Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 09:50 AM GMT

PDB ID	:	3JRM
Title	:	Crystal structure of archaeal 20S proteasome in complex with mutated P26 activator
Authors	:	Stadtmueller, B.M.; Whitby, F.G.; Hill, C.P.
Deposited on	:	2009-09-08
Resolution	:	2.90 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
http://wwpdb.org/validation/2016/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:

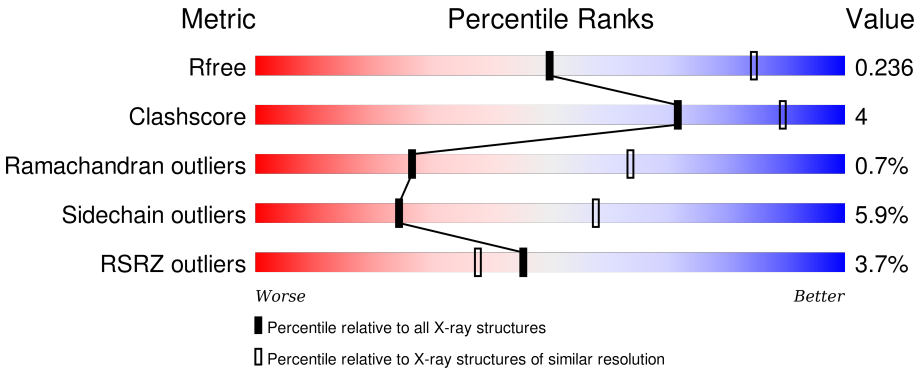
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

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 2.90 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}	91344	1451 (2.90-2.90)
Clashscore	102246	1668 (2.90-2.90)
Ramachandran outliers	100387	1630 (2.90-2.90)
Sidechain outliers	100360	1632 (2.90-2.90)
RSRZ outliers	91569	1456 (2.90-2.90)

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 on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. 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	227	7% 88% 9% ·
1	B	227	6% 86% 11% ·
1	C	227	4% 88% 9% ·
1	D	227	6% 89% 7% ·
1	E	227	5% 86% 10% ·

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Mol	Chain	Length	Quality of chain
1	F	227	7% 85% 11%
1	G	227	4% 85% 11%
2	H	203	2% 86% 12%
2	I	203	% 88% 9%
2	J	203	3% 89% 9%
2	K	203	3% 89% 9%
2	L	203	2% 88% 9%
2	M	203	2% 88% 9%
2	N	203	2% 87% 10%
3	O	228	3% 82% 13%
3	P	228	4% 85% 10%
3	Q	228	3% 85% 10%
3	R	228	4% 84% 11%
3	S	228	2% 86% 9%
3	T	228	2% 85% 11%
3	U	228	3% 84% 11%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 35035 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 Proteasome subunit alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	227	Total	C	N	O	S	0	0	0
			1768	1123	299	343	3			
1	B	227	Total	C	N	O	S	0	0	0
			1768	1123	299	343	3			
1	C	227	Total	C	N	O	S	0	0	0
			1768	1123	299	343	3			
1	D	227	Total	C	N	O	S	0	0	0
			1768	1123	299	343	3			
1	E	227	Total	C	N	O	S	0	0	0
			1768	1123	299	343	3			
1	F	227	Total	C	N	O	S	0	0	0
			1768	1123	299	343	3			
1	G	227	Total	C	N	O	S	0	0	0
			1768	1123	299	343	3			

- Molecule 2 is a protein called Proteasome subunit beta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	203	Total	C	N	O	S	0	0	0
			1557	985	264	297	11			
2	I	203	Total	C	N	O	S	0	0	0
			1557	985	264	297	11			
2	J	203	Total	C	N	O	S	0	0	0
			1557	985	264	297	11			
2	K	203	Total	C	N	O	S	0	0	0
			1557	985	264	297	11			
2	L	203	Total	C	N	O	S	0	0	0
			1557	985	264	297	11			
2	M	203	Total	C	N	O	S	0	0	0
			1557	985	264	297	11			
2	N	203	Total	C	N	O	S	0	0	0
			1557	985	264	297	11			

- Molecule 3 is a protein called Proteasome activator protein PA26.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	O	218	Total	C	N	O	S	0	0	0
			1680	1054	296	324	6			
3	P	218	Total	C	N	O	S	0	0	0
			1680	1054	296	324	6			
3	Q	218	Total	C	N	O	S	0	0	0
			1680	1054	296	324	6			
3	R	218	Total	C	N	O	S	0	0	0
			1680	1054	296	324	6			
3	S	218	Total	C	N	O	S	0	0	0
			1680	1054	296	324	6			
3	T	218	Total	C	N	O	S	0	0	0
			1680	1054	296	324	6			
3	U	218	Total	C	N	O	S	0	0	0
			1680	1054	296	324	6			

There are 27 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
O	49	VAL	THR	VARIANT	UNP Q9U8G2
O	102	ALA	GLU	ENGINEERED	UNP Q9U8G2
O	230	TYR	VAL	ENGINEERED	UNP Q9U8G2
O	226	THR	SER	ENGINEERED	UNP Q9U8G2
P	49	VAL	THR	VARIANT	UNP Q9U8G2
P	102	ALA	GLU	ENGINEERED	UNP Q9U8G2
P	230	TYR	VAL	ENGINEERED	UNP Q9U8G2
O	226	THR	SER	ENGINEERED	UNP Q9U8G2
Q	49	VAL	THR	VARIANT	UNP Q9U8G2
Q	102	ALA	GLU	ENGINEERED	UNP Q9U8G2
Q	230	TYR	VAL	ENGINEERED	UNP Q9U8G2
O	226	THR	SER	ENGINEERED	UNP Q9U8G2
R	49	VAL	THR	VARIANT	UNP Q9U8G2
R	102	ALA	GLU	ENGINEERED	UNP Q9U8G2
R	230	TYR	VAL	ENGINEERED	UNP Q9U8G2
O	226	THR	SER	ENGINEERED	UNP Q9U8G2
S	49	VAL	THR	VARIANT	UNP Q9U8G2
S	102	ALA	GLU	ENGINEERED	UNP Q9U8G2
S	230	TYR	VAL	ENGINEERED	UNP Q9U8G2
O	226	THR	SER	ENGINEERED	UNP Q9U8G2
T	49	VAL	THR	VARIANT	UNP Q9U8G2
T	102	ALA	GLU	ENGINEERED	UNP Q9U8G2
T	230	TYR	VAL	ENGINEERED	UNP Q9U8G2
O	226	THR	SER	ENGINEERED	UNP Q9U8G2

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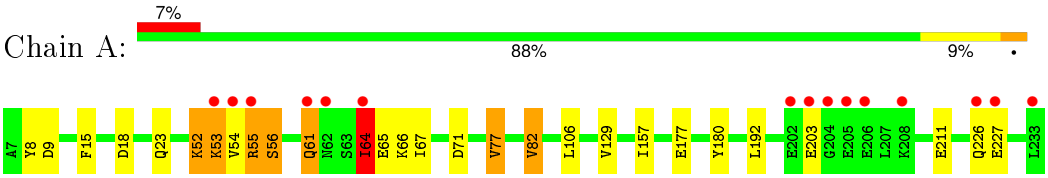
Chain	Residue	Modelled	Actual	Comment	Reference
U	49	VAL	THR	VARIANT	UNP Q9U8G2
U	102	ALA	GLU	ENGINEERED	UNP Q9U8G2
U	230	TYR	VAL	ENGINEERED	UNP Q9U8G2

3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

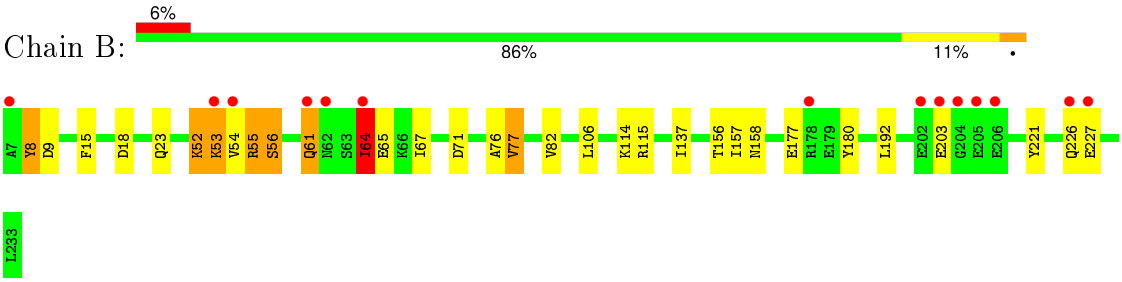
- Molecule 1: Proteasome subunit alpha

Chain A:



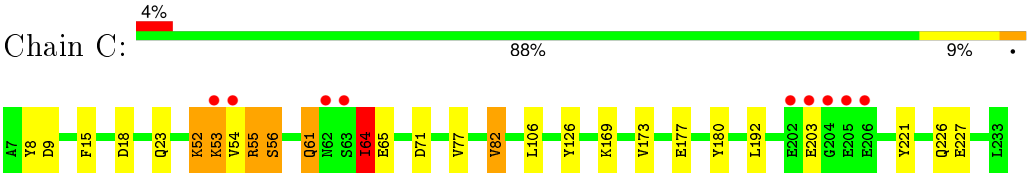
- Molecule 1: Proteasome subunit alpha

Chain B:



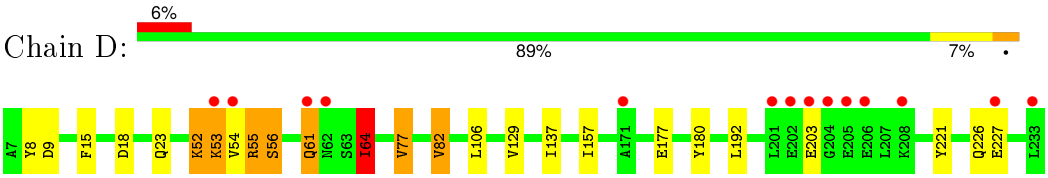
- Molecule 1: Proteasome subunit alpha

Chain C:



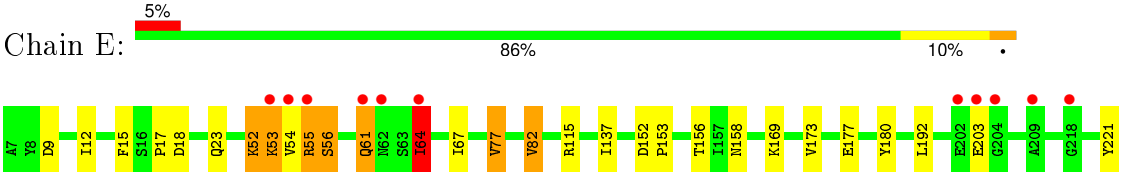
- Molecule 1: Proteasome subunit alpha

Chain D:



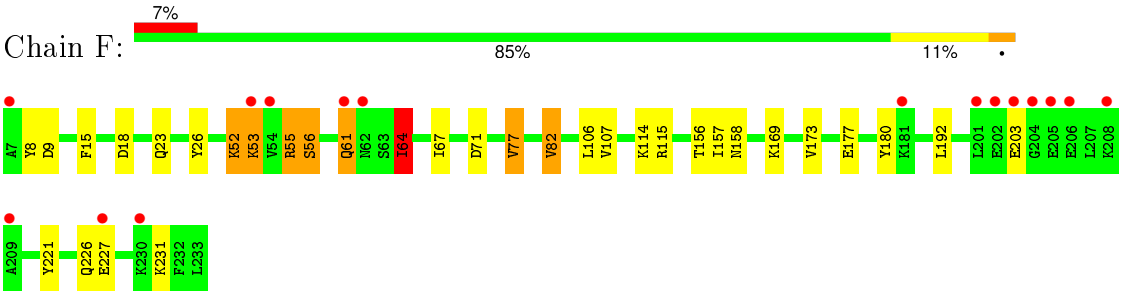
- Molecule 1: Proteasome subunit alpha

Chain E:



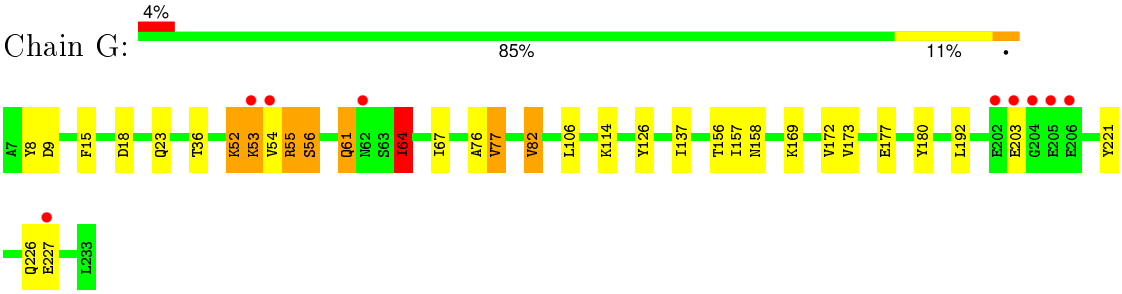
- Molecule 1: Proteasome subunit alpha

Chain F:



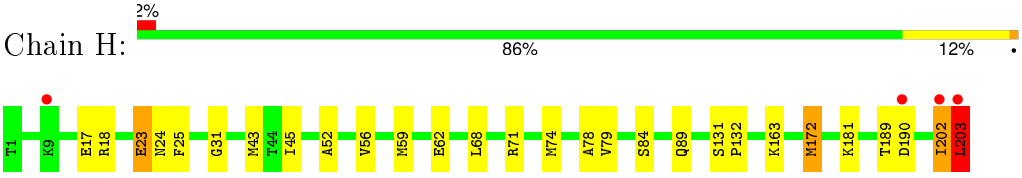
- Molecule 1: Proteasome subunit alpha

Chain G:



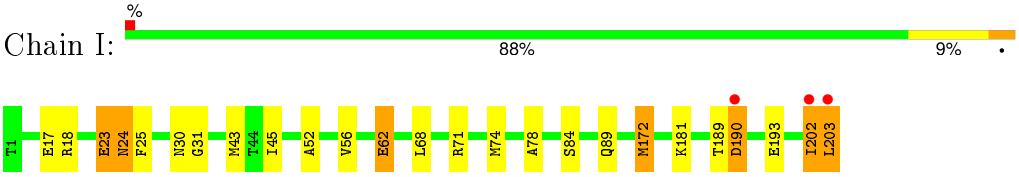
- Molecule 2: Proteasome subunit beta

Chain H:



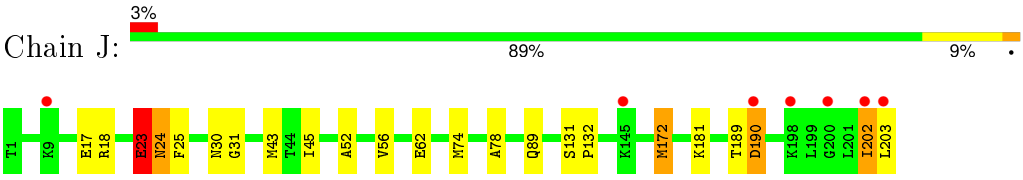
- Molecule 2: Proteasome subunit beta

Chain I:



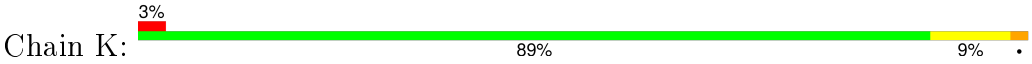
- Molecule 2: Proteasome subunit beta

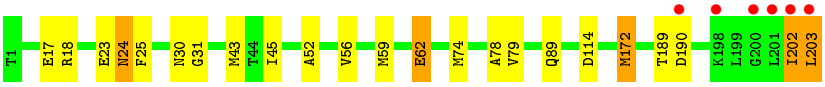
Chain J:



- Molecule 2: Proteasome subunit beta

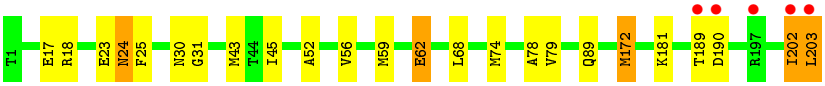
Chain K:





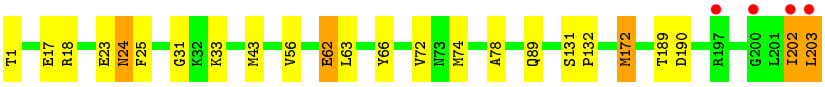
• Molecule 2: Proteasome subunit beta

Chain L:



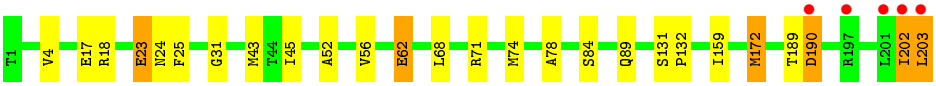
• Molecule 2: Proteasome subunit beta

Chain M:



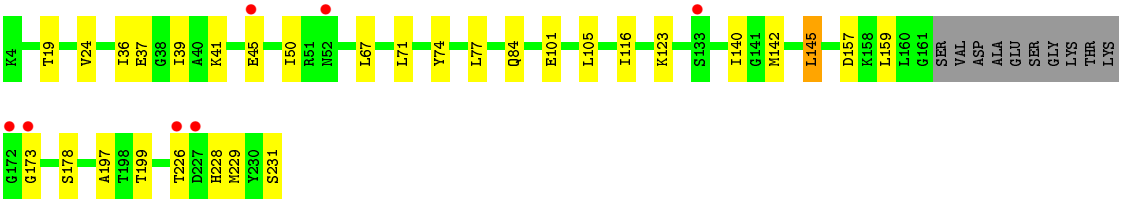
• Molecule 2: Proteasome subunit beta

Chain N:



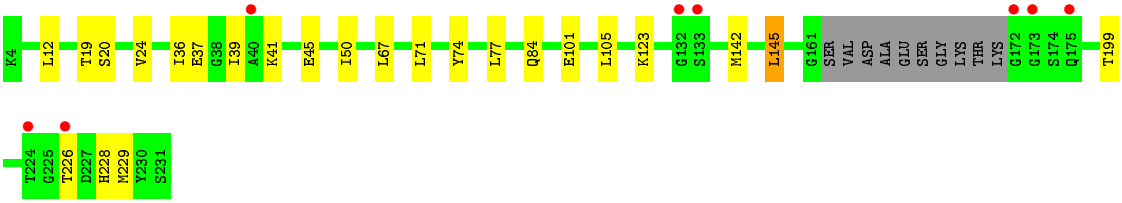
• Molecule 3: Proteasome activator protein PA26

Chain O:



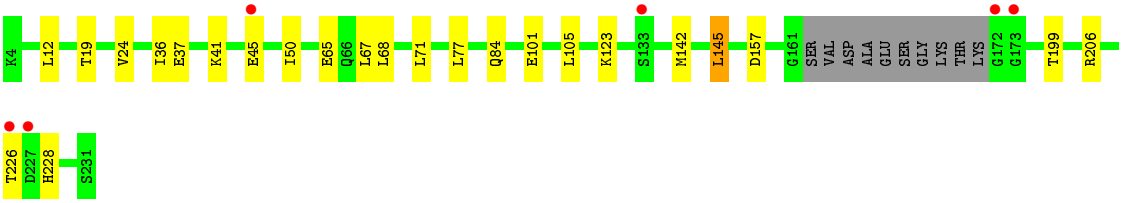
• Molecule 3: Proteasome activator protein PA26

Chain P:

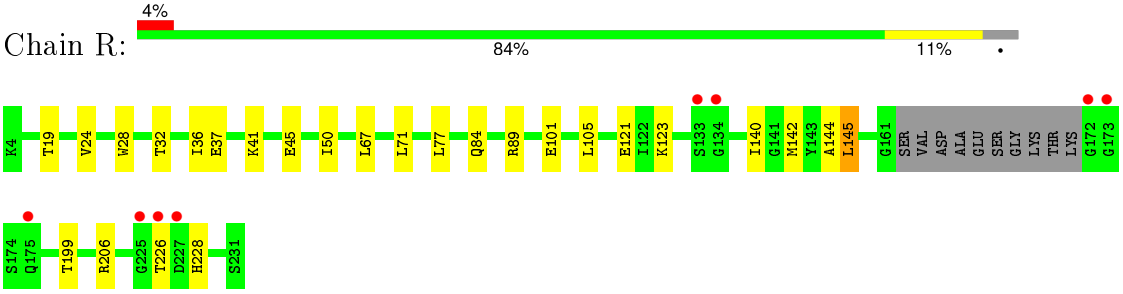


• Molecule 3: Proteasome activator protein PA26

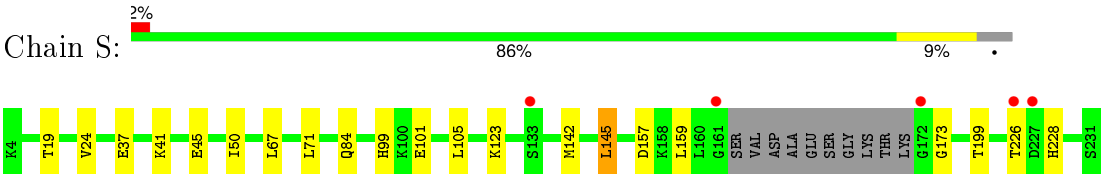
Chain Q:



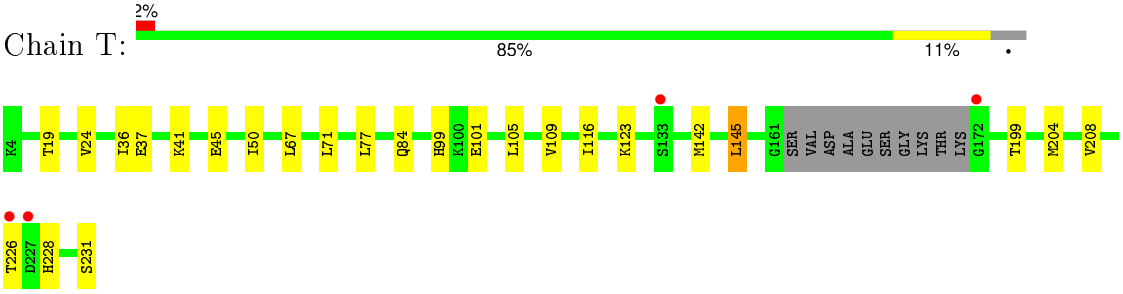
• Molecule 3: Proteasome activator protein PA26



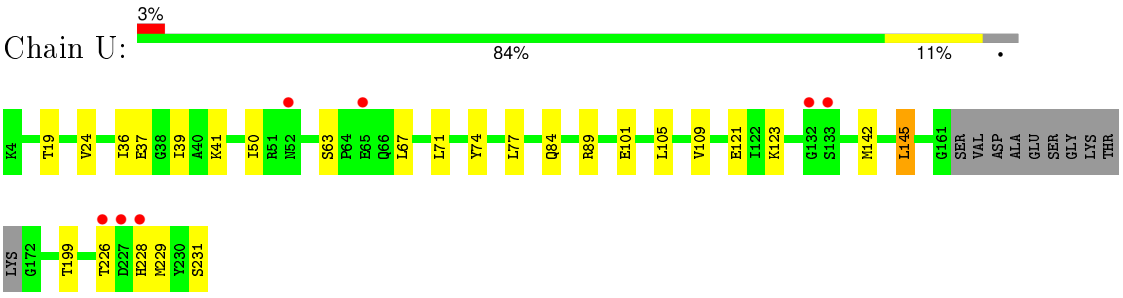
• Molecule 3: Proteasome activator protein PA26



• Molecule 3: Proteasome activator protein PA26



• Molecule 3: Proteasome activator protein PA26



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	255.07Å 126.36Å 180.78Å 90.00° 92.54° 90.00°	Depositor
Resolution (Å)	29.82 – 2.90 29.82 – 2.90	Depositor EDS
% Data completeness (in resolution range)	98.6 (29.82-2.90) 98.6 (29.82-2.90)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.82 (at 2.90Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, R_{free}	0.201 , 0.233 0.207 , 0.236	Depositor DCC
R_{free} test set	2516 reflections (2.05%)	DCC
Wilson B-factor (Å^2)	46.3	Xtriage
Anisotropy	0.048	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 24.8	EDS
Estimated twinning fraction	0.000 for -h,-k,l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.35$	Xtriage
Outliers	2 of 125182 reflections (0.002%)	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	35035	wwPDB-VP
Average B, all atoms (Å^2)	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.75% 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, 0.375 respectively for untwinned datasets, and 0.333, 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	0.71	0/1792	0.70	0/2416
1	B	0.72	0/1792	0.71	1/2416 (0.0%)
1	C	0.72	0/1792	0.71	0/2416
1	D	0.72	0/1792	0.70	0/2416
1	E	0.70	0/1792	0.71	1/2416 (0.0%)
1	F	0.71	0/1792	0.73	1/2416 (0.0%)
1	G	0.73	0/1792	0.70	0/2416
2	H	0.71	1/1576 (0.1%)	0.73	0/2129
2	I	0.73	2/1576 (0.1%)	0.74	0/2129
2	J	0.73	0/1576	0.74	0/2129
2	K	0.73	2/1576 (0.1%)	0.72	0/2129
2	L	0.72	2/1576 (0.1%)	0.73	0/2129
2	M	0.72	2/1576 (0.1%)	0.73	1/2129 (0.0%)
2	N	0.73	1/1576 (0.1%)	0.73	1/2129 (0.0%)
3	O	0.65	0/1704	0.67	0/2304
3	P	0.64	0/1704	0.66	0/2304
3	Q	0.66	0/1704	0.65	0/2304
3	R	0.65	0/1704	0.67	0/2304
3	S	0.65	0/1704	0.67	0/2304
3	T	0.66	0/1704	0.68	0/2304
3	U	0.64	0/1704	0.67	0/2304
All	All	0.70	10/35504 (0.0%)	0.70	5/47943 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
1	B	0	2
1	C	0	2
1	D	0	2

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Mol	Chain	#Chirality outliers	#Planarity outliers
1	E	0	1
1	F	0	1
1	G	0	2
All	All	0	12

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	L	62	GLU	CG-CD	5.95	1.60	1.51
2	I	62	GLU	CG-CD	5.77	1.60	1.51
2	N	62	GLU	CG-CD	5.62	1.60	1.51
2	K	203	LEU	N-CA	5.50	1.57	1.46
2	H	203	LEU	N-CA	5.35	1.57	1.46
2	M	62	GLU	CG-CD	5.34	1.59	1.51
2	L	203	LEU	N-CA	5.21	1.56	1.46
2	I	203	LEU	N-CA	5.17	1.56	1.46
2	K	62	GLU	CG-CD	5.14	1.59	1.51
2	M	203	LEU	N-CA	5.07	1.56	1.46

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	F	115	ARG	NE-CZ-NH1	6.97	123.79	120.30
1	B	115	ARG	NE-CZ-NH1	6.01	123.31	120.30
1	E	115	ARG	NE-CZ-NH1	5.13	122.87	120.30
2	N	203	LEU	CA-CB-CG	5.08	126.98	115.30
2	M	203	LEU	CA-CB-CG	5.04	126.90	115.30

There are no chirality outliers.

All (12) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	54	VAL	Peptide
1	A	8	TYR	Peptide
1	B	54	VAL	Peptide
1	B	8	TYR	Peptide
1	C	54	VAL	Peptide
1	C	8	TYR	Peptide
1	D	54	VAL	Peptide
1	D	8	TYR	Peptide
1	E	54	VAL	Peptide

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Mol	Chain	Res	Type	Group
1	F	8	TYR	Peptide
1	G	54	VAL	Peptide
1	G	8	TYR	Peptide

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1768	0	1800	17	0
1	B	1768	0	1800	18	0
1	C	1768	0	1800	17	0
1	D	1768	0	1800	19	0
1	E	1768	0	1800	24	0
1	F	1768	0	1800	28	0
1	G	1768	0	1800	21	0
2	H	1557	0	1609	17	0
2	I	1557	0	1609	16	0
2	J	1557	0	1609	15	0
2	K	1557	0	1609	12	0
2	L	1557	0	1609	15	0
2	M	1557	0	1609	15	0
2	N	1557	0	1609	15	0
3	O	1680	0	1701	19	0
3	P	1680	0	1701	15	0
3	Q	1680	0	1701	13	0
3	R	1680	0	1701	14	0
3	S	1680	0	1701	13	0
3	T	1680	0	1701	21	0
3	U	1680	0	1701	19	0
All	All	35035	0	35770	305	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 4.

All (305) 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)
3:R:50:ILE:HD11	3:R:67:LEU:HD21	1.64	0.77
3:Q:50:ILE:HD11	3:Q:67:LEU:HD21	1.67	0.77
2:I:43:MET:CE	2:I:56:VAL:HG22	2.15	0.76
3:S:50:ILE:HD11	3:S:67:LEU:HD21	1.67	0.76
3:O:50:ILE:HD11	3:O:67:LEU:HD21	1.69	0.75
3:Q:226:THR:HG21	3:Q:228:HIS:CD2	2.22	0.74
3:U:226:THR:HG21	3:U:228:HIS:CD2	2.23	0.73
3:O:226:THR:HG21	3:O:228:HIS:CD2	2.24	0.73
3:P:226:THR:HG21	3:P:228:HIS:CD2	2.24	0.73
3:R:226:THR:HG21	3:R:228:HIS:CD2	2.25	0.71
3:T:50:ILE:HD11	3:T:67:LEU:HD21	1.72	0.71
3:S:226:THR:HG21	3:S:228:HIS:CD2	2.25	0.71
3:T:226:THR:HG21	3:T:228:HIS:CD2	2.25	0.71
2:L:43:MET:CE	2:L:56:VAL:HG22	2.21	0.71
3:P:50:ILE:HD11	3:P:67:LEU:HD21	1.74	0.69
2:N:43:MET:CE	2:N:56:VAL:HG22	2.23	0.69
2:K:43:MET:CE	2:K:56:VAL:HG22	2.23	0.67
3:U:50:ILE:HD11	3:U:67:LEU:HD21	1.77	0.67
2:H:43:MET:CE	2:H:56:VAL:HG22	2.25	0.66
2:J:43:MET:CE	2:J:56:VAL:HG22	2.28	0.64
2:M:24:ASN:H	2:M:24:ASN:HD22	1.47	0.62
2:I:43:MET:HE3	2:I:56:VAL:HG22	1.81	0.62
2:L:43:MET:HE3	2:L:56:VAL:HG22	1.82	0.61
3:Q:226:THR:CG2	3:Q:228:HIS:CD2	2.85	0.60
1:E:82:VAL:HG22	3:U:229:MET:O	2.02	0.60
2:K:43:MET:HE3	2:K:56:VAL:HG22	1.82	0.60
2:N:24:ASN:H	2:N:24:ASN:HD22	1.50	0.59
3:O:226:THR:CG2	3:O:228:HIS:CD2	2.85	0.59
3:T:226:THR:CG2	3:T:228:HIS:CD2	2.86	0.59
3:S:101:GLU:HG2	3:T:105:LEU:HD22	1.85	0.59
3:U:226:THR:CG2	3:U:228:HIS:CD2	2.86	0.58
3:P:226:THR:CG2	3:P:228:HIS:CD2	2.85	0.58
3:R:226:THR:CG2	3:R:228:HIS:CD2	2.85	0.58
1:F:107:VAL:HG11	2:M:72:VAL:HG21	1.85	0.58
2:J:24:ASN:HD22	2:J:24:ASN:H	1.49	0.58
2:N:43:MET:HE3	2:N:56:VAL:HG22	1.85	0.58
2:M:43:MET:CE	2:M:56:VAL:HG22	2.34	0.57
3:O:105:LEU:HD22	3:U:101:GLU:HG2	1.86	0.57
2:L:24:ASN:H	2:L:24:ASN:HD22	1.52	0.57
3:S:226:THR:CG2	3:S:228:HIS:CD2	2.87	0.57
2:K:24:ASN:H	2:K:24:ASN:HD22	1.53	0.56
3:U:71:LEU:HB2	3:U:145:LEU:HD13	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:15:PHE:N	1:C:23:GLN:OE1	2.40	0.55
1:E:15:PHE:N	1:F:23:GLN:OE1	2.40	0.54
1:A:9:ASP:O	1:A:23:GLN:NE2	2.41	0.54
2:N:74:MET:HG2	2:N:78:ALA:HB3	1.90	0.54
1:E:17:PRO:HA	1:F:26:TYR:CG	2.44	0.53
1:G:9:ASP:O	1:G:23:GLN:NE2	2.42	0.53
3:R:36:ILE:HG12	3:R:77:LEU:HD21	1.90	0.53
3:Q:101:GLU:HG2	3:R:105:LEU:HD22	1.91	0.53
1:F:55:ARG:O	1:F:56:SER:CB	2.57	0.53
2:I:43:MET:HE1	2:I:56:VAL:HG22	1.90	0.52
2:H:43:MET:HE1	2:H:56:VAL:HG22	1.92	0.52
2:M:43:MET:HE3	2:M:56:VAL:HG22	1.91	0.52
2:I:24:ASN:H	2:I:24:ASN:HD22	1.54	0.52
1:D:82:VAL:HG13	3:T:231:SER:CB	2.39	0.52
3:O:71:LEU:HB2	3:O:145:LEU:HD13	1.90	0.52
3:R:101:GLU:HG2	3:S:105:LEU:HD22	1.91	0.52
1:E:9:ASP:O	1:E:23:GLN:NE2	2.43	0.52
1:D:9:ASP:O	1:D:23:GLN:NE2	2.43	0.52
1:G:64:ILE:HD12	1:G:64:ILE:N	2.25	0.51
1:F:9:ASP:O	1:F:23:GLN:NE2	2.43	0.51
1:D:15:PHE:N	1:E:23:GLN:OE1	2.42	0.51
2:K:74:MET:HG2	2:K:78:ALA:HB3	1.92	0.51
2:H:24:ASN:H	2:H:24:ASN:HD22	1.58	0.51
2:L:74:MET:HG2	2:L:78:ALA:HB3	1.93	0.51
1:C:64:ILE:HD12	1:C:64:ILE:N	2.24	0.51
2:I:74:MET:HG2	2:I:78:ALA:HB3	1.92	0.51
1:F:15:PHE:N	1:G:23:GLN:OE1	2.42	0.51
3:Q:71:LEU:HB2	3:Q:145:LEU:HD13	1.92	0.51
1:F:55:ARG:O	1:F:56:SER:HB2	2.11	0.51
3:P:71:LEU:HB2	3:P:145:LEU:HD13	1.92	0.50
3:P:101:GLU:HG2	3:Q:105:LEU:HD22	1.94	0.50
2:H:74:MET:HG2	2:H:78:ALA:HB3	1.93	0.50
1:A:23:GLN:OE1	1:G:15:PHE:N	2.41	0.50
3:T:101:GLU:HG2	3:U:105:LEU:HD22	1.91	0.50
3:U:71:LEU:CB	3:U:145:LEU:HD13	2.41	0.50
2:J:18:ARG:HD3	2:J:31:GLY:O	2.11	0.50
2:J:74:MET:HG2	2:J:78:ALA:HB3	1.93	0.50
1:F:53:LYS:O	1:F:55:ARG:HG2	2.12	0.50
1:F:64:ILE:N	1:F:64:ILE:HD12	2.27	0.50
2:H:43:MET:HE3	2:H:56:VAL:HG22	1.93	0.49
2:J:43:MET:HE3	2:J:56:VAL:HG22	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:82:VAL:HG22	3:O:229:MET:O	2.12	0.49
3:T:71:LEU:HB2	3:T:145:LEU:HD13	1.95	0.49
2:K:172:MET:HE3	2:K:189:THR:HG23	1.94	0.49
2:M:172:MET:CE	2:M:189:THR:HG23	2.43	0.49
2:H:18:ARG:HD3	2:H:31:GLY:O	2.13	0.49
2:L:172:MET:CE	2:L:189:THR:HG23	2.42	0.49
1:C:9:ASP:O	1:C:23:GLN:NE2	2.46	0.49
3:R:71:LEU:HB2	3:R:145:LEU:HD13	1.94	0.49
2:N:190:ASP:OD1	2:N:190:ASP:N	2.46	0.49
1:D:82:VAL:CG1	3:T:231:SER:HB2	2.43	0.48
1:D:82:VAL:CG1	3:T:231:SER:CB	2.91	0.48
1:E:158:ASN:HD22	1:F:64:ILE:HG12	1.79	0.48
1:E:82:VAL:CG1	3:U:231:SER:HB2	2.43	0.48
3:O:24:VAL:HG13	3:O:84:GLN:HB3	1.95	0.48
3:O:71:LEU:CB	3:O:145:LEU:HD13	2.44	0.48
1:A:53:LYS:O	1:A:55:ARG:HG2	2.13	0.48
1:C:15:PHE:N	1:D:23:GLN:OE1	2.41	0.48
1:A:64:ILE:HD12	1:A:64:ILE:N	2.29	0.48
3:U:50:ILE:HD11	3:U:67:LEU:HD11	1.96	0.48
3:Q:226:THR:HG22	3:Q:228:HIS:H	1.79	0.47
2:J:172:MET:CE	2:J:189:THR:HG23	2.44	0.47
1:F:156:THR:HG23	1:G:82:VAL:HG21	1.96	0.47
3:P:24:VAL:HG13	3:P:84:GLN:HB3	1.96	0.47
2:M:24:ASN:ND2	2:M:24:ASN:H	2.11	0.47
3:O:101:GLU:HG2	3:P:105:LEU:HD22	1.97	0.47
2:H:172:MET:CE	2:H:189:THR:HG23	2.44	0.47
1:D:53:LYS:O	1:D:55:ARG:HG2	2.14	0.47
1:E:169:LYS:O	1:E:173:VAL:HG23	2.14	0.47
2:L:43:MET:HE1	2:L:56:VAL:HA	1.95	0.47
2:J:43:MET:HE1	2:J:56:VAL:HG22	1.96	0.47
1:B:8:TYR:OH	1:C:9:ASP:OD2	2.22	0.47
3:P:71:LEU:CB	3:P:145:LEU:HD13	2.45	0.47
2:L:172:MET:HE3	2:L:189:THR:HG23	1.96	0.47
1:E:55:ARG:O	1:E:56:SER:CB	2.62	0.47
1:C:65:GLU:OE2	2:I:71:ARG:NH2	2.46	0.47
3:Q:71:LEU:CB	3:Q:145:LEU:HD13	2.45	0.47
1:E:156:THR:HG23	1:F:82:VAL:HG21	1.97	0.47
3:S:226:THR:HG22	3:S:228:HIS:H	1.80	0.46
2:K:172:MET:CE	2:K:189:THR:HG23	2.45	0.46
1:A:55:ARG:O	1:A:56:SER:CB	2.63	0.46
2:M:74:MET:HG2	2:M:78:ALA:HB3	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:53:LYS:O	1:C:55:ARG:HG2	2.15	0.46
3:R:24:VAL:HG13	3:R:84:GLN:HB3	1.97	0.46
1:D:82:VAL:HG13	3:T:231:SER:HB2	1.97	0.46
1:F:67:ILE:HG12	1:F:77:VAL:CG1	2.45	0.46
3:O:36:ILE:HG12	3:O:77:LEU:HD21	1.98	0.46
3:S:71:LEU:HB2	3:S:145:LEU:HD13	1.97	0.46
2:N:24:ASN:H	2:N:24:ASN:ND2	2.13	0.46
1:B:53:LYS:O	1:B:55:ARG:HG2	2.16	0.46
2:H:172:MET:HE3	2:H:189:THR:HG23	1.98	0.46
2:L:18:ARG:HD3	2:L:31:GLY:O	2.16	0.46
2:K:45:ILE:HB	2:K:52:ALA:HB1	1.97	0.46
1:E:55:ARG:O	1:E:56:SER:HB2	2.16	0.46
2:M:66:TYR:CD2	2:M:74:MET:HE2	2.51	0.46
3:O:178:SER:HG	3:U:63:SER:HG	1.63	0.46
1:G:52:LYS:NZ	1:G:61:GLN:HG2	2.31	0.46
1:F:158:ASN:HA	1:G:64:ILE:HG12	1.98	0.46
1:A:55:ARG:O	1:A:56:SER:HB2	2.16	0.45
1:B:55:ARG:O	1:B:56:SER:CB	2.64	0.45
1:E:64:ILE:HD12	1:E:64:ILE:N	2.32	0.45
2:H:43:MET:HE1	2:H:56:VAL:HA	1.97	0.45
1:B:64:ILE:N	1:B:64:ILE:HD12	2.32	0.45
1:D:64:ILE:HD12	1:D:64:ILE:N	2.31	0.45
3:S:99:HIS:HB3	3:T:109:VAL:HG22	1.99	0.45
3:Q:36:ILE:HG12	3:Q:77:LEU:HD21	1.99	0.45
1:G:53:LYS:O	1:G:55:ARG:HG2	2.17	0.45
3:R:71:LEU:CB	3:R:145:LEU:HD13	2.47	0.45
3:S:24:VAL:HG13	3:S:84:GLN:HB3	1.98	0.45
1:B:180:TYR:HA	1:B:192:LEU:HD21	1.99	0.45
1:A:65:GLU:OE2	2:N:71:ARG:NH2	2.47	0.45
2:J:172:MET:HE3	2:J:189:THR:HG23	1.99	0.45
3:U:24:VAL:HG13	3:U:84:GLN:HB3	1.97	0.45
3:U:226:THR:HG22	3:U:228:HIS:H	1.80	0.45
3:P:226:THR:HG22	3:P:228:HIS:H	1.81	0.45
1:E:17:PRO:HB3	3:P:105:LEU:HD11	1.98	0.45
1:D:55:ARG:O	1:D:56:SER:CB	2.65	0.45
1:B:156:THR:HG23	1:C:82:VAL:HG21	1.99	0.45
2:J:24:ASN:H	2:J:24:ASN:ND2	2.14	0.45
1:A:67:ILE:HG12	1:A:77:VAL:CG1	2.46	0.45
2:M:18:ARG:HD3	2:M:31:GLY:O	2.17	0.45
1:F:52:LYS:NZ	1:F:61:GLN:HG2	2.32	0.45
3:R:226:THR:HG22	3:R:228:HIS:H	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:82:VAL:CG1	3:U:231:SER:CB	2.95	0.44
1:F:82:VAL:CG1	3:O:231:SER:HB2	2.47	0.44
1:E:53:LYS:O	1:E:55:ARG:HG2	2.16	0.44
1:B:65:GLU:OE2	2:H:71:ARG:NH2	2.50	0.44
2:I:43:MET:HE1	2:I:56:VAL:HA	1.98	0.44
2:J:43:MET:HE1	2:J:56:VAL:HA	1.98	0.44
2:K:18:ARG:HD3	2:K:31:GLY:O	2.17	0.44
1:C:52:LYS:NZ	1:C:61:GLN:HG2	2.32	0.44
2:L:43:MET:CE	2:L:56:VAL:HA	2.47	0.44
3:P:36:ILE:HG12	3:P:77:LEU:HD21	1.99	0.44
3:T:36:ILE:HG12	3:T:77:LEU:HD21	2.00	0.44
1:G:67:ILE:HG12	1:G:77:VAL:CG1	2.47	0.44
2:I:18:ARG:HB3	2:I:30:ASN:HA	2.00	0.44
1:F:55:ARG:O	1:F:55:ARG:NH1	2.51	0.44
3:T:226:THR:HG22	3:T:228:HIS:H	1.83	0.43
3:U:36:ILE:HG12	3:U:77:LEU:HD21	1.99	0.43
1:B:77:VAL:HG23	1:B:137:ILE:HB	2.00	0.43
2:I:190:ASP:OD1	2:I:190:ASP:N	2.49	0.43
1:C:71:ASP:HA	2:I:68:LEU:HD11	2.00	0.43
1:C:126:TYR:CD1	1:D:129:VAL:HG12	2.53	0.43
2:N:43:MET:HE1	2:N:56:VAL:HA	1.99	0.43
3:S:101:GLU:CG	3:T:105:LEU:HD22	2.48	0.43
2:I:18:ARG:HD3	2:I:31:GLY:O	2.19	0.43
1:E:67:ILE:HG12	1:E:77:VAL:CG1	2.47	0.43
1:A:52:LYS:NZ	1:A:61:GLN:HG2	2.33	0.43
2:I:172:MET:HE1	2:I:193:GLU:HG3	1.98	0.43
3:T:99:HIS:HB3	3:U:109:VAL:HG22	1.99	0.43
1:C:55:ARG:O	1:C:56:SER:HB2	2.18	0.43
1:D:82:VAL:CG1	3:T:231:SER:HB3	2.49	0.43
1:G:82:VAL:HG22	3:P:229:MET:O	2.17	0.43
1:G:77:VAL:HG23	1:G:137:ILE:HB	2.01	0.43
1:D:77:VAL:HG23	1:D:137:ILE:HB	2.01	0.43
3:O:140:ILE:HG22	3:O:197:ALA:HB2	2.00	0.43
3:O:226:THR:HG22	3:O:228:HIS:H	1.84	0.43
3:T:71:LEU:CB	3:T:145:LEU:HD13	2.48	0.43
1:B:55:ARG:O	1:B:56:SER:HB2	2.19	0.43
1:G:180:TYR:HA	1:G:192:LEU:HD21	2.01	0.43
1:A:129:VAL:HG12	1:G:126:TYR:CD1	2.54	0.43
1:G:169:LYS:O	1:G:173:VAL:HG23	2.18	0.43
1:B:114:LYS:HA	1:B:157:ILE:HD11	1.99	0.43
1:A:71:ASP:HA	2:N:68:LEU:HD11	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:R:140:ILE:HD11	3:R:144:ALA:HB1	2.01	0.43
3:T:24:VAL:HG13	3:T:84:GLN:HB3	2.00	0.43
1:G:114:LYS:HA	1:G:157:ILE:HD11	2.00	0.43
3:O:159:LEU:O	3:O:173:GLY:HA3	2.19	0.43
2:K:18:ARG:HB3	2:K:30:ASN:HA	2.01	0.42
1:D:52:LYS:NZ	1:D:61:GLN:HG2	2.34	0.42
1:B:158:ASN:HA	1:C:64:ILE:HG12	2.01	0.42
1:C:55:ARG:O	1:C:56:SER:CB	2.67	0.42
1:D:180:TYR:HA	1:D:192:LEU:HD21	2.01	0.42
2:N:43:MET:HE1	2:N:56:VAL:HG22	2.02	0.42
1:D:55:ARG:O	1:D:56:SER:HB2	2.19	0.42
1:E:77:VAL:HG23	1:E:137:ILE:HB	2.00	0.42
1:D:55:ARG:NH1	1:D:55:ARG:O	2.52	0.42
1:C:55:ARG:HB2	1:C:55:ARG:CZ	2.50	0.42
1:E:152:ASP:HB2	1:E:153:PRO:HD2	2.01	0.42
1:A:157:ILE:HG21	1:A:157:ILE:HD13	1.84	0.42
1:G:55:ARG:O	1:G:56:SER:CB	2.67	0.42
1:A:180:TYR:HA	1:A:192:LEU:HD21	2.02	0.42
1:F:180:TYR:HA	1:F:192:LEU:HD21	2.02	0.42
3:P:39:ILE:HD13	3:P:74:TYR:HA	2.01	0.42
1:D:55:ARG:HB2	1:D:55:ARG:CZ	2.50	0.42
2:I:45:ILE:HB	2:I:52:ALA:HB1	2.01	0.42
3:P:50:ILE:HD11	3:P:67:LEU:HD11	2.00	0.42
2:H:23:GLU:HB3	2:H:24:ASN:H	1.69	0.42
1:B:9:ASP:O	1:B:23:GLN:NE2	2.52	0.42
3:U:89:ARG:HD3	3:U:121:GLU:OE2	2.19	0.42
1:F:169:LYS:O	1:F:173:VAL:HG23	2.19	0.42
3:P:12:LEU:HD22	3:Q:206:ARG:HD3	2.02	0.42
1:E:17:PRO:HA	1:F:26:TYR:CD2	2.54	0.42
1:A:64:ILE:HG12	1:G:158:ASN:HA	2.02	0.42
1:C:180:TYR:HA	1:C:192:LEU:HD21	2.02	0.42
2:J:190:ASP:OD1	2:J:190:ASP:N	2.52	0.42
2:H:163:LYS:NZ	2:H:203:LEU:HB3	2.34	0.42
2:K:43:MET:HE1	2:K:56:VAL:HA	2.02	0.41
1:C:169:LYS:O	1:C:173:VAL:HG23	2.20	0.41
3:Q:24:VAL:HG13	3:Q:84:GLN:HB3	2.01	0.41
1:A:82:VAL:HG21	1:G:156:THR:HG23	2.01	0.41
2:L:43:MET:HE1	2:L:56:VAL:HG22	1.98	0.41
1:F:107:VAL:HG11	2:M:72:VAL:CG2	2.50	0.41
1:B:67:ILE:HG12	1:B:77:VAL:CG1	2.49	0.41
2:L:45:ILE:HB	2:L:52:ALA:HB1	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:1:THR:HG1	2:M:33:LYS:HZ3	1.67	0.41
3:T:116:ILE:HG21	3:T:116:ILE:HD13	1.79	0.41
1:E:17:PRO:HA	1:F:26:TYR:CD1	2.55	0.41
2:I:24:ASN:ND2	2:I:24:ASN:H	2.18	0.41
2:M:63:LEU:CD2	2:M:74:MET:SD	3.09	0.41
2:L:18:ARG:HB3	2:L:30:ASN:HA	2.03	0.41
2:N:4:VAL:HG12	2:N:159:ILE:HD11	2.02	0.41
2:H:45:ILE:HB	2:H:52:ALA:HB1	2.02	0.41
3:O:116:ILE:HD13	3:O:116:ILE:HG21	1.86	0.41
2:N:45:ILE:HB	2:N:52:ALA:HB1	2.01	0.41
2:J:45:ILE:HB	2:J:52:ALA:HB1	2.03	0.41
2:H:43:MET:CE	2:H:56:VAL:HA	2.51	0.41
1:F:71:ASP:HA	2:L:68:LEU:HD11	2.03	0.41
2:N:131:SER:N	2:N:132:PRO:CD	2.84	0.41
3:S:159:LEU:O	3:S:173:GLY:HA3	2.21	0.41
3:O:105:LEU:HD22	3:U:101:GLU:CG	2.48	0.41
1:F:67:ILE:HG12	1:F:77:VAL:HG13	2.02	0.41
3:S:71:LEU:CB	3:S:145:LEU:HD13	2.50	0.41
1:F:114:LYS:HA	1:F:157:ILE:HD11	2.02	0.41
2:H:59:MET:CE	2:H:79:VAL:HG13	2.51	0.41
1:E:12:ILE:HD12	1:E:12:ILE:HA	1.93	0.41
3:O:50:ILE:HD11	3:O:67:LEU:HD11	2.02	0.41
2:H:131:SER:N	2:H:132:PRO:CD	2.84	0.41
2:J:131:SER:N	2:J:132:PRO:CD	2.84	0.41
3:R:89:ARG:HD3	3:R:121:GLU:OE2	2.21	0.41
1:E:180:TYR:HA	1:E:192:LEU:HD21	2.03	0.41
2:L:24:ASN:H	2:L:24:ASN:ND2	2.18	0.41
2:M:172:MET:HE2	2:M:189:THR:HG23	2.03	0.41
1:G:55:ARG:O	1:G:56:SER:HB2	2.20	0.41
2:K:114:ASP:OD1	2:K:114:ASP:C	2.60	0.41
3:T:226:THR:HG21	3:T:228:HIS:HD2	1.81	0.40
1:E:158:ASN:HA	1:F:64:ILE:HG12	2.03	0.40
2:I:172:MET:CE	2:I:193:GLU:HG3	2.51	0.40
2:L:59:MET:CE	2:L:79:VAL:HG13	2.51	0.40
1:E:52:LYS:NZ	1:E:61:GLN:HG2	2.35	0.40
3:Q:12:LEU:HD22	3:R:206:ARG:HD3	2.02	0.40
1:F:107:VAL:CG1	2:M:72:VAL:HG21	2.49	0.40
2:J:18:ARG:HB3	2:J:30:ASN:HA	2.02	0.40
1:A:66:LYS:N	1:A:211:GLU:OE1	2.52	0.40
1:B:71:ASP:HA	2:H:68:LEU:HD11	2.03	0.40
3:R:28:TRP:HA	3:R:32:THR:HB	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:59:MET:CE	2:K:79:VAL:HG13	2.51	0.40
3:S:226:THR:HG21	3:S:228:HIS:HD2	1.82	0.40
2:J:23:GLU:HB3	2:J:24:ASN:H	1.71	0.40
1:G:76:ALA:HA	1:G:137:ILE:O	2.22	0.40
1:B:76:ALA:HA	1:B:137:ILE:O	2.21	0.40
1:A:15:PHE:N	1:B:23:GLN:OE1	2.52	0.40
2:N:172:MET:CE	2:N:189:THR:HG23	2.52	0.40
3:U:39:ILE:HD13	3:U:74:TYR:HA	2.03	0.40
2:M:131:SER:N	2:M:132:PRO:CD	2.85	0.40
1:D:157:ILE:HD13	1:D:157:ILE:HG21	1.91	0.40
2:I:172:MET:CE	2:I:189:THR:HG23	2.52	0.40
3:T:204:MET:O	3:T:208:VAL:HG23	2.22	0.40
1:B:52:LYS:NZ	1:B:61:GLN:HG2	2.37	0.40
3:O:39:ILE:HD13	3:O:74:TYR:HA	2.03	0.40
2:N:18:ARG:HD3	2:N:31:GLY:O	2.21	0.40
1:G:36:THR:HG21	1:G:172:VAL:HG21	2.04	0.40
3:Q:65:GLU:HA	3:Q:68:LEU:HD12	2.04	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	225/227 (99%)	215 (96%)	7 (3%)	3 (1%)	15	46
1	B	225/227 (99%)	216 (96%)	6 (3%)	3 (1%)	15	46
1	C	225/227 (99%)	215 (96%)	7 (3%)	3 (1%)	15	46
1	D	225/227 (99%)	215 (96%)	7 (3%)	3 (1%)	15	46
1	E	225/227 (99%)	213 (95%)	9 (4%)	3 (1%)	15	46
1	F	225/227 (99%)	215 (96%)	6 (3%)	4 (2%)	11	37
1	G	225/227 (99%)	213 (95%)	9 (4%)	3 (1%)	15	46

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	H	201/203 (99%)	193 (96%)	7 (4%)	1 (0%)	34	71
2	I	201/203 (99%)	193 (96%)	6 (3%)	2 (1%)	19	54
2	J	201/203 (99%)	192 (96%)	7 (4%)	2 (1%)	19	54
2	K	201/203 (99%)	193 (96%)	7 (4%)	1 (0%)	34	71
2	L	201/203 (99%)	193 (96%)	7 (4%)	1 (0%)	34	71
2	M	201/203 (99%)	192 (96%)	8 (4%)	1 (0%)	34	71
2	N	201/203 (99%)	193 (96%)	6 (3%)	2 (1%)	19	54
3	O	214/228 (94%)	210 (98%)	4 (2%)	0	100	100
3	P	214/228 (94%)	210 (98%)	4 (2%)	0	100	100
3	Q	214/228 (94%)	210 (98%)	4 (2%)	0	100	100
3	R	214/228 (94%)	210 (98%)	4 (2%)	0	100	100
3	S	214/228 (94%)	210 (98%)	4 (2%)	0	100	100
3	T	214/228 (94%)	210 (98%)	4 (2%)	0	100	100
3	U	214/228 (94%)	210 (98%)	4 (2%)	0	100	100
All	All	4480/4606 (97%)	4321 (96%)	127 (3%)	32 (1%)	26	63

All (32) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	56	SER
1	B	56	SER
1	C	56	SER
1	D	56	SER
1	E	56	SER
1	F	56	SER
1	G	56	SER
1	A	53	LYS
1	B	53	LYS
1	C	53	LYS
1	D	53	LYS
1	G	53	LYS
1	E	53	LYS
1	F	53	LYS
1	F	64	ILE
1	B	64	ILE
1	G	64	ILE
2	H	202	ILE

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Mol	Chain	Res	Type
2	I	23	GLU
2	J	202	ILE
2	K	202	ILE
2	L	202	ILE
1	A	64	ILE
1	D	64	ILE
1	F	231	LYS
2	I	202	ILE
2	J	23	GLU
2	M	202	ILE
2	N	23	GLU
2	N	202	ILE
1	C	64	ILE
1	E	64	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	Percentiles	
1	A	188/188 (100%)	176 (94%)	12 (6%)	22	53
1	B	188/188 (100%)	175 (93%)	13 (7%)	19	48
1	C	188/188 (100%)	175 (93%)	13 (7%)	19	48
1	D	188/188 (100%)	175 (93%)	13 (7%)	19	48
1	E	188/188 (100%)	176 (94%)	12 (6%)	22	53
1	F	188/188 (100%)	175 (93%)	13 (7%)	19	48
1	G	188/188 (100%)	175 (93%)	13 (7%)	19	48
2	H	170/170 (100%)	159 (94%)	11 (6%)	21	52
2	I	170/170 (100%)	158 (93%)	12 (7%)	18	47
2	J	170/170 (100%)	159 (94%)	11 (6%)	21	52
2	K	170/170 (100%)	160 (94%)	10 (6%)	24	58
2	L	170/170 (100%)	159 (94%)	11 (6%)	21	52
2	M	170/170 (100%)	160 (94%)	10 (6%)	24	58

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
2	N	170/170 (100%)	160 (94%)	10 (6%)	24 58
3	O	178/186 (96%)	169 (95%)	9 (5%)	29 65
3	P	178/186 (96%)	169 (95%)	9 (5%)	29 65
3	Q	178/186 (96%)	169 (95%)	9 (5%)	29 65
3	R	178/186 (96%)	170 (96%)	8 (4%)	34 70
3	S	178/186 (96%)	169 (95%)	9 (5%)	29 65
3	T	178/186 (96%)	170 (96%)	8 (4%)	34 70
3	U	178/186 (96%)	171 (96%)	7 (4%)	39 75
All	All	3752/3808 (98%)	3529 (94%)	223 (6%)	24 58

All (223) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	18	ASP
1	A	52	LYS
1	A	55	ARG
1	A	61	GLN
1	A	64	ILE
1	A	77	VAL
1	A	82	VAL
1	A	106	LEU
1	A	177	GLU
1	A	203	GLU
1	A	226	GLN
1	A	227	GLU
1	B	18	ASP
1	B	52	LYS
1	B	55	ARG
1	B	61	GLN
1	B	64	ILE
1	B	77	VAL
1	B	82	VAL
1	B	106	LEU
1	B	177	GLU
1	B	203	GLU
1	B	221	TYR
1	B	226	GLN
1	B	227	GLU
1	C	18	ASP

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Mol	Chain	Res	Type
1	C	52	LYS
1	C	55	ARG
1	C	61	GLN
1	C	64	ILE
1	C	77	VAL
1	C	82	VAL
1	C	106	LEU
1	C	177	GLU
1	C	203	GLU
1	C	221	TYR
1	C	226	GLN
1	C	227	GLU
1	D	18	ASP
1	D	52	LYS
1	D	55	ARG
1	D	61	GLN
1	D	64	ILE
1	D	77	VAL
1	D	82	VAL
1	D	106	LEU
1	D	177	GLU
1	D	203	GLU
1	D	221	TYR
1	D	226	GLN
1	D	227	GLU
1	E	18	ASP
1	E	52	LYS
1	E	55	ARG
1	E	61	GLN
1	E	64	ILE
1	E	77	VAL
1	E	82	VAL
1	E	177	GLU
1	E	203	GLU
1	E	221	TYR
1	E	226	GLN
1	E	227	GLU
1	F	18	ASP
1	F	52	LYS
1	F	55	ARG
1	F	61	GLN
1	F	64	ILE

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Mol	Chain	Res	Type
1	F	77	VAL
1	F	82	VAL
1	F	106	LEU
1	F	177	GLU
1	F	203	GLU
1	F	221	TYR
1	F	226	GLN
1	F	227	GLU
1	G	18	ASP
1	G	52	LYS
1	G	55	ARG
1	G	61	GLN
1	G	64	ILE
1	G	77	VAL
1	G	82	VAL
1	G	106	LEU
1	G	177	GLU
1	G	203	GLU
1	G	221	TYR
1	G	226	GLN
1	G	227	GLU
2	H	17	GLU
2	H	23	GLU
2	H	25	PHE
2	H	62	GLU
2	H	84	SER
2	H	89	GLN
2	H	172	MET
2	H	181	LYS
2	H	190	ASP
2	H	202	ILE
2	H	203	LEU
2	I	17	GLU
2	I	23	GLU
2	I	24	ASN
2	I	25	PHE
2	I	62	GLU
2	I	84	SER
2	I	89	GLN
2	I	172	MET
2	I	181	LYS
2	I	190	ASP

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Mol	Chain	Res	Type
2	I	202	ILE
2	I	203	LEU
2	J	17	GLU
2	J	23	GLU
2	J	24	ASN
2	J	25	PHE
2	J	62	GLU
2	J	89	GLN
2	J	172	MET
2	J	181	LYS
2	J	190	ASP
2	J	202	ILE
2	J	203	LEU
2	K	17	GLU
2	K	23	GLU
2	K	24	ASN
2	K	25	PHE
2	K	62	GLU
2	K	89	GLN
2	K	172	MET
2	K	190	ASP
2	K	202	ILE
2	K	203	LEU
2	L	17	GLU
2	L	23	GLU
2	L	24	ASN
2	L	25	PHE
2	L	62	GLU
2	L	89	GLN
2	L	172	MET
2	L	181	LYS
2	L	190	ASP
2	L	202	ILE
2	L	203	LEU
2	M	17	GLU
2	M	23	GLU
2	M	24	ASN
2	M	25	PHE
2	M	62	GLU
2	M	89	GLN
2	M	172	MET
2	M	190	ASP

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Mol	Chain	Res	Type
2	M	202	ILE
2	M	203	LEU
2	N	17	GLU
2	N	23	GLU
2	N	25	PHE
2	N	62	GLU
2	N	84	SER
2	N	89	GLN
2	N	172	MET
2	N	190	ASP
2	N	202	ILE
2	N	203	LEU
3	O	19	THR
3	O	37	GLU
3	O	41	LYS
3	O	45	GLU
3	O	123	LYS
3	O	142	MET
3	O	145	LEU
3	O	157	ASP
3	O	199	THR
3	P	19	THR
3	P	20	SER
3	P	37	GLU
3	P	41	LYS
3	P	45	GLU
3	P	123	LYS
3	P	142	MET
3	P	145	LEU
3	P	199	THR
3	Q	19	THR
3	Q	37	GLU
3	Q	41	LYS
3	Q	45	GLU
3	Q	123	LYS
3	Q	142	MET
3	Q	145	LEU
3	Q	157	ASP
3	Q	199	THR
3	R	19	THR
3	R	37	GLU
3	R	41	LYS

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Mol	Chain	Res	Type
3	R	45	GLU
3	R	123	LYS
3	R	142	MET
3	R	145	LEU
3	R	199	THR
3	S	19	THR
3	S	37	GLU
3	S	41	LYS
3	S	45	GLU
3	S	123	LYS
3	S	142	MET
3	S	145	LEU
3	S	157	ASP
3	S	199	THR
3	T	19	THR
3	T	37	GLU
3	T	41	LYS
3	T	45	GLU
3	T	123	LYS
3	T	142	MET
3	T	145	LEU
3	T	199	THR
3	U	19	THR
3	U	37	GLU
3	U	41	LYS
3	U	123	LYS
3	U	142	MET
3	U	145	LEU
3	U	199	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (35) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	226	GLN
1	B	226	GLN
1	C	226	GLN
1	D	158	ASN
1	D	226	GLN
1	E	158	ASN
1	F	158	ASN
1	F	226	GLN
1	G	226	GLN

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Mol	Chain	Res	Type
2	H	24	ASN
2	I	24	ASN
2	I	191	GLN
2	J	24	ASN
2	K	24	ASN
2	K	191	GLN
2	L	24	ASN
2	M	24	ASN
2	N	24	ASN
3	O	75	GLN
3	O	79	HIS
3	O	228	HIS
3	P	75	GLN
3	P	79	HIS
3	P	228	HIS
3	Q	79	HIS
3	Q	228	HIS
3	R	79	HIS
3	R	228	HIS
3	S	75	GLN
3	S	79	HIS
3	S	228	HIS
3	T	75	GLN
3	T	228	HIS
3	U	79	HIS
3	U	228	HIS

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 carbohydrates 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	227/227 (100%)	-0.00	15 (6%)	22	16	26, 37, 61, 65	0
1	B	227/227 (100%)	0.05	14 (6%)	24	17	26, 37, 61, 65	0
1	C	227/227 (100%)	0.02	9 (3%)	42	35	26, 37, 61, 65	0
1	D	227/227 (100%)	0.05	14 (6%)	24	17	26, 37, 61, 65	0
1	E	227/227 (100%)	0.02	12 (5%)	30	23	26, 37, 61, 65	0
1	F	227/227 (100%)	0.03	16 (7%)	19	13	26, 37, 61, 65	0
1	G	227/227 (100%)	0.04	9 (3%)	42	35	26, 37, 61, 65	0
2	H	203/203 (100%)	-0.14	4 (1%)	68	64	25, 33, 47, 61	0
2	I	203/203 (100%)	-0.24	3 (1%)	76	74	25, 33, 47, 61	0
2	J	203/203 (100%)	-0.15	7 (3%)	49	41	25, 33, 47, 61	0
2	K	203/203 (100%)	-0.17	6 (2%)	54	47	25, 33, 47, 61	0
2	L	203/203 (100%)	-0.20	5 (2%)	61	55	25, 33, 47, 61	0
2	M	203/203 (100%)	-0.22	4 (1%)	68	64	25, 33, 47, 61	0
2	N	203/203 (100%)	-0.26	5 (2%)	61	55	25, 33, 47, 61	0
3	O	218/228 (95%)	-0.00	7 (3%)	51	43	31, 40, 51, 60	0
3	P	218/228 (95%)	-0.07	8 (3%)	45	38	30, 40, 51, 60	0
3	Q	218/228 (95%)	-0.06	6 (2%)	56	50	31, 40, 51, 60	0
3	R	218/228 (95%)	-0.01	8 (3%)	45	38	30, 40, 51, 60	0
3	S	218/228 (95%)	-0.13	5 (2%)	64	59	30, 40, 51, 60	0
3	T	218/228 (95%)	-0.05	4 (1%)	71	68	30, 40, 51, 60	0
3	U	218/228 (95%)	-0.07	7 (3%)	51	43	30, 40, 51, 60	0
All	All	4536/4606 (98%)	-0.07	168 (3%)	45	38	25, 37, 54, 65	0

All (168) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	I	202	ILE	10.2
2	J	202	ILE	7.3
2	K	202	ILE	7.0
2	M	202	ILE	6.4
2	H	202	ILE	6.3
2	N	202	ILE	6.3
2	M	203	LEU	6.1
2	L	202	ILE	5.6
2	K	203	LEU	5.4
2	L	203	LEU	5.2
1	F	62	ASN	5.2
1	B	204	GLY	4.9
3	O	172	GLY	4.9
2	I	203	LEU	4.9
1	C	204	GLY	4.8
1	A	54	VAL	4.8
1	G	204	GLY	4.6
1	D	206	GLU	4.6
1	F	203	GLU	4.6
2	H	203	LEU	4.6
1	G	203	GLU	4.6
2	N	203	LEU	4.5
1	G	206	GLU	4.3
1	B	54	VAL	4.3
2	K	200	GLY	4.2
3	R	133	SER	4.2
3	U	133	SER	4.2
1	B	206	GLU	4.2
1	E	203	GLU	4.1
1	A	203	GLU	4.1
3	R	226	THR	4.1
1	D	62	ASN	4.1
1	B	227	GLU	4.0
1	D	203	GLU	3.9
1	F	206	GLU	3.9
1	G	202	GLU	3.9
3	U	226	THR	3.9
1	E	204	GLY	3.9
1	C	202	GLU	3.9
1	E	54	VAL	3.9
1	F	54	VAL	3.9
3	Q	133	SER	3.8
1	E	62	ASN	3.8

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Mol	Chain	Res	Type	RSRZ
1	D	204	GLY	3.8
1	C	203	GLU	3.6
1	D	61	GLN	3.6
1	B	203	GLU	3.6
1	G	53	LYS	3.6
1	A	202	GLU	3.5
3	T	227	ASP	3.5
1	G	54	VAL	3.5
1	G	205	GLU	3.4
1	A	204	GLY	3.4
1	F	202	GLU	3.4
3	S	226	THR	3.4
3	T	133	SER	3.3
1	G	62	ASN	3.3
1	A	206	GLU	3.3
3	P	173	GLY	3.3
3	S	172	GLY	3.3
3	P	133	SER	3.2
1	C	63	SER	3.2
3	R	172	GLY	3.2
1	A	205	GLU	3.2
1	A	227	GLU	3.1
3	T	226	THR	3.1
3	P	172	GLY	3.1
1	D	208	LYS	3.1
1	B	202	GLU	3.1
1	E	202	GLU	3.1
3	Q	173	GLY	3.1
1	C	54	VAL	3.1
1	F	53	LYS	3.1
1	F	205	GLU	3.1
1	E	61	GLN	3.0
1	C	62	ASN	2.9
3	O	133	SER	2.9
3	R	227	ASP	2.9
2	J	9	LYS	2.9
3	R	225	GLY	2.9
1	A	62	ASN	2.9
2	J	190	ASP	2.9
2	K	190	ASP	2.8
3	U	227	ASP	2.8
1	E	226	GLN	2.8

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Mol	Chain	Res	Type	RSRZ
2	J	198	LYS	2.8
1	A	208	LYS	2.7
1	D	202	GLU	2.7
1	A	61	GLN	2.7
3	O	173	GLY	2.7
3	Q	172	GLY	2.7
1	D	205	GLU	2.7
2	K	198	LYS	2.7
2	L	190	ASP	2.7
1	F	208	LYS	2.6
1	G	227	GLU	2.6
1	B	53	LYS	2.6
1	F	61	GLN	2.6
1	B	64	ILE	2.6
1	E	64	ILE	2.6
1	F	7	ALA	2.6
1	C	53	LYS	2.6
1	C	206	GLU	2.5
3	O	226	THR	2.5
1	F	204	GLY	2.5
2	H	190	ASP	2.5
1	C	205	GLU	2.5
3	P	226	THR	2.5
2	J	203	LEU	2.5
1	B	7	ALA	2.5
3	Q	226	THR	2.5
1	A	226	GLN	2.5
1	B	61	GLN	2.5
1	B	205	GLU	2.4
1	A	53	LYS	2.4
1	A	233	LEU	2.4
1	D	227	GLU	2.4
1	E	53	LYS	2.4
1	F	201	LEU	2.4
1	F	209	ALA	2.4
3	P	132	GLY	2.4
1	D	233	LEU	2.3
3	S	227	ASP	2.3
1	A	55	ARG	2.3
1	F	227	GLU	2.3
3	R	175	GLN	2.3
2	I	190	ASP	2.3

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Mol	Chain	Res	Type	RSRZ
3	S	133	SER	2.3
3	U	132	GLY	2.3
3	U	228	HIS	2.3
3	Q	227	ASP	2.3
1	F	181	LYS	2.3
3	P	224	THR	2.3
1	B	226	GLN	2.3
1	B	62	ASN	2.2
3	O	45	GLU	2.2
3	U	65	GLU	2.2
1	D	54	VAL	2.2
2	J	145	LYS	2.2
1	E	209	ALA	2.2
3	P	175	GLN	2.2
1	D	171	ALA	2.2
2	H	9	LYS	2.2
3	R	173	GLY	2.2
3	U	52	ASN	2.2
3	O	227	ASP	2.2
2	M	200	GLY	2.2
3	T	172	GLY	2.2
1	A	64	ILE	2.2
2	J	200	GLY	2.2
1	B	178	ARG	2.2
3	S	161	GLY	2.2
2	N	201	LEU	2.2
2	N	190	ASP	2.1
3	R	134	GLY	2.1
3	O	52	ASN	2.1
2	N	197	ARG	2.1
3	Q	45	GLU	2.1
1	E	218	GLY	2.0
1	D	201	LEU	2.0
2	K	201	LEU	2.0
2	M	197	ARG	2.0
1	D	53	LYS	2.0
2	L	189	THR	2.0
1	E	55	ARG	2.0
1	F	230	LYS	2.0
3	P	40	ALA	2.0
2	L	197	ARG	2.0

6.2 Non-standard residues in protein, DNA, RNA chains

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates

There are no carbohydrates in this entry.

6.4 Ligands

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.