



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 20, 2026 – 05:23 AM UTC

PDB ID : 1YAU / pdb_00001yau
Title : Structure of Archeabacterial 20S proteasome- PA26 complex
Authors : Forster, A.; Masters, E.I.; Whitby, F.G.; Robinson, H.; Hill, C.P.
Deposited on : 2004-12-17
Resolution : 2.40 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

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

with specific help available everywhere you see the ⓘ 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
Mogul	:	2022.3.0, CSD as543be (2022)
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

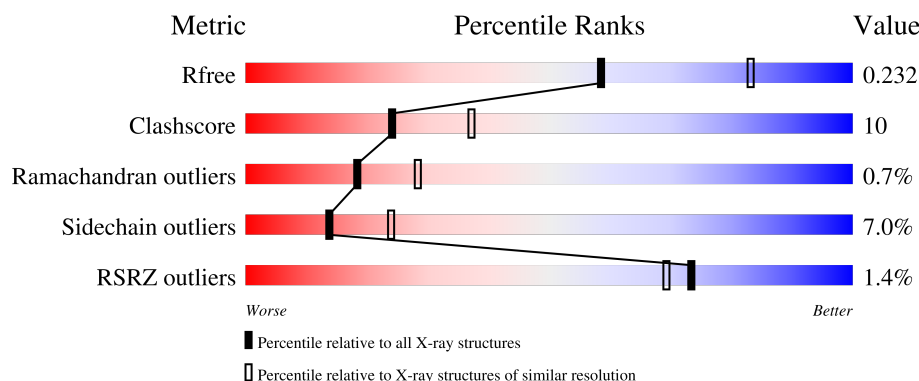
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



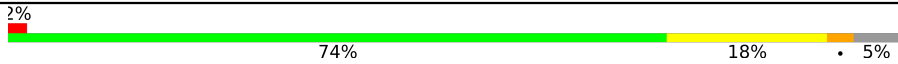
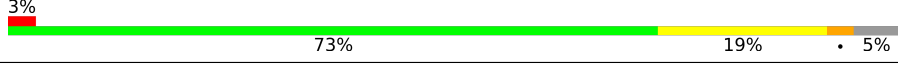
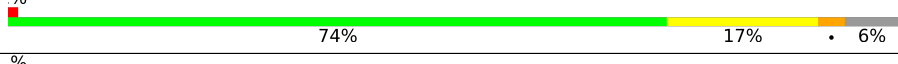
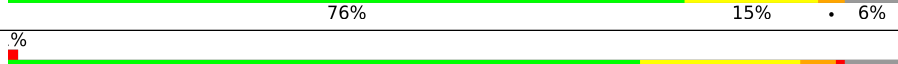
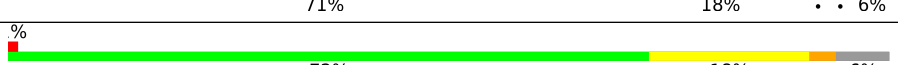
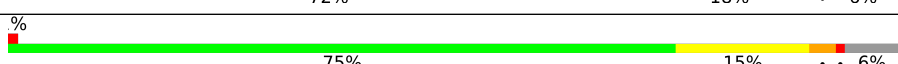
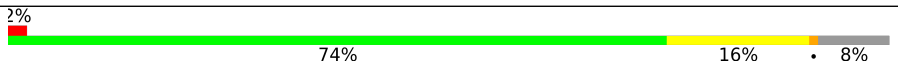
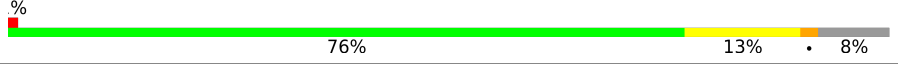
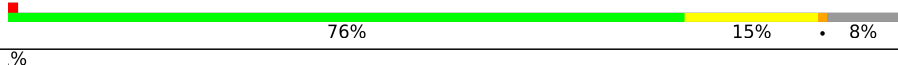
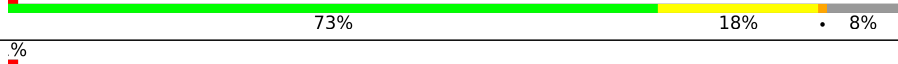
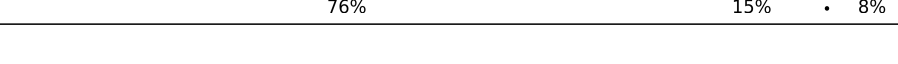
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	4912 (2.40-2.40)
Clashscore	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)
RSRZ outliers	180081	4916 (2.40-2.40)

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	233	67% 22% 6% 5%
1	B	233	69% 23% • 5%
1	C	233	76% 15% • • 5%
1	D	233	70% 21% • 5%
1	E	233	67% 22% 5% 5%

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Mol	Chain	Length	Quality of chain
1	F	233	
1	G	233	
2	H	217	
2	I	217	
2	J	217	
2	K	217	
2	L	217	
2	M	217	
2	N	217	
3	O	237	
3	P	237	
3	Q	237	
3	R	237	
3	S	237	
3	T	237	
3	U	237	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	SO4	A	3007	-	-	X	-

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 36610 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 alpha subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	222	Total	C	N	O	S	0	0	0
			1728	1098	291	336	3			
1	B	222	Total	C	N	O	S	0	0	0
			1728	1098	291	336	3			
1	C	222	Total	C	N	O	S	0	0	0
			1728	1098	291	336	3			
1	D	222	Total	C	N	O	S	0	0	0
			1728	1098	291	336	3			
1	E	222	Total	C	N	O	S	0	0	0
			1728	1098	291	336	3			
1	F	222	Total	C	N	O	S	0	0	0
			1728	1098	291	336	3			
1	G	222	Total	C	N	O	S	0	0	0
			1728	1098	291	336	3			

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	8	GLY	TYR	engineered mutation	UNP P25156
A	9	GLY	ASP	engineered mutation	UNP P25156
B	8	GLY	TYR	engineered mutation	UNP P25156
B	9	GLY	ASP	engineered mutation	UNP P25156
C	8	GLY	TYR	engineered mutation	UNP P25156
C	9	GLY	ASP	engineered mutation	UNP P25156
D	8	GLY	TYR	engineered mutation	UNP P25156
D	9	GLY	ASP	engineered mutation	UNP P25156
E	8	GLY	TYR	engineered mutation	UNP P25156
E	9	GLY	ASP	engineered mutation	UNP P25156
F	8	GLY	TYR	engineered mutation	UNP P25156
F	9	GLY	ASP	engineered mutation	UNP P25156
G	8	GLY	TYR	engineered mutation	UNP P25156
G	9	GLY	ASP	engineered mutation	UNP P25156

- Molecule 2 is a protein called Proteasome beta subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	203	Total	C	N	O	S	0	2	0
			1577	999	266	300	12			
2	I	203	Total	C	N	O	S	0	2	0
			1577	999	266	300	12			
2	J	203	Total	C	N	O	S	0	2	0
			1577	999	266	300	12			
2	K	203	Total	C	N	O	S	0	1	0
			1569	994	265	299	11			
2	L	203	Total	C	N	O	S	0	1	0
			1569	994	265	299	11			
2	M	203	Total	C	N	O	S	0	2	0
			1577	999	266	300	12			
2	N	203	Total	C	N	O	S	0	2	0
			1577	999	266	300	12			

There are 42 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
H	204	HIS	-	expression tag	UNP P28061
H	205	HIS	-	expression tag	UNP P28061
H	206	HIS	-	expression tag	UNP P28061
H	207	HIS	-	expression tag	UNP P28061
H	208	HIS	-	expression tag	UNP P28061
H	209	HIS	-	expression tag	UNP P28061
I	204	HIS	-	expression tag	UNP P28061
I	205	HIS	-	expression tag	UNP P28061
I	206	HIS	-	expression tag	UNP P28061
I	207	HIS	-	expression tag	UNP P28061
I	208	HIS	-	expression tag	UNP P28061
I	209	HIS	-	expression tag	UNP P28061
J	204	HIS	-	expression tag	UNP P28061
J	205	HIS	-	expression tag	UNP P28061
J	206	HIS	-	expression tag	UNP P28061
J	207	HIS	-	expression tag	UNP P28061
J	208	HIS	-	expression tag	UNP P28061
J	209	HIS	-	expression tag	UNP P28061
K	204	HIS	-	expression tag	UNP P28061
K	205	HIS	-	expression tag	UNP P28061
K	206	HIS	-	expression tag	UNP P28061
K	207	HIS	-	expression tag	UNP P28061
K	208	HIS	-	expression tag	UNP P28061
K	209	HIS	-	expression tag	UNP P28061

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Chain	Residue	Modelled	Actual	Comment	Reference
L	204	HIS	-	expression tag	UNP P28061
L	205	HIS	-	expression tag	UNP P28061
L	206	HIS	-	expression tag	UNP P28061
L	207	HIS	-	expression tag	UNP P28061
L	208	HIS	-	expression tag	UNP P28061
L	209	HIS	-	expression tag	UNP P28061
M	204	HIS	-	expression tag	UNP P28061
M	205	HIS	-	expression tag	UNP P28061
M	206	HIS	-	expression tag	UNP P28061
M	207	HIS	-	expression tag	UNP P28061
M	208	HIS	-	expression tag	UNP P28061
M	209	HIS	-	expression tag	UNP P28061
N	204	HIS	-	expression tag	UNP P28061
N	205	HIS	-	expression tag	UNP P28061
N	206	HIS	-	expression tag	UNP P28061
N	207	HIS	-	expression tag	UNP P28061
N	208	HIS	-	expression tag	UNP P28061
N	209	HIS	-	expression tag	UNP P28061

- 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
			1679	1051	296	326	6			
3	P	218	Total	C	N	O	S	0	0	0
			1679	1051	296	326	6			
3	Q	218	Total	C	N	O	S	0	0	0
			1679	1051	296	326	6			
3	R	218	Total	C	N	O	S	0	0	0
			1679	1051	296	326	6			
3	S	218	Total	C	N	O	S	0	0	0
			1679	1051	296	326	6			
3	T	218	Total	C	N	O	S	0	0	0
			1679	1051	296	326	6			
3	U	218	Total	C	N	O	S	0	0	0
			1679	1051	296	326	6			

There are 56 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
O	-5	MET	-	initiating methionine	GB 5757773
O	-4	HIS	-	expression tag	GB 5757773

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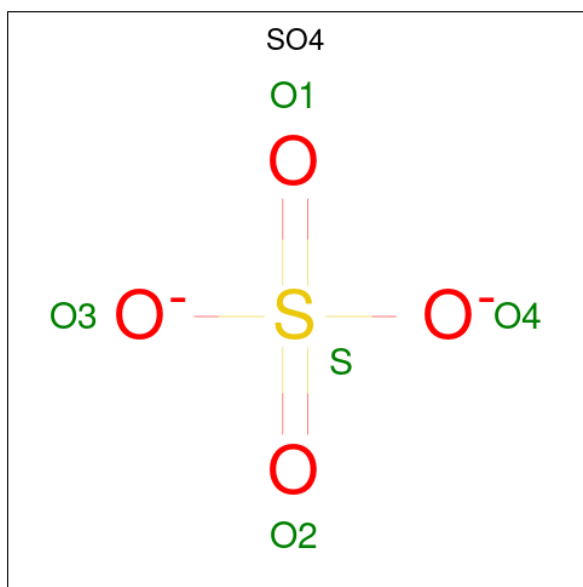
Chain	Residue	Modelled	Actual	Comment	Reference
O	-3	HIS	-	expression tag	GB 5757773
O	-2	HIS	-	expression tag	GB 5757773
O	-1	HIS	-	expression tag	GB 5757773
O	0	HIS	-	expression tag	GB 5757773
O	1	HIS	-	expression tag	GB 5757773
O	49	VAL	THR	variant	GB 5757773
P	-5	MET	-	initiating methionine	GB 5757773
P	-4	HIS	-	expression tag	GB 5757773
P	-3	HIS	-	expression tag	GB 5757773
P	-2	HIS	-	expression tag	GB 5757773
P	-1	HIS	-	expression tag	GB 5757773
P	0	HIS	-	expression tag	GB 5757773
P	1	HIS	-	expression tag	GB 5757773
P	49	VAL	THR	variant	GB 5757773
Q	-5	MET	-	initiating methionine	GB 5757773
Q	-4	HIS	-	expression tag	GB 5757773
Q	-3	HIS	-	expression tag	GB 5757773
Q	-2	HIS	-	expression tag	GB 5757773
Q	-1	HIS	-	expression tag	GB 5757773
Q	0	HIS	-	expression tag	GB 5757773
Q	1	HIS	-	expression tag	GB 5757773
Q	49	VAL	THR	variant	GB 5757773
R	-5	MET	-	initiating methionine	GB 5757773
R	-4	HIS	-	expression tag	GB 5757773
R	-3	HIS	-	expression tag	GB 5757773
R	-2	HIS	-	expression tag	GB 5757773
R	-1	HIS	-	expression tag	GB 5757773
R	0	HIS	-	expression tag	GB 5757773
R	1	HIS	-	expression tag	GB 5757773
R	49	VAL	THR	variant	GB 5757773
S	-5	MET	-	initiating methionine	GB 5757773
S	-4	HIS	-	expression tag	GB 5757773
S	-3	HIS	-	expression tag	GB 5757773
S	-2	HIS	-	expression tag	GB 5757773
S	-1	HIS	-	expression tag	GB 5757773
S	0	HIS	-	expression tag	GB 5757773
S	1	HIS	-	expression tag	GB 5757773
S	49	VAL	THR	variant	GB 5757773
T	-5	MET	-	initiating methionine	GB 5757773
T	-4	HIS	-	expression tag	GB 5757773
T	-3	HIS	-	expression tag	GB 5757773
T	-2	HIS	-	expression tag	GB 5757773

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Chain	Residue	Modelled	Actual	Comment	Reference
T	-1	HIS	-	expression tag	GB 5757773
T	0	HIS	-	expression tag	GB 5757773
T	1	HIS	-	expression tag	GB 5757773
T	49	VAL	THR	variant	GB 5757773
U	-5	MET	-	initiating methionine	GB 5757773
U	-4	HIS	-	expression tag	GB 5757773
U	-3	HIS	-	expression tag	GB 5757773
U	-2	HIS	-	expression tag	GB 5757773
U	-1	HIS	-	expression tag	GB 5757773
U	0	HIS	-	expression tag	GB 5757773
U	1	HIS	-	expression tag	GB 5757773
U	49	VAL	THR	variant	GB 5757773

- Molecule 4 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total O S 5 4 1	0	0
4	B	1	Total O S 5 4 1	0	0
4	C	1	Total O S 5 4 1	0	0
4	D	1	Total O S 5 4 1	0	0
4	E	1	Total O S 5 4 1	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	F	1	Total	O	S	0	0
			5	4	1		
4	G	1	Total	O	S	0	0
			5	4	1		
4	H	1	Total	O	S	0	0
			5	4	1		
4	H	1	Total	O	S	0	0
			5	4	1		
4	I	1	Total	O	S	0	0
			5	4	1		
4	I	1	Total	O	S	0	0
			5	4	1		
4	I	1	Total	O	S	0	0
			5	4	1		
4	J	1	Total	O	S	0	0
			5	4	1		
4	J	1	Total	O	S	0	0
			5	4	1		
4	K	1	Total	O	S	0	0
			5	4	1		
4	K	1	Total	O	S	0	0
			5	4	1		
4	L	1	Total	O	S	0	0
			5	4	1		
4	L	1	Total	O	S	0	0
			5	4	1		
4	M	1	Total	O	S	0	0
			5	4	1		
4	M	1	Total	O	S	0	0
			5	4	1		
4	M	1	Total	O	S	0	0
			5	4	1		
4	M	1	Total	O	S	0	0
			5	4	1		
4	N	1	Total	O	S	0	0
			5	4	1		
4	N	1	Total	O	S	0	0
			5	4	1		
4	N	1	Total	O	S	0	0
			5	4	1		

- Molecule 5 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	H	1	Total	C	O	0	0
			6	3	3		
5	I	1	Total	C	O	0	0
			6	3	3		
5	J	1	Total	C	O	0	0
			6	3	3		
5	K	1	Total	C	O	0	0
			6	3	3		
5	L	1	Total	C	O	0	0
			6	3	3		
5	M	1	Total	C	O	0	0
			6	3	3		
5	N	1	Total	C	O	0	0
			6	3	3		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	67	Total	O	0	0
			67	67		
6	B	58	Total	O	0	0
			58	58		
6	C	69	Total	O	0	0
			69	69		
6	D	49	Total	O	0	0
			49	49		
6	E	67	Total	O	0	0
			67	67		

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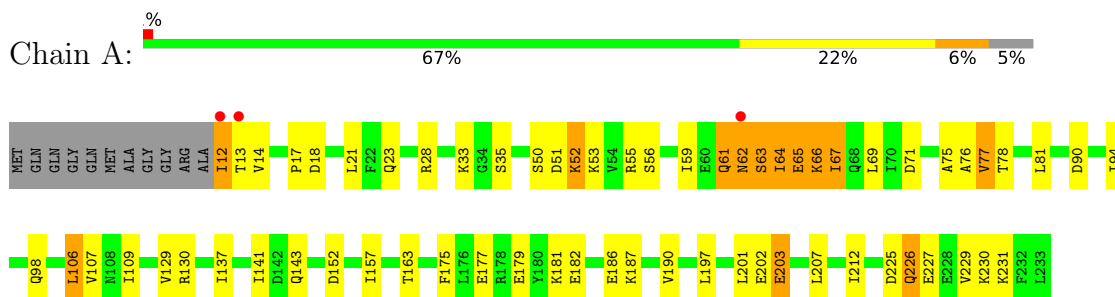
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	F	61	Total 61	O 61	0	0
6	G	51	Total 51	O 51	0	0
6	H	93	Total 93	O 93	0	0
6	I	100	Total 100	O 100	0	0
6	J	94	Total 94	O 94	0	0
6	K	85	Total 85	O 85	0	0
6	L	93	Total 93	O 93	0	0
6	M	100	Total 100	O 100	0	0
6	N	107	Total 107	O 107	0	0
6	O	52	Total 52	O 52	0	0
6	P	47	Total 47	O 47	0	0
6	Q	47	Total 47	O 47	0	0
6	R	69	Total 69	O 69	0	0
6	S	90	Total 90	O 90	0	0
6	T	97	Total 97	O 97	0	0
6	U	75	Total 75	O 75	0	0

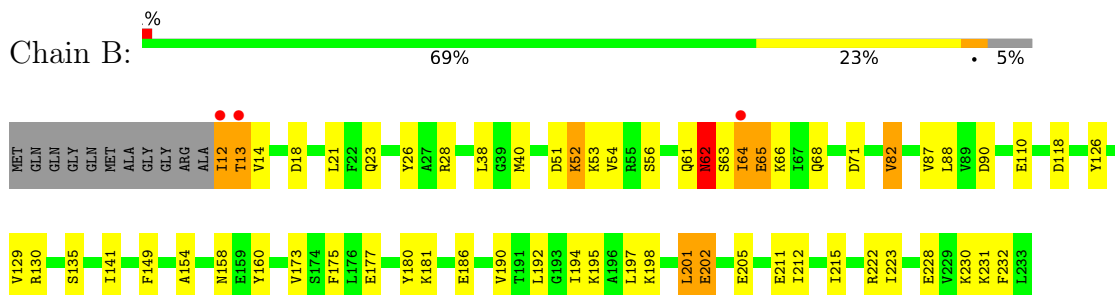
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

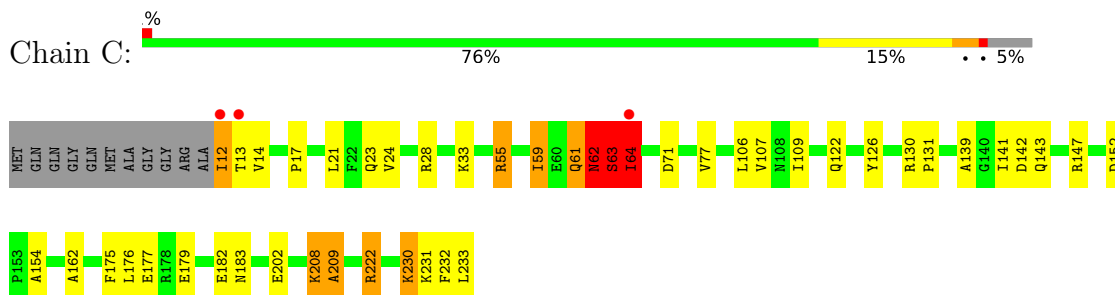
- Molecule 1: Proteasome alpha subunit



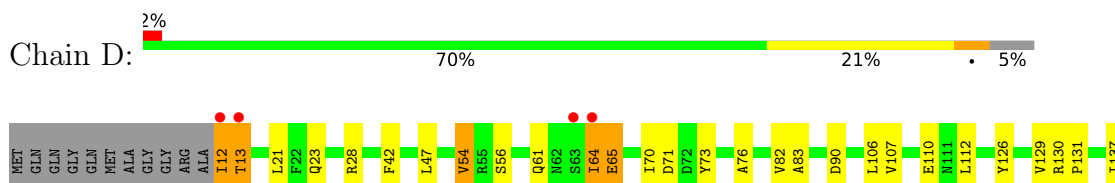
- Molecule 1: Proteasome alpha subunit



- Molecule 1: Proteasome alpha subunit



- Molecule 1: Proteasome alpha subunit

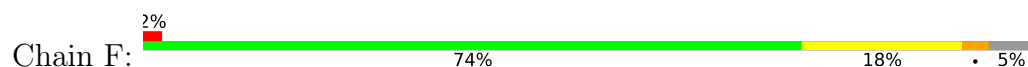




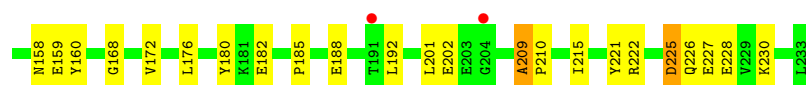
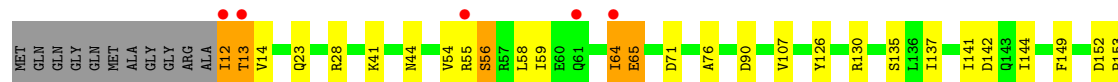
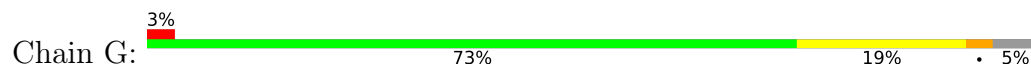
• Molecule 1: Proteasome alpha subunit



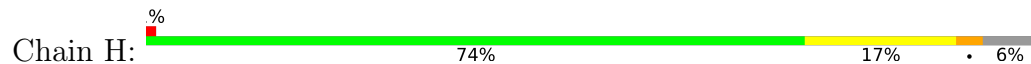
• Molecule 1: Proteasome alpha subunit



• Molecule 1: Proteasome alpha subunit

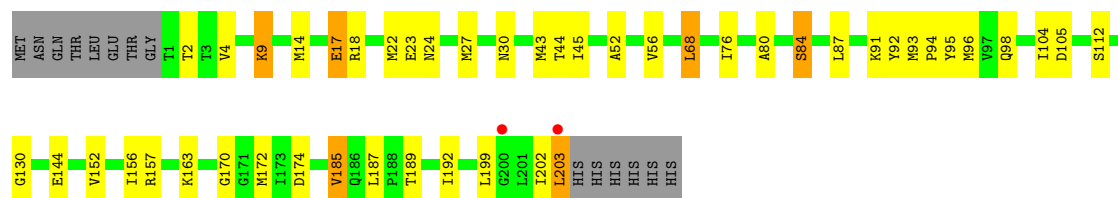


• Molecule 2: Proteasome beta subunit

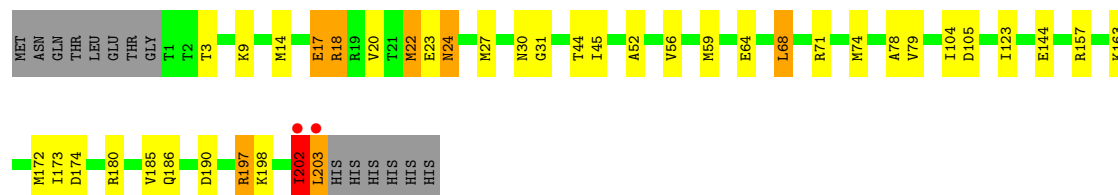
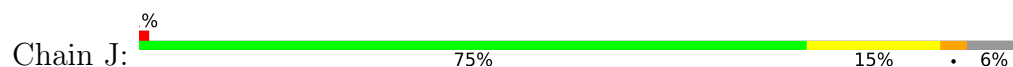


• Molecule 2: Proteasome beta subunit

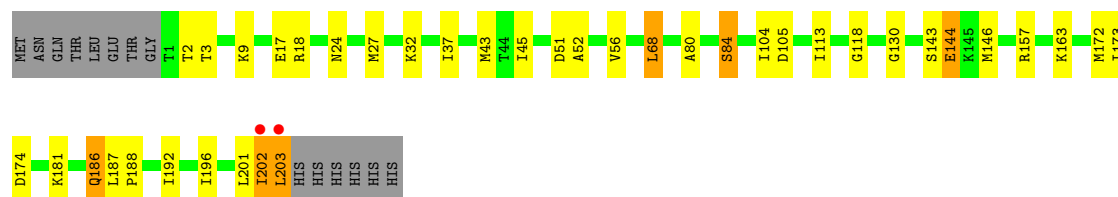
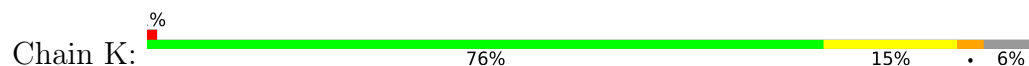




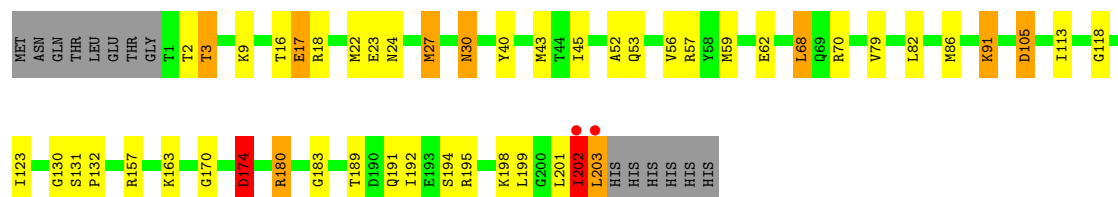
• Molecule 2: Proteasome beta subunit



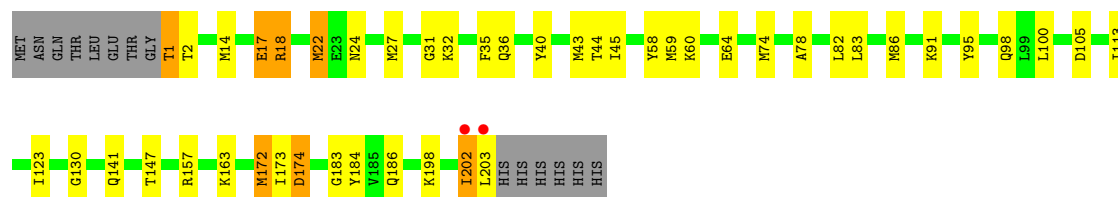
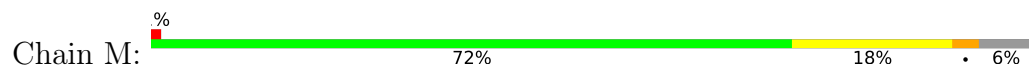
• Molecule 2: Proteasome beta subunit



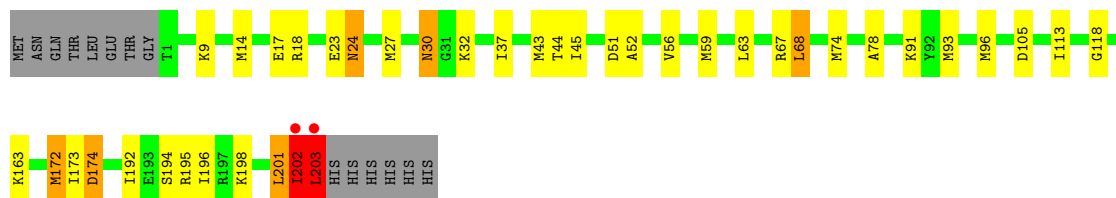
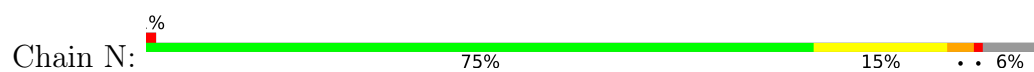
• Molecule 2: Proteasome beta subunit



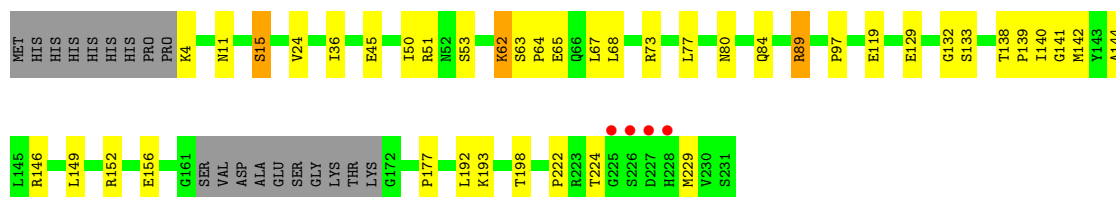
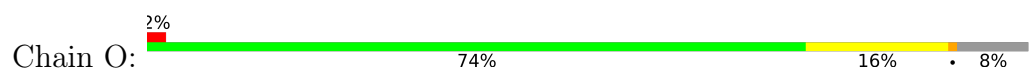
• Molecule 2: Proteasome beta subunit



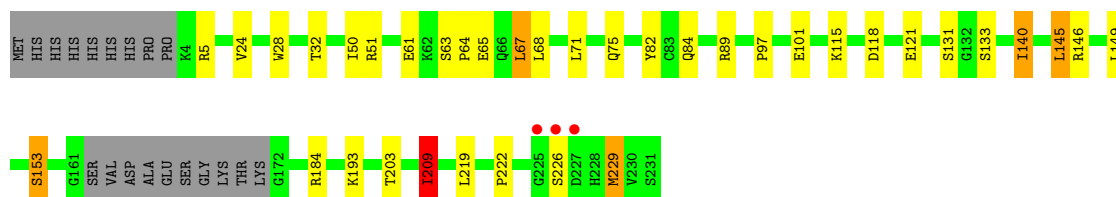
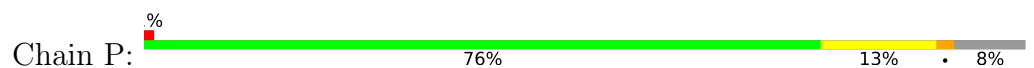
• Molecule 2: Proteasome beta subunit



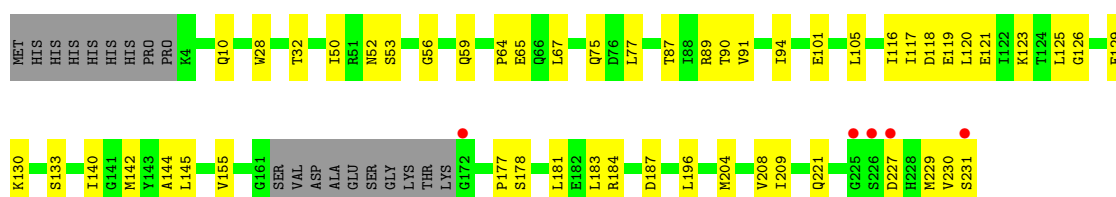
• Molecule 3: proteasome activator protein PA26



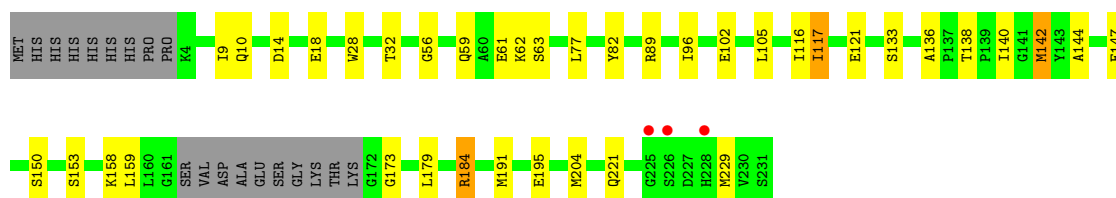
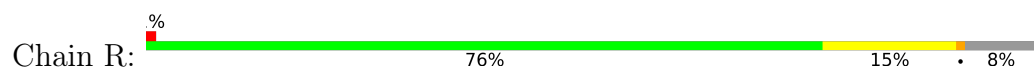
• Molecule 3: proteasome activator protein PA26



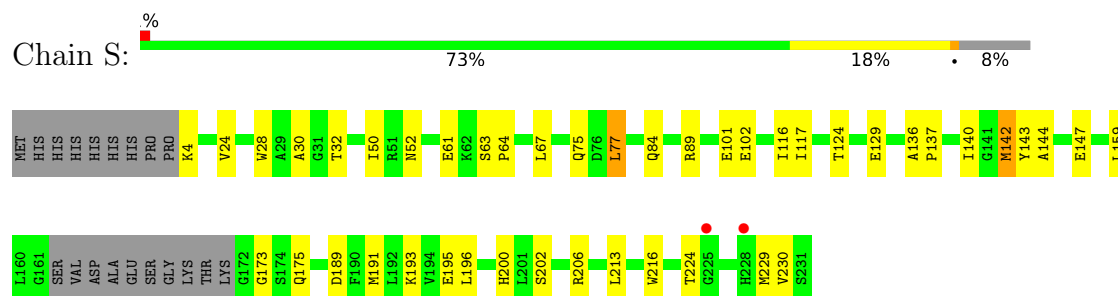
• Molecule 3: proteasome activator protein PA26



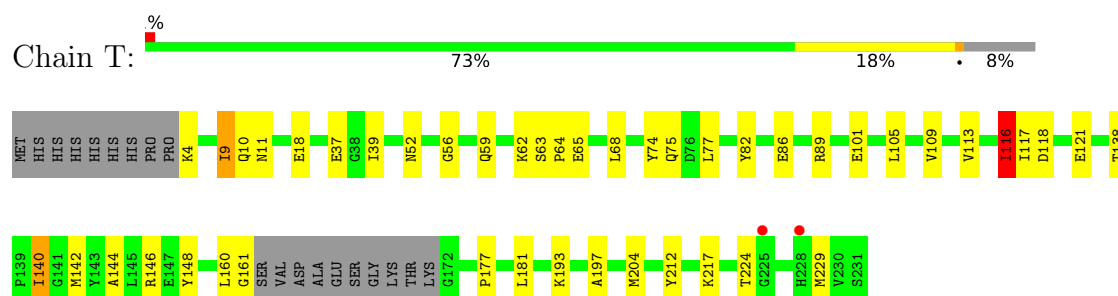
• Molecule 3: proteasome activator protein PA26



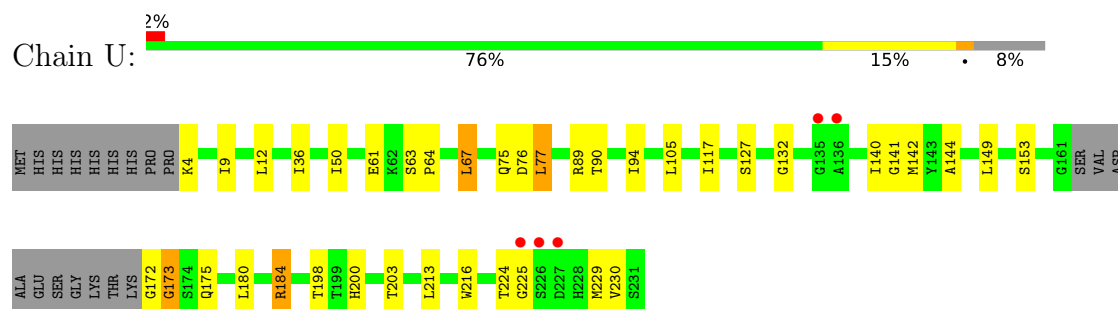
- Molecule 3: proteasome activator protein PA26



- 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	255.22Å 126.91Å 181.03Å 90.00° 92.42° 90.00°	Depositor
Resolution (Å)	8.00 – 2.40 8.00 – 2.40	Depositor EDS
% Data completeness (in resolution range)	99.8 (8.00-2.40) 97.0 (8.00-2.40)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.29 (at 2.40Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.180 , 0.233 0.180 , 0.232	Depositor DCC
R_{free} test set	1069 reflections (0.49%)	wwPDB-VP
Wilson B-factor (Å ²)	35.2	Xtriage
Anisotropy	0.028	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.48 , 67.2	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	0.95	EDS
Total number of atoms	36610	wwPDB-VP
Average B, all atoms (Å ²)	40.0	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.*

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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, SO4

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	1/1751 (0.1%)	1.06	1/2359 (0.0%)
1	B	1.02	2/1751 (0.1%)	1.12	3/2359 (0.1%)
1	C	1.00	1/1751 (0.1%)	1.06	3/2359 (0.1%)
1	D	0.97	3/1751 (0.2%)	1.12	1/2359 (0.0%)
1	E	0.97	0/1751	1.11	4/2359 (0.2%)
1	F	0.95	2/1751 (0.1%)	1.04	2/2359 (0.1%)
1	G	0.96	0/1751	1.08	2/2359 (0.1%)
2	H	1.09	2/1597 (0.1%)	1.09	2/2157 (0.1%)
2	I	1.06	2/1597 (0.1%)	1.10	0/2157
2	J	1.09	3/1597 (0.2%)	1.10	1/2157 (0.0%)
2	K	1.08	1/1589 (0.1%)	1.13	0/2147
2	L	1.07	3/1589 (0.2%)	1.10	2/2147 (0.1%)
2	M	1.10	2/1597 (0.1%)	1.12	3/2157 (0.1%)
2	N	1.09	6/1597 (0.4%)	1.11	3/2157 (0.1%)
3	O	0.85	0/1702	1.09	1/2299 (0.0%)
3	P	0.83	1/1702 (0.1%)	1.08	2/2299 (0.1%)
3	Q	0.85	1/1702 (0.1%)	1.07	0/2299
3	R	0.92	0/1702	1.11	2/2299 (0.1%)
3	S	0.98	1/1702 (0.1%)	1.10	2/2299 (0.1%)
3	T	0.99	3/1702 (0.2%)	1.11	1/2299 (0.0%)
3	U	0.96	1/1702 (0.1%)	1.07	3/2299 (0.1%)
All	All	0.99	35/35334 (0.1%)	1.09	38/47685 (0.1%)

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	C	0	1

All (35) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	N	105	ASP	CA-C	8.01	1.56	1.52
2	N	202	ILE	CA-C	7.92	1.62	1.52
2	M	105	ASP	CA-C	7.59	1.56	1.52
2	N	202	ILE	CA-CB	7.21	1.64	1.54
1	D	13	THR	CA-CB	6.96	1.64	1.53
1	B	82	VAL	CA-CB	6.88	1.62	1.54
2	L	105	ASP	CA-C	6.86	1.55	1.52
1	B	64	ILE	CA-CB	6.72	1.63	1.54
2	I	185	VAL	CA-CB	6.64	1.62	1.54
3	S	30	ALA	CA-C	6.31	1.55	1.52
1	D	64	ILE	CA-CB	6.19	1.62	1.54
1	C	64	ILE	CA-CB	5.92	1.62	1.54
2	L	192	ILE	CA-CB	5.92	1.61	1.54
3	Q	209	ILE	CA-CB	5.90	1.61	1.54
2	H	202	ILE	N-CA	5.84	1.52	1.46
2	N	202	ILE	N-CA	5.75	1.53	1.46
2	L	202	ILE	CA-CB	5.71	1.62	1.54
2	M	147	THR	CA-CB	5.58	1.62	1.53
2	J	185	VAL	CA-CB	5.51	1.61	1.54
1	F	141	ILE	CA-CB	5.48	1.61	1.54
2	I	76	ILE	CA-CB	5.45	1.61	1.54
2	J	20	VAL	CA-CB	5.44	1.60	1.53
2	H	105	ASP	CA-C	5.44	1.55	1.52
2	K	202	ILE	CA-CB	5.29	1.61	1.54
3	U	141	GLY	N-CA	5.24	1.48	1.44
3	T	9	ILE	CA-CB	5.22	1.60	1.54
3	P	209	ILE	CA-CB	5.18	1.60	1.54
2	N	203	LEU	N-CA	5.18	1.56	1.46
3	T	116	ILE	CA-CB	5.18	1.61	1.54
2	N	192	ILE	CA-CB	5.17	1.60	1.54
3	T	140	ILE	CA-CB	5.17	1.61	1.55
1	F	13	THR	CA-CB	5.16	1.60	1.53
1	D	82	VAL	CA-CB	5.13	1.61	1.54
2	J	104	ILE	CA-CB	5.13	1.60	1.54
1	A	163	THR	CA-CB	5.00	1.61	1.53

All (38) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	201	LEU	N-CA-C	7.73	119.34	111.07
1	B	13	THR	N-CA-C	-7.50	99.26	109.54
2	H	202	ILE	N-CA-C	7.25	119.68	108.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	R	96	ILE	N-CA-C	-7.17	101.14	108.96
1	D	13	THR	N-CA-C	-6.82	102.26	110.44
3	P	5	ARG	N-CA-C	6.53	118.20	111.14
2	M	202	ILE	N-CA-C	6.46	118.23	108.80
3	S	52	ASN	N-CA-C	6.30	120.69	113.19
2	N	202	ILE	N-CA-C	6.25	122.33	109.34
1	B	63	SER	N-CA-C	6.24	116.31	108.45
2	N	201	LEU	N-CA-C	6.08	117.87	109.29
3	U	141	GLY	N-CA-C	6.03	121.13	112.81
1	E	77	VAL	N-CA-C	-5.91	99.71	108.45
3	S	216	TRP	N-CA-C	5.91	117.72	111.28
2	J	202	ILE	N-CA-C	5.89	117.19	108.65
2	N	203	LEU	CA-CB-CG	5.84	136.73	116.30
1	G	13	THR	CA-C-N	-5.73	116.08	123.19
1	G	13	THR	C-N-CA	-5.73	116.08	123.19
2	M	95	TYR	N-CA-C	-5.52	101.48	109.59
1	C	77	VAL	N-CA-C	-5.51	99.89	108.81
1	A	63	SER	N-CA-C	-5.50	106.62	113.38
1	B	118	ASP	N-CA-C	5.49	117.27	111.28
1	C	63	SER	N-CA-C	5.42	117.21	109.14
3	P	229	MET	N-CA-C	5.41	117.25	111.36
2	M	45	ILE	N-CA-C	5.40	116.25	108.48
1	F	97	GLN	N-CA-C	5.23	116.98	111.28
1	E	157	ILE	N-CA-C	5.21	116.88	108.85
3	O	141	GLY	N-CA-C	5.19	120.19	112.41
2	L	202	ILE	N-CA-C	5.16	120.08	109.34
2	L	174	ASP	CB-CA-C	-5.15	101.26	109.75
1	F	14	VAL	N-CA-C	5.10	115.25	108.11
1	C	183	ASN	N-CA-C	5.07	118.73	112.24
3	R	117	ILE	N-CA-C	5.07	115.84	110.72
3	U	216	TRP	N-CA-C	5.06	116.80	111.28
1	E	70	ILE	N-CA-C	-5.04	106.76	111.45
3	T	217	LYS	N-CA-C	5.04	116.77	111.28
2	H	23	GLU	CB-CA-C	-5.03	110.39	117.23
3	U	127	SER	N-CA-C	5.01	118.54	112.23

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	62	ASN	Peptide

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	1728	0	1764	54	0
1	B	1728	0	1764	48	0
1	C	1728	0	1764	44	0
1	D	1728	0	1764	48	0
1	E	1728	0	1764	57	0
1	F	1728	0	1764	42	0
1	G	1728	0	1764	35	0
2	H	1577	0	1625	28	0
2	I	1577	0	1625	33	0
2	J	1577	0	1625	25	0
2	K	1569	0	1617	35	0
2	L	1569	0	1617	31	0
2	M	1577	0	1625	40	0
2	N	1577	0	1625	32	0
3	O	1679	0	1700	35	0
3	P	1679	0	1700	29	0
3	Q	1679	0	1700	36	0
3	R	1679	0	1700	36	0
3	S	1679	0	1700	36	0
3	T	1679	0	1700	40	0
3	U	1679	0	1700	37	0
4	A	5	0	0	2	0
4	B	5	0	0	0	0
4	C	5	0	0	0	0
4	D	5	0	0	1	0
4	E	5	0	0	0	0
4	F	5	0	0	0	0
4	G	5	0	0	0	0
4	H	10	0	0	0	0
4	I	15	0	0	1	0
4	J	10	0	0	1	0
4	K	10	0	0	0	0
4	L	10	0	0	1	0
4	M	20	0	0	1	0
4	N	15	0	0	1	0
5	H	6	0	8	0	0
5	I	6	0	8	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	J	6	0	8	0	0
5	K	6	0	8	0	0
5	L	6	0	8	2	0
5	M	6	0	8	0	0
5	N	6	0	8	0	0
6	A	67	0	0	7	0
6	B	58	0	0	2	0
6	C	69	0	0	2	0
6	D	49	0	0	3	0
6	E	67	0	0	10	0
6	F	61	0	0	5	0
6	G	51	0	0	4	0
6	H	93	0	0	4	0
6	I	100	0	0	8	0
6	J	94	0	0	13	0
6	K	85	0	0	12	0
6	L	93	0	0	1	0
6	M	100	0	0	6	0
6	N	107	0	0	8	0
6	O	52	0	0	3	0
6	P	47	0	0	2	0
6	Q	47	0	0	1	0
6	R	69	0	0	4	0
6	S	90	0	0	1	0
6	T	97	0	0	1	0
6	U	75	0	0	5	0
All	All	36610	0	35663	705	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 10.

All (705) 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:U:184:ARG:HG2	3:U:184:ARG:HH11	0.95	1.11
1:E:143:GLN:HG3	6:E:3051:HOH:O	1.49	1.10
1:D:28:ARG:HH22	3:U:229:MET:HG2	1.02	1.08
2:L:27:MET:HG2	6:M:3108:HOH:O	1.53	1.08
1:G:28:ARG:HH22	3:Q:229:MET:HG2	1.20	1.05
1:E:28:ARG:HH22	3:O:229:MET:HG2	1.16	1.04
3:R:184:ARG:HB3	3:R:184:ARG:HH11	1.18	1.03

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:O:89:ARG:HH11	3:O:89:ARG:HB3	1.20	1.03
1:E:106:LEU:HD21	6:E:3071:HOH:O	1.60	1.01
2:I:22:MET:HE1	6:J:3103:HOH:O	1.60	1.00
3:S:144:ALA:HB3	6:S:320:HOH:O	1.59	1.00
1:E:208:LYS:CD	1:E:208:LYS:H	1.73	0.99
1:C:13:THR:O	1:D:130:ARG:HB3	1.63	0.98
3:U:184:ARG:HG2	3:U:184:ARG:NH1	1.72	0.98
1:A:106:LEU:HD21	6:A:3049:HOH:O	1.63	0.97
2:I:27:MET:HE1	6:J:3098:HOH:O	1.65	0.96
3:O:89:ARG:HB3	3:O:89:ARG:NH1	1.81	0.96
2:I:9:LYS:HE3	6:I:3095:HOH:O	1.66	0.96
1:B:28:ARG:HH22	3:S:229:MET:HG3	1.30	0.95
1:A:12:ILE:HG13	1:A:13:THR:HG23	1.45	0.95
1:B:62:ASN:H	1:B:62:ASN:HD22	1.00	0.94
1:E:208:LYS:H	1:E:208:LYS:HD2	1.32	0.93
2:J:203:LEU:HD21	6:J:3101:HOH:O	1.68	0.91
1:B:90:ASP:HB3	6:H:3078:HOH:O	1.69	0.91
1:D:28:ARG:NH2	3:U:229:MET:HG2	1.86	0.91
2:M:59:MET:HE1	2:M:86:MET:HE1	1.51	0.90
1:D:28:ARG:HH22	3:U:229:MET:CG	1.85	0.90
2:J:22:MET:HB2	2:J:27:MET:SD	2.11	0.90
2:J:203:LEU:CD2	6:J:3101:HOH:O	2.20	0.89
1:C:61:GLN:CD	1:C:61:GLN:H	1.80	0.88
3:R:184:ARG:HH11	3:R:184:ARG:CB	1.86	0.88
1:G:12:ILE:HA	1:G:23:GLN:HG3	1.56	0.87
3:T:89:ARG:HD2	3:U:203:THR:HG21	1.56	0.86
1:B:12:ILE:HG13	1:B:13:THR:HG23	1.56	0.86
1:E:28:ARG:HH22	3:O:229:MET:CG	1.89	0.85
1:E:201:LEU:O	1:E:202:GLU:HB2	1.76	0.85
2:L:22:MET:HB2	2:L:27:MET:SD	2.17	0.84
2:M:59:MET:CE	2:M:86:MET:HE1	2.07	0.84
2:H:9:LYS:HG3	6:H:3025:HOH:O	1.76	0.83
1:B:62:ASN:HD22	1:B:62:ASN:N	1.71	0.83
1:F:13:THR:O	1:G:130:ARG:HB3	1.78	0.82
3:R:184:ARG:HB3	3:R:184:ARG:NH1	1.93	0.82
2:I:9:LYS:HG3	6:I:3107:HOH:O	1.78	0.82
1:G:90:ASP:HB3	6:M:3091:HOH:O	1.80	0.81
2:M:58[A]:TYR:CD2	2:M:59:MET:HE2	2.16	0.80
3:Q:119:GLU:HG3	3:Q:123:LYS:HE3	1.63	0.80
1:B:28:ARG:NH2	3:S:229:MET:HG3	1.97	0.80
1:B:175:PHE:CZ	1:B:195:LYS:HG2	2.15	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:65:GLU:HA	6:D:3022:HOH:O	1.80	0.79
1:A:12:ILE:HG23	6:A:3029:HOH:O	1.82	0.79
2:M:58[A]:TYR:HD2	2:M:59:MET:HE2	1.46	0.79
1:A:130:ARG:HB3	1:G:13:THR:O	1.81	0.79
1:F:21:LEU:HD12	3:P:229:MET:HE1	1.66	0.78
1:F:28:ARG:HH22	3:P:229:MET:CG	1.95	0.78
1:A:13:THR:O	1:B:130:ARG:HB3	1.82	0.78
6:F:3054:HOH:O	1:G:64:ILE:HD12	1.83	0.78
3:T:116:ILE:HG12	3:T:204:MET:CE	2.14	0.78
1:D:13:THR:O	1:E:130:ARG:HB3	1.83	0.77
6:H:3018:HOH:O	2:N:27:MET:HE1	1.84	0.77
1:F:12:ILE:HG13	1:F:13:THR:HG23	1.66	0.77
1:B:222:ARG:NH1	1:B:228:GLU:OE1	2.18	0.77
2:M:186:GLN:OE1	6:M:3124:HOH:O	2.02	0.77
2:N:172:MET:HE2	2:N:173:ILE:H	1.48	0.77
2:K:186:GLN:HG3	6:K:3072:HOH:O	1.84	0.76
2:L:191:GLN:HE21	2:L:195:ARG:HE	1.33	0.76
1:B:62:ASN:H	1:B:62:ASN:ND2	1.77	0.76
1:D:12:ILE:HG13	1:D:13:THR:HG23	1.67	0.75
2:I:27:MET:CE	6:J:3098:HOH:O	2.28	0.75
1:G:64:ILE:HG12	6:G:3019:HOH:O	1.86	0.74
1:D:12:ILE:HA	1:D:23:GLN:HG3	1.69	0.74
1:G:12:ILE:HG13	1:G:13:THR:HG23	1.67	0.74
1:F:12:ILE:HA	1:F:23:GLN:HG3	1.68	0.74
1:D:90:ASP:HB3	6:J:3069:HOH:O	1.87	0.73
2:M:172:MET:HE3	2:M:172:MET:HA	1.71	0.72
1:C:107:VAL:HG13	1:C:143:GLN:HG3	1.70	0.72
2:J:27:MET:HG2	6:K:3044:HOH:O	1.90	0.72
4:J:3017:SO4:O1	6:J:3110:HOH:O	2.08	0.71
3:O:132:GLY:HA3	6:O:255:HOH:O	1.90	0.71
1:A:52:LYS:NZ	1:A:66:LYS:HD2	2.06	0.70
3:R:144:ALA:HB3	6:R:286:HOH:O	1.91	0.70
1:E:28:ARG:NH2	6:E:3056:HOH:O	2.23	0.70
2:M:58[A]:TYR:HD2	2:M:59:MET:CE	2.03	0.70
2:N:24:ASN:H	2:N:24:ASN:HD22	1.37	0.70
1:E:222:ARG:NH1	1:E:228:GLU:OE2	2.16	0.70
1:A:81:LEU:HD23	3:Q:230:VAL:HG22	1.73	0.70
3:Q:89:ARG:NH1	3:Q:118:ASP:OD1	2.25	0.70
2:J:157:ARG:HD2	6:J:3028:HOH:O	1.92	0.69
3:R:56:GLY:H	3:R:59:GLN:HE21	1.40	0.69
1:C:12:ILE:HG13	1:C:13:THR:HG23	1.73	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:163:LYS:NZ	2:I:203:LEU:HB3	2.08	0.69
2:N:67:ARG:HD2	6:N:3075:HOH:O	1.91	0.69
3:Q:133:SER:HB3	3:R:133:SER:HB2	1.72	0.69
1:A:187:LYS:HE3	1:A:231:LYS:NZ	2.07	0.69
2:J:197:ARG:HG2	6:J:3107:HOH:O	1.92	0.69
6:G:3010:HOH:O	3:Q:229:MET:SD	2.51	0.69
3:U:184:ARG:HH11	3:U:184:ARG:CG	1.89	0.68
1:F:28:ARG:HH22	3:P:229:MET:HG2	1.57	0.68
2:H:18:ARG:CZ	2:H:174:ASP:OD1	2.41	0.68
2:N:202:ILE:HG13	2:N:203:LEU:H	1.59	0.68
3:R:221:GLN:HG3	6:R:289:HOH:O	1.93	0.68
1:F:12:ILE:N	6:F:3046:HOH:O	2.26	0.68
2:M:58[A]:TYR:CD2	2:M:59:MET:CE	2.76	0.68
3:O:97:PRO:HG3	3:O:222:PRO:HG2	1.76	0.68
1:E:61:GLN:NE2	1:E:62:ASN:H	1.92	0.68
4:I:3016:SO4:O4	6:I:3118:HOH:O	2.09	0.67
2:N:172:MET:CE	2:N:173:ILE:H	2.07	0.67
2:M:157:ARG:HD2	6:M:3046:HOH:O	1.93	0.67
2:H:163:LYS:NZ	2:H:203:LEU:HB3	2.08	0.67
3:T:116:ILE:HG12	3:T:204:MET:HE3	1.77	0.66
1:C:28:ARG:HH12	3:T:229:MET:HG3	1.59	0.66
2:I:9:LYS:HG2	6:I:3040:HOH:O	1.93	0.66
1:A:203:GLU:CD	1:A:203:GLU:H	2.03	0.66
3:P:63:SER:OG	3:Q:178:SER:OG	2.14	0.66
1:G:28:ARG:NH2	3:Q:229:MET:HG2	2.04	0.66
2:I:187:LEU:HB2	2:I:192:ILE:HD11	1.78	0.66
1:E:28:ARG:NH2	3:O:229:MET:HG2	2.01	0.66
2:H:32:LYS:HE2	6:H:3087:HOH:O	1.95	0.65
1:E:51:ASP:OD1	6:E:3066:HOH:O	2.14	0.65
1:C:33:LYS:HB2	3:S:230:VAL:HG11	1.78	0.65
3:T:116:ILE:HG12	3:T:204:MET:HE1	1.77	0.65
2:K:144:GLU:HG2	6:K:3068:HOH:O	1.97	0.65
1:B:12:ILE:HA	1:B:23:GLN:HG3	1.79	0.65
3:T:146:ARG:HD3	6:U:240:HOH:O	1.97	0.65
3:P:64:PRO:HB2	3:P:67:LEU:HG	1.78	0.64
2:L:43:MET:HE3	2:L:56:VAL:HG22	1.79	0.64
3:Q:129:GLU:HG2	3:R:138:THR:O	1.97	0.64
1:D:230:LYS:HA	1:D:233:LEU:HD12	1.79	0.64
3:T:11:ASN:OD1	6:T:322:HOH:O	2.15	0.64
1:B:28:ARG:NH2	3:S:229:MET:CG	2.61	0.64
3:P:149:LEU:O	3:P:153:SER:HB3	1.97	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:12:ILE:HA	1:C:23:GLN:HG3	1.80	0.64
2:N:201:LEU:O	6:N:3123:HOH:O	2.15	0.64
3:T:64:PRO:O	3:T:68:LEU:HG	1.98	0.64
1:A:90:ASP:HB3	6:N:3111:HOH:O	1.98	0.63
1:E:71:ASP:HA	2:K:68:LEU:HD21	1.81	0.63
1:C:209:ALA:CB	1:C:233:LEU:HD11	2.29	0.63
2:L:191:GLN:HB2	6:L:3104:HOH:O	1.98	0.63
1:C:106:LEU:HD21	6:C:3071:HOH:O	1.99	0.63
1:C:62:ASN:H	1:C:62:ASN:ND2	1.96	0.63
2:K:18:ARG:HG3	2:K:172:MET:O	1.99	0.63
2:L:18:ARG:NH1	2:L:30:ASN:OD1	2.30	0.62
2:L:105:ASP:O	2:L:180:ARG:NH1	2.31	0.62
2:H:43:MET:HE3	2:H:56:VAL:HG22	1.80	0.62
2:J:157:ARG:CD	6:J:3028:HOH:O	2.47	0.62
1:F:62:ASN:H	1:F:62:ASN:HD22	1.47	0.62
1:E:41:LYS:NZ	1:F:60:GLU:OE2	2.32	0.61
1:F:28:ARG:HH22	3:P:229:MET:HG3	1.65	0.61
2:K:172:MET:HE1	2:K:192:ILE:HG22	1.81	0.61
2:M:172:MET:HE2	2:M:173:ILE:H	1.65	0.61
3:S:189:ASP:O	3:S:193:LYS:HG3	1.99	0.61
1:A:65:GLU:HA	4:A:3007:SO4:O1	2.00	0.61
1:F:67:ILE:HD12	1:F:211:GLU:HG2	1.82	0.61
3:O:192:LEU:HD21	3:U:142:MET:HE1	1.81	0.61
3:P:28:TRP:HA	3:P:32:THR:HB	1.83	0.61
1:D:178:ARG:HG2	1:D:179:GLU:HG2	1.82	0.61
1:D:187:LYS:HE3	1:D:232:PHE:CE2	2.34	0.61
1:A:21:LEU:HD12	3:R:229:MET:HE1	1.81	0.61
2:H:91:LYS:HE2	2:N:51:ASP:OD1	2.00	0.61
2:H:24:ASN:HD22	2:H:24:ASN:H	1.48	0.61
1:C:61:GLN:C	1:C:63:SER:H	2.09	0.60
1:D:12:ILE:HG13	1:D:13:THR:CG2	2.30	0.60
3:R:89:ARG:HD3	3:R:121:GLU:OE2	2.01	0.60
1:B:21:LEU:HD12	3:S:229:MET:HE1	1.84	0.60
2:N:202:ILE:CG1	2:N:203:LEU:H	2.13	0.60
1:E:208:LYS:HD2	1:E:208:LYS:N	2.12	0.60
1:F:81:LEU:HD22	3:O:229:MET:HE2	1.83	0.60
2:J:17:GLU:C	2:J:18:ARG:HG2	2.26	0.60
1:E:61:GLN:CD	1:E:61:GLN:H	2.09	0.60
1:C:209:ALA:HA	1:C:233:LEU:HD11	1.84	0.60
2:M:40:TYR:CD1	2:M:183:GLY:HA2	2.37	0.60
2:H:18:ARG:NH2	2:H:174:ASP:OD1	2.35	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:222:ARG:HH12	1:B:228:GLU:CD	2.10	0.59
1:G:141:ILE:HD12	1:G:215:ILE:HG12	1.84	0.59
2:I:98:GLN:HB3	6:I:3119:HOH:O	2.01	0.59
1:C:55:ARG:CZ	1:C:55:ARG:HA	2.32	0.59
2:J:203:LEU:HD23	6:J:3101:HOH:O	1.97	0.59
3:R:184:ARG:HH11	3:R:184:ARG:CG	2.15	0.59
1:B:202:GLU:O	1:B:205:GLU:HB3	2.02	0.59
1:G:201:LEU:HD21	6:G:3040:HOH:O	2.02	0.59
1:D:13:THR:HG21	1:D:126:TYR:C	2.27	0.59
1:G:28:ARG:HH22	3:Q:229:MET:CG	2.07	0.59
1:A:52:LYS:HZ2	1:A:66:LYS:HD2	1.65	0.59
3:T:86:GLU:OE2	3:T:121:GLU:OE1	2.20	0.59
1:A:66:LYS:HE3	1:A:66:LYS:HA	1.83	0.59
1:F:62:ASN:HD22	1:F:62:ASN:N	2.01	0.59
1:A:12:ILE:CG1	1:A:13:THR:HG23	2.26	0.58
1:A:187:LYS:HE3	1:A:231:LYS:HZ3	1.65	0.58
1:C:28:ARG:NH2	1:C:152:ASP:OD2	2.31	0.58
1:A:12:ILE:HD12	1:A:12:ILE:O	2.03	0.58
1:D:107:VAL:O	1:D:142:ASP:HB2	2.03	0.58
1:G:12:ILE:HA	1:G:23:GLN:CG	2.31	0.58
1:A:28:ARG:NH2	1:A:152:ASP:OD2	2.34	0.58
1:D:21:LEU:HD12	3:U:229:MET:HE1	1.85	0.58
2:K:2:THR:OG1	2:K:130:GLY:HA3	2.04	0.58
6:A:3033:HOH:O	1:B:82:VAL:HG11	2.03	0.58
1:F:51:ASP:HB2	1:F:197:LEU:HD11	1.85	0.58
1:F:106:LEU:HD21	6:F:3060:HOH:O	2.02	0.58
3:O:192:LEU:HD21	3:U:142:MET:CE	2.33	0.58
2:N:24:ASN:H	2:N:24:ASN:ND2	2.00	0.58
2:N:43:MET:HE3	2:N:56:VAL:HG22	1.84	0.58
3:R:140:ILE:CD1	3:R:144:ALA:HB1	2.33	0.58
3:S:50:ILE:HD11	3:S:67:LEU:HD21	1.85	0.58
2:L:18:ARG:NE	2:L:174:ASP:OD1	2.33	0.58
3:U:50:ILE:HD11	3:U:67:LEU:HD21	1.85	0.58
1:D:12:ILE:HG12	1:D:129:VAL:O	2.03	0.58
1:E:13:THR:HG22	6:E:3011:HOH:O	2.04	0.58
3:S:143:TYR:O	3:S:147:GLU:HG3	2.03	0.58
2:L:43:MET:CE	2:L:56:VAL:HG22	2.32	0.57
1:F:201:LEU:O	1:F:202:GLU:O	2.22	0.57
1:C:21:LEU:HD12	3:T:229:MET:HE1	1.85	0.57
2:J:18:ARG:HH21	2:J:30:ASN:HD21	1.52	0.57
2:N:91:LYS:HE2	6:N:3110:HOH:O	2.03	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:208:LYS:H	1:E:208:LYS:HD3	1.66	0.57
2:J:18:ARG:HD2	2:J:31:GLY:O	2.05	0.57
2:H:163:LYS:HZ1	2:H:203:LEU:HB3	1.66	0.57
2:K:24:ASN:HD22	2:K:24:ASN:H	1.53	0.57
1:A:186:GLU:O	1:A:190:VAL:HG23	2.05	0.56
2:H:194:SER:O	2:H:198:LYS:HG2	2.04	0.56
1:A:107:VAL:HG13	1:A:143:GLN:HG3	1.86	0.56
1:B:28:ARG:HH22	3:S:229:MET:CG	2.09	0.56
3:Q:50:ILE:HD11	3:Q:67:LEU:HD11	1.87	0.56
3:O:73:ARG:HD2	6:O:247:HOH:O	2.06	0.56
2:N:163:LYS:HZ1	2:N:203:LEU:HB3	1.69	0.56
1:C:13:THR:HG21	1:C:126:TYR:C	2.31	0.56
1:E:156:THR:HG23	1:F:82:VAL:HG21	1.87	0.56
1:E:227:GLU:O	1:E:231:LYS:HD3	2.06	0.56
3:T:89:ARG:NH2	3:T:118:ASP:OD1	2.39	0.56
2:H:147:THR:OG1	2:H:150:GLU:HG2	2.05	0.56
1:A:28:ARG:HH22	3:R:229:MET:HG3	1.71	0.55
1:B:175:PHE:HZ	1:B:195:LYS:HG2	1.69	0.55
2:I:2:THR:OG1	2:I:130:GLY:HA3	2.06	0.55
2:M:18:ARG:HG3	2:M:172:MET:O	2.06	0.55
1:A:94:ILE:O	1:A:98:GLN:HG3	2.05	0.55
2:J:24:ASN:HD22	2:J:24:ASN:H	1.53	0.55
3:P:65:GLU:HA	3:P:68:LEU:HD12	1.88	0.55
1:D:180:TYR:HA	1:D:192:LEU:HD21	1.87	0.55
1:E:67:ILE:HD12	1:E:211:GLU:HB3	1.86	0.55
2:J:157:ARG:NE	6:J:3097:HOH:O	2.38	0.55
1:E:100:LYS:NZ	6:E:3033:HOH:O	2.38	0.55
1:F:142:ASP:OD2	1:F:147:ARG:NH1	2.37	0.55
2:H:24:ASN:H	2:H:24:ASN:ND2	2.05	0.55
3:O:89:ARG:NH1	3:O:89:ARG:CB	2.63	0.55
3:P:140:ILE:HG23	3:P:193:LYS:HD3	1.88	0.55
1:D:107:VAL:HG13	1:D:143:GLN:CG	2.37	0.55
2:M:17:GLU:C	2:M:18:ARG:HG2	2.32	0.55
3:S:101:GLU:HG3	3:T:105:LEU:CD2	2.37	0.55
3:T:89:ARG:CD	3:U:203:THR:HG21	2.33	0.55
1:E:33:LYS:HB2	3:U:230:VAL:HG11	1.89	0.54
2:K:43:MET:HE3	2:K:56:VAL:HG22	1.89	0.54
2:M:18:ARG:NH1	2:M:174:ASP:OD2	2.40	0.54
2:I:172:MET:HE2	2:I:189:THR:HG23	1.89	0.54
2:I:30:ASN:CG	6:I:3038:HOH:O	2.50	0.54
2:M:1:THR:HB	4:M:3010:SO4:O3	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:172:MET:HE3	2:N:172:MET:HA	1.90	0.54
1:B:62:ASN:N	1:B:62:ASN:ND2	2.43	0.54
1:E:209:ALA:HA	1:E:233:LEU:HD11	1.88	0.54
1:F:71:ASP:HA	2:L:68:LEU:HD21	1.89	0.54
1:A:63:SER:HB2	1:G:159:GLU:OE1	2.07	0.54
1:C:61:GLN:O	1:C:63:SER:N	2.38	0.54
1:F:13:THR:HG21	1:F:126:TYR:C	2.32	0.54
3:P:24:VAL:HG13	3:P:84:GLN:HB3	1.90	0.54
3:R:28:TRP:HA	3:R:32:THR:HB	1.89	0.54
3:U:89:ARG:HD3	3:U:117:ILE:HG22	1.89	0.54
1:A:12:ILE:N	6:A:3074:HOH:O	2.40	0.54
1:A:175:PHE:CZ	1:A:179:GLU:HG3	2.43	0.54
6:Q:274:HOH:O	3:R:18:GLU:HG2	2.07	0.54
3:O:11:ASN:O	3:O:15:SER:HB3	2.08	0.54
3:O:133:SER:N	3:P:133:SER:O	2.39	0.54
1:F:12:ILE:HG13	1:F:13:THR:CG2	2.38	0.53
3:O:65:GLU:HA	3:O:68:LEU:HD12	1.89	0.53
3:U:75:GLN:HG3	3:U:142:MET:O	2.08	0.53
3:O:73:ARG:CD	6:O:247:HOH:O	2.55	0.53
1:D:126:TYR:HH	1:E:123:TYR:HH	1.56	0.53
3:T:89:ARG:NH1	3:T:118:ASP:OD1	2.38	0.53
1:C:222:ARG:HH11	1:C:222:ARG:HB2	1.74	0.53
3:O:51:ARG:NH2	3:U:76:ASP:OD1	2.41	0.53
2:I:94:PRO:HG2	2:I:96[A]:MET:HE3	1.90	0.53
3:Q:75:GLN:HG3	3:Q:142:MET:O	2.08	0.53
3:Q:181:LEU:O	3:Q:184:ARG:HB3	2.09	0.53
3:S:101:GLU:HG3	3:T:105:LEU:HD22	1.91	0.52
1:C:13:THR:O	1:D:130:ARG:CB	2.47	0.52
1:F:55:ARG:O	1:F:56:SER:CB	2.56	0.52
2:H:37:ILE:HG21	2:H:43:MET:HE2	1.90	0.52
2:K:18:ARG:HD3	2:K:174:ASP:OD2	2.10	0.52
2:N:37:ILE:HG21	2:N:43:MET:HE2	1.92	0.52
1:E:156:THR:HG23	1:F:82:VAL:CG2	2.40	0.52
3:Q:50:ILE:HD13	3:Q:187:ASP:HB3	1.91	0.52
1:F:12:ILE:HA	1:F:23:GLN:CG	2.39	0.52
2:H:172:MET:HE2	2:H:189:THR:HG23	1.92	0.52
2:M:82:LEU:HG	2:M:86:MET:CE	2.39	0.52
3:R:82:TYR:CD2	3:S:196:LEU:HD22	2.45	0.52
1:D:12:ILE:CD1	1:D:13:THR:HG22	2.40	0.52
2:J:52:ALA:O	2:J:56:VAL:HG23	2.09	0.52
1:C:208:LYS:O	1:C:209:ALA:CB	2.57	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:32:LYS:HE3	6:N:3047:HOH:O	2.09	0.52
1:A:61:GLN:O	1:A:62:ASN:CB	2.57	0.52
3:P:97:PRO:HG3	3:P:222:PRO:HG2	1.92	0.52
3:T:65:GLU:HA	3:T:68:LEU:HD12	1.92	0.52
6:F:3054:HOH:O	1:G:64:ILE:HG23	2.10	0.51
3:Q:101:GLU:HG3	3:R:105:LEU:CD2	2.41	0.51
3:P:28:TRP:HB3	3:P:209:ILE:HD11	1.92	0.51
2:J:18:ARG:NH2	2:J:30:ASN:HD21	2.08	0.51
1:B:173:VAL:O	1:B:177:GLU:HG3	2.10	0.51
1:D:203:GLU:N	1:D:203:GLU:CD	2.69	0.51
2:K:80:ALA:O	2:K:84:SER:HB3	2.10	0.51
3:R:56:GLY:H	3:R:59:GLN:NE2	2.07	0.51
1:E:61:GLN:O	1:E:62:ASN:C	2.53	0.51
1:D:107:VAL:HG13	1:D:143:GLN:HG3	1.93	0.51
1:G:71:ASP:HB2	2:M:64:GLU:OE2	2.11	0.51
3:S:101:GLU:CG	3:T:105:LEU:HD22	2.41	0.51
1:A:65:GLU:HB3	4:A:3007:SO4:O4	2.11	0.51
2:I:163:LYS:HZ1	2:I:203:LEU:HB3	1.76	0.51
2:L:24:ASN:H	2:L:24:ASN:HD22	1.59	0.51
2:M:18:ARG:HD2	2:M:31:GLY:O	2.11	0.51
3:O:36:ILE:HG23	3:O:198:THR:HB	1.93	0.51
1:E:201:LEU:O	1:E:202:GLU:CB	2.53	0.51
3:R:144:ALA:O	3:R:147:GLU:HB2	2.11	0.51
3:S:61:GLU:C	3:T:177:PRO:HG3	2.36	0.51
2:J:45:ILE:HB	2:J:52:ALA:HB1	1.93	0.50
3:S:129:GLU:HG3	3:T:138:THR:O	2.11	0.50
3:T:160:LEU:O	3:T:161:GLY:C	2.51	0.50
1:A:13:THR:O	1:B:130:ARG:CB	2.57	0.50
1:A:76:ALA:HA	1:A:137:ILE:O	2.11	0.50
1:C:61:GLN:C	1:C:63:SER:N	2.69	0.50
1:D:152:ASP:HB2	1:D:153:PRO:HD2	1.92	0.50
1:E:77:VAL:HG12	1:E:137:ILE:HB	1.92	0.50
1:A:12:ILE:HB	6:A:3031:HOH:O	2.10	0.50
1:E:64:ILE:HA	6:E:3065:HOH:O	2.10	0.50
2:I:80:ALA:O	2:I:84:SER:HB3	2.10	0.50
2:M:24:ASN:HD22	2:M:24:ASN:H	1.59	0.50
1:G:41:LYS:NZ	6:G:3055:HOH:O	2.44	0.50
2:I:163:LYS:HZ3	2:I:203:LEU:HB3	1.75	0.50
2:M:59:MET:HE3	2:M:86:MET:HE1	1.93	0.50
1:A:33:LYS:HB2	3:Q:230:VAL:HG11	1.94	0.50
2:M:82:LEU:HG	2:M:86:MET:HE2	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:R:9:ILE:HD11	3:S:213:LEU:HB2	1.93	0.50
3:U:184:ARG:NH1	3:U:184:ARG:CG	2.57	0.50
1:B:13:THR:HG21	1:B:126:TYR:C	2.36	0.50
1:D:12:ILE:HD12	1:D:12:ILE:O	2.12	0.50
2:K:45:ILE:HB	2:K:52:ALA:HB1	1.93	0.50
1:A:13:THR:O	1:B:130:ARG:HD3	2.12	0.50
1:D:71:ASP:HB2	2:J:64:GLU:OE2	2.12	0.50
1:G:55:ARG:O	1:G:56:SER:CB	2.60	0.50
2:L:62:GLU:HG2	2:L:82:LEU:HD21	1.93	0.50
3:S:28:TRP:HA	3:S:32:THR:HB	1.93	0.50
2:I:87:LEU:HD23	2:I:95:TYR:CD1	2.47	0.49
2:L:45:ILE:HB	2:L:52:ALA:HB1	1.93	0.49
1:C:28:ARG:HH22	3:T:229:MET:CG	2.25	0.49
1:D:203:GLU:CD	1:D:203:GLU:H	2.19	0.49
3:Q:64:PRO:HB2	3:Q:67:LEU:HG	1.94	0.49
1:A:212:ILE:HD12	1:A:229:VAL:HG22	1.93	0.49
3:U:36:ILE:HG23	3:U:198:THR:HB	1.94	0.49
3:U:225:GLY:HA3	6:U:290:HOH:O	2.11	0.49
1:A:50:SER:OG	1:A:66:LYS:HG2	2.13	0.49
2:M:2:THR:OG1	2:M:130:GLY:HA3	2.13	0.49
1:D:71:ASP:HA	2:J:68:LEU:HD21	1.94	0.49
2:K:18:ARG:HD2	6:K:3054:HOH:O	2.12	0.49
3:O:140:ILE:CD1	3:O:144:ALA:HB1	2.43	0.49
3:R:116:ILE:O	3:R:204:MET:HE3	2.12	0.49
1:F:55:ARG:O	1:F:56:SER:HB2	2.12	0.49
2:I:24:ASN:H	2:I:24:ASN:HD22	1.61	0.49
2:K:172:MET:HE1	2:K:192:ILE:CG2	2.43	0.49
1:C:55:ARG:HA	1:C:55:ARG:NH1	2.28	0.49
1:C:209:ALA:HB2	1:C:233:LEU:HD11	1.94	0.49
1:F:12:ILE:HG23	6:F:3039:HOH:O	2.13	0.49
2:J:14:MET:HE2	2:J:44:THR:HG23	1.94	0.49
3:Q:90:THR:O	3:Q:94:ILE:HG12	2.12	0.49
1:B:12:ILE:CG1	1:B:13:THR:HG23	2.38	0.48
2:I:45:ILE:HB	2:I:52:ALA:HB1	1.94	0.48
2:N:163:LYS:NZ	2:N:203:LEU:CB	2.76	0.48
2:H:124:TYR:CD1	2:H:138:LEU:HD13	2.48	0.48
2:K:51:ASP:OD1	2:L:91:LYS:HE2	2.13	0.48
1:B:230:LYS:C	1:B:232:PHE:H	2.20	0.48
1:A:21:LEU:HD12	3:R:229:MET:CE	2.43	0.48
1:E:210:PRO:HD2	1:E:229:VAL:CG1	2.43	0.48
2:N:174:ASP:CG	6:N:3129:HOH:O	2.57	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:202:ILE:HD13	2:J:202:ILE:H	1.79	0.48
2:M:32:LYS:HE3	2:M:35:PHE:CE1	2.48	0.48
2:N:18:ARG:HG3	2:N:172:MET:O	2.14	0.48
1:E:65:GLU:O	1:E:68:GLN:NE2	2.46	0.48
1:B:198:LYS:HA	1:B:201:LEU:HD22	1.95	0.48
1:F:176:LEU:O	1:F:180:TYR:CB	2.62	0.48
1:F:176:LEU:O	1:F:180:TYR:HB2	2.14	0.48
1:C:209:ALA:CA	1:C:233:LEU:HD11	2.44	0.48
1:E:83:ALA:HB3	6:E:3026:HOH:O	2.14	0.48
1:F:12:ILE:HD12	1:F:12:ILE:O	2.14	0.48
2:K:163:LYS:HB3	2:K:203:LEU:HD22	1.96	0.48
1:A:63:SER:CB	1:G:159:GLU:OE1	2.62	0.48
1:G:180:TYR:HA	1:G:192:LEU:HD21	1.95	0.48
2:M:74:MET:HG2	2:M:78:ALA:HB3	1.96	0.48
3:U:4:LYS:HA	6:U:289:HOH:O	2.14	0.48
2:J:172:MET:HE3	6:J:3093:HOH:O	2.13	0.47
2:K:9:LYS:HG3	6:K:3029:HOH:O	2.13	0.47
3:T:105:LEU:O	3:T:109:VAL:HG23	2.14	0.47
1:A:187:LYS:HE3	1:A:231:LYS:HZ1	1.79	0.47
2:M:36:GLN:O	2:M:60:LYS:HE2	2.15	0.47
3:Q:120:LEU:HB2	3:Q:204:MET:HE3	1.96	0.47
1:B:110:GLU:HG3	1:B:149:PHE:CE2	2.50	0.47
3:S:140:ILE:HB	3:S:193:LYS:HB3	1.97	0.47
2:L:53:GLN:HB3	5:L:2001:GOL:H12	1.97	0.47
3:O:24:VAL:HG13	3:O:84:GLN:HB3	1.96	0.47
3:Q:140:ILE:HG13	3:Q:144:ALA:HB2	1.95	0.47
3:U:172:GLY:O	3:U:173:GLY:C	2.56	0.47
1:A:18:ASP:HB2	3:R:102:GLU:OE1	2.14	0.47
3:R:140:ILE:HD11	3:R:144:ALA:HB1	1.96	0.47
3:S:124:THR:HG23	3:S:200:HIS:HD2	1.80	0.47
1:B:65:GLU:O	1:B:68:GLN:NE2	2.48	0.47
1:C:24:VAL:HG11	1:C:154:ALA:HB2	1.95	0.47
1:F:209:ALA:HA	1:F:233:LEU:HD11	1.96	0.47
2:I:91:LYS:HE3	2:I:92:TYR:CE1	2.49	0.47
2:I:93:MET:HE1	6:I:3116:HOH:O	2.14	0.47
2:K:37:ILE:HG21	2:K:43:MET:HE2	1.96	0.47
2:M:27:MET:HG2	6:N:3066:HOH:O	2.15	0.47
3:O:177:PRO:HG3	3:U:61:GLU:C	2.40	0.47
3:P:71:LEU:HB2	3:P:145:LEU:HD13	1.97	0.47
3:U:132:GLY:HA3	6:U:264:HOH:O	2.14	0.47
1:G:149:PHE:HA	1:G:158:ASN:O	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:154:ALA:HB1	3:S:229:MET:HE3	1.96	0.47
1:E:66:LYS:HB2	6:E:3062:HOH:O	2.15	0.47
3:O:50:ILE:HD11	3:O:67:LEU:HD21	1.96	0.47
2:I:87:LEU:HD23	2:I:95:TYR:HD1	1.80	0.47
2:L:22:MET:HE1	6:M:3121:HOH:O	2.15	0.47
2:M:163:LYS:NZ	2:M:203:LEU:HB3	2.29	0.47
1:B:180:TYR:HA	1:B:192:LEU:HD21	1.97	0.46
1:D:13:THR:HG21	1:D:126:TYR:O	2.16	0.46
6:E:3038:HOH:O	1:F:12:ILE:HB	2.15	0.46
2:I:14:MET:HE2	2:I:44:THR:HG23	1.97	0.46
1:F:43:ALA:HA	1:F:183:ASN:OD1	2.15	0.46
2:H:82:LEU:O	2:H:86:MET:HG3	2.15	0.46
2:I:152:VAL:O	2:I:156:ILE:HD12	2.14	0.46
2:K:157:ARG:HD2	6:K:3051:HOH:O	2.15	0.46
3:P:89:ARG:NH1	3:P:118:ASP:OD1	2.48	0.46
3:T:86:GLU:OE2	3:T:121:GLU:CD	2.58	0.46
1:A:67:ILE:HG12	1:A:77:VAL:CG1	2.45	0.46
1:A:201:LEU:HD11	1:A:207:LEU:HB2	1.96	0.46
1:B:186:GLU:O	1:B:190:VAL:HG23	2.14	0.46
2:N:59:MET:O	2:N:63:LEU:HG	2.16	0.46
3:S:64:PRO:HB2	3:S:67:LEU:HG	1.98	0.46
1:E:81:LEU:HD23	3:U:230:VAL:CG2	2.46	0.46
2:J:59:MET:CE	2:J:79:VAL:HG13	2.45	0.46
2:K:201:LEU:O	2:K:202:ILE:HG23	2.15	0.46
2:K:203:LEU:HD11	6:K:3097:HOH:O	2.15	0.46
3:O:133:SER:HB3	3:P:133:SER:HB2	1.97	0.46
3:P:82:TYR:CD2	3:Q:196:LEU:HD22	2.50	0.46
6:R:267:HOH:O	3:S:175:GLN:HG3	2.16	0.46
1:D:110:GLU:CD	6:D:3051:HOH:O	2.58	0.46
2:K:24:ASN:H	2:K:24:ASN:ND2	2.14	0.46
1:A:225:ASP:OD2	1:A:227:GLU:HG2	2.15	0.46
1:D:42:PHE:HB2	1:D:184:LEU:O	2.16	0.46
2:N:18:ARG:HB3	2:N:30:ASN:HA	1.96	0.46
3:Q:89:ARG:HD3	3:Q:121:GLU:OE2	2.15	0.46
3:U:64:PRO:HB2	3:U:67:LEU:HG	1.98	0.46
1:B:51:ASP:HB2	1:B:197:LEU:HD11	1.98	0.46
1:B:66:LYS:HB2	1:B:211:GLU:OE2	2.15	0.46
1:C:162:ALA:HB1	1:C:176:LEU:HD13	1.97	0.46
1:C:208:LYS:O	1:C:209:ALA:HB2	2.16	0.46
1:G:152:ASP:HB2	1:G:153:PRO:HD2	1.98	0.46
1:C:55:ARG:HB2	1:C:59:ILE:HG13	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:158:ASN:HB2	1:E:160:TYR:CE1	2.50	0.45
1:F:42:PHE:HB2	1:F:184:LEU:O	2.15	0.45
2:I:43:MET:HE3	2:I:56:VAL:HG22	1.98	0.45
2:M:22:MET:HE3	2:M:27:MET:HE1	1.98	0.45
1:C:61:GLN:OE1	1:C:62:ASN:ND2	2.50	0.45
1:G:158:ASN:HB2	1:G:160:TYR:CE1	2.51	0.45
1:G:185:PRO:HG2	1:G:188:GLU:HB2	1.98	0.45
2:L:191:GLN:O	2:L:195:ARG:HG3	2.16	0.45
1:D:186:GLU:O	1:D:190:VAL:HG23	2.16	0.45
2:H:23:GLU:HB3	2:H:24:ASN:H	1.52	0.45
2:N:163:LYS:NZ	2:N:203:LEU:HB3	2.31	0.45
3:P:28:TRP:CB	3:P:209:ILE:HD11	2.46	0.45
1:D:65:GLU:HG2	4:D:3003:SO4:O4	2.17	0.45
1:G:107:VAL:O	1:G:142:ASP:HB2	2.16	0.45
1:A:12:ILE:HA	1:A:23:GLN:HG3	1.97	0.45
1:E:76:ALA:HA	1:E:137:ILE:O	2.16	0.45
3:P:75:GLN:NE2	6:P:270:HOH:O	2.48	0.45
1:E:24:VAL:HG11	1:E:154:ALA:HB2	1.99	0.45
2:M:22:MET:HB2	2:M:27:MET:SD	2.57	0.45
3:O:68:LEU:HD21	3:O:149:LEU:HD21	1.98	0.45
3:S:142:MET:HE2	3:S:142:MET:HB2	1.46	0.45
1:B:180:TYR:O	1:B:181:LYS:HD2	2.16	0.45
3:P:50:ILE:HD11	3:P:67:LEU:HD21	1.98	0.45
3:S:63:SER:HA	3:S:64:PRO:HD3	1.80	0.45
2:I:172:MET:CE	2:I:192:ILE:HB	2.46	0.45
2:L:163:LYS:HE2	2:L:203:LEU:HD13	1.99	0.45
2:M:98:GLN:HB3	6:M:3107:HOH:O	2.16	0.45
3:S:191:MET:O	3:S:195:GLU:HG3	2.16	0.45
3:T:68:LEU:HD23	3:T:148:TYR:HE2	1.80	0.45
3:T:113:VAL:O	3:T:117:ILE:HG12	2.17	0.45
1:A:61:GLN:O	1:A:62:ASN:HB2	2.15	0.45
1:C:64:ILE:HG22	1:C:64:ILE:O	2.16	0.45
1:D:47:LEU:C	1:D:47:LEU:HD12	2.42	0.45
1:D:76:ALA:HA	1:D:137:ILE:O	2.17	0.45
2:L:43:MET:HE1	2:L:56:VAL:HA	1.98	0.45
2:L:70:ARG:NH1	4:L:3019:SO4:O1	2.49	0.45
2:M:163:LYS:HZ1	2:M:203:LEU:HB3	1.82	0.45
1:A:51:ASP:HB2	1:A:197:LEU:HD11	1.98	0.45
1:B:71:ASP:HA	2:H:68:LEU:HD21	1.99	0.45
1:E:36:THR:HA	1:E:165:ILE:O	2.17	0.45
1:G:13:THR:HG21	1:G:126:TYR:C	2.42	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:O:80:ASN:O	3:O:84:GLN:HG3	2.17	0.45
1:B:64:ILE:HG22	1:B:64:ILE:O	2.17	0.44
3:T:116:ILE:O	3:T:204:MET:CE	2.65	0.44
1:A:28:ARG:HH22	3:R:229:MET:CG	2.30	0.44
1:B:141:ILE:HD12	1:B:215:ILE:HG12	1.99	0.44
1:E:47:LEU:HD12	1:E:47:LEU:C	2.41	0.44
1:G:56:SER:C	1:G:58:LEU:H	2.25	0.44
1:G:168:GLY:O	1:G:172:VAL:HG23	2.17	0.44
2:L:17:GLU:HB2	2:L:170:GLY:O	2.17	0.44
3:T:140:ILE:HG12	3:T:144:ALA:HB2	1.98	0.44
1:A:107:VAL:O	1:A:143:GLN:HG2	2.17	0.44
1:C:28:ARG:HH22	3:T:229:MET:HG3	1.82	0.44
2:I:17:GLU:HB2	2:I:170:GLY:O	2.18	0.44
2:K:187:LEU:HA	2:K:188:PRO:HD3	1.87	0.44
2:K:196:ILE:HG23	2:K:201:LEU:HB2	1.98	0.44
2:K:203:LEU:HD21	6:K:3097:HOH:O	2.17	0.44
3:T:18:GLU:OE1	3:T:212:TYR:OH	2.28	0.44
1:C:109:ILE:HG13	1:C:142:ASP:HB3	1.98	0.44
1:D:152:ASP:HB2	1:D:153:PRO:CD	2.48	0.44
1:E:109:ILE:HG13	1:E:142:ASP:HB3	1.99	0.44
2:H:163:LYS:NZ	2:H:171:GLY:O	2.51	0.44
2:H:171:GLY:H	2:H:203:LEU:HD13	1.82	0.44
2:N:45:ILE:HB	2:N:52:ALA:HB1	1.99	0.44
2:N:172:MET:HE1	2:N:196:ILE:CD1	2.47	0.44
3:T:86:GLU:OE2	3:T:121:GLU:OE2	2.35	0.44
1:B:18:ASP:HB2	3:S:102:GLU:OE1	2.17	0.44
3:O:140:ILE:HB	3:O:193:LYS:HB3	1.98	0.44
1:D:141:ILE:HD13	1:D:146:PRO:HA	1.99	0.44
1:F:164:ALA:O	1:F:169:LYS:HG3	2.18	0.44
3:Q:89:ARG:CG	3:Q:117:ILE:HG21	2.48	0.44
3:T:140:ILE:HG22	3:T:197:ALA:HB2	1.99	0.44
1:E:61:GLN:HE21	1:E:62:ASN:H	1.62	0.44
2:I:18:ARG:HG3	2:I:172:MET:O	2.18	0.44
2:L:3:THR:HB	2:L:16:THR:HG22	2.00	0.44
2:H:13:ILE:HG12	2:H:177:VAL:HG22	1.99	0.44
2:K:18:ARG:CD	6:K:3054:HOH:O	2.65	0.44
2:L:131:SER:N	2:L:132:PRO:HD2	2.33	0.44
1:A:71:ASP:HA	2:N:68:LEU:HD21	2.00	0.43
1:B:52:LYS:HB2	6:B:3033:HOH:O	2.18	0.43
2:J:74:MET:HG2	2:J:78:ALA:HB3	1.99	0.43
2:N:43:MET:HE1	2:N:56:VAL:HA	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Q:101:GLU:HG3	3:R:105:LEU:HD22	2.00	0.43
3:S:75:GLN:HG3	3:S:142:MET:O	2.18	0.43
2:I:91:LYS:HD2	6:I:3093:HOH:O	2.16	0.43
2:K:172:MET:HE3	2:K:173:ILE:O	2.17	0.43
3:T:82:TYR:OH	3:U:200:HIS:HB2	2.18	0.43
1:B:38:LEU:C	1:B:38:LEU:HD12	2.43	0.43
2:H:51:ASP:CG	2:I:91:LYS:HZ3	2.26	0.43
2:M:43:MET:HA	2:M:100:LEU:O	2.18	0.43
3:P:89:ARG:HD3	3:P:121:GLU:OE2	2.18	0.43
2:I:157:ARG:HE	2:I:199:LEU:HD22	1.82	0.43
2:L:18:ARG:HB3	2:L:30:ASN:HA	2.00	0.43
2:M:184:TYR:CD1	2:M:184:TYR:C	2.96	0.43
3:Q:125:LEU:O	3:Q:126:GLY:C	2.61	0.43
1:B:194:ILE:HD11	1:B:212:ILE:HD11	2.00	0.43
1:E:201:LEU:HD12	1:E:201:LEU:HA	1.79	0.43
2:I:172:MET:HE1	2:I:192:ILE:HB	2.01	0.43
3:O:64:PRO:HB2	3:O:67:LEU:HG	2.01	0.43
3:R:117:ILE:O	3:R:121:GLU:HG3	2.18	0.43
1:C:122:GLN:HG3	6:C:3065:HOH:O	2.18	0.43
2:L:40:TYR:CD1	2:L:183:GLY:HA2	2.54	0.43
3:Q:101:GLU:CG	3:R:105:LEU:HD22	2.49	0.43
1:D:106:LEU:C	1:D:106:LEU:HD23	2.44	0.43
1:E:222:ARG:HH12	1:E:228:GLU:CD	2.18	0.43
2:K:43:MET:HE1	2:K:56:VAL:HA	2.00	0.43
3:Q:155:VAL:HG12	3:Q:183:LEU:HD13	1.99	0.43
2:K:43:MET:CE	2:K:56:VAL:HG22	2.49	0.43
3:R:158:LYS:HB3	3:R:179:LEU:HD21	2.00	0.43
3:U:184:ARG:O	3:U:184:ARG:HG3	2.16	0.43
2:L:59:MET:CE	2:L:79:VAL:HG13	2.48	0.43
3:Q:28:TRP:HA	3:Q:32:THR:HB	2.01	0.43
3:S:136:ALA:HA	3:S:137:PRO:HD3	1.84	0.43
1:D:12:ILE:HD13	1:D:131:PRO:HD3	1.99	0.42
1:G:55:ARG:O	1:G:56:SER:HB3	2.19	0.42
2:H:3:THR:HB	2:H:16:THR:HG22	2.01	0.42
2:L:86:MET:HE2	2:L:86:MET:HB3	1.92	0.42
1:A:17:PRO:HA	1:B:26:TYR:CD2	2.54	0.42
1:E:81:LEU:HD23	3:U:230:VAL:HG23	2.00	0.42
1:F:175:PHE:CZ	1:F:195:LYS:HB3	2.54	0.42
2:M:40:TYR:HD1	2:M:183:GLY:HA2	1.83	0.42
1:C:230:LYS:C	1:C:232:PHE:H	2.27	0.42
1:E:12:ILE:HB	1:E:23:GLN:HG3	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:O:63:SER:HA	3:O:64:PRO:HD3	1.87	0.42
3:O:89:ARG:NH1	3:P:203:THR:HG21	2.34	0.42
1:B:52:LYS:HA	1:B:52:LYS:HE2	2.02	0.42
1:D:185:PRO:HD2	1:D:188:GLU:HG3	2.02	0.42
1:E:13:THR:HG21	1:E:126:TYR:C	2.43	0.42
1:G:152:ASP:HB2	1:G:153:PRO:CD	2.50	0.42
1:G:225:ASP:OD1	1:G:227:GLU:HG3	2.18	0.42
2:K:187:LEU:HB2	2:K:192:ILE:HD11	2.02	0.42
4:N:3021:SO4:O1	6:N:3128:HOH:O	2.21	0.42
1:B:154:ALA:CB	3:S:229:MET:HE3	2.49	0.42
1:F:12:ILE:HG12	1:F:129:VAL:O	2.20	0.42
1:F:90:ASP:O	1:F:94:ILE:HG12	2.20	0.42
1:F:97:GLN:OE1	1:F:97:GLN:HA	2.18	0.42
1:G:209:ALA:HA	1:G:210:PRO:HD2	1.95	0.42
2:L:2:THR:OG1	2:L:130:GLY:HA3	2.19	0.42
2:L:157:ARG:HE	2:L:199:LEU:HD22	1.83	0.42
3:R:184:ARG:NH1	3:R:184:ARG:CG	2.82	0.42
3:U:225:GLY:CA	6:U:290:HOH:O	2.67	0.42
1:A:143:GLN:CG	6:A:3017:HOH:O	2.67	0.42
1:B:158:ASN:HB2	1:B:160:TYR:CE1	2.55	0.42
1:C:61:GLN:CD	1:C:61:GLN:N	2.58	0.42
1:G:222:ARG:HH12	1:G:228:GLU:CD	2.26	0.42
2:H:2:THR:OG1	2:H:130:GLY:HA3	2.19	0.42
1:A:107:VAL:HG22	1:A:143:GLN:HE21	1.84	0.42
1:B:13:THR:HB	1:C:130:ARG:HG2	2.00	0.42
1:D:70:ILE:HG21	1:D:112:LEU:HD21	2.00	0.42
1:E:96:ALA:O	1:E:100:LYS:HG3	2.19	0.42
1:F:150:ASP:C	1:F:150:ASP:OD1	2.62	0.42
2:N:74:MET:HG2	2:N:78:ALA:HB3	2.01	0.42
3:R:221:GLN:CG	6:R:289:HOH:O	2.62	0.42
1:G:76:ALA:HA	1:G:137:ILE:O	2.20	0.42
2:H:43:MET:HE1	2:H:56:VAL:HA	2.02	0.42
2:N:195:ARG:HG2	2:N:198:LYS:HE3	2.02	0.42
3:S:63:SER:OG	3:T:181:LEU:HD12	2.19	0.42
1:A:67:ILE:HG12	1:A:77:VAL:HG13	2.00	0.42
1:F:158:ASN:HB2	1:F:160:TYR:CE1	2.54	0.42
3:O:62:LYS:HE3	3:O:62:LYS:HB2	1.77	0.42
1:C:71:ASP:HA	2:I:68:LEU:HD21	2.01	0.42
1:C:139:ALA:HA	1:C:147:ARG:O	2.20	0.42
3:Q:87:THR:O	3:Q:91:VAL:HG23	2.20	0.42
3:T:9:ILE:HD11	3:U:213:LEU:HB2	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:64:ILE:O	1:D:64:ILE:HG22	2.20	0.41
1:D:175:PHE:HZ	1:D:195:LYS:HD3	1.85	0.41
1:E:172:VAL:HG13	1:E:196:ALA:HB1	2.02	0.41
2:K:24:ASN:HB3	6:K:3095:HOH:O	2.19	0.41
2:L:57:ARG:HG3	5:L:2001:GOL:H2	2.01	0.41
3:O:89:ARG:HH12	3:P:203:THR:HG21	1.84	0.41
1:B:40:MET:HE2	1:B:40:MET:HB3	1.97	0.41
1:C:62:ASN:H	1:C:62:ASN:HD22	1.67	0.41
2:K:172:MET:CE	2:K:192:ILE:CG2	2.98	0.41
3:O:138:THR:HA	3:O:139:PRO:HD3	1.97	0.41
3:Q:56:GLY:H	3:Q:59:GLN:HE21	1.67	0.41
3:Q:130:LYS:O	3:R:136:ALA:N	2.43	0.41
1:B:52:LYS:CB	6:B:3033:HOH:O	2.67	0.41
1:E:12:ILE:HA	1:E:23:GLN:CG	2.49	0.41
3:T:56:GLY:H	3:T:59:GLN:NE2	2.18	0.41
3:T:75:GLN:HG3	3:T:142:MET:O	2.20	0.41
3:T:101:GLU:HG3	3:U:105:LEU:HD22	2.02	0.41
3:U:36:ILE:HG13	3:U:77:LEU:HD11	2.02	0.41
1:D:107:VAL:HG13	1:D:143:GLN:HG2	2.02	0.41
1:F:201:LEU:O	1:F:202:GLU:C	2.64	0.41
2:K:113:ILE:HA	2:K:118:GLY:O	2.20	0.41
2:L:113:ILE:HA	2:L:118:GLY:O	2.20	0.41
2:N:113:ILE:HA	2:N:118:GLY:O	2.21	0.41
3:O:152:ARG:NH1	3:O:156:GLU:OE2	2.50	0.41
3:U:149:LEU:O	3:U:153:SER:HB2	2.20	0.41
1:A:66:LYS:HE2	1:A:78:THR:H	1.86	0.41
1:C:12:ILE:HD13	1:C:131:PRO:HD3	2.03	0.41
1:D:83:ALA:HB3	6:D:3009:HOH:O	2.20	0.41
1:E:173:VAL:O	1:E:177:GLU:HG3	2.20	0.41
1:E:201:LEU:O	1:E:205:GLU:OE1	2.39	0.41
2:H:66:TYR:CD2	2:H:74:MET:HE2	2.55	0.41
2:H:172:MET:HE3	2:H:192:ILE:HG21	2.02	0.41
2:J:163:LYS:NZ	2:J:203:LEU:HB3	2.36	0.41
2:M:141:GLN:OE1	2:M:157:ARG:NH2	2.53	0.41
3:R:142:MET:HE2	3:R:142:MET:HB2	1.75	0.41
1:C:17:PRO:HB3	3:U:105:LEU:HD11	2.03	0.41
1:F:160:TYR:CE2	1:G:59:ILE:HD13	2.56	0.41
2:M:58[A]:TYR:CE2	2:M:59:MET:CE	3.03	0.41
3:Q:116:ILE:HG12	3:Q:208:VAL:HG22	2.02	0.41
1:C:175:PHE:CZ	1:C:179:GLU:HG3	2.56	0.41
2:K:157:ARG:CD	6:K:3051:HOH:O	2.67	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:24:ASN:H	2:M:24:ASN:ND2	2.18	0.41
3:Q:142:MET:HE2	3:Q:142:MET:HB2	1.90	0.41
3:S:159:LEU:O	3:S:173:GLY:HA3	2.21	0.41
3:S:202:SER:O	3:S:206:ARG:HG3	2.20	0.41
2:H:19:ARG:HD3	2:H:26:ILE:HG12	2.03	0.41
2:K:143:SER:HB3	2:K:146:MET:HG3	2.01	0.41
3:U:9:ILE:O	3:U:12:LEU:HB2	2.21	0.41
1:A:69:LEU:HD23	1:A:75:ALA:HB2	2.03	0.41
1:D:73:TYR:O	1:D:140:GLY:HA3	2.20	0.41
3:P:51:ARG:O	3:P:184:ARG:NH2	2.54	0.41
3:P:146:ARG:HD3	6:P:259:HOH:O	2.20	0.41
3:R:159:LEU:O	3:R:173:GLY:HA3	2.20	0.41
3:T:140:ILE:HB	3:T:193:LYS:HB3	2.03	0.41
3:U:90:THR:O	3:U:94:ILE:HG12	2.21	0.41
1:E:12:ILE:HA	1:E:23:GLN:HG3	2.03	0.41
1:E:107:VAL:O	1:E:142:ASP:HB2	2.21	0.41
3:P:101:GLU:HG3	3:Q:105:LEU:CD2	2.51	0.41
1:A:143:GLN:HB3	6:A:3017:HOH:O	2.20	0.40
3:P:89:ARG:HH11	3:P:89:ARG:HD2	1.75	0.40
3:R:191:MET:O	3:R:195:GLU:HG3	2.21	0.40
3:S:77:LEU:O	3:S:77:LEU:HG	2.15	0.40
1:E:21:LEU:HD12	3:O:229:MET:HE1	2.03	0.40
2:N:202:ILE:CG1	2:N:203:LEU:N	2.82	0.40
3:Q:116:ILE:HG13	3:Q:204:MET:HE1	2.02	0.40
1:C:175:PHE:CD1	1:C:175:PHE:C	2.99	0.40
1:D:54:VAL:HG13	1:D:61:GLN:NE2	2.37	0.40
2:K:32:LYS:HE2	6:K:3092:HOH:O	2.21	0.40
2:M:14:MET:HE2	2:M:44:THR:HG23	2.03	0.40
2:N:14:MET:HE2	2:N:44:THR:HG23	2.03	0.40
2:N:202:ILE:CD1	2:N:203:LEU:H	2.34	0.40
3:O:77:LEU:C	3:O:77:LEU:HD13	2.46	0.40
3:R:10:GLN:NE2	3:R:14:ASP:OD1	2.48	0.40
3:S:89:ARG:HD3	3:S:117:ILE:HG22	2.03	0.40
1:E:208:LYS:CD	1:E:208:LYS:N	2.55	0.40
2:J:172:MET:CE	2:J:173:ILE:H	2.34	0.40
2:M:22:MET:HE3	2:M:27:MET:CE	2.52	0.40
3:S:24:VAL:HG13	3:S:84:GLN:HB3	2.04	0.40
3:T:39:ILE:HD13	3:T:74:TYR:HA	2.03	0.40
2:M:83:LEU:HA	2:M:86:MET:HE3	2.03	0.40
3:P:61:GLU:C	3:Q:177:PRO:HG3	2.47	0.40
3:T:116:ILE:O	3:T:204:MET:HE2	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:U:140:ILE:CD1	3:U:144:ALA:HB1	2.52	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	220/233 (94%)	208 (94%)	6 (3%)	6 (3%)	4	4
1	B	220/233 (94%)	204 (93%)	13 (6%)	3 (1%)	9	13
1	C	220/233 (94%)	211 (96%)	5 (2%)	4 (2%)	6	9
1	D	220/233 (94%)	202 (92%)	16 (7%)	2 (1%)	14	22
1	E	220/233 (94%)	210 (96%)	8 (4%)	2 (1%)	14	22
1	F	220/233 (94%)	206 (94%)	11 (5%)	3 (1%)	9	13
1	G	220/233 (94%)	205 (93%)	10 (4%)	5 (2%)	5	6
2	H	203/217 (94%)	195 (96%)	8 (4%)	0	100	100
2	I	203/217 (94%)	196 (97%)	7 (3%)	0	100	100
2	J	203/217 (94%)	194 (96%)	9 (4%)	0	100	100
2	K	202/217 (93%)	196 (97%)	6 (3%)	0	100	100
2	L	202/217 (93%)	197 (98%)	4 (2%)	1 (0%)	24	37
2	M	203/217 (94%)	196 (97%)	7 (3%)	0	100	100
2	N	203/217 (94%)	195 (96%)	7 (3%)	1 (0%)	24	37
3	O	214/237 (90%)	208 (97%)	6 (3%)	0	100	100
3	P	214/237 (90%)	209 (98%)	4 (2%)	1 (0%)	24	37
3	Q	214/237 (90%)	206 (96%)	8 (4%)	0	100	100
3	R	214/237 (90%)	206 (96%)	8 (4%)	0	100	100
3	S	214/237 (90%)	206 (96%)	8 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	T	214/237 (90%)	208 (97%)	6 (3%)	0	100	100
3	U	214/237 (90%)	208 (97%)	5 (2%)	1 (0%)	24	37
All	All	4457/4809 (93%)	4266 (96%)	162 (4%)	29 (1%)	18	28

All (29) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	226	GLN
1	C	62	ASN
1	C	209	ALA
1	D	54	VAL
1	D	56	SER
1	F	56	SER
1	F	202	GLU
1	G	182	GLU
1	A	62	ASN
1	B	231	LYS
1	E	202	GLU
1	E	203	GLU
1	G	56	SER
2	N	202	ILE
3	U	173	GLY
1	A	55	ARG
1	B	62	ASN
1	G	65	GLU
3	P	226	SER
1	B	56	SER
1	A	109	ILE
1	C	231	LYS
1	A	67	ILE
2	L	202	ILE
1	A	64	ILE
1	G	209	ALA
1	F	64	ILE
1	G	64	ILE
1	C	64	ILE

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	185/191 (97%)	162 (88%)	23 (12%)	4	6
1	B	185/191 (97%)	170 (92%)	15 (8%)	11	18
1	C	185/191 (97%)	171 (92%)	14 (8%)	12	21
1	D	185/191 (97%)	171 (92%)	14 (8%)	12	21
1	E	185/191 (97%)	168 (91%)	17 (9%)	8	14
1	F	185/191 (97%)	174 (94%)	11 (6%)	18	31
1	G	185/191 (97%)	172 (93%)	13 (7%)	14	24
2	H	172/183 (94%)	161 (94%)	11 (6%)	16	28
2	I	172/183 (94%)	158 (92%)	14 (8%)	11	18
2	J	172/183 (94%)	152 (88%)	20 (12%)	5	8
2	K	171/183 (93%)	160 (94%)	11 (6%)	16	28
2	L	171/183 (93%)	154 (90%)	17 (10%)	7	11
2	M	172/183 (94%)	161 (94%)	11 (6%)	16	28
2	N	172/183 (94%)	158 (92%)	14 (8%)	11	18
3	O	179/196 (91%)	168 (94%)	11 (6%)	17	30
3	P	179/196 (91%)	171 (96%)	8 (4%)	24	42
3	Q	179/196 (91%)	170 (95%)	9 (5%)	22	38
3	R	179/196 (91%)	171 (96%)	8 (4%)	24	42
3	S	179/196 (91%)	174 (97%)	5 (3%)	38	60
3	T	179/196 (91%)	170 (95%)	9 (5%)	22	38
3	U	179/196 (91%)	172 (96%)	7 (4%)	28	48
All	All	3750/3990 (94%)	3488 (93%)	262 (7%)	14	24

All (262) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	12	ILE
1	A	14	VAL
1	A	35	SER
1	A	52	LYS
1	A	53	LYS

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Mol	Chain	Res	Type
1	A	56	SER
1	A	59	ILE
1	A	61	GLN
1	A	64	ILE
1	A	65	GLU
1	A	66	LYS
1	A	77	VAL
1	A	106	LEU
1	A	129	VAL
1	A	141	ILE
1	A	157	ILE
1	A	177	GLU
1	A	181	LYS
1	A	182	GLU
1	A	202	GLU
1	A	203	GLU
1	A	226	GLN
1	A	230	LYS
1	B	12	ILE
1	B	14	VAL
1	B	52	LYS
1	B	53	LYS
1	B	54	VAL
1	B	61	GLN
1	B	62	ASN
1	B	65	GLU
1	B	87	VAL
1	B	88	LEU
1	B	129	VAL
1	B	135	SER
1	B	201	LEU
1	B	202	GLU
1	B	223	ILE
1	C	12	ILE
1	C	14	VAL
1	C	55	ARG
1	C	59	ILE
1	C	61	GLN
1	C	62	ASN
1	C	63	SER
1	C	141	ILE
1	C	177	GLU

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Mol	Chain	Res	Type
1	C	182	GLU
1	C	202	GLU
1	C	208	LYS
1	C	222	ARG
1	C	230	LYS
1	D	12	ILE
1	D	65	GLU
1	D	143	GLN
1	D	157	ILE
1	D	174	SER
1	D	179	GLU
1	D	181	LYS
1	D	182	GLU
1	D	187	LYS
1	D	203	GLU
1	D	212	ILE
1	D	226	GLN
1	D	227	GLU
1	D	233	LEU
1	E	12	ILE
1	E	13	THR
1	E	14	VAL
1	E	35	SER
1	E	47	LEU
1	E	54	VAL
1	E	61	GLN
1	E	63	SER
1	E	64	ILE
1	E	66	LYS
1	E	106	LEU
1	E	153	PRO
1	E	157	ILE
1	E	188	GLU
1	E	201	LEU
1	E	208	LYS
1	E	211	GLU
1	F	12	ILE
1	F	14	VAL
1	F	52	LYS
1	F	55	ARG
1	F	62	ASN
1	F	157	ILE

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Mol	Chain	Res	Type
1	F	188	GLU
1	F	202	GLU
1	F	203	GLU
1	F	227	GLU
1	F	231	LYS
1	G	12	ILE
1	G	14	VAL
1	G	44	ASN
1	G	54	VAL
1	G	65	GLU
1	G	135	SER
1	G	144	ILE
1	G	176	LEU
1	G	202	GLU
1	G	221	TYR
1	G	225	ASP
1	G	226	GLN
1	G	230	LYS
2	H	3	THR
2	H	17	GLU
2	H	30	ASN
2	H	68	LEU
2	H	91	LYS
2	H	112	SER
2	H	144	GLU
2	H	174	ASP
2	H	190	ASP
2	H	202	ILE
2	H	203	LEU
2	I	4	VAL
2	I	9	LYS
2	I	17	GLU
2	I	23	GLU
2	I	68	LEU
2	I	84	SER
2	I	104	ILE
2	I	105	ASP
2	I	112	SER
2	I	144	GLU
2	I	174	ASP
2	I	185	VAL
2	I	202	ILE

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Mol	Chain	Res	Type
2	I	203	LEU
2	J	3	THR
2	J	9	LYS
2	J	17	GLU
2	J	18	ARG
2	J	22	MET
2	J	23	GLU
2	J	24	ASN
2	J	68	LEU
2	J	71	ARG
2	J	105	ASP
2	J	123	ILE
2	J	144	GLU
2	J	174	ASP
2	J	180	ARG
2	J	186	GLN
2	J	190	ASP
2	J	197	ARG
2	J	198	LYS
2	J	202	ILE
2	J	203	LEU
2	K	3	THR
2	K	17	GLU
2	K	27	MET
2	K	68	LEU
2	K	84	SER
2	K	104	ILE
2	K	105	ASP
2	K	144	GLU
2	K	181	LYS
2	K	186	GLN
2	K	203	LEU
2	L	3	THR
2	L	9	LYS
2	L	17	GLU
2	L	23	GLU
2	L	27	MET
2	L	30	ASN
2	L	68	LEU
2	L	91	LYS
2	L	123	ILE
2	L	174	ASP

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Mol	Chain	Res	Type
2	L	180	ARG
2	L	189	THR
2	L	194	SER
2	L	198	LYS
2	L	201	LEU
2	L	202	ILE
2	L	203	LEU
2	M	1	THR
2	M	17	GLU
2	M	18	ARG
2	M	22	MET
2	M	91	LYS
2	M	113	ILE
2	M	123	ILE
2	M	172	MET
2	M	174	ASP
2	M	198	LYS
2	M	202	ILE
2	N	9	LYS
2	N	17	GLU
2	N	23	GLU
2	N	24	ASN
2	N	30	ASN
2	N	68	LEU
2	N	93	MET
2	N	96[A]	MET
2	N	96[B]	MET
2	N	172	MET
2	N	174	ASP
2	N	194	SER
2	N	202	ILE
2	N	203	LEU
3	O	4	LYS
3	O	15	SER
3	O	45	GLU
3	O	53	SER
3	O	62	LYS
3	O	89	ARG
3	O	119	GLU
3	O	129	GLU
3	O	142	MET
3	O	146	ARG

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Mol	Chain	Res	Type
3	O	224	THR
3	P	67	LEU
3	P	115	LYS
3	P	131	SER
3	P	140	ILE
3	P	145	LEU
3	P	153	SER
3	P	209	ILE
3	P	219	LEU
3	Q	10	GLN
3	Q	52	ASN
3	Q	53	SER
3	Q	65	GLU
3	Q	77	LEU
3	Q	145	LEU
3	Q	221	GLN
3	Q	227	ASP
3	Q	231	SER
3	R	61	GLU
3	R	62	LYS
3	R	63	SER
3	R	77	LEU
3	R	142	MET
3	R	150	SER
3	R	153	SER
3	R	184	ARG
3	S	4	LYS
3	S	77	LEU
3	S	116	ILE
3	S	142	MET
3	S	224	THR
3	T	4	LYS
3	T	10	GLN
3	T	37	GLU
3	T	52	ASN
3	T	62	LYS
3	T	63	SER
3	T	77	LEU
3	T	116	ILE
3	T	224	THR
3	U	63	SER
3	U	67	LEU

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Mol	Chain	Res	Type
3	U	77	LEU
3	U	175	GLN
3	U	180	LEU
3	U	184	ARG
3	U	224	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (55) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	219	ASN
1	A	226	GLN
1	B	62	ASN
1	C	62	ASN
1	C	226	GLN
1	D	61	GLN
1	D	62	ASN
1	D	183	ASN
1	D	219	ASN
1	D	226	GLN
1	E	61	GLN
1	E	62	ASN
1	E	122	GLN
1	E	226	GLN
1	F	62	ASN
1	F	219	ASN
1	F	226	GLN
1	G	68	GLN
2	H	24	ASN
2	H	141	GLN
2	I	24	ASN
2	I	191	GLN
2	J	24	ASN
2	J	30	ASN
2	J	141	GLN
2	J	191	GLN
2	K	24	ASN
2	K	141	GLN
2	L	24	ASN
2	L	141	GLN
2	L	191	GLN
2	M	24	ASN
2	M	191	GLN

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Mol	Chain	Res	Type
2	N	24	ASN
2	N	164	GLN
2	N	186	GLN
2	N	191	GLN
3	P	10	GLN
3	P	75	GLN
3	P	79	HIS
3	P	185	GLN
3	Q	47	HIS
3	Q	59	GLN
3	Q	79	HIS
3	Q	200	HIS
3	R	59	GLN
3	R	79	HIS
3	R	80	ASN
3	R	228	HIS
3	S	47	HIS
3	S	75	GLN
3	S	79	HIS
3	S	200	HIS
3	T	59	GLN
3	U	175	GLN

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](#)

32 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and

the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
5	GOL	I	2005	-	5,5,5	0.31	0	5,5,5	0.87	0
5	GOL	J	2006	-	5,5,5	0.48	0	5,5,5	0.40	0
4	SO4	N	3021	-	4,4,4	0.20	0	6,6,6	0.35	0
5	GOL	K	2007	-	5,5,5	0.78	0	5,5,5	1.28	1 (20%)
5	GOL	N	2003	-	5,5,5	0.35	0	5,5,5	0.36	0
4	SO4	N	3009	-	4,4,4	0.20	0	6,6,6	0.64	0
4	SO4	N	3022	-	4,4,4	0.29	0	6,6,6	0.21	0
4	SO4	M	3020	-	4,4,4	0.24	0	6,6,6	0.49	0
5	GOL	L	2001	-	5,5,5	0.34	0	5,5,5	0.78	0
4	SO4	E	3004	-	4,4,4	0.29	0	6,6,6	0.21	0
4	SO4	K	3013	-	4,4,4	0.22	0	6,6,6	0.49	0
4	SO4	F	3005	-	4,4,4	0.36	0	6,6,6	0.14	0
4	SO4	H	3008	-	4,4,4	0.36	0	6,6,6	0.61	0
4	SO4	I	3011	-	4,4,4	0.26	0	6,6,6	0.57	0
4	SO4	L	3019	-	4,4,4	0.11	0	6,6,6	0.53	0
4	SO4	J	3017	-	4,4,4	0.24	0	6,6,6	0.34	0
4	SO4	B	3001	-	4,4,4	0.25	0	6,6,6	0.14	0
4	SO4	C	3002	-	4,4,4	0.24	0	6,6,6	0.12	0
4	SO4	H	3015	-	4,4,4	0.18	0	6,6,6	0.98	0
4	SO4	L	3014	-	4,4,4	0.23	0	6,6,6	0.47	0
4	SO4	M	3010	-	4,4,4	0.33	0	6,6,6	0.66	0
4	SO4	A	3007	-	4,4,4	0.24	0	6,6,6	0.16	0
4	SO4	D	3003	-	4,4,4	0.23	0	6,6,6	0.23	0
4	SO4	K	3018	-	4,4,4	0.27	0	6,6,6	0.57	0
4	SO4	I	3016	-	4,4,4	0.28	0	6,6,6	0.71	0
5	GOL	H	2004	-	5,5,5	0.39	0	5,5,5	1.04	0
4	SO4	I	3023	-	4,4,4	0.39	0	6,6,6	0.18	0
4	SO4	M	3024	-	4,4,4	0.33	0	6,6,6	0.23	0
4	SO4	G	3006	-	4,4,4	0.26	0	6,6,6	0.14	0
4	SO4	J	3012	-	4,4,4	0.24	0	6,6,6	0.37	0
4	SO4	M	3025	-	4,4,4	0.27	0	6,6,6	0.34	0
5	GOL	M	2002	-	5,5,5	0.55	0	5,5,5	0.93	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	GOL	I	2005	-	-	3/4/4/4	-
5	GOL	J	2006	-	-	2/4/4/4	-
5	GOL	K	2007	-	-	2/4/4/4	-
5	GOL	H	2004	-	-	4/4/4/4	-
5	GOL	N	2003	-	-	2/4/4/4	-
5	GOL	L	2001	-	-	1/4/4/4	-
5	GOL	M	2002	-	-	4/4/4/4	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	K	2007	GOL	O3-C3-C2	-2.28	100.10	110.38

There are no chirality outliers.

All (18) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	H	2004	GOL	C1-C2-C3-O3
5	H	2004	GOL	O2-C2-C3-O3
5	I	2005	GOL	C1-C2-C3-O3
5	I	2005	GOL	O2-C2-C3-O3
5	J	2006	GOL	O1-C1-C2-C3
5	K	2007	GOL	C1-C2-C3-O3
5	K	2007	GOL	O2-C2-C3-O3
5	M	2002	GOL	O1-C1-C2-C3
5	N	2003	GOL	O1-C1-C2-O2
5	N	2003	GOL	O1-C1-C2-C3
5	M	2002	GOL	C1-C2-C3-O3
5	I	2005	GOL	O1-C1-C2-O2
5	J	2006	GOL	O1-C1-C2-O2
5	M	2002	GOL	O1-C1-C2-O2
5	M	2002	GOL	O2-C2-C3-O3
5	H	2004	GOL	O1-C1-C2-O2
5	H	2004	GOL	O1-C1-C2-C3
5	L	2001	GOL	O2-C2-C3-O3

There are no ring outliers.

8 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	N	3021	SO4	1	0
5	L	2001	GOL	2	0
4	L	3019	SO4	1	0
4	J	3017	SO4	1	0
4	M	3010	SO4	1	0
4	A	3007	SO4	2	0
4	D	3003	SO4	1	0
4	I	3016	SO4	1	0

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	222/233 (95%)	-0.64	3 (1%) 73 69	21, 36, 77, 85	0
1	B	222/233 (95%)	-0.65	3 (1%) 73 69	21, 36, 72, 86	0
1	C	222/233 (95%)	-0.62	3 (1%) 73 69	21, 36, 73, 86	0
1	D	222/233 (95%)	-0.55	4 (1%) 67 63	23, 39, 76, 87	0
1	E	222/233 (95%)	-0.70	3 (1%) 73 69	23, 35, 66, 78	0
1	F	222/233 (95%)	-0.60	4 (1%) 67 63	24, 39, 77, 88	0
1	G	222/233 (95%)	-0.53	7 (3%) 50 46	24, 38, 75, 88	0
2	H	203/217 (93%)	-0.91	2 (0%) 79 76	14, 28, 48, 78	2 (0%)
2	I	203/217 (93%)	-0.87	2 (0%) 79 76	13, 29, 50, 71	2 (0%)
2	J	203/217 (93%)	-0.84	2 (0%) 79 76	13, 30, 51, 76	2 (0%)
2	K	203/217 (93%)	-0.85	2 (0%) 79 76	15, 30, 51, 74	1 (0%)
2	L	203/217 (93%)	-0.81	2 (0%) 79 76	14, 30, 50, 73	1 (0%)
2	M	203/217 (93%)	-0.88	2 (0%) 79 76	14, 29, 46, 69	2 (0%)
2	N	203/217 (93%)	-0.86	2 (0%) 79 76	12, 29, 49, 71	2 (0%)
3	O	218/237 (91%)	-0.48	4 (1%) 67 63	30, 46, 72, 80	0
3	P	218/237 (91%)	-0.44	3 (1%) 73 69	32, 49, 77, 86	0
3	Q	218/237 (91%)	-0.40	5 (2%) 61 57	30, 50, 76, 93	0
3	R	218/237 (91%)	-0.49	3 (1%) 73 69	25, 44, 76, 85	0
3	S	218/237 (91%)	-0.65	2 (0%) 81 78	23, 37, 72, 85	0
3	T	218/237 (91%)	-0.63	2 (0%) 81 78	24, 38, 69, 84	0
3	U	218/237 (91%)	-0.59	5 (2%) 61 57	25, 38, 73, 87	0
All	All	4501/4809 (93%)	-0.66	65 (1%) 73 69	12, 36, 72, 93	12 (0%)

All (65) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	L	203	LEU	5.8
2	N	203	LEU	5.5
1	D	12	ILE	5.3
1	B	12	ILE	5.3
2	I	203	LEU	5.2
2	M	203	LEU	5.1
1	D	13	THR	5.0
2	H	203	LEU	4.7
1	F	13	THR	4.5
3	R	225	GLY	4.5
1	G	12	ILE	4.4
1	G	13	THR	4.2
3	O	225	GLY	4.1
2	J	203	LEU	4.1
1	C	12	ILE	4.0
1	A	13	THR	4.0
3	Q	227	ASP	3.9
1	B	13	THR	3.9
1	C	13	THR	3.8
1	F	12	ILE	3.8
3	Q	225	GLY	3.7
2	H	202	ILE	3.6
1	B	64	ILE	3.5
1	C	64	ILE	3.4
3	P	225	GLY	3.3
3	P	226	SER	3.3
2	K	203	LEU	3.3
3	R	226	SER	3.3
1	D	64	ILE	3.3
3	U	226	SER	3.2
1	F	64	ILE	3.2
3	T	225	GLY	3.1
3	U	225	GLY	3.1
1	E	12	ILE	3.0
2	J	202	ILE	2.9
1	A	12	ILE	2.8
1	G	64	ILE	2.8
1	G	204	GLY	2.7
1	F	55	ARG	2.6
3	S	228	HIS	2.6
3	O	226	SER	2.5
1	E	13	THR	2.5
3	P	227	ASP	2.4

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Mol	Chain	Res	Type	RSRZ
3	T	228	HIS	2.4
3	Q	172	GLY	2.4
2	N	202	ILE	2.4
1	D	63	SER	2.3
2	L	202	ILE	2.3
3	R	228	HIS	2.3
1	G	191	THR	2.3
3	S	225	GLY	2.2
2	I	200	GLY	2.2
3	U	227	ASP	2.2
1	A	62	ASN	2.1
3	U	135	GLY	2.1
2	K	202	ILE	2.1
2	M	202	ILE	2.1
1	E	55	ARG	2.1
1	G	55	ARG	2.0
3	Q	226	SER	2.0
3	Q	231	SER	2.0
1	G	61	GLN	2.0
3	U	136	ALA	2.0
3	O	227	ASP	2.0
3	O	228	HIS	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](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	SO4	E	3004	5/5	0.64	0.15	120,121,121,121	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	SO4	F	3005	5/5	0.82	0.12	112,112,113,113	0
4	SO4	B	3001	5/5	0.84	0.11	128,128,128,128	0
4	SO4	G	3006	5/5	0.86	0.10	114,114,114,114	0
4	SO4	A	3007	5/5	0.87	0.10	116,117,117,117	0
4	SO4	I	3023	5/5	0.87	0.12	83,83,84,84	0
4	SO4	D	3003	5/5	0.89	0.09	105,105,105,106	0
4	SO4	M	3024	5/5	0.89	0.10	82,84,85,86	0
4	SO4	C	3002	5/5	0.91	0.10	110,110,110,110	0
4	SO4	M	3025	5/5	0.91	0.12	77,77,79,79	0
4	SO4	N	3022	5/5	0.91	0.10	89,90,91,91	0
5	GOL	N	2003	6/6	0.92	0.05	44,45,46,46	0
5	GOL	K	2007	6/6	0.93	0.06	38,39,41,42	0
5	GOL	M	2002	6/6	0.93	0.05	49,51,52,52	0
5	GOL	I	2005	6/6	0.93	0.04	36,38,41,44	0
5	GOL	J	2006	6/6	0.94	0.05	37,41,46,50	0
5	GOL	L	2001	6/6	0.94	0.05	41,41,42,44	0
4	SO4	H	3015	5/5	0.95	0.08	47,49,51,51	0
4	SO4	M	3020	5/5	0.96	0.07	63,64,64,65	0
5	GOL	H	2004	6/6	0.96	0.05	42,42,44,44	0
4	SO4	N	3021	5/5	0.97	0.06	54,55,58,59	0
4	SO4	L	3019	5/5	0.97	0.07	56,58,58,59	0
4	SO4	I	3016	5/5	0.97	0.06	51,52,56,56	0
4	SO4	H	3008	5/5	0.98	0.06	47,47,50,52	0
4	SO4	M	3010	5/5	0.98	0.07	50,53,55,55	0
4	SO4	I	3011	5/5	0.98	0.05	38,40,43,46	0
4	SO4	J	3017	5/5	0.98	0.05	49,50,50,52	0
4	SO4	K	3013	5/5	0.98	0.07	42,43,47,49	0
4	SO4	K	3018	5/5	0.98	0.06	56,57,57,57	0
4	SO4	L	3014	5/5	0.98	0.07	46,47,50,51	0
4	SO4	N	3009	5/5	0.99	0.07	46,47,50,50	0
4	SO4	J	3012	5/5	0.99	0.04	44,44,47,48	0

6.5 Other polymers

There are no such residues in this entry.