

Full wwPDB X-ray Structure Validation Report (i)

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PDB ID	:	6XVI
Title	:	Crystal structure of Megabody Mb-Nb207-c7HopQ_A12
Authors	:	Steyaert, J.; Uchanski, T.; Fischer, B.
Deposited on	:	2020-01-22
Resolution	:	2.60 Å(reported)
Title Authors Deposited on Resolution	: : :	Crystal structure of Megabody Mb-Nb207-c7HopQ_A1 Steyaert, J.; Uchanski, T.; Fischer, B. 2020-01-22 2.60 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 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	:	2.16
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)	:	2.16

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 2.60 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 $(\#Entries, resolution, range(Å))$		
\mathbf{R}_{free}	130704	3163 (2.60-2.60)		
Clashscore	141614	3518 (2.60-2.60)		
Ramachandran outliers	138981	$3455\ (2.60-2.60)$		
Sidechain outliers	138945	3455(2.60-2.60)		
RSRZ outliers	127900	3104 (2.60-2.60)		

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	521	% • 70%	13%		16%
1	В	521	^{2%} 70%	11%	•	19%
1	С	521	4% 69%	13%	•	17%
1	D	521	68%	12%		20%



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2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 13015 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

• Molecule 1 is a protein called Outer membrane protein, Outer membrane protein,Mb-Nb207 $-\rm c7HopQ_A12.$

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace	
1	Λ	437	Total	С	Ν	Ο	\mathbf{S}	0	0	0
	л	407	3310	2050	585	662	13	0	0	0
1	р	494	Total	С	Ν	Ο	S	0	0	0
	D	424	3207	1988	564	642	13	0	0	0
1	C	420	Total	С	Ν	Ο	S	0	0	0
		430	3255	2012	576	654	13	0	0	0
1	П	418	Total	С	Ν	Ο	S	0	0	0
	418	3167	1960	557	637	13	U	0	0	

There are 52 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
А	1	GLN	-	expression tag	UNP B5Z8H1
А	2	VAL	-	expression tag	UNP B5Z8H1
А	3	GLN	-	expression tag	UNP B5Z8H1
А	4	LEU	-	expression tag	UNP B5Z8H1
А	5	VAL	-	expression tag	UNP B5Z8H1
А	6	GLU	-	expression tag	UNP B5Z8H1
А	7	SER	-	expression tag	UNP B5Z8H1
А	8	GLY	-	expression tag	UNP B5Z8H1
А	9	GLY	-	expression tag	UNP B5Z8H1
А	10	GLY	-	expression tag	UNP B5Z8H1
А	11	LEU	-	expression tag	UNP B5Z8H1
А	12	VAL	-	expression tag	UNP B5Z8H1
А	13	ARG	-	expression tag	UNP B5Z8H1
В	1	GLN	-	expression tag	UNP B5Z8H1
В	2	VAL	-	expression tag	UNP B5Z8H1
В	3	GLN	-	expression tag	UNP B5Z8H1
В	4	LEU	-	expression tag	UNP B5Z8H1
В	5	VAL	-	expression tag	UNP B5Z8H1
В	6	GLU	-	expression tag	UNP B5Z8H1
В	7	SER	-	expression tag	UNP B5Z8H1



Chain	Residue	Modelled	Actual	Comment	Reference
В	8	GLY	-	expression tag	UNP B5Z8H1
В	9	GLY	-	expression tag	UNP B5Z8H1
В	10	GLY	_	expression tag	UNP B5Z8H1
В	11	LEU	_	expression tag	UNP B5Z8H1
В	12	VAL	-	expression tag	UNP B5Z8H1
В	13	ARG	-	expression tag	UNP B5Z8H1
С	1	GLN	-	expression tag	UNP B5Z8H1
С	2	VAL	-	expression tag	UNP B5Z8H1
С	3	GLN	-	expression tag	UNP B5Z8H1
С	4	LEU	-	expression tag	UNP B5Z8H1
С	5	VAL	-	expression tag	UNP B5Z8H1
С	6	GLU	-	expression tag	UNP B5Z8H1
С	7	SER	-	expression tag	UNP B5Z8H1
С	8	GLY	-	expression tag	UNP B5Z8H1
С	9	GLY	-	expression tag	UNP B5Z8H1
С	10	GLY	-	expression tag	UNP B5Z8H1
С	11	LEU	-	expression tag	UNP B5Z8H1
С	12	VAL	-	expression tag	UNP B5Z8H1
С	13	ARG	-	expression tag	UNP B5Z8H1
D	1	GLN	-	expression tag	UNP B5Z8H1
D	2	VAL	-	expression tag	UNP B5Z8H1
D	3	GLN	-	expression tag	UNP B5Z8H1
D	4	LEU	-	expression tag	UNP B5Z8H1
D	5	VAL	-	expression tag	UNP B5Z8H1
D	6	GLU	-	expression tag	UNP B5Z8H1
D	7	SER	-	expression tag	UNP B5Z8H1
D	8	GLY	-	expression tag	UNP B5Z8H1
D	9	GLY	-	expression tag	UNP B5Z8H1
D	10	GLY	-	expression tag	UNP B5Z8H1
D	11	LEU	-	expression tag	UNP B5Z8H1
D	12	VAL	-	expression tag	UNP B5Z8H1
D	13	ARG	-	expression tag	UNP B5Z8H1

• Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	А	36	Total O 36 36	0	0
2	В	21	Total O 21 21	0	0
2	С	9	Total O 9 9	0	0



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	D	10	Total O 10 10	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: Outer membrane protein, Outer membrane protein, Mb-Nb207-c7HopQ_A12







4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants	96.05Å 117.38Å 96.84 Å	Deneiten
a, b, c, α , β , γ	90.00° 90.72° 90.00°	Depositor
$\mathbf{P}_{\text{assolution}}(\hat{\mathbf{A}})$	29.62 - 2.60	Depositor
Resolution (A)	29.62 - 2.60	EDS
% Data completeness	94.6 (29.62-2.60)	Depositor
(in resolution range $)$	$94.6\ (29.62-2.60)$	EDS
R _{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	$1.10 (at 2.61 \text{\AA})$	Xtriage
Refinement program	PHENIX 1.12_2829	Depositor
R R.	0.224 , 0.250	Depositor
n, n_{free}	0.224 , 0.251	DCC
R_{free} test set	3141 reflections $(5.00%)$	wwPDB-VP
Wilson B-factor $(Å^2)$	66.2	Xtriage
Anisotropy	0.039	Xtriage
Bulk solvent $k_{sol}(e/A^3), B_{sol}(A^2)$	0.31 , 33.7	EDS
L-test for $twinning^2$	$< L >=0.48, < L^2>=0.31$	Xtriage
	0.000 for l,k,-h	
Estimated twinning fraction	0.074 for h,-k,-l	Xtriage
	0.019 for l,-k,h	
F_o, F_c correlation	0.94	EDS
Total number of atoms	13015	wwPDB-VP
Average B, all atoms $(Å^2)$	76.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 3.60% 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)

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	lengths	Bond angles		
	Unam	RMSZ	# Z > 5	RMSZ	# Z > 5	
1	А	0.64	0/3358	0.72	0/4547	
1	В	0.62	0/3253	0.68	0/4402	
1	С	0.62	0/3300	0.71	0/4466	
1	D	0.57	0/3212	0.71	0/4348	
All	All	0.61	0/13123	0.71	0/17763	

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	А	3310	0	3246	45	0
1	В	3207	0	3136	36	0
1	С	3255	0	3184	53	0
1	D	3167	0	3091	59	0
2	А	36	0	0	1	0
2	В	21	0	0	0	0
2	С	9	0	0	1	0
2	D	10	0	0	0	0
All	All	13015	0	12657	189	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 7.



A 1 -		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:D:306:TYR:CD2	1:D:351:LYS:HA	1.57	1.37
1:D:215:ILE:HD11	1:D:266:ARG:NH1	1.72	1.03
1:D:306:TYR:CE2	1:D:351:LYS:HA	1.95	1.01
1:D:306:TYR:CD2	1:D:351:LYS:CA	2.49	0.95
1:D:215:ILE:HD11	1:D:266:ARG:HH12	1.25	0.94
1:D:306:TYR:HD2	1:D:351:LYS:HA	1.22	0.93
1:C:253:ALA:O	1:C:256:ILE:HG22	1.70	0.91
1:D:215:ILE:CD1	1:D:266:ARG:HH12	1.85	0.89
1:C:253:ALA:O	1:C:256:ILE:CG2	2.25	0.85
1:D:306:TYR:HE2	1:D:351:LYS:CB	1.89	0.85
1:D:306:TYR:CE2	1:D:351:LYS:CA	2.63	0.80
1:B:221:LEU:HD21	1:B:256:ILE:HG12	1.62	0.79
1:C:22:THR:HG22	2:C:609:HOH:O	1.81	0.79
1:D:266:ARG:HG2	1:D:266:ARG:HH11	1.49	0.78
1:B:350:LEU:HD12	1:B:351:LYS:H	1.47	0.78
1:D:214:GLN:HB3	1:D:262:ASN:HD21	1.50	0.77
1:C:34:GLN:HG3	1:C:90:ILE:HG21	1.67	0.76
1:D:306:TYR:CE2	1:D:351:LYS:CB	2.69	0.76
1:D:306:TYR:HE2	1:D:351:LYS:HB3	1.50	0.76
1:A:119:LEU:H	1:A:119:LEU:HD12	1.50	0.76
1:D:215:ILE:CD1	1:D:266:ARG:NH1	2.44	0.75
1:C:254:GLN:NE2	1:C:254:GLN:HA	1.99	0.75
1:A:121:SER:HB2	1:A:122:PRO:HD3	1.70	0.72
1:A:354:LYS:HG3	1:A:355:ASN:ND2	2.05	0.72
1:B:214:GLN:HB2	1:B:262:ASN:HD21	1.54	0.72
1:D:306:TYR:HD2	1:D:350:LEU:O	1.73	0.70
1:A:320:TYR:HB2	1:A:328:THR:HG23	1.74	0.70
1:C:254:GLN:HE21	1:C:254:GLN:HA	1.57	0.70
1:D:34:GLN:HG3	1:D:90:ILE:HG21	1.73	0.69
1:C:253:ALA:C	1:C:256:ILE:HG22	2.12	0.68
1:D:306:TYR:HD2	1:D:351:LYS:CA	1.98	0.68
1:D:375:LYS:NZ	1:D:379:GLN:OE1	2.26	0.68
1:D:306:TYR:HB3	1:D:350:LEU:O	1.96	0.66
1:D:216:ASN:O	1:D:219:GLN:HG2	1.96	0.66
1:C:253:ALA:HA	1:C:256:ILE:HG22	1.78	0.65
1:C:256:ILE:HG23	1:C:257:ASN:N	2.12	0.65
1:A:375:LYS:NZ	1:A:379:GLN:OE1	2.29	0.65
1:B:438:TRP:O	1:B:457:ARG:NH2	2.30	0.64
1:A:121:SER:CB	1:A:122:PRO:HD3	2.26	0.64
1:D:354:LYS:HG2	1:D:355:ASN:ND2	2.13	0.63

All (189) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.



		Interatomic	Clash
Atom-1	Atom-2	distance $(Å)$	overlap(Å)
1:B:34:GLN:HG3	1:B:90:ILE:HG21	1.81	0.62
1:B:214:GLN:HB2	1:B:262:ASN:ND2	2.14	0.62
1:D:306:TYB:CD2	1:D:350:LEU:O	2 51	0.62
1:B:89:MET:HE1	1:B:156:LEU:HD22	1.82	0.61
1:D:306:TYR:HD2	1:D:350:LEU:C	2.03	0.61
1:C:253:ALA:HA	1:C:256:ILE:CG2	2.31	0.60
1:C:323:GLU:HA	1:C:323:GLU:OE1	2.01	0.60
1:D:208:PHE:CE2	1:D:270:LEU:HD13	2.36	0.60
1:B:22:THR:HG21	1:B:372:ILE:HG23	1.84	0.60
1:C:15:THR:HG23	1:C:397:THR:HG23	1.83	0.59
1:A:22:THR:HG21	1:A:372:ILE:HG23	1.85	0.58
1:B:404:ARG:HD2	1:B:467:GLN:OE1	2.04	0.57
1:C:111:ILE:HG12	1:C:125:LEU:HD11	1.85	0.57
1:C:483:ALA:HB3	1:C:500:TYR:HB2	1.85	0.57
1:B:312:GLU:HA	1:B:312:GLU:OE1	2.04	0.57
1:C:253:ALA:CA	1:C:256:ILE:HG22	2.35	0.57
1:B:211:GLN:HB3	1:B:214:GLN:NE2	2.19	0.57
1:C:256:ILE:HG23	1:C:257:ASN:H	1.68	0.57
1:C:305:GLY:HA2	1:C:350:LEU:O	2.04	0.57
1:D:367:HIS:O	1:D:371:GLN:HG2	2.05	0.56
1:D:22:THR:HG21	1:D:372:ILE:HG23	1.87	0.56
1:C:213:PRO:CG	1:D:351:LYS:HD3	2.35	0.56
1:A:82:GLU:HG2	1:A:161:LEU:HD23	1.87	0.56
1:C:284:LEU:O	1:C:288:ARG:HG2	2.05	0.56
1:D:46:ILE:HB	1:D:302:ILE:HD12	1.86	0.56
1:C:213:PRO:HG2	1:D:351:LYS:CD	2.36	0.55
1:C:165:ILE:O	1:C:190:GLY:HA3	2.06	0.55
1:C:2:VAL:HG22	1:C:411:GLY:HA3	1.89	0.55
1:A:473:PRO:HA	1:A:509:VAL:HG23	1.88	0.54
1:B:187:TRP:HE1	1:B:328:THR:HG21	1.73	0.54
1:C:253:ALA:O	1:C:256:ILE:HG23	2.07	0.54
1:A:291:LEU:HD13	1:A:373:LEU:HD23	1.90	0.53
1:C:130:GLN:HA	1:C:130:GLN:OE1	2.07	0.53
1:D:3:GLN:H	1:D:410:SER:HB3	1.74	0.53
1:C:291:LEU:HD22	1:C:377:LEU:HD12	1.90	0.53
1:B:2:VAL:HG11	1:B:500:TYR:CZ	2.43	0.53
1:A:485:ARG:NH1	1:A:500:TYR:CZ	2.78	0.52
1:C:82:GLU:HG2	1:C:161:LEU:HD23	1.91	0.52
1:C:349:THR:HG23	1:C:349:THR:O	2.09	0.52
1:C:213:PRO:HG2	1:D:351:LYS:HD3	1.92	0.51
1:D:46:ILE:HA	1:D:74:ASN:HA	1.92	0.51



	Interatomic Clash					
Atom-1	Atom-2	distance (Å)	overlap (Å)			
1:B:274:THR:HG23	1:B:280:TYR:CE2	2.45	0.51			
1:C:89:MET:HE1	1:C:156:LEU:HD22	1.92	0.51			
1:A:90:ILE:HD13	1:A:286:ALA:HB1	1.93	0.50			
1:D:266:ARG:CG	1:D:266:ARG:HH11	2.21	0.50			
1:D:266:ARG:NH1	1:D:266:ARG:HG2	2.20	0.50			
1:B:353:ASP:OD1	1:B:354:LYS:N	2.41	0.50			
1:B:471:LEU:HB3	1:B:509:VAL:HG21	1.93	0.50			
1:B:192:ALA:O	1:B:288:ARG:HD3	2.11	0.50			
1:A:472:LYS:O	1:A:509:VAL:HG21	2.11	0.50			
1:A:215:ILE:HD11	1:A:266:ARG:HG3	1.94	0.49			
1:A:157:SER:O	1:A:162:LYS:HA	2.12	0.49			
1:C:260:VAL:HG12	1:C:261:ASN:N	2.27	0.49			
1:B:306:TYR:CD1	1:B:306:TYR:C	2.87	0.49			
1:A:305:GLY:HA3	1:A:352:ALA:HB2	1.95	0.49			
1:A:214:GLN:NE2	1:A:266:ARG:HD3	2.28	0.48			
1:C:192:ALA:O	1:C:288:ARG:HD3	2.12	0.48			
1:C:413:THR:HB	1:C:438:TRP:NE1	2.28	0.48			
1:C:46:ILE:HA	1:C:74:ASN:HA	1.94	0.48			
1:B:212:THR:O	1:B:215:ILE:HG13	2.13	0.48			
1:D:359:SER:OG	1:D:361:GLU:OE1	2.32	0.48			
1:A:370:TYR:CD1	1:A:370:TYR:C	2.86	0.48			
1:D:306:TYR:CB	1:D:350:LEU:O	2.62	0.48			
1:C:417:ALA:HB3	1:C:485:ARG:HA	1.95	0.48			
1:D:97:VAL:O	1:D:100:THR:HG22	2.14	0.48			
1:D:192:ALA:O	1:D:288:ARG:HD3	2.14	0.48			
1:B:211:GLN:O	1:B:214:GLN:HG2	2.14	0.47			
1:D:123:SER:O	1:D:126:THR:HG22	2.14	0.47			
1:A:387:SER:O	1:A:388:LYS:HE2	2.13	0.47			
1:D:165:ILE:O	1:D:190:GLY:HA3	2.14	0.47			
1:D:208:PHE:HA	1:D:266:ARG:HH21	1.80	0.47			
1:D:26:ALA:HB2	1:D:382:LEU:HD11	1.97	0.47			
1:A:449:ALA:HB1	1:A:453:PHE:HB2	1.97	0.46			
1:D:353:ASP:O	1:D:356:VAL:HG12	2.15	0.46			
1:A:485:ARG:NH1	1:A:500:TYR:OH	2.39	0.46			
1:A:407:CYS:HB3	1:A:464:VAL:HG12	1.97	0.46			
1:A:43:TYR:CE2	1:A:362:GLN:NE2	2.83	0.46			
1:C:484:ARG:HD3	1:C:492:PRO:HG3	1.97	0.46			
1:D:20:ILE:O	1:D:393:GLU:HA	$2.\overline{16}$	0.46			
1:D:266:ARG:NH1	1:D:266:ARG:CG	2.79	0.46			
1:B:132:MET:HG3	1:B:222:ALA:HB2	1.97	0.45			
1:B:320:TYR:CZ	1:B:367:HIS:HD2	$2.\overline{34}$	$0.\overline{45}$			



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:C:322:ASP:HB3	1:C:324:ASN:ND2	2.31	0.45
1:A:119:LEU:CD1	1:A:119:LEU:H	2.16	0.45
1:A:250:LYS:O	1:A:250:LYS:HG3	2.16	0.45
1:A:106:ASN:O	1:A:108:PRO:HD3	2.15	0.45
1:A:89:MET:CE	1:A:153:PHE:HA	2.46	0.45
1:C:82:GLU:HG2	1:C:161:LEU:CD2	2.47	0.45
1:A:379:GLN:O	1:A:379:GLN:HG3	2.16	0.45
1:A:305:GLY:HA2	1:A:350:LEU:O	2.17	0.45
1:A:27:GLN:O	1:A:31:THR:HG23	2.17	0.45
1:B:305:GLY:HA3	1:B:352:ALA:HB2	1.99	0.44
1:A:291:LEU:HD12	1:A:291:LEU:HA	1.77	0.44
1:C:124:SER:O	1:C:127:ALA:N	2.50	0.44
1:A:390:GLU:HG3	2:A:619:HOH:O	2.16	0.44
1:C:92:ASN:O	1:C:96:ILE:HG12	2.17	0.44
1:D:306:TYR:HD2	1:D:351:LYS:N	2.15	0.44
1:A:354:LYS:HG2	1:A:354:LYS:O	2.16	0.44
1:B:316:LYS:HE3	1:B:364:GLU:OE2	2.18	0.44
1:A:85:ALA:O	1:A:89:MET:HG3	2.17	0.44
1:A:220:ASN:O	1:A:224:THR:HG23	2.18	0.44
1:B:402:SER:HB2	1:B:467:GLN:HE21	1.83	0.44
1:D:28:ASN:O	1:D:32:GLN:HG2	2.17	0.44
1:D:215:ILE:HD11	1:D:266:ARG:HH11	1.74	0.43
1:B:318:PHE:CD1	1:B:318:PHE:N	2.87	0.43
1:C:133:LEU:CD2	1:C:219:GLN:HG3	2.48	0.43
1:C:287:LEU:O	1:C:290:VAL:HG22	2.19	0.43
1:C:213:PRO:CB	1:D:351:LYS:HD3	2.48	0.43
1:B:306:TYR:O	1:B:306:TYR:CD1	2.70	0.43
1:D:24:ASN:HB2	1:D:381:GLY:O	2.18	0.43
1:D:306:TYR:CE2	1:D:351:LYS:HB3	2.39	0.43
1:C:256:ILE:CG2	1:C:257:ASN:N	2.81	0.43
1:D:34:GLN:HG3	1:D:90:ILE:CG2	2.47	0.43
1:D:6:GLU:HA	1:D:407:CYS:HA	1.99	0.43
1:A:208:PHE:CE2	1:A:270:LEU:HD13	2.54	0.43
1:C:124:SER:O	1:C:127:ALA:HB3	2.19	0.43
1:C:297:MET:HG3	1:C:298:GLY:N	2.33	0.43
1:D:212:THR:O	1:D:216:ASN:ND2	2.52	0.43
1:A:317:ASP:HB3	1:A:329:THR:HG23	2.01	0.43
1:A:164:TYR:O	1:A:167:LYS:HG2	2.18	0.42
1:B:6:GLU:OE2	1:B:502:GLY:HA3	2.19	0.42
1:A:104:SER:HA	1:A:107:GLN:HE21	1.84	0.42
1:A:284:LEU:HD12	1:A:284:LEU:HA	1.83	0.42



Atom 1	Atom 2	Interatomic	Clash	
Atom-1	Atom-2	${ m distance}~({ m \AA})$	overlap (Å)	
1:B:157:SER:O	1:B:162:LYS:HA	2.20	0.42	
1:B:39:THR:HG21	1:B:366:ILE:HD11	2.01	0.42	
1:B:331:ASN:OD1	1:B:332:CYS:N	2.52	0.42	
1:C:212:THR:O	1:C:215:ILE:HG13	2.19	0.42	
1:A:356:VAL:HG13	1:A:357:SER:H	1.85	0.42	
1:C:33:ALA:HB1	1:C:290:VAL:HG21	2.01	0.42	
1:C:305:GLY:C	1:C:352:ALA:HB2	2.40	0.42	
1:A:2:VAL:HG11	1:A:500:TYR:CZ	2.54	0.42	
1:A:121:SER:N	1:A:122:PRO:CD	2.82	0.42	
1:B:435:GLY:HA3	1:B:444:TYR:CZ	2.55	0.42	
1:D:167:LYS:O	1:D:189:ASN:HB3	2.20	0.41	
1:D:425:ALA:HB1	1:D:426:PRO:HD2	2.03	0.41	
1:C:186:ASN:HB2	1:C:322:ASP:OD1	2.21	0.41	
1:B:139:GLN:NE2	1:B:267:ALA:HB2	2.35	0.41	
1:B:211:GLN:OE1	1:B:214:GLN:NE2	2.53	0.41	
1:B:293:LEU:O	1:B:297:MET:HG3	2.21	0.41	
1:C:6:GLU:OE2	1:C:502:GLY:HA3	2.20	0.41	
1:D:97:VAL:O	1:D:101:GLN:HG3	2.21	0.41	
1:A:44:CYS:O	1:A:74:ASN:HB2	2.21	0.41	
1:C:90:ILE:HD13	1:C:286:ALA:HB1	2.03	0.40	
1:D:225:LEU:HA	1:D:225:LEU:HD23	1.90	0.40	
1:C:66:TRP:HB3	1:C:160:HIS:HB3	2.03	0.40	
1:C:322:ASP:CB	1:C:324:ASN:ND2	2.84	0.40	
1:A:331:ASN:OD1	1:A:332:CYS:N	2.54	0.40	
1:B:4:LEU:HD13	1:B:481:CYS:SG	2.61	0.40	
1:D:136:ALA:HB2	1:D:263:LEU:HD21	2.02	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	Perce	ntiles
1	А	423/521~(81%)	412 (97%)	11 (3%)	0	100	100
1	В	408/521~(78%)	397~(97%)	11 (3%)	0	100	100
1	С	416/521~(80%)	401 (96%)	15~(4%)	0	100	100
1	D	404/521~(78%)	397~(98%)	6(2%)	1 (0%)	47	71
All	All	1651/2084~(79%)	1607 (97%)	43 (3%)	1 (0%)	51	75

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	71	GLY

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	А	355/427~(83%)	350~(99%)	5(1%)	67 85
1	В	342/427~(80%)	337~(98%)	5(2%)	65 83
1	С	347/427~(81%)	338~(97%)	9(3%)	46 72
1	D	338/427~(79%)	332~(98%)	6 (2%)	59 80
All	All	1382/1708~(81%)	1357 (98%)	25 (2%)	59 80

All (25) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	А	65	SER
1	А	119	LEU
1	А	228	GLU
1	А	457	ARG
1	А	479	TYR
1	В	102	GLN
1	В	306	TYR
1	В	350	LEU
1	В	416	THR
1	В	457	ARG



Mol	Chain	Res	Type
1	С	254	GLN
1	С	258	GLN
1	С	307	THR
1	С	349	THR
1	С	350	LEU
1	С	429	GLU
1	С	457	ARG
1	С	472	LYS
1	С	498	TYR
1	D	266	ARG
1	D	306	TYR
1	D	320	TYR
1	D	457	ARG
1	D	479	TYR
1	D	498	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	А	107	GLN
1	С	254	GLN
1	С	326	ASN
1	С	462	ASN
1	D	262	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)

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 (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, 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	2	$\mathbf{OWAB}(\mathbf{\AA}^2)$	$Q{<}0.9$
1	А	437/521~(83%)	0.36	4 (0%) 84	82	37,68,105,155	0
1	В	424/521~(81%)	0.42	8 (1%) 66	62	43,69,110,139	0
1	С	430/521~(82%)	0.55	23 (5%) 26	20	42, 72, 126, 147	0
1	D	418/521~(80%)	0.58	25 (5%) 21	16	46, 78, 131, 182	0
All	All	1709/2084~(82%)	0.47	60 (3%) 44	36	37, 72, 121, 182	0

All (60) RSRZ outliers are listed below:

Mol	Chain	\mathbf{Res}	Type	RSRZ
1	D	217	GLN	7.2
1	С	132	MET	6.1
1	D	310	PRO	5.7
1	А	311	GLY	4.9
1	С	312	GLU	4.8
1	С	2	VAL	4.7
1	D	351	LYS	4.7
1	D	324	ASN	4.4
1	D	132	MET	4.3
1	D	125	LEU	4.0
1	D	256	ILE	3.9
1	С	313	ASN	3.7
1	D	352	ALA	3.7
1	С	256	ILE	3.5
1	В	256	ILE	3.4
1	С	111	ILE	3.4
1	С	356	VAL	3.4
1	С	252	SER	3.4
1	В	132	MET	3.4
1	D	122	PRO	3.3
1	В	263	LEU	3.3



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Mol	Chain	Res	Type	RSRZ
1	С	225	LEU	3.2
1	С	350	LEU	3.2
1	С	379	GLN	3.2
1	А	310	PRO	3.2
1	В	334	GLY	3.1
1	В	125	LEU	3.0
1	С	112	THR	3.0
1	D	48	ILE	3.0
1	D	486	ARG	2.9
1	D	127	ALA	2.7
1	D	271	ALA	2.7
1	D	350	LEU	2.5
1	А	132	MET	2.5
1	В	507	VAL	2.5
1	D	266	ARG	2.5
1	D	464	VAL	2.5
1	С	263	LEU	2.4
1	С	218	ALA	2.4
1	С	217	GLN	2.4
1	С	108	PRO	2.3
1	С	437	TYR	2.3
1	В	308	LYS	2.3
1	D	450	LYS	2.3
1	С	253	ALA	2.3
1	С	131	LYS	2.2
1	С	349	THR	2.2
1	D	134	LYS	2.2
1	D	305	GLY	2.2
1	D	104	SER	2.2
1	В	169	ASP	2.2
1	А	225	LEU	2.2
1	D	306	TYR	2.2
1	D	224	THR	2.1
1	С	301	VAL	2.1
1	D	474	GLU	2.1
1	С	3	GLN	2.1
1	D	136	ALA	2.1
1	D	257	ASN	2.0
1	С	127	ALA	2.0

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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.

