84:ARG:NH2	2.45	0.48
3:K:29:ILE:HD11	3:K:90:GLN:HG2	1.95	0.48
3:T:187:GLU:O	3:T:211:ARG:NH1	2.47	0.48
1:X:56:GLY:O	1:X:232:ARG:NH2	2.46	0.48
3:Q:29:ILE:HG22	3:Q:68:GLY:O	2.12	0.48
2:E:67:ARG:NH2	2:E:90:ASP:OD2	2.46	0.48
1:U:156:LEU:HD23	1:U:214:TRP:CH2	2.48	0.47
2:G:44:ARG:HG3	3:H:100:GLN:HA	1.96	0.47
3:K:90:GLN:OE1	3:K:92:ASN:N	2.44	0.47
3:W:29:ILE:HD11	3:W:90:GLN:O	2.13	0.47
1:A:67:GLY:N	1:A:88:GLU:OE2	2.47	0.47
2:J:6:GLN:OE1	2:J:115:GLY:N	2.42	0.47
3:H:29:ILE:HD11	3:H:90:GLN:O	2.14	0.47



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:L:47:VAL:HG12	1:L:91:LEU:HD13	1.96	0.47
1:A:56:GLY:O	1:A:232:ARG:NH2	2.46	0.47
1:R:158:TYR:O	1:R:189:ARG:NH1	2.46	0.47
2:G:67:ARG:NH2	2:G:90:ASP:OD2	2.48	0.47
3:Q:124:GLN:OE1	3:Q:131:SER:N	2.48	0.47
2:M:6:GLN:OE1	2:M:115:GLY:N	2.47	0.46
1:X:94:GLN:O	1:X:98:LEU:HD22	2.16	0.46
1:D:70:SER:O	1:D:73:ARG:NH1	2.48	0.46
1:X:93:LEU:HD11	1:X:164:PHE:CD2	2.51	0.46
3:N:1:ASP:HB2	3:N:2:ILE:HD12	1.97	0.46
3:N:33:LEU:O	3:N:51:GLY:N	2.43	0.45
1:U:47:VAL:HG12	1:U:91:LEU:HD13	1.98	0.45
2:V:61:ASN:OD1	2:V:62:GLU:N	2.50	0.45
3:C:2:ILE:HG21	3:C:90:GLN:HG3	1.99	0.44
3:T:29:ILE:HD11	3:T:90:GLN:HG2	1.99	0.44
3:Q:108:ARG:NE	3:Q:170:ASP:O	2.50	0.44
1:L:19:ASP:OD1	1:L:21:ASP:N	2.51	0.44
3:W:4:MET:HE1	3:W:25:ALA:CB	2.47	0.44
3:W:29:ILE:HG22	3:W:68:GLY:O	2.18	0.44
3:C:29:ILE:HG22	3:C:68:GLY:O	2.18	0.43
1:L:158:TYR:O	1:L:189:ARG:NH1	2.48	0.43
1:D:86:ASP:N	1:D:86:ASP:OD1	2.52	0.43
2:J:61:ASN:OD1	2:J:62:GLU:N	2.51	0.43
1:L:50:ASP:OD2	1:L:53:THR:OG1	2.22	0.43
3:W:4:MET:HE2	3:W:4:MET:CA	2.40	0.43
1:0:94:GLN:0	1:O:98:LEU:HD22	2.19	0.42
3:K:4:MET:HE2	3:K:24:ARG:O	2.20	0.42
2:V:212:SER:OG	2:V:214:THR:OG1	2.37	0.42
1:X:64:ARG:NH1	1:X:212:ILE:HG23	2.34	0.42
1:I:64:ARG:NH1	1:I:212:ILE:HG23	2.33	0.42
1:X:21:ASP:N	1:X:21:ASP:OD1	2.53	0.42
3:T:12:SER:OG	3:T:140:TYR:OH	2.35	0.42
3:F:186:TYR:O	3:F:192:TYR:OH	2.32	0.42
3:N:29:ILE:HG22	3:N:68:GLY:O	2.19	0.42
1:D:20:CYS:CB	1:D:59:THR:HG22	2.50	0.42
1:L:21:ASP:N	1:L:21:ASP:OD1	2.52	0.42
2:S:4:LEU:HD23	2:S:111:VAL:CG1	2.50	0.42
1:A:24:TYR:HH	2:E:107:TRP:HE1	1.67	0.41
3:C:2:ILE:HD11	3:C:93:GLU:CD	2.40	0.41
1:U:94:GLN:O	1:U:98:LEU:HD22	2.20	0.41
1:U:21:ASP:N	1:U:21:ASP:OD1	2.53	0.41



Atom 1	Atom 2	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
2:E:4:LEU:HD23	2:E:111:VAL:HG12	2.01	0.41
2:P:4:LEU:HD23	2:P:111:VAL:CG1	2.51	0.41
1:R:94:GLN:O	1:R:98:LEU:HD22	2.20	0.41
2:M:61:ASN:OD1	2:M:62:GLU:N	2.53	0.41
2:P:61:ASN:OD1	2:P:62:GLU:N	2.54	0.41
3:N:4:MET:HE2	3:N:4:MET:CA	2.40	0.41
1:R:19:ASP:OD2	1:R:233:ARG:NH1	2.52	0.41
1:D:131:ASN:ND2	1:I:86:ASP:OD1	2.54	0.41
2:M:67:ARG:NH2	2:M:90:ASP:OD2	2.54	0.41
2:E:212:SER:OG	2:E:214:THR:OG1	2.34	0.41
3:T:90:GLN:OE1	3:T:92:ASN:N	2.53	0.41
3:C:124:GLN:OE1	3:C:131:SER:N	2.54	0.41
1:L:166:THR:HG22	1:L:167:PHE:N	2.36	0.41
3:T:186:TYR:O	3:T:192:TYR:OH	2.36	0.40
2:E:107:TRP:CZ2	3:F:94:TYR:HE2	2.39	0.40
1:X:31:ASP:N	1:X:31:ASP:OD1	2.52	0.40
1:A:93:LEU:HD12	1:A:140:TYR:HB3	2.02	0.40
2:B:4:LEU:HD23	2:B:111:VAL:HG12	2.04	0.40
2:E:114:GLN:N	2:E:114:GLN:OE1	2.55	0.40
1:I:64:ARG:NH1	1:I:212:ILE:CG2	2.85	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:M:144:THR:OG1	3:Q:202:SER:OG[3_555]	1.98	0.22

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	А	219/255~(86%)	209 (95%)	9~(4%)	1 (0%)	29 61



Mol	Chain	Analysed	Favoured	Allowed	Outliers	Perce	entiles
1	D	218/255~(86%)	209~(96%)	8 (4%)	1 (0%)	29	61
1	Ι	217/255~(85%)	207~(95%)	9 (4%)	1 (0%)	29	61
1	L	219/255~(86%)	211 (96%)	7(3%)	1 (0%)	29	61
1	Ο	219/255~(86%)	209~(95%)	9 (4%)	1 (0%)	29	61
1	R	217/255~(85%)	208~(96%)	8 (4%)	1 (0%)	29	61
1	U	219/255~(86%)	208~(95%)	9~(4%)	2(1%)	17	49
1	Х	218/255~(86%)	208~(95%)	9~(4%)	1 (0%)	29	61
2	В	220/222 (99%)	207~(94%)	13 (6%)	0	100	100
2	Е	220/222 (99%)	206 (94%)	14 (6%)	0	100	100
2	G	220/222 (99%)	206~(94%)	14 (6%)	0	100	100
2	J	220/222~(99%)	207~(94%)	13 (6%)	0	100	100
2	М	219/222~(99%)	207~(94%)	12 (6%)	0	100	100
2	Р	220/222 (99%)	208 (94%)	12 (6%)	0	100	100
2	S	220/222 (99%)	209~(95%)	11 (5%)	0	100	100
2	V	219/222 (99%)	207~(94%)	12 (6%)	0	100	100
3	С	212/214~(99%)	201 (95%)	9 (4%)	2(1%)	17	49
3	F	212/214~(99%)	201 (95%)	9 (4%)	2(1%)	17	49
3	Н	212/214~(99%)	201~(95%)	9~(4%)	2(1%)	17	49
3	Κ	212/214~(99%)	201~(95%)	8 (4%)	3~(1%)	11	37
3	Ν	212/214~(99%)	201 (95%)	9 (4%)	2(1%)	17	49
3	Q	$2\overline{12/214}\ (99\%)$	201~(95%)	10 (5%)	1 (0%)	29	61
3	Т	212/214 (99%)	201 (95%)	8 (4%)	3 (1%)	11	37
3	W	$2\overline{12/214}\ (99\%)$	200 (94%)	10 (5%)	2(1%)	17	49
All	All	5200/5528~(94%)	4933 (95%)	241 (5%)	26 (0%)	29	61

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All (26) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	А	65	PHE
1	D	65	PHE
1	Ι	65	PHE
1	L	65	PHE
1	0	65	PHE
1	R	65	PHE



Mol	Chain	Res	Type
1		1005	CIN
1	U	15	GLN
1	U	65	PHE
3	W	213	GLU
1	Х	65	PHE
3	N	96	PHE
3	Ν	138	ASN
3	Т	96	PHE
3	С	96	PHE
3	F	138	ASN
3	Н	138	ASN
3	K	138	ASN
3	Q	138	ASN
3	Т	91	HIS
3	W	96	PHE
3	К	2	ILE
3	С	94	TYR
3	F	94	TYR
3	Н	94	TYR
3	К	94	TYR
3	Т	2	ILE

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	Perce	ntiles
1	А	182/210~(87%)	176 (97%)	6 (3%)	38	66
1	D	181/210~(86%)	176~(97%)	5(3%)	43	70
1	Ι	180/210~(86%)	178 (99%)	2(1%)	73	86
1	L	182/210~(87%)	177 (97%)	5(3%)	44	70
1	О	182/210~(87%)	177 (97%)	5(3%)	44	70
1	R	180/210~(86%)	178 (99%)	2(1%)	73	86
1	U	182/210~(87%)	178 (98%)	4 (2%)	52	75
1	Х	181/210~(86%)	176 (97%)	5(3%)	43	70



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Mol	Chain	Analysed	Rotameric	Outliers	Perce	ntiles	;
2	В	194/194~(100%)	192~(99%)	2(1%)	76	88	
2	Е	194/194~(100%)	191 (98%)	3(2%)	65	82	
2	G	194/194~(100%)	192 (99%)	2(1%)	76	88	
2	J	194/194~(100%)	190 (98%)	4 (2%)	53	76	
2	М	193/194~(100%)	191 (99%)	2(1%)	76	88	
2	Р	194/194~(100%)	190 (98%)	4 (2%)	53	76	
2	S	194/194~(100%)	192 (99%)	2(1%)	76	88	
2	V	193/194~(100%)	191 (99%)	2(1%)	76	88	
3	С	188/188~(100%)	185~(98%)	3(2%)	62	81	
3	F	188/188~(100%)	184 (98%)	4 (2%)	53	76	
3	Н	188/188~(100%)	184 (98%)	4 (2%)	53	76	
3	K	188/188~(100%)	185~(98%)	3~(2%)	62	81	
3	Ν	188/188~(100%)	184 (98%)	4 (2%)	53	76	
3	Q	188/188~(100%)	184 (98%)	4 (2%)	53	76	
3	Т	188/188 (100%)	184 (98%)	4 (2%)	53	76	
3	W	188/188~(100%)	$1\overline{83}\ (97\%)$	5(3%)	44	70	
All	All	$450\overline{4/4736}\ (95\%)$	4418 (98%)	86 (2%)	57	78	

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All (86) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	А	63	LYS
1	А	73	ARG
1	А	147	PHE
1	А	186	PHE
1	А	210	ASN
1	А	232	ARG
2	В	101	TRP
2	В	147	LEU
3	С	81	GLU
3	С	90	GLN
3	С	94	TYR
1	D	63	LYS
1	D	73	ARG
1	D	147	PHE
1	D	186	PHE



Mol	Chain	Res	Type
1	D	232	ARG
2	Е	101	TRP
2	Е	114	GLN
2	Е	147	LEU
3	F	81	GLU
3	F	88	CYS
3	F	90	GLN
3	F	94	TYR
2	G	101	TRP
2	G	147	LEU
3	Н	81	GLU
3	Н	88	CYS
3	Н	90	GLN
3	Н	94	TYR
1	Ι	84	ARG
1	Ι	147	PHE
2	J	101	TRP
2	J	108	TYR
2	J	114	GLN
2	J	147	LEU
3	K	88	CYS
3	K	90	GLN
3	K	94	TYR
1	L	63	LYS
1	L	84	ARG
1	L	147	PHE
1	L	222	TYR
1	L	232	ARG
2	М	101	TRP
2	М	147	LEU
3	N	88	CYS
3	N	90	GLN
3	N	94	TYR
3	N	211	ARG
1	0	63	LYS
1	0	73	ARG
1	Ο	147	PHE
1	0	210	ASN
1	0	232	ARG
2	Р	22	CYS
2	P	101	TRP
2	Р	114	GLN



Mol	Chain	Res	Type
2	Р	147	LEU
3	Q	81	GLU
3	Q	88	CYS
3	Q	90	GLN
3	Q	94	TYR
1	R	63	LYS
1	R	147	PHE
2	S	101	TRP
2	S	147	LEU
3	Т	88	CYS
3	Т	90	GLN
3	Т	94	TYR
3	Т	211	ARG
1	U	63	LYS
1	U	73	ARG
1	U	147	PHE
1	U	186	PHE
2	V	101	TRP
2	V	147	LEU
3	W	46	LEU
3	W	81	GLU
3	W	88	CYS
3	W	90	GLN
3	W	94	TYR
1	Х	21	ASP
1	Х	63	LYS
1	Х	84	ARG
1	Х	147	PHE
1	Х	210	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	D	210	ASN
1	D	213	ASN
1	U	210	ASN
1	U	213	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 8 ligands modelled in this entry, 8 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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	$\langle RSRZ \rangle$	#RSRZ>2	$\mathbf{OWAB}(\mathrm{\AA}^2)$	$Q{<}0.9$
1	А	221/255~(86%)	0.39	1 (0%) 91 90	65, 90, 115, 187	0
1	D	220/255~(86%)	0.37	0 100 100	77,102,131,192	0
1	Ι	219/255~(85%)	0.26	1 (0%) 91 90	87, 122, 150, 197	0
1	L	221/255~(86%)	0.24	0 100 100	70, 91, 121, 178	0
1	Ο	221/255~(86%)	0.41	3 (1%) 75 74	78, 113, 156, 186	0
1	R	219/255~(85%)	0.30	2 (0%) 84 83	71, 104, 140, 176	0
1	U	221/255~(86%)	0.45	8 (3%) 42 42	79, 109, 143, 183	0
1	Х	220/255~(86%)	0.24	1 (0%) 91 90	70, 93, 124, 201	0
2	В	222/222 (100%)	0.60	14 (6%) 20 21	109, 138, 182, 291	0
2	Е	222/222 (100%)	0.37	5 (2%) 60 59	90, 123, 177, 262	0
2	G	222/222 (100%)	0.54	14 (6%) 20 21	87, 127, 168, 371	0
2	J	222/222 (100%)	0.18	4 (1%) 68 67	85, 126, 178, 266	0
2	М	221/222 (99%)	0.84	30 (13%) 3 3	120, 158, 197, 320	0
2	Р	222/222 (100%)	0.65	23 (10%) 6 8	88, 142, 200, 343	0
2	S	222/222 (100%)	1.10	44 (19%) 1 1	101, 164, 278, 351	0
2	V	221/222 (99%)	0.65	22 (9%) 7 8	91, 160, 241, 276	0
3	С	214/214~(100%)	0.26	6 (2%) 53 51	92, 116, 176, 226	0
3	F	214/214~(100%)	0.23	1 (0%) 91 90	89, 111, 139, 174	0
3	Н	214/214~(100%)	0.24	3 (1%) 75 74	88, 131, 167, 214	0
3	K	214/214~(100%)	0.34	6 (2%) 53 51	83, 128, 180, 218	0
3	N	$2\overline{14/214}\ (100\%)$	0.69	22 (10%) 6 8	122, 158, 198, 216	0
3	Q	$2\overline{14/214}\ (100\%)$	0.46	12 (5%) 24 25	95, 148, 215, 250	0
3	Т	214/214~(100%)	0.92	36 (16%) 1 2	115, 184, 246, 306	0
3	W	214/214 (100%)	0.92	35~(16%) 1 2	98, 190, 249, 286	0



Mol	Chain	Analysed	< RSRZ >	#RSRZ>2	$\mathbf{OWAB}(\mathbf{\AA}^2)$	Q<0.9
All	All	5248/5528~(94%)	0.49	293 (5%) 24 25	65, 126, 212, 371	0

All (293) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	М	139	SER	11.5
2	S	142	GLY	11.2
2	М	138	LYS	8.3
2	G	142	GLY	8.0
3	W	133	VAL	7.6
3	W	194	CYS	7.4
2	G	140	THR	7.3
2	М	137	SER	7.3
2	Р	140	THR	7.2
2	G	139	SER	7.0
3	Т	132	VAL	6.9
3	Т	152	ASN	6.8
3	N	214	CYS	6.2
2	Р	139	SER	6.2
2	S	199	GLY	6.1
2	S	141	SER	6.1
2	Р	150	LEU	6.0
3	W	114	SER	6.0
2	G	141	SER	5.8
2	S	144	THR	5.6
2	V	118	VAL	5.6
2	S	195	SER	5.5
2	S	135	PRO	5.4
3	W	177	SER	5.2
2	S	143	GLY	5.2
3	Т	180	THR	5.2
2	М	141	SER	5.2
2	S	148	GLY	5.1
2	J	139	SER	5.1
2	М	142	GLY	5.1
2	S	161	VAL	5.0
3	W	137	ASN	4.9
3	Т	204	PRO	4.8
3	W	156	SER	4.8
3	K	214	CYS	4.8
3	Т	149	LYS	4.8
3	W	196	VAL	4.6



Mol	Chain	Res	Type	RSRZ
3	W	205	VAL	4.5
2	V	1	GLN	4.4
2	V	221	GLU	4.4
3	N	17	ASP	4.3
2	В	140	THR	4.3
3	Т	116	PHE	4.2
2	S	210	LYS	4.2
2	J	140	THR	4.2
2	S	145	ALA	4.2
2	G	190	VAL	4.1
3	Т	133	VAL	4.1
2	В	128	PRO	4.1
3	W	206	THR	4.0
3	W	146	VAL	4.0
2	G	138	LYS	4.0
2	S	173	HIS	4.0
2	S	150	LEU	4.0
1	R	16	GLN	4.0
3	Q	214	CYS	3.9
2	М	193	VAL	3.9
2	V	217	ASP	3.9
2	Е	139	SER	3.9
2	М	109	PHE	3.9
2	S	134	ALA	3.9
2	М	143	GLY	3.9
3	Ν	202	SER	3.8
2	В	189	SER	3.8
2	G	188	SER	3.8
2	S	196	SER	3.8
2	S	137	SER	3.7
2	М	140	THR	3.7
2	S	168	LEU	3.7
2	S	200	THR	3.7
2	G	189	SER	3.7
3	Т	203	SER	3.7
3	Т	199	GLN	3.7
3	W	134	CYS	3.6
3	W	121	SER	3.6
2	V	130	VAL	3.6
3	N	204	PRO	3.5
3	W	178	THR	3.5
3	W	201	LEU	3.5



7ZMK

Mol	Chain	Res	Type	RSRZ
3	W	135	LEU	3.5
3	W	131	SER	3.4
2	S	37	VAL	3.4
2	S	170	SER	3.4
3	W	214	CYS	3.4
3	Т	195	GLU	3.4
3	С	1	ASP	3.4
2	V	132	PRO	3.4
2	М	36	TRP	3.4
2	М	136	SER	3.4
2	М	120	VAL	3.3
2	S	208	ASN	3.3
2	S	139	SER	3.3
2	М	81	MET	3.3
2	G	145	ALA	3.3
2	S	211	PRO	3.3
1	Х	15	GLN	3.3
3	Т	117	ILE	3.3
2	М	53	PRO	3.3
2	М	29	PHE	3.2
3	W	199	GLN	3.2
2	В	139	SER	3.2
3	W	116	PHE	3.2
3	W	117	ILE	3.2
3	W	183	LYS	3.2
2	В	129	SER	3.2
2	М	68	VAL	3.1
1	R	42	SER	3.1
3	Q	146	VAL	3.1
2	Р	131	PHE	3.1
2	Р	128	PRO	3.1
3	Т	113	PRO	3.1
2	J	62	GLU	3.1
2	S	94	TYR	3.0
2	S	86	LEU	3.0
2	Р	149	CYS	3.0
3	N	8	PRO	3.0
2	Р	200	THR	3.0
3	Т	155	GLN	3.0
3	Т	214	CYS	3.0
1	0	209	ALA	3.0
2	Р	119	THR	3.0



Mol	Chain	Res	Type	RSRZ
3	Q	88	CYS	3.0
2	Р	151	VAL	2.9
2	S	207	VAL	2.9
2	S	136	SER	2.9
2	G	130	VAL	2.9
2	V	119	THR	2.9
3	W	195	GLU	2.9
2	М	19	LYS	2.9
2	М	69	THR	2.8
3	Н	118	PHE	2.8
3	Q	86	TYR	2.8
3	Q	122	ASP	2.8
2	В	219	LYS	2.8
2	М	144	THR	2.8
2	V	120	VAL	2.8
2	М	60	TYR	2.8
2	Е	200	THR	2.8
3	N	82	ASP	2.8
2	В	168	LEU	2.7
2	V	150	LEU	2.7
2	М	151	VAL	2.7
2	S	83	LEU	2.7
3	Т	148	TRP	2.7
2	S	193	VAL	2.7
2	М	207	VAL	2.7
3	Т	110	VAL	2.7
3	Q	204	PRO	2.7
2	S	198	LEU	2.7
2	J	37	VAL	2.7
2	S	216	VAL	2.7
3	N	113	PRO	2.7
2	S	95	TYR	2.6
3	Т	127	SER	2.6
3	Ν	108	ARG	2.6
3	W	145	LYS	2.6
1	U	144	VAL	2.6
2	М	37	VAL	2.6
3	С	98	PHE	2.6
2	В	147	LEU	2.6
3	Т	154	LEU	2.6
3	W	27	LYS	2.6
3	F	147	GLN	2.6



Mol	Chain	Res	Type	RSRZ
3	Q	36	TYR	2.6
2	Р	45	LEU	2.6
3	Ν	199	GLN	2.5
2	Р	130	VAL	2.5
2	V	202	THR	2.5
2	S	171	GLY	2.5
3	Т	205	VAL	2.5
3	W	176	SER	2.5
2	М	82	GLU	2.5
2	Р	46	GLU	2.5
3	Q	131	SER	2.5
3	Ν	143	GLU	2.5
3	Ν	116	PHE	2.5
2	М	48	ILE	2.5
1	U	14	LEU	2.5
2	V	164	ASN	2.5
2	V	2	MET	2.5
2	Р	137	SER	2.5
3	W	113	PRO	2.4
3	Ν	14	SER	2.4
3	С	24	ARG	2.4
3	С	146	VAL	2.4
3	Q	116	PHE	2.4
3	W	93	GLU	2.4
2	V	193	VAL	2.4
3	Т	182	SER	2.4
3	W	213	GLU	2.4
2	G	200	THR	2.4
3	Т	206	THR	2.4
3	Т	201	LEU	2.4
3	N	183	LYS	2.4
2	S	1	GLN	2.4
2	P	18	VAL	2.4
3	N	19	VAL	2.4
3	N	144	ALA	2.4
3	K	122	ASP	2.3
1	А	14	LEU	2.3
2	S	147	LEU	2.3
2	S	172	VAL	2.3
2	S	129	SER	2.3
2	P	207	VAL	2.3
3	Т	171	SER	2.3



Mol	Chain	Res	Type	RSRZ
2	S	151	VAL	2.3
3	Q	123	GLU	2.3
2	V	48	ILE	2.3
1	U	196	LEU	2.3
2	Р	83	LEU	2.3
3	С	135	LEU	2.3
3	Ν	104	LEU	2.3
3	Т	130	ALA	2.3
3	Т	185	ASP	2.3
3	Ν	115	VAL	2.3
3	W	170	ASP	2.3
3	W	202	SER	2.3
2	В	166	GLY	2.3
2	V	62	GLU	2.3
2	V	218	LYS	2.3
3	Т	126	LYS	2.3
3	Т	135	LEU	2.3
2	Ε	48	ILE	2.3
2	В	204	ILE	2.3
2	М	202	THR	2.3
2	V	175	PHE	2.3
3	Κ	34	ALA	2.3
3	Т	115	VAL	2.3
2	V	147	LEU	2.2
3	Ν	12	SER	2.2
3	Т	144	ALA	2.2
1	U	72	PHE	2.2
2	Р	95	TYR	2.2
3	W	148	TRP	2.2
2	S	18	VAL	2.2
3	K	193	ALA	2.2
3	Т	192	TYR	2.2
3	W	181	LEU	2.2
2	E	195	SER	2.2
2	М	27	PHE	2.2
3	Т	153	ALA	2.2
2	Р	84	ARG	2.2
2	V	166	GLY	2.2
2	Р	94	TYR	2.2
2	Р	219	LYS	2.2
2	M	84	ARG	2.2
2	М	145	ALA	2.2



Mol	Chain	Res	Type	RSRZ
2	Р	138	LYS	2.2
3	Ν	203	SER	2.2
1	U	110	ASP	2.2
1	Ι	16	GLN	2.1
2	В	109	PHE	2.1
3	Q	97	THR	2.1
3	Ν	11	LEU	2.1
2	В	37	VAL	2.1
2	S	38	ARG	2.1
3	С	100	GLN	2.1
3	Н	36	TYR	2.1
2	V	135	PRO	2.1
3	W	111	ALA	2.1
3	Т	109	THR	2.1
2	S	109	PHE	2.1
2	V	204	ILE	2.1
2	В	190	VAL	2.1
3	Q	126	LYS	2.1
3	W	115	VAL	2.1
2	G	147	LEU	2.1
1	U	112	GLU	2.1
3	Ν	107	LYS	2.1
2	S	140	THR	2.1
2	М	132	PRO	2.1
1	0	196	LEU	2.1
3	W	11	LEU	2.1
1	U	145	ALA	2.0
2	Р	202	THR	2.0
2	V	151	VAL	2.0
2	В	148	GLY	2.0
2	G	143	GLY	2.0
3	Н	202	SER	2.0
3	K	21	ILE	2.0
1	0	29	GLN	2.0
2	Е	47	TRP	2.0
2	S	153	ASP	2.0
3	K	103	LYS	2.0
3	Т	191	VAL	2.0
2	G	204	ILE	2.0
2	Р	147	LEU	2.0
1	U	186	PHE	2.0
3	Т	147	GLN	2.0



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Mol	Chain	Res	Type	RSRZ
2	S	85	SER	2.0
3	Ν	146	VAL	2.0
3	Т	177	SER	2.0
3	Т	190	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)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	$\mathbf{B} ext{-factors}(\mathbf{A}^2)$	Q<0.9
4	CA	U	501	1/1	0.86	0.21	97,97,97,97	0
4	CA	Ι	501	1/1	0.95	0.17	129,129,129,129	0
4	CA	А	501	1/1	0.95	0.17	82,82,82,82	0
4	CA	0	501	1/1	0.97	0.19	97,97,97,97	0
4	CA	Х	501	1/1	0.97	0.19	84,84,84,84	0
4	CA	L	501	1/1	0.98	0.20	83,83,83,83	0
4	CA	D	501	1/1	0.99	0.24	95,95,95,95	0
4	CA	R	501	1/1	0.99	0.19	111,111,111,111	0

6.5 Other polymers (i)

There are no such residues in this entry.

