



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 17, 2026 – 07:06 PM UTC

PDB ID : 3JSE / pdb_00003jse
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 : 2009-09-10
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

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

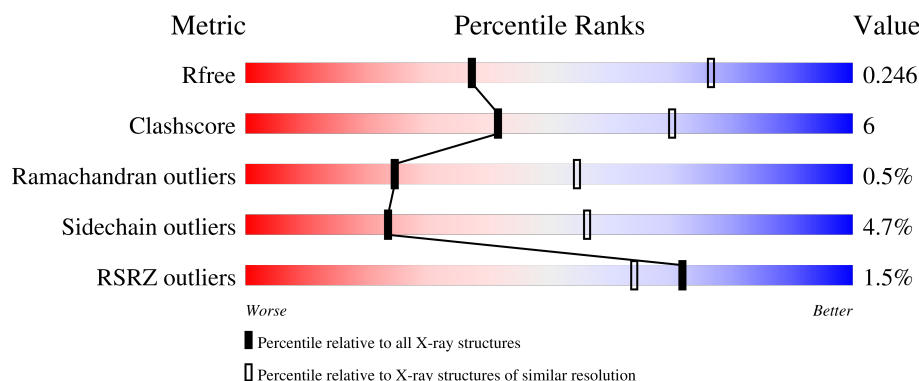
1 Overall quality at a glance

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.



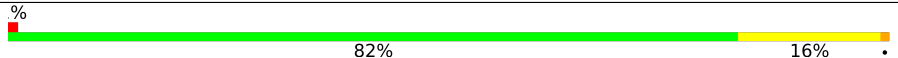
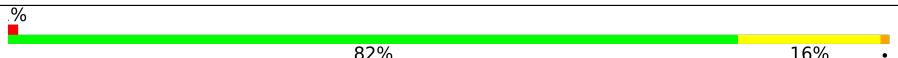
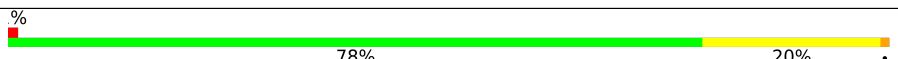
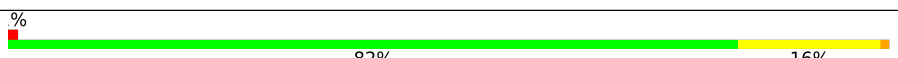
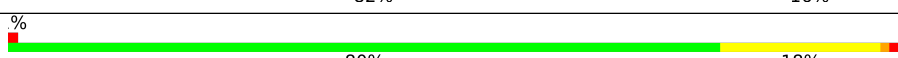
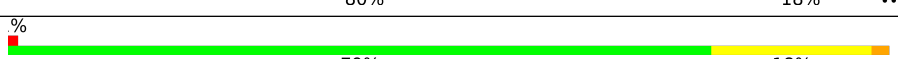
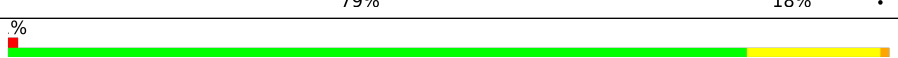
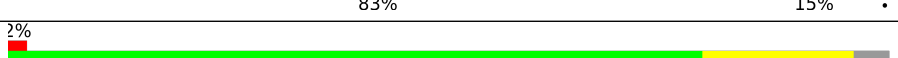
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	2481 (2.90-2.90)
Clashscore	190562	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (2.90-2.90)
RSRZ outliers	180081	2481 (2.90-2.90)

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 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 $\leq 5\%$. 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	 83% 15% 2% 0%
1	B	227	 82% 16% 2% 0%
1	C	227	 86% 12% 2% 0%
1	D	227	 87% 12% 1% 0%
1	E	227	 81% 17% 2% 0%

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Mol	Chain	Length	Quality of chain	
1	F	227		.
1	G	227		.
2	H	203		.
2	I	203		.
2	J	203		.
2	K	203		.
2	L	203		..
2	M	203		.
2	N	203		.
3	O	228		.
3	P	228		.
3	Q	228		.
3	R	228		.
3	S	228		.
3	T	228		.
3	U	228		.

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 35056 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
			1683	1056	296	325	6			
3	P	218	Total	C	N	O	S	0	0	0
			1683	1056	296	325	6			
3	Q	218	Total	C	N	O	S	0	0	0
			1683	1056	296	325	6			
3	R	218	Total	C	N	O	S	0	0	0
			1683	1056	296	325	6			
3	S	218	Total	C	N	O	S	0	0	0
			1683	1056	296	325	6			
3	T	218	Total	C	N	O	S	0	0	0
			1683	1056	296	325	6			
3	U	218	Total	C	N	O	S	0	0	0
			1683	1056	296	325	6			

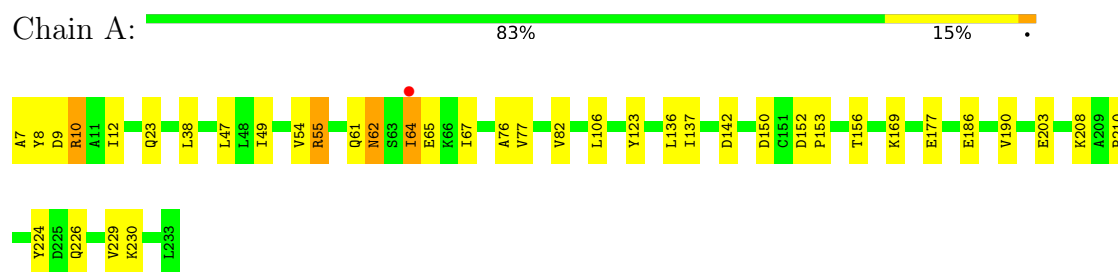
There are 21 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
O	49	VAL	THR	variant	UNP Q9U8G2
O	230	PHE	VAL	engineered mutation	UNP Q9U8G2
O	226	THR	SER	engineered mutation	UNP Q9U8G2
P	49	VAL	THR	variant	UNP Q9U8G2
P	230	PHE	VAL	engineered mutation	UNP Q9U8G2
O	226	THR	SER	engineered mutation	UNP Q9U8G2
Q	49	VAL	THR	variant	UNP Q9U8G2
Q	230	PHE	VAL	engineered mutation	UNP Q9U8G2
O	226	THR	SER	engineered mutation	UNP Q9U8G2
R	49	VAL	THR	variant	UNP Q9U8G2
R	230	PHE	VAL	engineered mutation	UNP Q9U8G2
O	226	THR	SER	engineered mutation	UNP Q9U8G2
S	49	VAL	THR	variant	UNP Q9U8G2
S	230	PHE	VAL	engineered mutation	UNP Q9U8G2
O	226	THR	SER	engineered mutation	UNP Q9U8G2
T	49	VAL	THR	variant	UNP Q9U8G2
T	230	PHE	VAL	engineered mutation	UNP Q9U8G2
O	226	THR	SER	engineered mutation	UNP Q9U8G2
U	49	VAL	THR	variant	UNP Q9U8G2
U	230	PHE	VAL	engineered mutation	UNP Q9U8G2
O	226	THR	SER	engineered mutation	UNP Q9U8G2

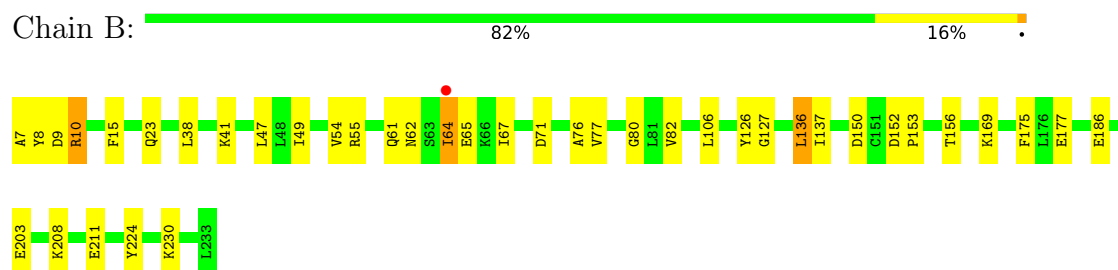
3 Residue-property plots

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.

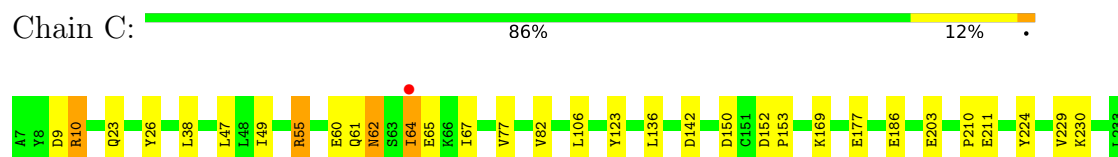
• Molecule 1: Proteasome subunit alpha



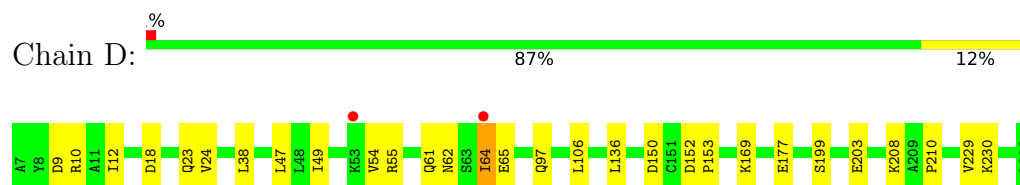
• Molecule 1: Proteasome subunit alpha



• Molecule 1: Proteasome subunit alpha

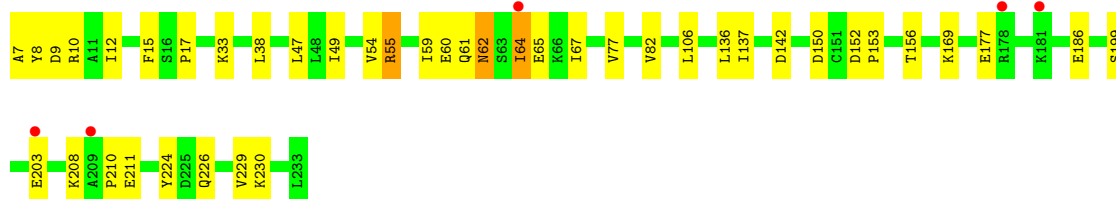


• Molecule 1: Proteasome subunit alpha



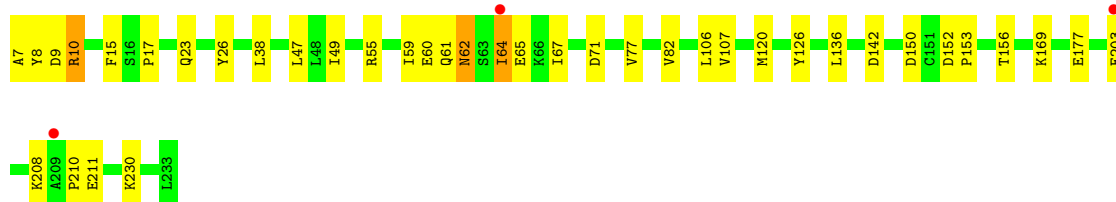
• Molecule 1: Proteasome subunit alpha

Chain E:  2% 81% 17%



- Molecule 1: Proteasome subunit alpha

Chain F:  1% 83% 16%



- Molecule 1: Proteasome subunit alpha

Chain G:  2% 82% 17%



- Molecule 2: Proteasome subunit beta

Chain H:  2% 82% 16%



- Molecule 2: Proteasome subunit beta

Chain I:  2% 82% 16%



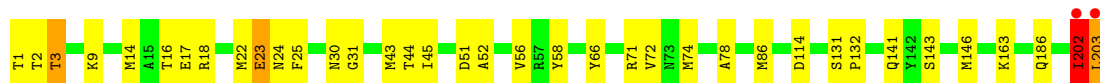
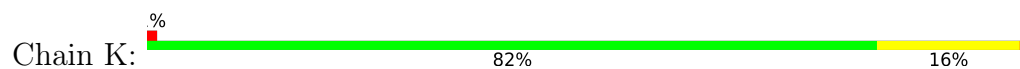
- Molecule 2: Proteasome subunit beta

Chain J:  2% 78% 20%

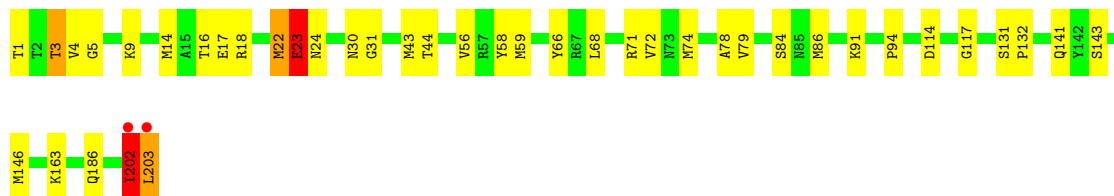
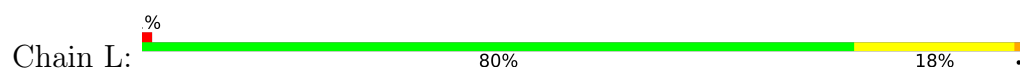




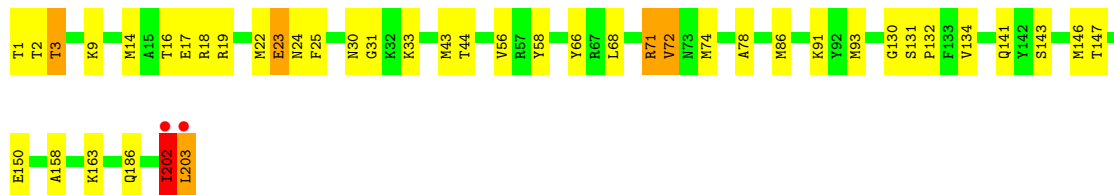
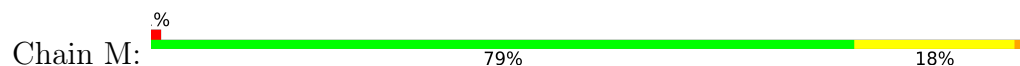
- Molecule 2: Proteasome subunit beta



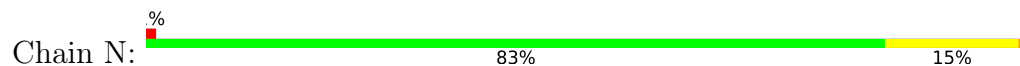
- Molecule 2: Proteasome subunit beta



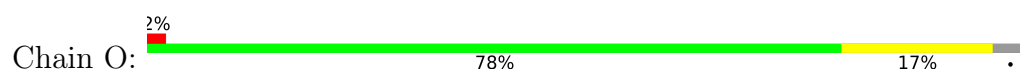
- Molecule 2: Proteasome subunit beta



- Molecule 2: Proteasome subunit beta

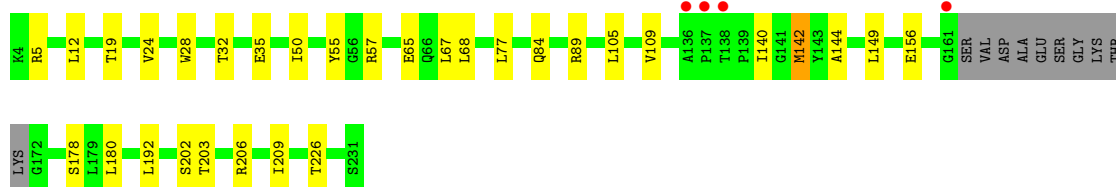
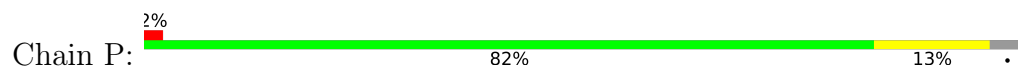


- Molecule 3: Proteasome activator protein PA26

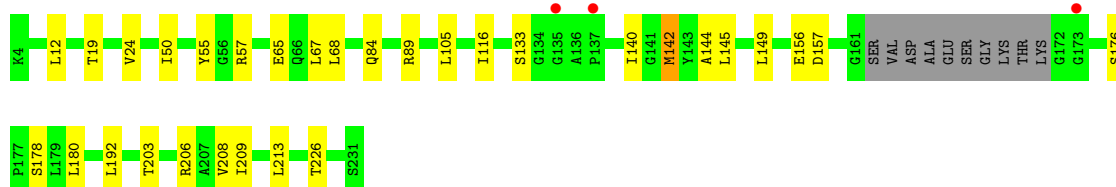
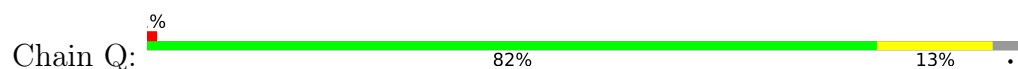




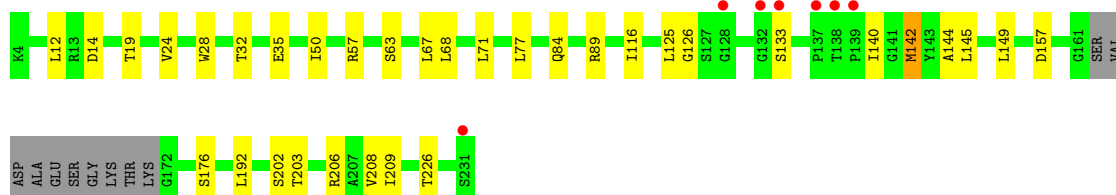
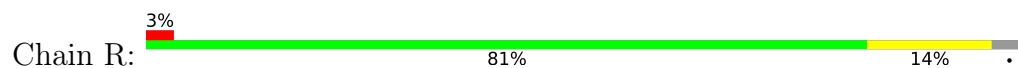
• Molecule 3: Proteasome activator protein PA26



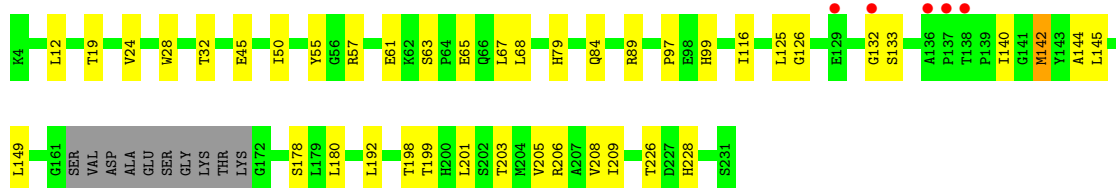
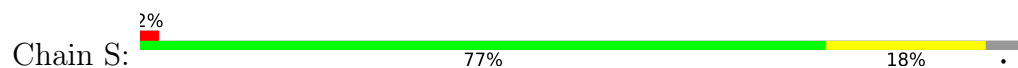
• Molecule 3: Proteasome activator protein PA26



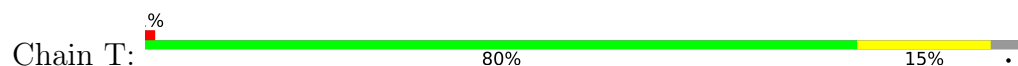
• Molecule 3: Proteasome activator protein PA26

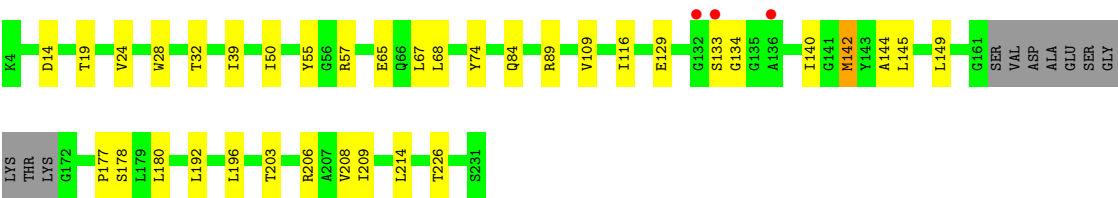


• Molecule 3: Proteasome activator protein PA26

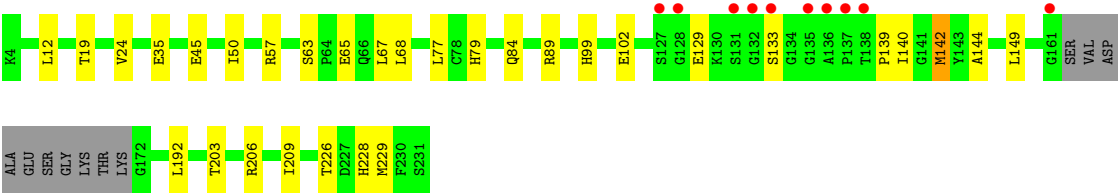
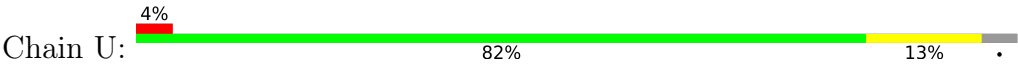


• Molecule 3: Proteasome activator protein PA26





● Molecule 3: Proteasome activator protein PA26



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	254.70Å 126.10Å 180.39Å 90.00° 92.00° 90.00°	Depositor
Resolution (Å)	19.86 – 2.90 19.86 – 2.90	Depositor EDS
% Data completeness (in resolution range)	93.0 (19.86-2.90) 92.7 (19.86-2.90)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.26 (at 2.88Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.212 , 0.241 0.218 , 0.246	Depositor DCC
R_{free} test set	2328 reflections (1.85%)	wwPDB-VP
Wilson B-factor (Å ²)	61.7	Xtriage
Anisotropy	0.101	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 19.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.000 for -h,-k,l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	35056	wwPDB-VP
Average B, all atoms (Å ²)	57.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.53% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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.

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).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.99	1/1792 (0.1%)	0.95	0/2416
1	B	1.01	2/1792 (0.1%)	0.95	1/2416 (0.0%)
1	C	1.03	1/1792 (0.1%)	0.93	0/2416
1	D	1.02	1/1792 (0.1%)	0.95	0/2416
1	E	1.01	1/1792 (0.1%)	0.99	1/2416 (0.0%)
1	F	0.97	1/1792 (0.1%)	0.95	0/2416
1	G	0.99	1/1792 (0.1%)	0.94	0/2416
2	H	1.03	3/1576 (0.2%)	0.94	0/2129
2	I	1.03	3/1576 (0.2%)	0.97	0/2129
2	J	1.04	3/1576 (0.2%)	0.95	0/2129
2	K	1.03	3/1576 (0.2%)	0.95	0/2129
2	L	1.05	3/1576 (0.2%)	0.97	0/2129
2	M	1.05	3/1576 (0.2%)	1.00	2/2129 (0.1%)
2	N	1.04	3/1576 (0.2%)	0.99	2/2129 (0.1%)
3	O	0.99	0/1707	0.96	1/2307 (0.0%)
3	P	0.94	0/1707	0.91	0/2307
3	Q	0.96	0/1707	0.96	0/2307
3	R	0.96	0/1707	0.93	0/2307
3	S	0.97	0/1707	0.94	0/2307
3	T	0.96	0/1707	0.96	0/2307
3	U	0.99	0/1707	0.97	0/2307
All	All	1.00	29/35525 (0.1%)	0.96	7/47964 (0.0%)

All (29) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	I	202	ILE	CA-CB	8.62	1.66	1.54
2	L	202	ILE	CA-CB	8.22	1.65	1.54
1	B	64	ILE	CA-CB	8.07	1.65	1.54
2	H	202	ILE	CA-CB	8.04	1.65	1.54
2	N	202	ILE	CA-CB	8.00	1.65	1.54
1	D	64	ILE	CA-CB	7.93	1.65	1.54
2	J	202	ILE	CA-CB	7.90	1.65	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	K	202	ILE	CA-CB	7.70	1.65	1.54
2	I	202	ILE	CA-C	7.39	1.62	1.52
2	M	202	ILE	CA-CB	7.29	1.64	1.54
1	A	64	ILE	CA-CB	7.17	1.64	1.54
1	G	64	ILE	CA-CB	7.08	1.64	1.54
1	F	64	ILE	CA-CB	6.87	1.63	1.54
2	J	202	ILE	CA-C	6.70	1.61	1.52
2	N	202	ILE	CA-C	6.35	1.60	1.52
2	L	202	ILE	CA-C	6.30	1.60	1.52
2	H	202	ILE	CA-C	6.30	1.60	1.52
2	K	202	ILE	CA-C	6.30	1.60	1.52
1	C	64	ILE	CA-CB	6.16	1.62	1.54
1	E	64	ILE	CA-CB	6.05	1.62	1.54
2	M	202	ILE	CA-C	6.00	1.60	1.52
2	M	202	ILE	N-CA	5.91	1.53	1.46
2	J	202	ILE	N-CA	5.80	1.53	1.46
1	B	80	GLY	C-O	-5.49	1.20	1.24
2	K	202	ILE	N-CA	5.46	1.53	1.46
2	N	202	ILE	N-CA	5.42	1.53	1.46
2	L	202	ILE	N-CA	5.28	1.52	1.46
2	I	202	ILE	N-CA	5.15	1.52	1.46
2	H	202	ILE	N-CA	5.07	1.52	1.46

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	N	93	MET	CA-C-N	6.26	126.45	120.31
2	N	93	MET	C-N-CA	6.26	126.45	120.31
3	O	141	GLY	N-CA-C	5.17	120.17	112.41
1	B	127	GLY	N-CA-C	-5.15	105.95	112.54
2	M	93	MET	CA-C-N	5.14	125.15	120.21
2	M	93	MET	C-N-CA	5.14	125.15	120.21
1	E	9	ASP	N-CA-CB	-5.00	103.97	110.88

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen

atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1768	0	1800	25	0
1	B	1768	0	1800	29	0
1	C	1768	0	1800	23	0
1	D	1768	0	1800	15	0
1	E	1768	0	1800	27	0
1	F	1768	0	1800	32	0
1	G	1768	0	1800	29	0
2	H	1557	0	1609	21	0
2	I	1557	0	1609	23	0
2	J	1557	0	1609	28	0
2	K	1557	0	1609	24	0
2	L	1557	0	1609	27	0
2	M	1557	0	1609	27	0
2	N	1557	0	1609	23	0
3	O	1683	0	1702	30	0
3	P	1683	0	1702	24	0
3	Q	1683	0	1702	23	0
3	R	1683	0	1702	25	1
3	S	1683	0	1702	33	1
3	T	1683	0	1702	30	1
3	U	1683	0	1702	24	1
All	All	35056	0	35777	452	2

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 6.

All (452) 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)
1:E:8:TYR:OH	1:F:9:ASP:OD2	1.96	0.84
3:T:89:ARG:HD3	3:U:203:THR:HG21	1.64	0.79
2:K:14:MET:HE2	2:K:44:THR:HG23	1.69	0.73
1:F:8:TYR:OH	1:G:9:ASP:OD2	2.01	0.73
3:O:68:LEU:HD21	3:O:149:LEU:HD21	1.70	0.72
3:U:140:ILE:HD11	3:U:144:ALA:HB1	1.72	0.71
3:S:68:LEU:HD21	3:S:149:LEU:HD21	1.72	0.71
3:R:68:LEU:HD21	3:R:149:LEU:HD21	1.71	0.71
3:T:140:ILE:HD11	3:T:144:ALA:HB1	1.73	0.71
2:H:43:MET:HE3	2:H:56:VAL:HG22	1.72	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Q:140:ILE:HD11	3:Q:144:ALA:HB1	1.76	0.68
3:U:68:LEU:HD21	3:U:149:LEU:HD21	1.75	0.68
2:I:163:LYS:NZ	2:I:203:LEU:HB3	2.08	0.68
2:K:43:MET:HE3	2:K:56:VAL:HG22	1.76	0.68
2:H:43:MET:HE1	2:H:56:VAL:HA	1.75	0.67
2:L:43:MET:HE3	2:L:56:VAL:HG22	1.77	0.67
3:Q:68:LEU:HD21	3:Q:149:LEU:HD21	1.76	0.67
3:P:140:ILE:HD11	3:P:144:ALA:HB1	1.77	0.67
3:S:89:ARG:HD3	3:T:203:THR:HG21	1.76	0.67
2:L:14:MET:HE2	2:L:44:THR:HG23	1.78	0.66
3:S:133:SER:N	3:T:133:SER:O	2.27	0.66
3:R:140:ILE:HD11	3:R:144:ALA:HB1	1.78	0.66
2:H:14:MET:HE2	2:H:44:THR:HG23	1.77	0.66
2:N:43:MET:HE3	2:N:56:VAL:HG22	1.78	0.65
3:P:50:ILE:HD11	3:P:67:LEU:HD21	1.79	0.65
2:N:14:MET:HE2	2:N:44:THR:HG23	1.78	0.65
3:T:68:LEU:HD21	3:T:149:LEU:HD21	1.78	0.65
1:E:82:VAL:HG22	3:U:229:MET:O	1.98	0.64
3:Q:50:ILE:HD11	3:Q:67:LEU:HD21	1.79	0.64
2:H:43:MET:CE	2:H:56:VAL:HG22	2.28	0.64
3:P:68:LEU:HD21	3:P:149:LEU:HD21	1.80	0.63
2:I:14:MET:HE2	2:I:44:THR:HG23	1.79	0.63
3:T:50:ILE:HD11	3:T:67:LEU:HD21	1.81	0.63
2:J:43:MET:HE3	2:J:56:VAL:HG22	1.81	0.62
3:U:140:ILE:CD1	3:U:144:ALA:HB1	2.29	0.62
2:J:43:MET:HE1	2:J:56:VAL:HA	1.82	0.62
2:L:43:MET:CE	2:L:56:VAL:HG22	2.29	0.62
3:O:140:ILE:HD11	3:O:144:ALA:HB1	1.81	0.62
3:S:50:ILE:HD11	3:S:67:LEU:HD21	1.82	0.62
1:C:150:ASP:OD1	1:C:150:ASP:C	2.43	0.62
1:E:156:THR:HG23	1:F:82:VAL:HG21	1.82	0.62
2:I:43:MET:HE1	2:I:56:VAL:HA	1.83	0.61
1:B:47:LEU:HD12	1:B:47:LEU:C	2.25	0.61
2:K:43:MET:HE1	2:K:56:VAL:HA	1.83	0.61
2:H:163:LYS:NZ	2:H:203:LEU:HB3	2.16	0.61
2:K:43:MET:CE	2:K:56:VAL:HG22	2.30	0.61
2:I:43:MET:HE3	2:I:56:VAL:HG22	1.83	0.60
1:E:38:LEU:HD11	1:E:49:ILE:HD12	1.83	0.60
1:B:8:TYR:OH	1:C:9:ASP:OD2	2.09	0.60
2:M:14:MET:HE2	2:M:44:THR:HG23	1.84	0.60
1:E:7:ALA:HB1	1:F:10:ARG:NH1	2.17	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:T:140:ILE:CD1	3:T:144:ALA:HB1	2.33	0.59
3:T:142:MET:HE2	3:U:192:LEU:HD21	1.85	0.59
2:M:163:LYS:NZ	2:M:203:LEU:HB3	2.17	0.58
3:S:140:ILE:HD11	3:S:144:ALA:HB1	1.84	0.58
2:J:14:MET:HE2	2:J:44:THR:HG23	1.86	0.58
3:O:89:ARG:HD3	3:P:203:THR:HG21	1.84	0.58
1:F:126:TYR:HH	1:G:123:TYR:HH	1.52	0.57
3:R:50:ILE:HD11	3:R:67:LEU:HD21	1.85	0.57
2:I:74:MET:HG2	2:I:78:ALA:HB3	1.86	0.57
1:E:54:VAL:HG23	1:E:208:LYS:HZ1	1.68	0.57
1:B:150:ASP:OD1	1:B:150:ASP:C	2.47	0.57
3:S:142:MET:CE	3:T:192:LEU:HD21	2.34	0.57
2:N:3:THR:HB	2:N:16:THR:HG22	1.87	0.57
2:N:163:LYS:NZ	2:N:203:LEU:HB3	2.19	0.57
3:P:140:ILE:CD1	3:P:144:ALA:HB1	2.35	0.57
2:N:43:MET:HE1	2:N:56:VAL:HA	1.87	0.57
3:Q:140:ILE:CD1	3:Q:144:ALA:HB1	2.34	0.57
3:Q:12:LEU:HD22	3:R:206:ARG:HD3	1.88	0.56
1:F:150:ASP:C	1:F:150:ASP:OD1	2.48	0.56
1:C:55:ARG:HE	3:S:228:HIS:CE1	2.24	0.56
2:H:202:ILE:HG22	2:H:203:LEU:H	1.70	0.56
3:P:89:ARG:HD3	3:Q:203:THR:HG21	1.86	0.56
3:Q:206:ARG:HA	3:Q:209:ILE:HD12	1.87	0.56
2:K:163:LYS:NZ	2:K:203:LEU:HB3	2.21	0.56
3:O:203:THR:HG21	3:U:89:ARG:HD3	1.88	0.56
3:T:142:MET:CE	3:U:192:LEU:HD21	2.36	0.56
1:B:65:GLU:OE1	1:B:65:GLU:HA	2.05	0.56
2:L:202:ILE:HG22	2:L:203:LEU:H	1.71	0.56
1:A:65:GLU:HA	1:A:65:GLU:OE1	2.06	0.55
1:A:150:ASP:C	1:A:150:ASP:OD1	2.49	0.55
1:G:150:ASP:OD1	1:G:150:ASP:C	2.50	0.55
2:L:163:LYS:NZ	2:L:203:LEU:HB3	2.21	0.55
2:M:202:ILE:HG22	2:M:203:LEU:H	1.71	0.55
1:E:65:GLU:OE1	1:E:65:GLU:HA	2.07	0.55
3:U:50:ILE:HD11	3:U:67:LEU:HD21	1.89	0.55
1:E:15:PHE:N	1:F:23:GLN:OE1	2.40	0.54
3:Q:142:MET:HE2	3:R:192:LEU:HD21	1.90	0.54
2:J:141:GLN:O	2:J:146:MET:HE3	2.06	0.54
3:R:116:ILE:HD12	3:R:208:VAL:HG22	1.89	0.54
3:O:206:ARG:HA	3:O:209:ILE:HD12	1.88	0.54
1:E:17:PRO:HA	1:F:26:TYR:CG	2.42	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:65:GLU:OE1	1:C:65:GLU:HA	2.08	0.54
3:Q:55:TYR:O	3:Q:180:LEU:HD21	2.08	0.54
1:E:150:ASP:OD1	1:E:150:ASP:C	2.50	0.54
3:O:140:ILE:CD1	3:O:144:ALA:HB1	2.38	0.54
2:H:163:LYS:HE3	2:H:203:LEU:HD13	1.90	0.54
2:J:43:MET:CE	2:J:56:VAL:HG22	2.37	0.54
2:L:43:MET:HE1	2:L:56:VAL:HA	1.89	0.54
2:M:24:ASN:HD22	2:M:24:ASN:H	1.56	0.54
1:C:186:GLU:OE2	1:C:224:TYR:OH	2.25	0.54
2:N:43:MET:CE	2:N:56:VAL:HG22	2.38	0.54
3:R:140:ILE:CD1	3:R:144:ALA:HB1	2.38	0.53
1:G:65:GLU:OE1	1:G:65:GLU:HA	2.08	0.53
1:F:65:GLU:HA	1:F:65:GLU:OE1	2.09	0.53
2:N:18:ARG:HD3	2:N:31:GLY:O	2.08	0.53
3:O:133:SER:O	3:U:133:SER:N	2.41	0.53
1:D:54:VAL:HG23	1:D:208:LYS:HZ1	1.74	0.53
2:K:202:ILE:HG22	2:K:203:LEU:H	1.73	0.53
3:R:63:SER:HG	3:S:178:SER:HG	1.55	0.53
1:B:38:LEU:C	1:B:38:LEU:HD12	2.34	0.53
1:D:65:GLU:HA	1:D:65:GLU:OE1	2.08	0.53
2:N:74:MET:HG2	2:N:78:ALA:HB3	1.91	0.52
3:T:206:ARG:HA	3:T:209:ILE:HD12	1.91	0.52
3:U:50:ILE:HD11	3:U:67:LEU:HD11	1.91	0.52
2:I:18:ARG:HB3	2:I:30:ASN:HA	1.92	0.52
3:S:140:ILE:CD1	3:S:144:ALA:HB1	2.40	0.52
2:H:18:ARG:HB3	2:H:30:ASN:HA	1.91	0.52
3:S:79:HIS:HD2	3:T:196:LEU:HD21	1.73	0.52
2:J:114:ASP:OD1	2:J:114:ASP:C	2.51	0.52
1:B:41:LYS:NZ	1:C:60:GLU:OE2	2.40	0.52
1:E:67:ILE:HG12	1:E:77:VAL:CG1	2.39	0.52
2:I:202:ILE:HG22	2:I:203:LEU:H	1.74	0.52
3:Q:89:ARG:HD3	3:R:203:THR:HG21	1.91	0.52
2:J:163:LYS:NZ	2:J:203:LEU:HB3	2.24	0.52
2:M:163:LYS:HE3	2:M:203:LEU:HD13	1.91	0.52
3:S:24:VAL:HG13	3:S:84:GLN:HB3	1.92	0.52
3:S:99:HIS:HB3	3:T:109:VAL:HG22	1.90	0.52
1:A:38:LEU:HD11	1:A:49:ILE:HD12	1.92	0.52
3:R:89:ARG:HD3	3:S:203:THR:HG21	1.92	0.52
1:D:9:ASP:O	1:D:23:GLN:NE2	2.43	0.52
2:N:143:SER:HB3	2:N:146:MET:HG3	1.91	0.52
1:D:38:LEU:HD11	1:D:49:ILE:HD12	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:S:142:MET:HE2	3:T:192:LEU:HD21	1.91	0.52
1:C:38:LEU:HD12	1:C:38:LEU:C	2.35	0.51
1:E:17:PRO:HB3	3:P:105:LEU:HD11	1.91	0.51
1:F:156:THR:HG23	1:G:82:VAL:HG21	1.92	0.51
3:O:99:HIS:HB3	3:P:109:VAL:HG22	1.92	0.51
3:O:206:ARG:HD3	3:U:12:LEU:HD22	1.92	0.51
3:R:142:MET:CE	3:S:192:LEU:HD21	2.40	0.51
3:S:55:TYR:O	3:S:180:LEU:HD21	2.09	0.51
1:B:156:THR:HG23	1:C:82:VAL:HG21	1.91	0.51
2:J:18:ARG:HD3	2:J:31:GLY:O	2.10	0.51
1:G:65:GLU:HB3	1:G:211:GLU:OE2	2.10	0.51
3:Q:65:GLU:HA	3:Q:68:LEU:HD12	1.92	0.51
3:R:68:LEU:HD23	3:R:145:LEU:HD11	1.93	0.51
2:J:18:ARG:HB3	2:J:30:ASN:HA	1.91	0.51
3:P:55:TYR:O	3:P:180:LEU:HD21	2.10	0.51
3:U:206:ARG:HA	3:U:209:ILE:HD12	1.91	0.51
2:J:143:SER:HB3	2:J:146:MET:HG3	1.93	0.51
2:M:141:GLN:O	2:M:146:MET:HE3	2.11	0.51
2:L:59:MET:CE	2:L:79:VAL:HG13	2.41	0.51
3:P:12:LEU:HD22	3:Q:206:ARG:HD3	1.91	0.51
2:K:163:LYS:HE3	2:K:203:LEU:HD13	1.92	0.50
2:L:18:ARG:HB3	2:L:30:ASN:HA	1.93	0.50
2:M:3:THR:HB	2:M:16:THR:HG22	1.93	0.50
2:N:24:ASN:H	2:N:24:ASN:HD22	1.60	0.50
3:T:68:LEU:HD23	3:T:145:LEU:HD11	1.93	0.50
1:F:38:LEU:HD12	1:F:38:LEU:C	2.36	0.50
1:F:67:ILE:HG12	1:F:77:VAL:CG1	2.42	0.50
2:K:74:MET:HG2	2:K:78:ALA:HB3	1.94	0.50
3:T:116:ILE:HD12	3:T:208:VAL:HG22	1.93	0.50
2:J:163:LYS:HE3	2:J:203:LEU:HD13	1.93	0.50
2:N:18:ARG:HB3	2:N:30:ASN:HA	1.93	0.50
2:I:141:GLN:O	2:I:146:MET:HE3	2.12	0.50
1:G:67:ILE:HG12	1:G:77:VAL:HG12	1.94	0.50
3:P:24:VAL:HG13	3:P:84:GLN:HB3	1.94	0.50
2:I:43:MET:CE	2:I:56:VAL:HG22	2.42	0.50
2:I:163:LYS:HZ1	2:I:203:LEU:HB3	1.76	0.50
3:P:206:ARG:HA	3:P:209:ILE:HD12	1.94	0.50
1:E:47:LEU:HD12	1:E:47:LEU:C	2.36	0.50
3:O:116:ILE:HD12	3:O:208:VAL:HG22	1.93	0.50
2:N:202:ILE:HG22	2:N:203:LEU:H	1.77	0.49
3:R:24:VAL:HG13	3:R:84:GLN:HB3	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:163:LYS:HE3	2:N:203:LEU:HD13	1.93	0.49
3:Q:142:MET:CE	3:R:192:LEU:HD21	2.42	0.49
2:J:202:ILE:HG22	2:J:203:LEU:H	1.77	0.49
2:H:74:MET:HG2	2:H:78:ALA:HB3	1.92	0.49
2:H:143:SER:HB3	2:H:146:MET:HG3	1.94	0.49
2:I:163:LYS:HE3	2:I:203:LEU:HD13	1.93	0.49
3:O:24:VAL:HG13	3:O:84:GLN:HB3	1.95	0.49
1:G:67:ILE:HG12	1:G:77:VAL:CG1	2.43	0.49
2:K:18:ARG:HD3	2:K:31:GLY:O	2.13	0.49
2:L:18:ARG:HD3	2:L:31:GLY:O	2.12	0.49
2:M:18:ARG:HB3	2:M:30:ASN:HA	1.95	0.49
1:B:54:VAL:HG23	1:B:208:LYS:HZ1	1.78	0.49
1:A:82:VAL:HG21	1:G:156:THR:HG23	1.94	0.48
2:J:74:MET:HG2	2:J:78:ALA:HB3	1.95	0.48
3:O:196:LEU:HD21	3:U:79:HIS:HD2	1.78	0.48
1:F:17:PRO:HB3	3:Q:105:LEU:HD11	1.95	0.48
3:O:178:SER:OG	3:U:63:SER:OG	2.22	0.48
2:N:141:GLN:O	2:N:146:MET:HE3	2.13	0.48
3:Q:156:GLU:OE1	3:R:176:SER:OG	2.26	0.48
3:R:35:GLU:HG3	3:R:77:LEU:HD13	1.95	0.48
3:S:206:ARG:HA	3:S:209:ILE:HD12	1.96	0.48
1:B:7:ALA:HB1	1:C:10:ARG:NH1	2.28	0.48
1:C:38:LEU:HD11	1:C:49:ILE:HD12	1.96	0.48
1:E:38:LEU:HD12	1:E:38:LEU:C	2.39	0.48
2:L:74:MET:HG2	2:L:78:ALA:HB3	1.95	0.48
1:G:142:ASP:OD1	1:G:142:ASP:C	2.57	0.48
1:G:54:VAL:HG23	1:G:208:LYS:HZ1	1.79	0.48
2:N:18:ARG:CD	2:N:31:GLY:O	2.62	0.48
1:F:208:LYS:O	1:F:210:PRO:HD3	2.14	0.47
2:H:24:ASN:HD22	2:H:24:ASN:H	1.62	0.47
2:K:24:ASN:HD22	2:K:24:ASN:H	1.62	0.47
1:A:47:LEU:C	1:A:47:LEU:HD12	2.39	0.47
1:A:186:GLU:OE2	1:A:224:TYR:OH	2.22	0.47
2:H:163:LYS:HZ1	2:H:203:LEU:HB3	1.78	0.47
2:I:58:TYR:HD1	2:I:86:MET:HE1	1.80	0.47
1:F:7:ALA:HB1	1:G:10:ARG:NH1	2.29	0.47
1:F:38:LEU:HD11	1:F:49:ILE:HD12	1.96	0.47
3:T:142:MET:HE2	3:T:142:MET:HB3	1.79	0.47
2:K:141:GLN:O	2:K:146:MET:HE3	2.14	0.47
1:B:186:GLU:OE2	1:B:224:TYR:OH	2.31	0.47
1:F:47:LEU:C	1:F:47:LEU:HD12	2.39	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:O:50:ILE:HD11	3:O:67:LEU:HD21	1.96	0.47
1:A:152:ASP:HB2	1:A:153:PRO:CD	2.45	0.47
1:E:17:PRO:HA	1:F:26:TYR:CD2	2.49	0.47
2:H:18:ARG:HD3	2:H:31:GLY:O	2.15	0.47
2:M:43:MET:HE1	2:M:56:VAL:HA	1.95	0.47
3:U:24:VAL:HG13	3:U:84:GLN:HB3	1.97	0.47
1:F:67:ILE:HG12	1:F:77:VAL:HG12	1.96	0.47
2:I:143:SER:HB3	2:I:146:MET:HG3	1.97	0.47
2:K:18:ARG:HB3	2:K:30:ASN:HA	1.96	0.46
1:A:54:VAL:HG23	1:A:208:LYS:HZ1	1.80	0.46
1:D:150:ASP:C	1:D:150:ASP:OD1	2.58	0.46
1:E:152:ASP:HB2	1:E:153:PRO:CD	2.45	0.46
2:L:66:TYR:CD2	2:L:74:MET:HE2	2.50	0.46
1:D:18:ASP:O	1:E:33:LYS:HE2	2.16	0.46
1:E:152:ASP:HB2	1:E:153:PRO:HD2	1.96	0.46
1:F:15:PHE:N	1:G:23:GLN:OE1	2.47	0.46
3:O:202:SER:O	3:O:206:ARG:HG3	2.15	0.46
3:S:125:LEU:O	3:S:126:GLY:C	2.58	0.46
2:L:143:SER:HB3	2:L:146:MET:HG3	1.97	0.46
3:O:136:ALA:HB3	3:U:129:GLU:HB2	1.97	0.46
1:A:23:GLN:OE1	1:G:15:PHE:N	2.45	0.46
2:J:18:ARG:CD	2:J:31:GLY:O	2.64	0.46
3:Q:68:LEU:HD23	3:Q:145:LEU:HD11	1.97	0.46
1:D:18:ASP:HB2	3:U:102:GLU:OE1	2.15	0.46
1:A:7:ALA:HB1	1:B:10:ARG:NH1	2.31	0.46
1:A:67:ILE:HG12	1:A:77:VAL:CG1	2.45	0.46
1:F:59:ILE:CG2	1:F:60:GLU:N	2.79	0.46
2:K:3:THR:HB	2:K:16:THR:HG22	1.97	0.46
2:L:114:ASP:C	2:L:114:ASP:OD1	2.58	0.46
2:M:2:THR:OG1	2:M:130:GLY:HA3	2.16	0.46
1:G:38:LEU:HD11	1:G:49:ILE:HD12	1.98	0.46
2:M:43:MET:HE3	2:M:56:VAL:HG22	1.97	0.46
2:M:143:SER:HB3	2:M:146:MET:HG3	1.97	0.46
3:P:65:GLU:HA	3:P:68:LEU:HD12	1.98	0.46
1:A:10:ARG:NH1	1:G:7:ALA:HB1	2.31	0.46
1:C:152:ASP:HB2	1:C:153:PRO:CD	2.46	0.46
2:J:24:ASN:HD22	2:J:24:ASN:H	1.62	0.46
2:H:3:THR:HB	2:H:16:THR:HG22	1.97	0.45
3:R:206:ARG:HA	3:R:209:ILE:HD12	1.98	0.45
1:C:152:ASP:HB2	1:C:153:PRO:HD2	1.97	0.45
2:I:18:ARG:HD3	2:I:31:GLY:O	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Q:116:ILE:HD12	3:Q:208:VAL:HG22	1.99	0.45
2:N:172:MET:CE	2:N:192:ILE:CG2	2.94	0.45
1:D:47:LEU:C	1:D:47:LEU:HD12	2.42	0.45
2:K:1:THR:CG2	2:K:2:THR:N	2.79	0.45
2:L:4:VAL:HG22	2:L:5:GLY:N	2.31	0.45
2:K:58:TYR:HD1	2:K:86:MET:HE1	1.81	0.45
1:A:67:ILE:HG12	1:A:77:VAL:HG12	1.98	0.45
1:A:123:TYR:HH	1:G:126:TYR:HH	1.62	0.45
1:F:65:GLU:HB3	1:F:211:GLU:OE2	2.17	0.45
2:L:141:GLN:O	2:L:146:MET:HE3	2.17	0.45
1:G:59:ILE:CG2	1:G:60:GLU:N	2.79	0.45
1:G:65:GLU:HG2	2:M:71:ARG:HH21	1.80	0.45
2:L:3:THR:HB	2:L:16:THR:HG22	1.99	0.45
3:O:12:LEU:HD22	3:P:206:ARG:HD3	1.99	0.45
3:O:55:TYR:O	3:O:180:LEU:HD21	2.16	0.45
1:F:82:VAL:HG22	3:O:229:MET:O	2.17	0.45
2:L:24:ASN:H	2:L:24:ASN:HD22	1.64	0.45
3:O:39:ILE:HD13	3:O:74:TYR:HA	1.98	0.45
3:P:5:ARG:HG2	3:Q:213:LEU:HD22	1.98	0.45
3:R:12:LEU:HD22	3:S:206:ARG:HD3	1.99	0.45
2:L:163:LYS:HE3	2:L:203:LEU:HD13	1.98	0.45
1:B:67:ILE:HG12	1:B:77:VAL:CG1	2.47	0.44
1:F:152:ASP:HB2	1:F:153:PRO:HD2	1.99	0.44
1:B:65:GLU:HB3	1:B:211:GLU:OE2	2.17	0.44
2:L:84:SER:OG	2:L:117:GLY:O	2.33	0.44
2:L:86:MET:HE2	2:L:86:MET:HB3	1.91	0.44
2:M:18:ARG:HD3	2:M:31:GLY:O	2.17	0.44
2:N:131:SER:N	2:N:132:PRO:CD	2.80	0.44
3:O:35:GLU:HG3	3:O:77:LEU:HD13	1.98	0.44
3:R:142:MET:HE2	3:S:192:LEU:HD21	1.99	0.44
3:S:116:ILE:HD12	3:S:208:VAL:HG22	2.00	0.44
3:U:65:GLU:HA	3:U:68:LEU:HD12	1.99	0.44
1:C:67:ILE:HG12	1:C:77:VAL:CG1	2.48	0.44
1:E:55:ARG:HE	3:U:228:HIS:CE1	2.35	0.44
1:E:186:GLU:OE2	1:E:224:TYR:OH	2.34	0.44
2:H:131:SER:N	2:H:132:PRO:CD	2.80	0.44
2:I:3:THR:HB	2:I:16:THR:HG22	1.99	0.44
2:N:114:ASP:C	2:N:114:ASP:OD1	2.60	0.44
1:D:152:ASP:HB2	1:D:153:PRO:HD2	1.98	0.44
1:D:208:LYS:O	1:D:210:PRO:HD3	2.18	0.44
3:R:202:SER:O	3:R:206:ARG:HG3	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:131:SER:N	2:M:132:PRO:CD	2.81	0.44
3:O:65:GLU:HA	3:O:68:LEU:HD12	1.99	0.44
3:S:61:GLU:C	3:T:177:PRO:HG3	2.43	0.44
3:S:65:GLU:HA	3:S:68:LEU:HD12	2.00	0.44
1:A:152:ASP:HB2	1:A:153:PRO:HD2	1.99	0.44
1:D:12:ILE:HD11	1:D:24:VAL:CG2	2.48	0.44
1:D:152:ASP:HB2	1:D:153:PRO:CD	2.48	0.44
1:G:71:ASP:HA	2:M:68:LEU:HD11	1.99	0.44
3:S:28:TRP:HA	3:S:32:THR:HB	1.98	0.44
3:S:68:LEU:HD23	3:S:145:LEU:HD11	2.00	0.44
3:S:142:MET:HE1	3:T:192:LEU:HD21	1.99	0.44
1:B:65:GLU:OE1	1:B:65:GLU:CA	2.65	0.44
2:J:45:ILE:HB	2:J:52:ALA:HB1	2.00	0.44
3:O:109:VAL:HG22	3:U:99:HIS:HB3	1.99	0.44
3:R:28:TRP:HA	3:R:32:THR:HB	2.00	0.44
3:T:129:GLU:HG3	3:U:139:PRO:O	2.18	0.44
2:K:143:SER:HB3	2:K:146:MET:HG3	2.00	0.44
2:N:58:TYR:HD1	2:N:86:MET:HE1	1.83	0.44
2:N:163:LYS:HZ3	2:N:203:LEU:HB3	1.83	0.44
3:T:65:GLU:HA	3:T:68:LEU:HD12	1.99	0.44
1:E:142:ASP:OD1	1:E:142:ASP:C	2.61	0.43
2:K:25:PHE:CD1	2:K:25:PHE:C	2.96	0.43
3:S:97:PRO:HA	3:T:214:LEU:HD13	2.00	0.43
3:P:142:MET:CE	3:Q:192:LEU:HD21	2.49	0.43
3:T:28:TRP:HA	3:T:32:THR:HB	2.01	0.43
1:B:38:LEU:HD11	1:B:49:ILE:HD12	2.00	0.43
1:B:15:PHE:N	1:C:23:GLN:OE1	2.46	0.43
1:F:71:ASP:HA	2:L:68:LEU:HD11	2.01	0.43
1:B:136:LEU:N	1:B:136:LEU:HD12	2.34	0.43
2:H:58:TYR:HD1	2:H:86:MET:HE1	1.84	0.43
2:L:94:PRO:O	2:M:91:LYS:NZ	2.51	0.43
3:P:35:GLU:HG3	3:P:77:LEU:HD13	2.01	0.43
3:R:71:LEU:HB2	3:R:145:LEU:HD13	2.01	0.43
1:B:77:VAL:CG2	1:B:137:ILE:HB	2.48	0.43
2:M:58:TYR:HD1	2:M:86:MET:HE1	1.83	0.43
3:S:63:SER:OG	3:T:178:SER:OG	2.12	0.43
3:T:24:VAL:HG13	3:T:84:GLN:HB3	2.01	0.43
3:T:55:TYR:O	3:T:180:LEU:HD21	2.18	0.43
1:A:8:TYR:OH	1:B:9:ASP:OD2	2.30	0.43
2:J:2:THR:OG1	2:J:130:GLY:HA3	2.19	0.43
2:L:22:MET:O	2:L:23:GLU:CB	2.67	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Q:24:VAL:HG13	3:Q:84:GLN:HB3	2.01	0.43
2:J:172:MET:CE	2:J:192:ILE:CG2	2.97	0.42
2:L:18:ARG:CD	2:L:31:GLY:O	2.67	0.42
2:N:172:MET:CE	2:N:192:ILE:HG22	2.49	0.42
3:U:35:GLU:HG3	3:U:77:LEU:HD13	2.01	0.42
1:E:12:ILE:HD12	1:E:12:ILE:HA	1.87	0.42
1:G:208:LYS:O	1:G:210:PRO:HD3	2.19	0.42
2:I:66:TYR:CD2	2:I:74:MET:HE2	2.54	0.42
1:B:67:ILE:HG12	1:B:77:VAL:HG12	2.01	0.42
1:G:77:VAL:CG2	1:G:137:ILE:HB	2.49	0.42
2:M:74:MET:HG2	2:M:78:ALA:HB3	2.00	0.42
3:S:132:GLY:HA2	3:T:134:GLY:C	2.44	0.42
1:A:12:ILE:HD12	1:A:12:ILE:HA	1.89	0.42
1:C:47:LEU:C	1:C:47:LEU:HD12	2.44	0.42
1:G:152:ASP:OD1	1:G:152:ASP:C	2.63	0.42
3:Q:133:SER:N	3:R:133:SER:O	2.50	0.42
3:S:12:LEU:HD22	3:T:206:ARG:HD3	2.00	0.42
1:C:65:GLU:HB3	1:C:211:GLU:OE2	2.19	0.42
2:M:19:ARG:O	2:M:33:LYS:NZ	2.48	0.42
1:G:152:ASP:HB2	1:G:153:PRO:HD2	2.02	0.42
1:C:67:ILE:HG12	1:C:77:VAL:HG12	2.02	0.42
1:D:38:LEU:C	1:D:38:LEU:HD12	2.44	0.42
1:E:210:PRO:HD2	1:E:229:VAL:HG11	2.02	0.42
1:F:126:TYR:OH	1:G:123:TYR:OH	2.30	0.42
1:F:152:ASP:HB2	1:F:153:PRO:CD	2.50	0.42
2:H:59:MET:CE	2:H:79:VAL:HG13	2.50	0.42
2:J:66:TYR:CD2	2:J:74:MET:HE2	2.54	0.42
1:C:142:ASP:C	1:C:142:ASP:OD1	2.63	0.42
1:C:210:PRO:HD2	1:C:229:VAL:CG1	2.50	0.42
1:G:152:ASP:HB2	1:G:153:PRO:CD	2.50	0.42
2:I:113:ILE:HA	2:I:118:GLY:O	2.19	0.42
2:K:66:TYR:CD2	2:K:74:MET:HE2	2.55	0.42
3:P:202:SER:O	3:P:206:ARG:HG3	2.19	0.42
1:A:210:PRO:HD2	1:A:229:VAL:HG11	2.01	0.42
1:B:9:ASP:O	1:B:23:GLN:NE2	2.53	0.42
2:J:86:MET:HE2	2:J:86:MET:HB3	1.98	0.42
2:K:14:MET:HE2	2:K:44:THR:CG2	2.45	0.42
2:M:25:PHE:CD1	2:M:25:PHE:C	2.98	0.42
3:O:142:MET:HE2	3:P:192:LEU:HD21	2.01	0.42
1:A:65:GLU:OE1	1:A:65:GLU:CA	2.68	0.42
1:E:65:GLU:HB3	1:E:211:GLU:OE2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:120:MET:HE2	1:F:152:ASP:O	2.19	0.42
3:R:125:LEU:O	3:R:126:GLY:C	2.63	0.42
3:T:39:ILE:HD13	3:T:74:TYR:HA	2.02	0.42
1:B:152:ASP:HB2	1:B:153:PRO:HD2	2.02	0.41
2:J:131:SER:N	2:J:132:PRO:CD	2.83	0.41
1:G:76:ALA:HA	1:G:137:ILE:O	2.21	0.41
2:H:45:ILE:HB	2:H:52:ALA:HB1	2.03	0.41
2:J:58:TYR:HD1	2:J:86:MET:HE1	1.84	0.41
2:K:18:ARG:CD	2:K:31:GLY:O	2.68	0.41
2:K:51:ASP:OD2	2:L:91:LYS:NZ	2.45	0.41
2:M:66:TYR:CD2	2:M:74:MET:HE2	2.55	0.41
1:C:9:ASP:OD1	1:C:26:TYR:OH	2.32	0.41
1:C:210:PRO:HD2	1:C:229:VAL:HG11	2.02	0.41
1:F:59:ILE:HG22	1:F:60:GLU:N	2.34	0.41
2:M:147:THR:HG23	2:M:150:GLU:OE2	2.20	0.41
3:O:63:SER:OG	3:P:178:SER:OG	2.37	0.41
3:P:28:TRP:HA	3:P:32:THR:HB	2.02	0.41
3:S:198:THR:O	3:S:199:THR:C	2.63	0.41
1:B:126:TYR:HH	1:C:123:TYR:HH	1.57	0.41
2:I:1:THR:CG2	2:I:2:THR:N	2.82	0.41
2:J:25:PHE:CD1	2:J:25:PHE:C	2.98	0.41
2:K:131:SER:N	2:K:132:PRO:CD	2.83	0.41
3:O:28:TRP:HA	3:O:32:THR:HB	2.02	0.41
1:A:9:ASP:O	1:A:23:GLN:NE2	2.54	0.41
1:A:142:ASP:OD1	1:A:142:ASP:C	2.64	0.41
1:G:48:LEU:HD13	1:G:77:VAL:HG13	2.01	0.41
2:J:3:THR:HB	2:J:16:THR:HG22	2.02	0.41
1:B:77:VAL:HG22	1:B:137:ILE:HB	2.03	0.41
2:N:172:MET:HE1	2:N:192:ILE:HG22	2.02	0.41
3:O:50:ILE:HD11	3:O:67:LEU:HD11	2.02	0.41
3:O:142:MET:HE2	3:O:142:MET:HB3	1.87	0.41
3:P:156:GLU:OE1	3:Q:176:SER:OG	2.36	0.41
1:A:156:THR:HG23	1:B:82:VAL:HG21	2.02	0.41
1:F:142:ASP:OD1	1:F:142:ASP:C	2.63	0.41
2:I:45:ILE:HB	2:I:52:ALA:HB1	2.02	0.41
2:L:131:SER:N	2:L:132:PRO:CD	2.83	0.41
1:A:47:LEU:HD22	1:A:190:VAL:HG22	2.03	0.41
1:C:65:GLU:OE1	1:C:65:GLU:CA	2.69	0.41
2:I:131:SER:N	2:I:132:PRO:CD	2.84	0.41
2:K:114:ASP:OD1	2:K:114:ASP:C	2.63	0.41
2:L:58:TYR:HD1	2:L:86:MET:HE1	1.84	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:163:LYS:HZ3	2:M:203:LEU:HB3	1.86	0.41
3:O:142:MET:CE	3:P:192:LEU:HD21	2.51	0.41
3:S:133:SER:HB3	3:T:133:SER:HB2	2.03	0.41
3:U:142:MET:HE2	3:U:142:MET:HB3	1.93	0.41
1:A:62:ASN:OD1	1:A:62:ASN:N	2.52	0.41
1:B:152:ASP:HB2	1:B:153:PRO:CD	2.50	0.41
2:I:18:ARG:CD	2:I:31:GLY:O	2.69	0.41
3:P:156:GLU:OE2	3:Q:178:SER:OG	2.39	0.41
3:R:142:MET:HE2	3:R:142:MET:HB3	1.81	0.41
1:B:71:ASP:HA	2:H:68:LEU:HD11	2.03	0.40
1:E:59:ILE:CG2	1:E:60:GLU:N	2.84	0.40
1:E:77:VAL:CG2	1:E:137:ILE:HB	2.51	0.40
2:I:24:ASN:H	2:I:24:ASN:HD22	1.66	0.40
2:J:187:LEU:HA	2:J:188:PRO:HD3	1.94	0.40
2:K:45:ILE:HB	2:K:52:ALA:HB1	2.03	0.40
1:D:97:GLN:HB3	2:J:61:ALA:HB1	2.03	0.40
1:D:210:PRO:HD2	1:D:229:VAL:HG11	2.03	0.40
1:F:107:VAL:HG11	2:M:72:VAL:HG21	2.03	0.40
2:H:25:PHE:C	2:H:25:PHE:CD1	2.99	0.40
2:H:91:LYS:NZ	2:N:94:PRO:O	2.54	0.40
2:J:113:ILE:HA	2:J:118:GLY:O	2.20	0.40
2:M:134:VAL:HG13	2:M:158:ALA:HB1	2.03	0.40
1:B:76:ALA:HA	1:B:137:ILE:O	2.21	0.40
1:E:7:ALA:CB	1:F:10:ARG:NH1	2.82	0.40
3:O:68:LEU:HD23	3:O:145:LEU:HD11	2.04	0.40
1:A:76:ALA:HA	1:A:137:ILE:O	2.22	0.40
1:B:175:PHE:CD1	1:B:175:PHE:C	3.00	0.40
1:G:47:LEU:C	1:G:47:LEU:HD12	2.47	0.40
2:I:25:PHE:CD1	2:I:25:PHE:C	2.98	0.40
2:J:141:GLN:O	2:J:146:MET:CE	2.69	0.40
2:M:43:MET:CE	2:M:56:VAL:HG22	2.52	0.40
3:S:201:LEU:O	3:S:205:VAL:HG23	2.22	0.40

All (2) 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)
3:R:14:ASP:OD1	3:U:45:GLU:OE1[4_555]	1.45	0.75
3:S:45:GLU:OE1	3:T:14:ASP:OD1[4_555]	1.80	0.40

5.3 Torsion angles

5.3.1 Protein backbone

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%)	209 (93%)	14 (6%)	2 (1%)	14	41
1	B	225/227 (99%)	209 (93%)	14 (6%)	2 (1%)	14	41
1	C	225/227 (99%)	211 (94%)	12 (5%)	2 (1%)	14	41
1	D	225/227 (99%)	209 (93%)	14 (6%)	2 (1%)	14	41
1	E	225/227 (99%)	210 (93%)	13 (6%)	2 (1%)	14	41
1	F	225/227 (99%)	213 (95%)	10 (4%)	2 (1%)	14	41
1	G	225/227 (99%)	212 (94%)	11 (5%)	2 (1%)	14	41
2	H	201/203 (99%)	193 (96%)	7 (4%)	1 (0%)	24	54
2	I	201/203 (99%)	193 (96%)	7 (4%)	1 (0%)	24	54
2	J	201/203 (99%)	194 (96%)	6 (3%)	1 (0%)	24	54
2	K	201/203 (99%)	194 (96%)	6 (3%)	1 (0%)	24	54
2	L	201/203 (99%)	194 (96%)	6 (3%)	1 (0%)	24	54
2	M	201/203 (99%)	192 (96%)	8 (4%)	1 (0%)	24	54
2	N	201/203 (99%)	192 (96%)	8 (4%)	1 (0%)	24	54
3	O	214/228 (94%)	207 (97%)	7 (3%)	0	100	100
3	P	214/228 (94%)	208 (97%)	6 (3%)	0	100	100
3	Q	214/228 (94%)	208 (97%)	6 (3%)	0	100	100
3	R	214/228 (94%)	207 (97%)	7 (3%)	0	100	100
3	S	214/228 (94%)	208 (97%)	6 (3%)	0	100	100
3	T	214/228 (94%)	209 (98%)	5 (2%)	0	100	100
3	U	214/228 (94%)	208 (97%)	6 (3%)	0	100	100
All	All	4480/4606 (97%)	4280 (96%)	179 (4%)	21 (0%)	24	54

All (21) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	64	ILE
1	B	64	ILE
1	D	64	ILE
1	E	64	ILE
1	F	64	ILE
1	G	64	ILE
1	C	64	ILE
2	L	23	GLU
2	H	23	GLU
2	I	23	GLU
2	J	23	GLU
2	K	23	GLU
2	M	23	GLU
2	N	23	GLU
1	E	62	ASN
1	G	62	ASN
1	B	62	ASN
1	C	62	ASN
1	F	62	ASN
1	A	55	ARG
1	D	62	ASN

5.3.2 Protein sidechains ⓘ

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%)	177 (94%)	11 (6%)	18	48
1	B	188/188 (100%)	179 (95%)	9 (5%)	23	55
1	C	188/188 (100%)	178 (95%)	10 (5%)	20	52
1	D	188/188 (100%)	178 (95%)	10 (5%)	20	52
1	E	188/188 (100%)	176 (94%)	12 (6%)	16	44
1	F	188/188 (100%)	178 (95%)	10 (5%)	20	52
1	G	188/188 (100%)	176 (94%)	12 (6%)	16	44
2	H	170/170 (100%)	160 (94%)	10 (6%)	18	48

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	I	170/170 (100%)	160 (94%)	10 (6%)	18	48
2	J	170/170 (100%)	160 (94%)	10 (6%)	18	48
2	K	170/170 (100%)	160 (94%)	10 (6%)	18	48
2	L	170/170 (100%)	159 (94%)	11 (6%)	15	44
2	M	170/170 (100%)	159 (94%)	11 (6%)	15	44
2	N	170/170 (100%)	159 (94%)	11 (6%)	15	44
3	O	179/187 (96%)	174 (97%)	5 (3%)	38	72
3	P	179/187 (96%)	175 (98%)	4 (2%)	45	77
3	Q	179/187 (96%)	174 (97%)	5 (3%)	38	72
3	R	179/187 (96%)	174 (97%)	5 (3%)	38	72
3	S	179/187 (96%)	175 (98%)	4 (2%)	45	77
3	T	179/187 (96%)	175 (98%)	4 (2%)	45	77
3	U	179/187 (96%)	175 (98%)	4 (2%)	45	77
All	All	3759/3815 (98%)	3581 (95%)	178 (5%)	23	56

All (178) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10	ARG
1	A	55	ARG
1	A	61	GLN
1	A	62	ASN
1	A	106	LEU
1	A	136	LEU
1	A	169	LYS
1	A	177	GLU
1	A	203	GLU
1	A	226	GLN
1	A	230	LYS
1	B	10	ARG
1	B	55	ARG
1	B	61	GLN
1	B	106	LEU
1	B	136	LEU
1	B	169	LYS
1	B	177	GLU
1	B	203	GLU

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Mol	Chain	Res	Type
1	B	230	LYS
1	C	10	ARG
1	C	55	ARG
1	C	61	GLN
1	C	62	ASN
1	C	106	LEU
1	C	136	LEU
1	C	169	LYS
1	C	177	GLU
1	C	203	GLU
1	C	230	LYS
1	D	10	ARG
1	D	55	ARG
1	D	61	GLN
1	D	106	LEU
1	D	136	LEU
1	D	169	LYS
1	D	177	GLU
1	D	199	SER
1	D	203	GLU
1	D	230	LYS
1	E	10	ARG
1	E	55	ARG
1	E	61	GLN
1	E	62	ASN
1	E	106	LEU
1	E	136	LEU
1	E	169	LYS
1	E	177	GLU
1	E	199	SER
1	E	203	GLU
1	E	226	GLN
1	E	230	LYS
1	F	10	ARG
1	F	55	ARG
1	F	61	GLN
1	F	62	ASN
1	F	106	LEU
1	F	136	LEU
1	F	169	LYS
1	F	177	GLU
1	F	203	GLU

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Mol	Chain	Res	Type
1	F	230	LYS
1	G	10	ARG
1	G	55	ARG
1	G	61	GLN
1	G	62	ASN
1	G	106	LEU
1	G	136	LEU
1	G	169	LYS
1	G	177	GLU
1	G	199	SER
1	G	203	GLU
1	G	226	GLN
1	G	230	LYS
2	H	1	THR
2	H	9	LYS
2	H	17	GLU
2	H	22	MET
2	H	23	GLU
2	H	71	ARG
2	H	72	VAL
2	H	186	GLN
2	H	202	ILE
2	H	203	LEU
2	I	1	THR
2	I	9	LYS
2	I	17	GLU
2	I	22	MET
2	I	23	GLU
2	I	71	ARG
2	I	72	VAL
2	I	186	GLN
2	I	202	ILE
2	I	203	LEU
2	J	1	THR
2	J	9	LYS
2	J	17	GLU
2	J	22	MET
2	J	23	GLU
2	J	71	ARG
2	J	72	VAL
2	J	186	GLN
2	J	202	ILE

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Mol	Chain	Res	Type
2	J	203	LEU
2	K	3	THR
2	K	9	LYS
2	K	17	GLU
2	K	22	MET
2	K	23	GLU
2	K	71	ARG
2	K	72	VAL
2	K	186	GLN
2	K	202	ILE
2	K	203	LEU
2	L	1	THR
2	L	3	THR
2	L	9	LYS
2	L	17	GLU
2	L	22	MET
2	L	23	GLU
2	L	71	ARG
2	L	72	VAL
2	L	186	GLN
2	L	202	ILE
2	L	203	LEU
2	M	1	THR
2	M	3	THR
2	M	9	LYS
2	M	17	GLU
2	M	22	MET
2	M	23	GLU
2	M	71	ARG
2	M	72	VAL
2	M	186	GLN
2	M	202	ILE
2	M	203	LEU
2	N	1	THR
2	N	3	THR
2	N	9	LYS
2	N	17	GLU
2	N	22	MET
2	N	23	GLU
2	N	71	ARG
2	N	72	VAL
2	N	186	GLN

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Mol	Chain	Res	Type
2	N	202	ILE
2	N	203	LEU
3	O	19	THR
3	O	57	ARG
3	O	142	MET
3	O	157	ASP
3	O	226	THR
3	P	19	THR
3	P	57	ARG
3	P	142	MET
3	P	226	THR
3	Q	19	THR
3	Q	57	ARG
3	Q	142	MET
3	Q	157	ASP
3	Q	226	THR
3	R	19	THR
3	R	57	ARG
3	R	142	MET
3	R	157	ASP
3	R	226	THR
3	S	19	THR
3	S	57	ARG
3	S	142	MET
3	S	226	THR
3	T	19	THR
3	T	57	ARG
3	T	142	MET
3	T	226	THR
3	U	19	THR
3	U	57	ARG
3	U	142	MET
3	U	226	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (50) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	44	ASN
1	D	44	ASN
1	E	111	ASN
2	H	24	ASN
2	H	36	GLN

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Mol	Chain	Res	Type
2	I	24	ASN
2	I	73	ASN
2	I	191	GLN
2	J	24	ASN
2	J	191	GLN
2	K	24	ASN
2	K	191	GLN
2	L	24	ASN
2	L	191	GLN
2	M	24	ASN
2	M	73	ASN
2	N	24	ASN
2	N	191	GLN
3	O	47	HIS
3	O	75	GLN
3	O	79	HIS
3	O	228	HIS
3	P	47	HIS
3	P	52	ASN
3	P	75	GLN
3	P	175	GLN
3	P	228	HIS
3	Q	47	HIS
3	Q	75	GLN
3	Q	79	HIS
3	Q	175	GLN
3	Q	228	HIS
3	R	47	HIS
3	R	52	ASN
3	R	75	GLN
3	R	79	HIS
3	R	228	HIS
3	S	47	HIS
3	S	75	GLN
3	S	79	HIS
3	S	175	GLN
3	S	228	HIS
3	T	47	HIS
3	T	75	GLN
3	T	175	GLN
3	T	228	HIS
3	U	47	HIS

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Mol	Chain	Res	Type
3	U	75	GLN
3	U	79	HIS
3	U	228	HIS

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	227/227 (100%)	-0.14	1 (0%) 88 85	43, 55, 79, 87	0
1	B	227/227 (100%)	-0.17	1 (0%) 88 85	43, 55, 79, 87	0
1	C	227/227 (100%)	-0.11	1 (0%) 88 85	43, 55, 79, 87	0
1	D	227/227 (100%)	-0.13	2 (0%) 81 75	43, 55, 79, 87	0
1	E	227/227 (100%)	-0.05	5 (2%) 62 53	43, 55, 79, 87	0
1	F	227/227 (100%)	-0.13	3 (1%) 75 67	43, 55, 79, 87	0
1	G	227/227 (100%)	-0.21	4 (1%) 67 59	43, 55, 79, 87	0
2	H	203/203 (100%)	-0.29	2 (0%) 79 73	44, 50, 65, 76	0
2	I	203/203 (100%)	-0.32	2 (0%) 79 73	44, 50, 65, 76	0
2	J	203/203 (100%)	-0.32	2 (0%) 79 73	44, 50, 65, 76	0
2	K	203/203 (100%)	-0.37	2 (0%) 79 73	44, 50, 65, 76	0
2	L	203/203 (100%)	-0.34	2 (0%) 79 73	44, 50, 65, 76	0
2	M	203/203 (100%)	-0.23	2 (0%) 79 73	44, 50, 65, 76	0
2	N	203/203 (100%)	-0.31	2 (0%) 79 73	44, 50, 65, 76	0
3	O	218/228 (95%)	0.03	4 (1%) 67 59	46, 60, 80, 91	0
3	P	218/228 (95%)	-0.05	4 (1%) 67 59	46, 60, 80, 91	0
3	Q	218/228 (95%)	0.02	3 (1%) 73 65	46, 60, 80, 91	0
3	R	218/228 (95%)	0.06	7 (3%) 50 41	46, 60, 80, 91	0
3	S	218/228 (95%)	0.01	5 (2%) 61 52	46, 60, 80, 91	0
3	T	218/228 (95%)	-0.01	3 (1%) 73 65	46, 60, 80, 91	0
3	U	218/228 (95%)	0.14	10 (4%) 37 29	46, 60, 80, 91	0
All	All	4536/4606 (98%)	-0.13	67 (1%) 72 64	43, 55, 78, 91	0

All (67) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	64	ILE	5.3
1	D	64	ILE	5.3
1	B	64	ILE	5.2
3	R	132	GLY	4.7
2	I	203	LEU	4.6
1	G	64	ILE	4.5
2	M	203	LEU	4.3
2	L	203	LEU	3.9
1	F	64	ILE	3.8
1	C	64	ILE	3.8
3	O	137	PRO	3.6
2	H	203	LEU	3.5
2	K	203	LEU	3.4
3	R	137	PRO	3.3
1	D	53	LYS	3.3
3	P	136	ALA	3.2
2	N	203	LEU	3.2
3	O	134	GLY	3.1
3	S	137	PRO	3.0
1	E	64	ILE	2.9
3	P	138	THR	2.9
3	U	128	GLY	2.9
3	U	132	GLY	2.9
3	R	133	SER	2.9
2	L	202	ILE	2.8
3	P	161	GLY	2.8
3	S	132	GLY	2.7
2	H	202	ILE	2.7
1	E	181	LYS	2.7
1	E	178	ARG	2.7
2	I	202	ILE	2.7
3	U	137	PRO	2.6
3	S	138	THR	2.6
2	M	202	ILE	2.6
3	R	138	THR	2.6
1	E	209	ALA	2.5
2	J	203	LEU	2.5
1	G	203	GLU	2.5
3	U	136	ALA	2.5
3	P	137	PRO	2.4
3	S	136	ALA	2.4
3	U	135	GLY	2.4
2	K	202	ILE	2.4

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Mol	Chain	Res	Type	RSRZ
2	N	202	ILE	2.4
3	U	131	SER	2.4
2	J	202	ILE	2.4
3	Q	137	PRO	2.4
3	T	132	GLY	2.4
1	F	209	ALA	2.4
3	U	138	THR	2.4
3	R	128	GLY	2.3
3	R	231	SER	2.3
3	O	138	THR	2.3
3	R	139	PRO	2.3
1	G	204	GLY	2.3
1	G	227	GLU	2.2
3	U	127	SER	2.2
3	U	133	SER	2.2
3	U	161	GLY	2.2
3	Q	173	GLY	2.2
3	T	136	ALA	2.1
3	S	129	GLU	2.1
3	O	157	ASP	2.1
3	T	133	SER	2.1
3	Q	135	GLY	2.1
1	E	203	GLU	2.1
1	F	203	GLU	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 oligosaccharides 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.