



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 14, 2026 – 03:16 PM UTC

PDB ID : 3SDI / pdb_00003sdi
Title : Structure of yeast 20S open-gate proteasome with Compound 20
Authors : Sintchak, M.D.
Deposited on : 2011-06-09
Resolution : 2.65 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
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
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

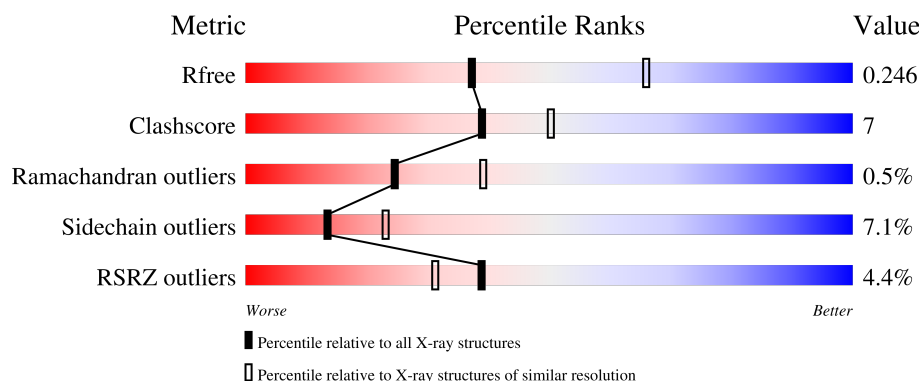
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.65 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	1110 (2.66-2.66)
Clashscore	190562	1141 (2.66-2.66)
Ramachandran outliers	187476	1126 (2.66-2.66)
Sidechain outliers	187428	1126 (2.66-2.66)
RSRZ outliers	180081	1110 (2.66-2.66)

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	250	2% 86% 12% .
1	O	250	2% 80% 17% ..
2	B	235	7% 75% 21% .
2	P	235	9% 76% 23% .
3	C	241	14% 80% 16% ..

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Mol	Chain	Length	Quality of chain
3	Q	241	
4	D	260	
4	R	260	
5	E	233	
5	S	233	
6	F	242	
6	T	242	
7	G	243	
7	U	243	
8	H	222	
8	V	222	
9	I	204	
9	W	204	
10	J	198	
10	X	198	
11	K	212	
11	Y	212	
12	L	222	
12	Z	222	
13	1	233	
13	M	233	
14	2	196	
14	N	196	

2 Entry composition

There are 18 unique types of molecules in this entry. The entry contains 49012 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 component Y7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	246	Total	C	N	O	S	0	0	0
			1881	1200	308	370	3			
1	O	246	Total	C	N	O	S	0	0	0
			1881	1200	308	370	3			

- Molecule 2 is a protein called Proteasome component Y13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	235	Total	C	N	O	S	0	0	0
			1827	1157	303	364	3			
2	P	235	Total	C	N	O	S	0	0	0
			1827	1157	303	364	3			

- Molecule 3 is a protein called Proteasome component PRE6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	238	Total	C	N	O	S	0	0	0
			1861	1163	325	369	4			
3	Q	238	Total	C	N	O	S	0	0	0
			1861	1163	325	369	4			

- Molecule 4 is a protein called Proteasome component PUP2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	228	Total	C	N	O	S	0	0	0
			1747	1094	291	355	7			
4	R	229	Total	C	N	O	S	0	0	0
			1752	1097	292	356	7			

- Molecule 5 is a protein called Proteasome component PRE5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	230	Total	C	N	O	S	0	0	0
			1755	1103	304	344	4			
5	S	230	Total	C	N	O	S	0	0	0
			1755	1103	304	344	4			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	127	ALA	TYR	conflict	UNP P40302
S	127	ALA	TYR	conflict	UNP P40302

- Molecule 6 is a protein called Proteasome component C1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	242	Total	C	N	O	S	0	0	0
			1886	1199	328	355	4			
6	T	242	Total	C	N	O	S	0	0	0
			1886	1199	328	355	4			

- Molecule 7 is a protein called Proteasome component C7-alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	G	240	Total	C	N	O	S	0	0	0
			1897	1206	319	364	8			
7	U	240	Total	C	N	O	S	0	0	0
			1897	1206	319	364	8			

- Molecule 8 is a protein called Proteasome component PUP1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	H	222	Total	C	N	O	S	0	0	0
			1685	1061	293	324	7			
8	V	222	Total	C	N	O	S	0	0	0
			1685	1061	293	324	7			

- Molecule 9 is a protein called Proteasome component PUP3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	I	204	Total	C	N	O	S	0	0	0
			1581	1010	258	305	8			
9	W	204	Total	C	N	O	S	0	0	0
			1581	1010	258	305	8			

- Molecule 10 is a protein called Proteasome component C11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	J	198	Total	C	N	O	S	0	0	0
			1582	1003	269	305	5			
10	X	198	Total	C	N	O	S	0	0	0
			1582	1003	269	305	5			

- Molecule 11 is a protein called Proteasome component PRE2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	K	212	Total	C	N	O	S	0	0	0
			1644	1045	280	312	7			
11	Y	212	Total	C	N	O	S	0	0	0
			1644	1045	280	312	7			

- Molecule 12 is a protein called Proteasome component C5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	L	222	Total	C	N	O	S	0	0	0
			1757	1115	303	335	4			
12	Z	222	Total	C	N	O	S	0	0	0
			1757	1115	303	335	4			

- Molecule 13 is a protein called Proteasome component PRE4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	M	233	Total	C	N	O	S	0	0	0
			1824	1154	312	351	7			
13	1	233	Total	C	N	O	S	0	0	0
			1824	1154	312	351	7			

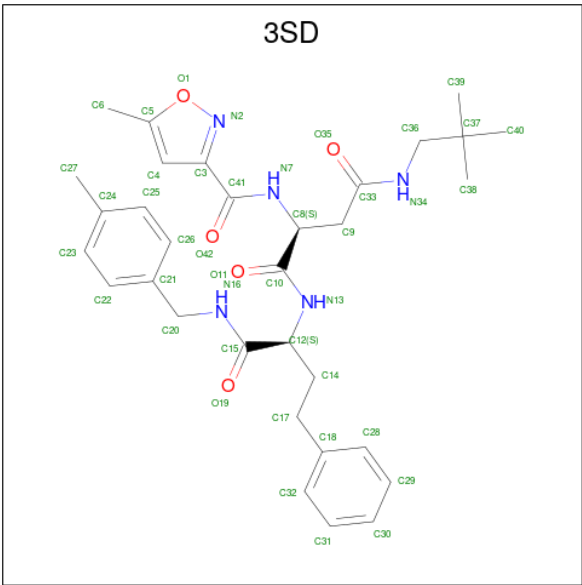
- Molecule 14 is a protein called Proteasome component PRE3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	N	196	Total	C	N	O	S	0	0	0
			1512	955	250	300	7			
14	2	196	Total	C	N	O	S	0	0	0
			1512	955	250	300	7			

- Molecule 15 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

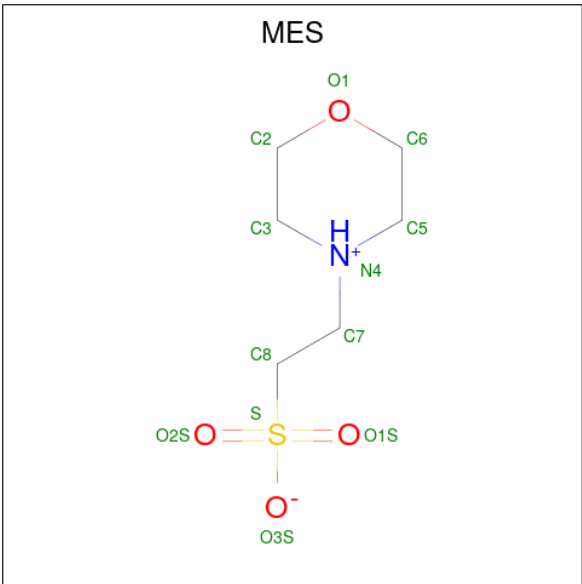
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
15	F	2	Total Mg 2 2	0	0
15	G	1	Total Mg 1 1	0	0
15	H	1	Total Mg 1 1	0	0
15	I	2	Total Mg 2 2	0	0
15	K	1	Total Mg 1 1	0	0
15	L	2	Total Mg 2 2	0	0
15	N	1	Total Mg 1 1	0	0
15	T	2	Total Mg 2 2	0	0
15	U	1	Total Mg 1 1	0	0
15	V	1	Total Mg 1 1	0	0
15	W	2	Total Mg 2 2	0	0
15	Y	1	Total Mg 1 1	0	0
15	Z	2	Total Mg 2 2	0	0
15	2	1	Total Mg 1 1	0	0

- Molecule 16 is N 4 -(2,2-dimethylpropyl)-N 1 -{(2S)-1-[(4-methylbenzyl)amino]-1-oxo-4-phenylbutan-2-yl}-N 2 -[(5-methyl-1,2-oxazol-3-yl)carbonyl]-L-aspartamide (CCD ID: 3SD) (formula: C₃₂H₄₁N₅O₅).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
16	K	1	Total	C	N	O	0	0
			42	32	5	5		
16	Y	1	Total	C	N	O	0	0
			42	32	5	5		

- Molecule 17 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (CCD ID: MES) (formula: C₆H₁₃NO₄S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
17	K	1	Total	C	N	O	S	0	0
			12	6	1	4	1		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
17	Y	1	Total	C	N	O	S	0	0
			12	6	1	4	1		

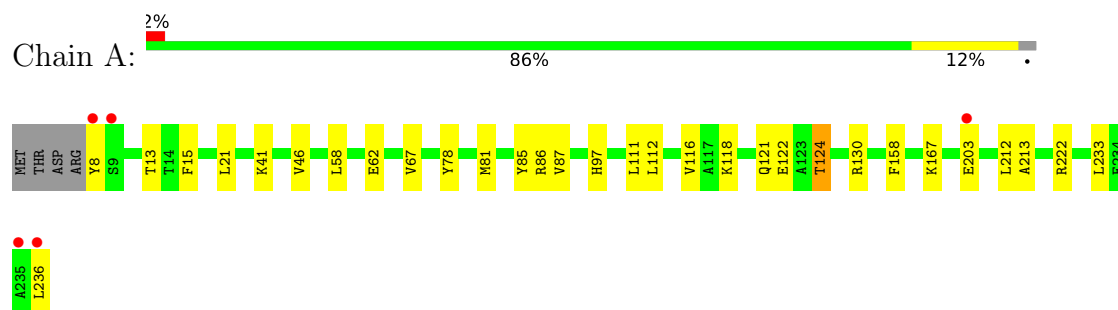
- Molecule 18 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
18	L	1	Total	O	0	0
			1	1		

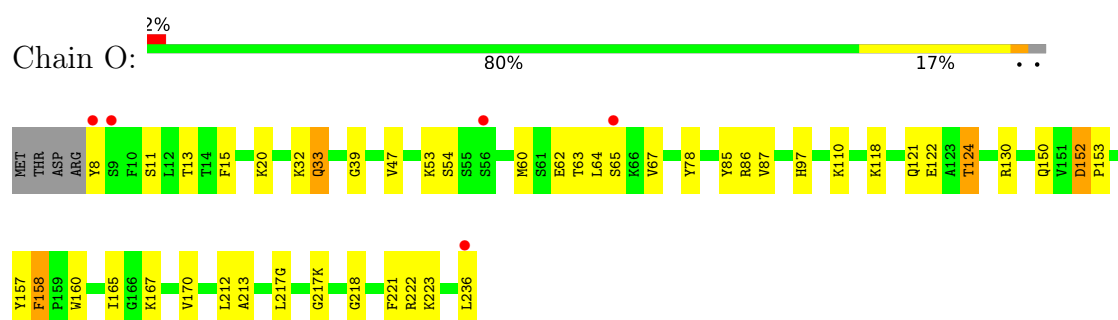
3 Residue-property plots [i](#)

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.

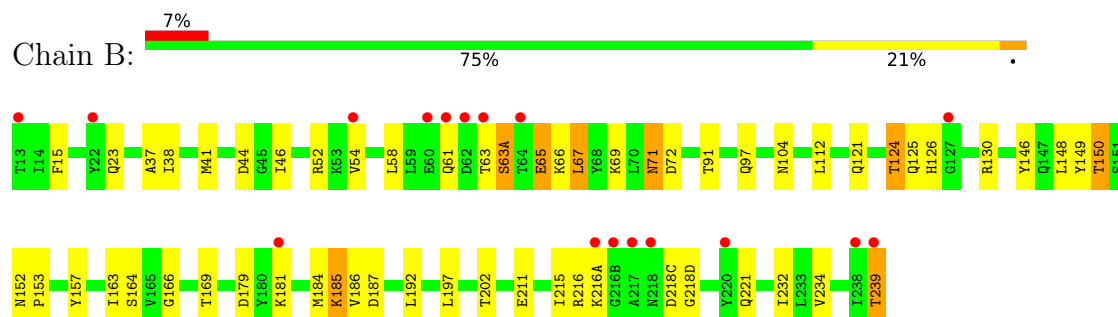
- Molecule 1: Proteasome component Y7



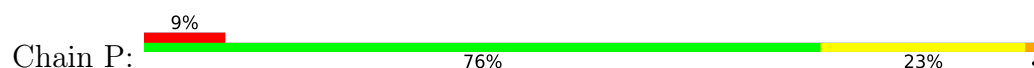
- Molecule 1: Proteasome component Y7

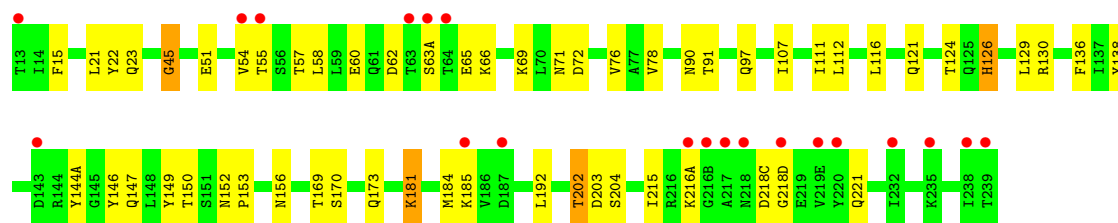


- Molecule 2: Proteasome component Y13

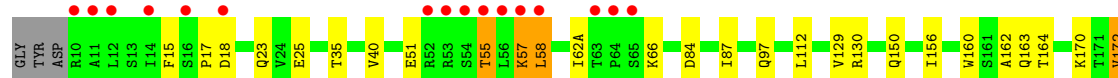
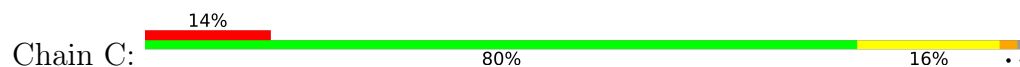


- Molecule 2: Proteasome component Y13

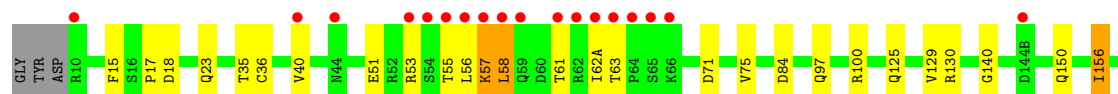
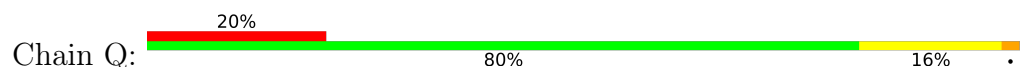




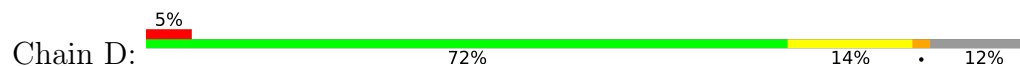
• Molecule 3: Proteasome component PRE6



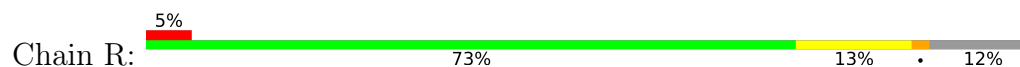
• Molecule 3: Proteasome component PRE6



• Molecule 4: Proteasome component PUP2

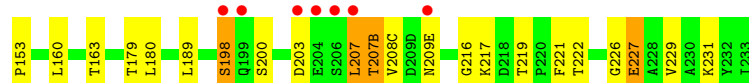
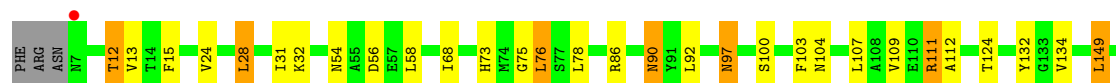
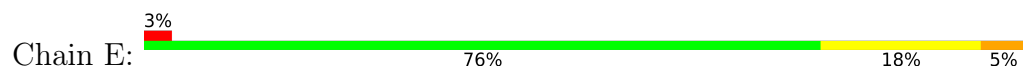


• Molecule 4: Proteasome component PUP2

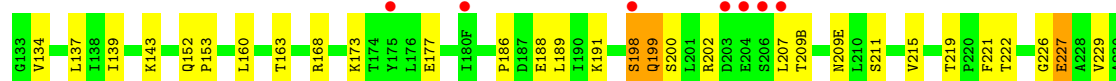
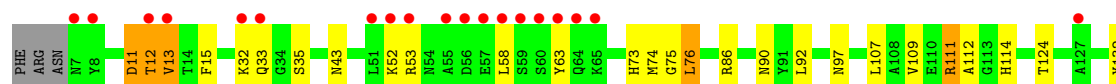
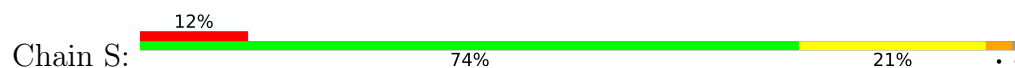




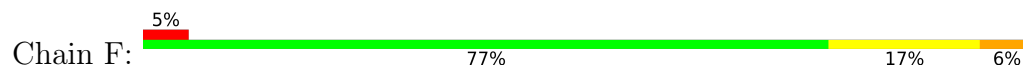
• Molecule 5: Proteasome component PRE5



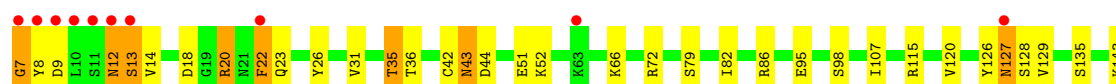
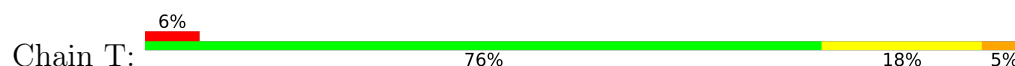
• Molecule 5: Proteasome component PRE5

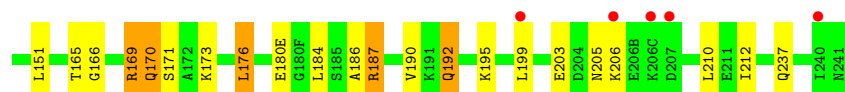


• Molecule 6: Proteasome component C1

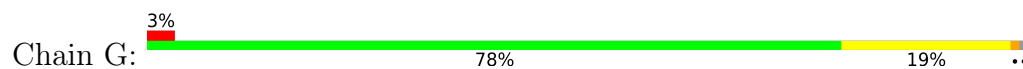


• Molecule 6: Proteasome component C1

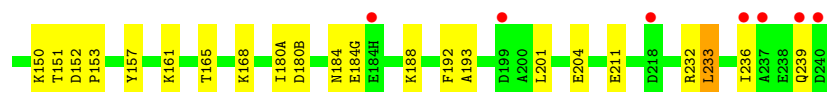
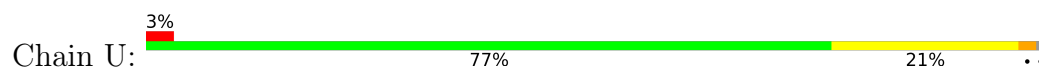




• Molecule 7: Proteasome component C7-alpha



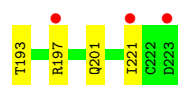
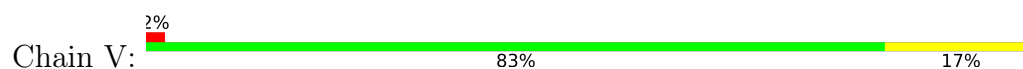
• Molecule 7: Proteasome component C7-alpha



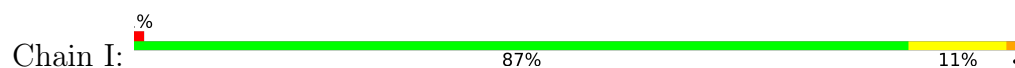
• Molecule 8: Proteasome component PUP1

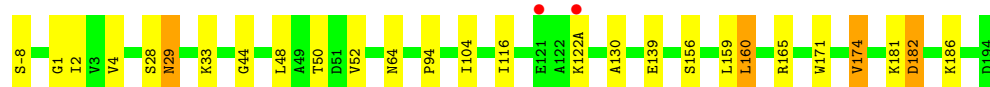


• Molecule 8: Proteasome component PUP1

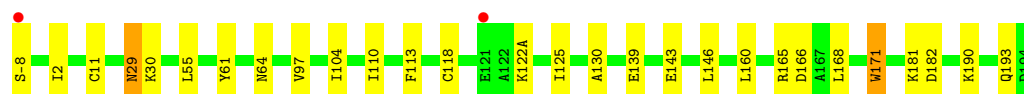
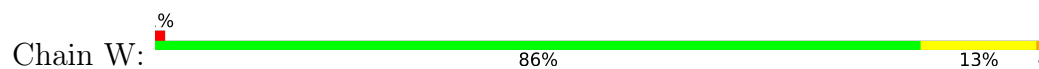


• Molecule 9: Proteasome component PUP3

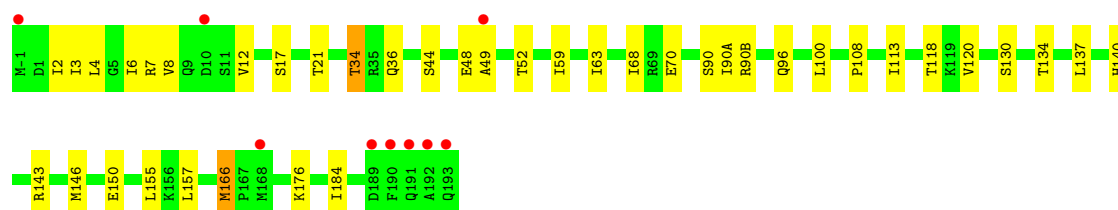
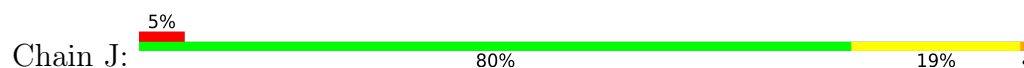




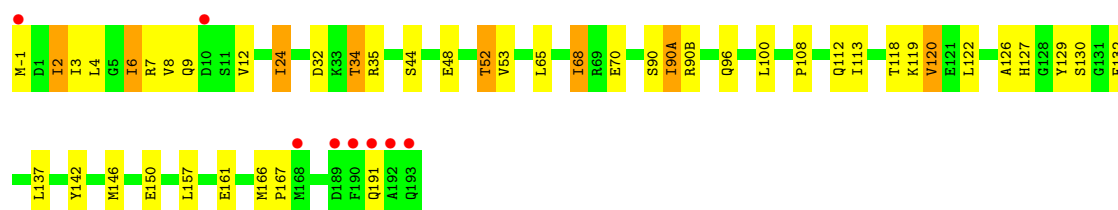
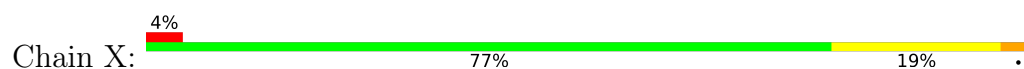
• Molecule 9: Proteasome component PUP3



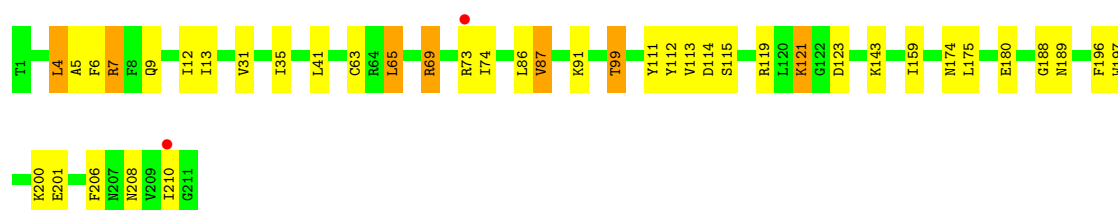
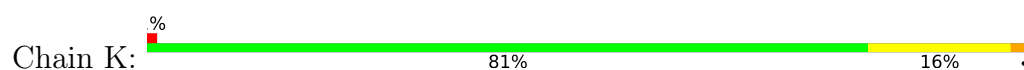
• Molecule 10: Proteasome component C11



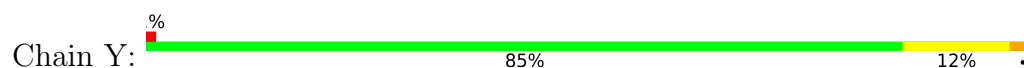
• Molecule 10: Proteasome component C11



• Molecule 11: Proteasome component PRE2

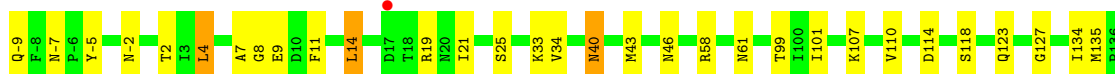
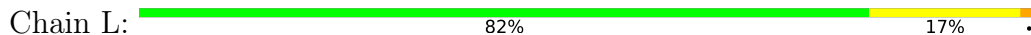


• Molecule 11: Proteasome component PRE2

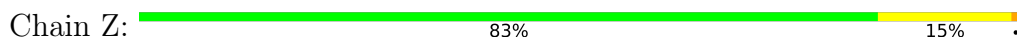




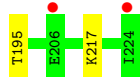
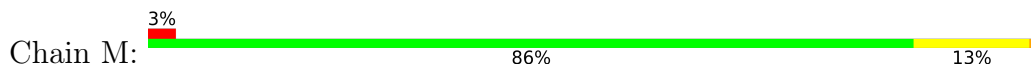
• Molecule 12: Proteasome component C5



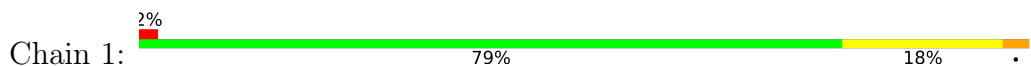
• Molecule 12: Proteasome component C5



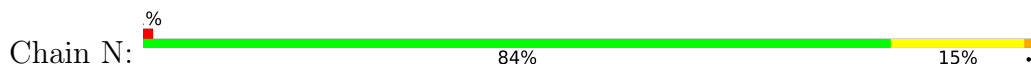
• Molecule 13: Proteasome component PRE4

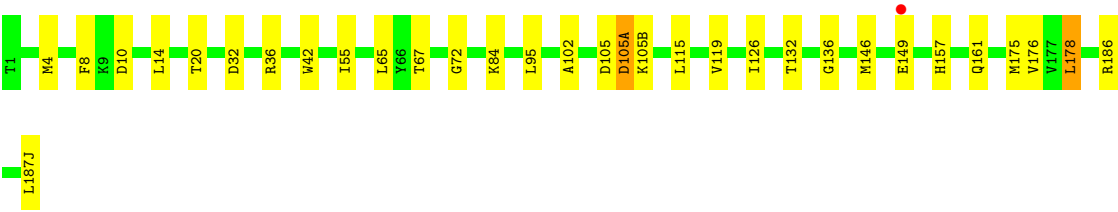


• Molecule 13: Proteasome component PRE4

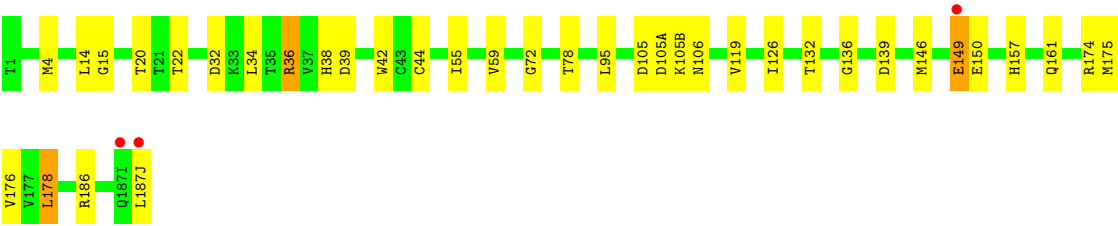
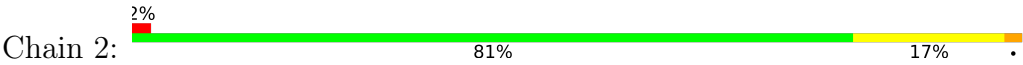


• Molecule 14: Proteasome component PRE3





● Molecule 14: Proteasome component PRE3



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	136.60Å 299.45Å 145.48Å 90.00° 113.17° 90.00°	Depositor
Resolution (Å)	30.00 – 2.65 30.00 – 2.65	Depositor EDS
% Data completeness (in resolution range)	95.4 (30.00-2.65) 95.6 (30.00-2.65)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.44 (at 2.64Å)	Xtriage
Refinement program	REFMAC 5.5.0110	Depositor
R, R_{free}	0.219 , 0.253 0.215 , 0.246	Depositor DCC
R_{free} test set	5996 reflections (2.02%)	wwPDB-VP
Wilson B-factor (Å ²)	49.8	Xtriage
Anisotropy	0.120	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 23.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	49012	wwPDB-VP
Average B, all atoms (Å ²)	47.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.25% 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: MES, 3SD, MG

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	0.58	0/1918	0.84	0/2597
1	O	0.58	0/1918	0.86	2/2597 (0.1%)
2	B	0.58	0/1856	0.87	1/2513 (0.0%)
2	P	0.60	0/1856	0.89	2/2513 (0.1%)
3	C	0.57	0/1889	0.88	0/2557
3	Q	0.59	0/1889	0.88	1/2557 (0.0%)
4	D	0.59	0/1770	0.86	2/2387 (0.1%)
4	R	0.57	0/1775	0.86	1/2394 (0.0%)
5	E	0.58	0/1781	0.83	1/2407 (0.0%)
5	S	0.57	0/1781	0.86	2/2407 (0.1%)
6	F	0.62	1/1926 (0.1%)	0.85	1/2599 (0.0%)
6	T	0.67	2/1926 (0.1%)	0.88	1/2599 (0.0%)
7	G	0.63	0/1934	0.83	0/2618
7	U	0.64	1/1934 (0.1%)	0.88	0/2618
8	H	0.64	0/1716	0.88	1/2326 (0.0%)
8	V	0.61	0/1716	0.85	0/2326
9	I	0.65	1/1611 (0.1%)	0.84	1/2174 (0.0%)
9	W	0.71	0/1611	0.85	0/2174
10	J	0.63	0/1610	0.90	1/2170 (0.0%)
10	X	0.70	1/1610 (0.1%)	0.91	3/2170 (0.1%)
11	K	0.61	0/1681	0.88	1/2274 (0.0%)
11	Y	0.59	0/1681	0.84	0/2274
12	L	0.64	0/1795	0.83	0/2420
12	Z	0.65	0/1795	0.85	3/2420 (0.1%)
13	1	0.72	1/1855 (0.1%)	0.98	4/2514 (0.2%)
13	M	0.79	2/1855 (0.1%)	0.89	2/2514 (0.1%)
14	2	0.69	1/1541 (0.1%)	0.90	1/2087 (0.0%)
14	N	0.72	0/1541	0.85	1/2087 (0.0%)
All	All	0.63	10/49771 (0.0%)	0.87	32/67293 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if

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

Mol	Chain	#Chirality outliers	#Planarity outliers
13	1	0	1

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	T	82	ILE	CA-CB	8.04	1.58	1.54
10	X	-1	MET	C-N	-7.46	1.23	1.33
6	F	82	ILE	CA-CB	7.21	1.57	1.54
13	M	0	THR	C-O	-6.03	1.17	1.23
13	M	77	ALA	CA-CB	-5.98	1.44	1.53
9	I	1	GLY	C-O	-5.88	1.18	1.23
7	U	82	ILE	CA-CB	5.65	1.57	1.53
14	2	72	GLY	C-O	-5.37	1.18	1.24
13	1	77	ALA	CA-CB	-5.11	1.44	1.53
6	T	7	GLY	N-CA	5.01	1.53	1.45

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	1	74	ALA	O-C-N	-20.18	95.75	122.59
10	X	-1	MET	CA-C-N	9.66	137.43	121.39
10	X	-1	MET	C-N-CA	9.66	137.43	121.39
4	D	128	MET	N-CA-C	-7.23	90.76	111.00
10	J	49	ALA	N-CA-C	7.17	119.77	111.02
10	X	-1	MET	O-C-N	-6.64	112.38	123.00
3	Q	125	GLN	N-CA-C	6.39	118.60	110.61
5	S	152	GLN	CA-C-N	6.33	126.03	119.82
5	S	152	GLN	C-N-CA	6.33	126.03	119.82
1	O	152	ASP	CA-C-N	6.23	127.63	119.84
1	O	152	ASP	C-N-CA	6.23	127.63	119.84
8	H	180	ILE	N-CA-C	5.93	116.59	110.36
13	1	161	VAL	CB-CA-C	-5.89	104.32	112.04
9	I	52	VAL	N-CA-C	-5.83	105.05	110.53
12	Z	93	PHE	CA-C-N	5.79	125.76	120.03
12	Z	93	PHE	C-N-CA	5.79	125.76	120.03
4	D	169	SER	N-CA-C	5.68	118.41	111.82
2	P	45	GLY	N-CA-C	5.66	118.25	110.56
13	1	-2	THR	N-CA-C	5.63	118.25	109.52
6	F	161	LYS	N-CA-C	-5.53	105.65	112.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	P	126	HIS	N-CA-C	5.43	116.53	108.60
6	T	107	ILE	N-CA-C	5.40	114.84	108.96
14	N	105(A)	ASP	N-CA-C	5.34	117.10	111.28
5	E	216	GLY	N-CA-C	5.33	117.78	110.69
13	M	73	ASP	CA-C-N	-5.32	111.38	121.54
13	M	73	ASP	C-N-CA	-5.32	111.38	121.54
11	K	188	GLY	N-CA-C	5.26	118.18	112.29
13	1	186	PHE	N-CA-C	5.19	116.69	108.96
14	2	106	ASN	N-CA-C	5.07	119.56	113.17
4	R	128	MET	N-CA-C	-5.06	96.82	111.00
12	Z	116	VAL	N-CA-C	5.05	117.03	111.77
2	B	179	ASP	N-CA-C	5.03	119.40	113.16

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
13	1	74	ALA	Mainchain

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	1881	0	1893	25	0
1	O	1881	0	1893	28	0
2	B	1827	0	1824	36	0
2	P	1827	0	1824	39	0
3	C	1861	0	1873	32	0
3	Q	1861	0	1873	27	0
4	D	1747	0	1718	23	0
4	R	1752	0	1720	19	0
5	E	1755	0	1761	30	0
5	S	1755	0	1761	35	0
6	F	1886	0	1876	39	0
6	T	1886	0	1875	50	0
7	G	1897	0	1891	44	0
7	U	1897	0	1891	44	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	H	1685	0	1688	15	0
8	V	1685	0	1688	24	0
9	I	1581	0	1574	14	0
9	W	1581	0	1574	24	0
10	J	1582	0	1583	19	0
10	X	1582	0	1583	25	0
11	K	1644	0	1595	25	0
11	Y	1644	0	1595	21	0
12	L	1757	0	1711	24	0
12	Z	1757	0	1711	23	0
13	1	1824	0	1832	38	0
13	M	1824	0	1832	21	0
14	2	1512	0	1481	22	0
14	N	1512	0	1481	17	0
15	2	1	0	0	0	0
15	F	2	0	0	0	0
15	G	1	0	0	0	0
15	H	1	0	0	0	0
15	I	2	0	0	0	0
15	K	1	0	0	0	0
15	L	2	0	0	0	0
15	N	1	0	0	0	0
15	T	2	0	0	0	0
15	U	1	0	0	0	0
15	V	1	0	0	0	0
15	W	2	0	0	0	0
15	Y	1	0	0	0	0
15	Z	2	0	0	0	0
16	K	42	0	41	1	0
16	Y	42	0	41	2	0
17	K	12	0	13	1	0
17	Y	12	0	13	0	0
18	L	1	0	0	0	0
All	All	49012	0	48709	667	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 7.

All (667) 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)
14:N:161:GLN:HE21	14:2:136:GLY:HA2	1.17	1.09
7:U:96:ALA:HA	7:U:107:MET:HE2	1.32	1.06
7:G:96:ALA:HA	7:G:107:MET:HE2	1.37	1.05
3:C:163:GLN:NE2	3:C:164:THR:H	1.59	1.00
1:A:130:ARG:HH21	7:G:124:THR:CG2	1.76	0.97
3:C:163:GLN:HE21	3:C:164:THR:N	1.60	0.97
5:S:207:LEU:HA	5:S:209(E):ASN:HD22	1.27	0.96
1:A:130:ARG:HH21	7:G:124:THR:HG22	1.31	0.96
3:C:57:LYS:HD2	3:C:58:LEU:H	1.31	0.95
11:Y:174:ASN:HD21	11:Y:189:ASN:HD22	1.14	0.95
13:1:152:ARG:HH11	13:1:152:ARG:HG3	1.34	0.92
1:O:130:ARG:HH21	7:U:124:THR:HG22	1.35	0.91
12:L:135:MET:HE3	9:W:165:ARG:NH2	1.88	0.89
5:S:52:LYS:HB2	5:S:63:TYR:HB3	1.54	0.89
3:C:15:PHE:H	4:D:23:GLN:HE22	1.15	0.89
6:T:170:GLN:CD	6:T:170:GLN:H	1.80	0.89
1:O:130:ARG:HH21	7:U:124:THR:CG2	1.87	0.87
12:L:4:LEU:HD13	12:L:138:LEU:HD21	1.55	0.87
14:N:136:GLY:HA2	14:2:161:GLN:HE21	1.40	0.86
1:O:86:ARG:HE	7:U:118:ASN:HD21	1.24	0.85
6:F:35:THR:HG21	6:F:51:GLU:O	1.77	0.84
13:1:69:ASN:ND2	13:1:72:ALA:HA	1.91	0.84
1:A:86:ARG:HE	7:G:118:ASN:HD21	1.22	0.84
6:F:95:GLU:HG2	6:F:115:ARG:HB3	1.60	0.83
11:Y:174:ASN:ND2	11:Y:189:ASN:HD22	1.76	0.83
8:V:80:LEU:HD12	8:V:113:ILE:HD11	1.61	0.82
7:G:184(G):GLU:HG2	7:G:188:LYS:HB3	1.61	0.82
12:Z:166:HIS:HD2	12:Z:168:GLN:H	1.27	0.81
14:N:161:GLN:NE2	14:2:136:GLY:HA2	1.94	0.81
11:K:174:ASN:HD21	11:K:189:ASN:HD22	1.29	0.81
3:C:163:GLN:HE21	3:C:164:THR:H	0.83	0.81
5:S:97:ASN:HD21	12:Z:61:ASN:HD21	1.26	0.80
5:E:97:ASN:HD21	12:L:61:ASN:HD21	1.29	0.80
3:Q:163:GLN:HE21	3:Q:164:THR:H	1.27	0.79
2:B:181:LYS:O	2:B:184:MET:HG3	1.83	0.79
14:2:157:HIS:HD2	14:2:187(J):LEU:HD13	1.47	0.79
5:E:15:PHE:H	6:F:23:GLN:HE22	1.32	0.77
7:G:184(G):GLU:HG2	7:G:188:LYS:CB	2.14	0.77
7:G:96:ALA:HA	7:G:107:MET:CE	2.14	0.77
7:U:121:GLN:O	7:U:124:THR:HB	1.86	0.76
2:P:124:THR:HG22	3:Q:130:ARG:HH21	1.50	0.75
6:T:187:ARG:HH11	6:T:187:ARG:CG	1.99	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:97:GLN:HE22	9:I:64:ASN:HD22	1.34	0.75
11:Y:143:LYS:HB2	11:Y:146:LEU:HD13	1.68	0.75
1:O:15:PHE:H	2:P:23:GLN:HE22	1.33	0.74
1:A:86:ARG:HE	7:G:118:ASN:ND2	1.85	0.74
12:L:40:ASN:HD21	12:L:183:GLY:HA2	1.51	0.73
1:O:124:THR:CG2	2:P:130:ARG:HH21	2.01	0.73
1:A:124:THR:HG22	2:B:130:ARG:HH21	1.53	0.73
6:T:95:GLU:HG2	6:T:115:ARG:HB3	1.69	0.72
3:C:57:LYS:HD2	3:C:58:LEU:N	2.03	0.72
4:D:97:VAL:HG21	11:K:65:LEU:HD13	1.70	0.72
12:L:33:LYS:HE3	12:L:46:ASN:ND2	2.04	0.72
3:Q:15:PHE:H	4:R:23:GLN:HE22	1.36	0.72
2:B:124:THR:HG22	3:C:130:ARG:HH21	1.52	0.72
2:B:126:HIS:HB3	3:C:129:VAL:HG12	1.71	0.72
1:A:15:PHE:H	2:B:23:GLN:HE22	1.35	0.72
2:P:121:GLN:O	2:P:124:THR:HB	1.90	0.72
14:2:157:HIS:CD2	14:2:187(J):LEU:HD13	2.25	0.72
11:K:4:LEU:CD1	11:K:159:ILE:HD11	2.20	0.72
7:G:170:GLN:HE21	7:G:174:THR:HG23	1.54	0.71
13:M:170:ASN:HD22	13:M:173:ARG:HH11	1.36	0.71
3:C:57:LYS:O	3:C:58:LEU:HB2	1.91	0.71
4:D:179:GLU:HB3	4:D:192:LEU:HD21	1.70	0.71
6:F:36:THR:HG22	6:F:51:GLU:OE2	1.90	0.71
1:O:124:THR:HG22	2:P:130:ARG:HH21	1.54	0.71
4:D:215:ILE:HG22	4:D:221:PHE:HD2	1.54	0.71
1:O:86:ARG:HH21	7:U:118:ASN:HD22	1.39	0.71
7:U:184(G):GLU:HG2	7:U:188:LYS:HB2	1.72	0.70
12:L:14:LEU:HD13	12:L:34:VAL:HG13	1.73	0.70
5:E:207:LEU:HA	5:E:209(E):ASN:HD22	1.56	0.70
3:C:163:GLN:HE22	3:C:173:ARG:HE	1.39	0.70
8:H:128:GLY:O	8:H:131:SER:HB2	1.91	0.70
2:P:97:GLN:HE22	9:W:64:ASN:HD22	1.38	0.69
7:U:96:ALA:HA	7:U:107:MET:CE	2.16	0.69
12:Z:4:LEU:HD13	12:Z:138:LEU:HD21	1.74	0.69
2:B:71:ASN:HD22	2:B:72:ASP:H	1.41	0.69
2:B:38:ILE:HD12	2:B:197:LEU:HG	1.75	0.69
14:N:136:GLY:HA2	14:2:161:GLN:NE2	2.08	0.68
2:B:121:GLN:O	2:B:124:THR:HB	1.93	0.68
13:M:152:ARG:HG3	13:M:152:ARG:HH11	1.57	0.68
2:P:51:GLU:OE2	2:P:202:THR:HG23	1.94	0.68
2:P:124:THR:CG2	3:Q:130:ARG:HH21	2.07	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:71:ASN:ND2	2:B:72:ASP:H	1.90	0.68
13:M:170:ASN:HD22	13:M:173:ARG:NH1	1.91	0.67
6:T:192:GLN:HE21	6:T:195:LYS:CE	2.06	0.67
6:F:12:ASN:HD21	6:F:124:THR:HA	1.58	0.67
5:S:15:PHE:H	6:T:23:GLN:HE22	1.40	0.67
2:B:71:ASN:ND2	2:B:72:ASP:N	2.41	0.67
11:K:208:ASN:O	9:W:29:ASN:ND2	2.27	0.67
6:F:95:GLU:HG3	6:F:115:ARG:HH11	1.59	0.67
13:1:0:THR:HG23	13:1:1:SER:N	2.11	0.66
2:B:65:GLU:HG3	2:B:66:LYS:HG3	1.78	0.65
1:A:130:ARG:NH2	7:G:124:THR:HG22	2.07	0.65
14:N:157:HIS:HD2	14:N:187(J):LEU:HD13	1.61	0.65
1:O:130:ARG:NH2	7:U:124:THR:HG22	2.11	0.65
14:N:55:ILE:HD11	14:N:95:LEU:HD13	1.77	0.65
11:K:4:LEU:HD13	11:K:159:ILE:HD11	1.77	0.65
2:B:67:LEU:HD22	2:B:211:GLU:HB3	1.77	0.65
12:L:4:LEU:CD1	12:L:138:LEU:HD21	2.26	0.64
5:S:35:SER:HB2	5:S:53:ARG:HB2	1.78	0.64
2:B:124:THR:CG2	3:C:130:ARG:HH21	2.11	0.64
13:1:152:ARG:HH11	13:1:152:ARG:CG	2.10	0.64
13:M:147:ARG:HH11	8:V:165:ASN:HD22	1.46	0.64
6:T:35:THR:HG21	6:T:51:GLU:O	1.98	0.64
5:E:227:GLU:CD	5:E:227:GLU:H	2.06	0.64
6:T:31:VAL:HG11	6:T:135:SER:HB2	1.78	0.63
7:G:49:ILE:CD1	7:G:193:ALA:HB1	2.28	0.63
3:Q:163:GLN:NE2	3:Q:164:THR:H	1.95	0.63
1:O:121:GLN:O	1:O:124:THR:HB	1.98	0.63
5:S:97:ASN:HD21	12:Z:61:ASN:ND2	1.94	0.63
7:G:49:ILE:CD1	7:G:193:ALA:CB	2.77	0.63
10:X:32:ASP:OD2	10:X:34:THR:HG22	1.98	0.63
8:V:197:ARG:HH21	9:W:139:GLU:HG3	1.63	0.63
1:O:86:ARG:HH21	7:U:118:ASN:ND2	1.95	0.62
4:D:40:ILE:HD12	4:D:193:VAL:HG23	1.80	0.62
6:F:169:ARG:HG3	6:F:173:LYS:HE3	1.81	0.62
12:L:134:ILE:HD11	12:L:162:ALA:HB2	1.82	0.62
12:Z:34:VAL:HG12	12:Z:176:LEU:HD22	1.81	0.62
7:G:87:ASN:C	7:G:87:ASN:HD22	2.08	0.62
2:P:69:LYS:HG3	2:P:221:GLN:OE1	2.00	0.62
1:O:86:ARG:HE	7:U:118:ASN:ND2	1.96	0.61
7:U:67:ILE:HD12	7:U:211:GLU:HG2	1.81	0.61
6:T:166:GLY:O	6:T:169:ARG:HB3	2.01	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:T:192:GLN:HE21	6:T:195:LYS:HE2	1.65	0.61
10:J:143:ARG:O	10:J:146:MET:HG3	2.00	0.61
5:S:73:HIS:HE1	5:S:107:LEU:O	1.83	0.61
7:U:184(G):GLU:HG2	7:U:188:LYS:CB	2.30	0.61
12:L:43:MET:HG3	12:L:101:ILE:HG22	1.82	0.61
2:P:97:GLN:HE21	9:W:61:TYR:HA	1.66	0.61
9:I:165:ARG:NH2	12:Z:135:MET:HE2	2.15	0.61
14:2:176:VAL:HG12	14:2:178:LEU:HD13	1.82	0.61
7:U:87:ASN:C	7:U:87:ASN:HD22	2.08	0.60
5:E:24:VAL:O	5:E:28:LEU:HD12	2.01	0.60
7:G:77:VAL:CG1	7:G:137:THR:HB	2.30	0.60
9:I:29:ASN:ND2	11:Y:208:ASN:O	2.34	0.60
2:P:65:GLU:HG3	2:P:66:LYS:HG3	1.84	0.60
14:2:55:ILE:HD11	14:2:95:LEU:HD13	1.82	0.60
1:A:97:HIS:HD2	8:H:61:SER:OG	1.84	0.60
4:D:140:GLY:HA2	4:D:215:ILE:HG12	1.81	0.60
7:G:77:VAL:HG12	7:G:137:THR:HB	1.84	0.60
6:T:187:ARG:HH11	6:T:187:ARG:HG2	1.66	0.60
10:X:146:MET:HE2	10:X:150:GLU:HB3	1.83	0.60
6:T:169:ARG:HG3	6:T:173:LYS:HE3	1.84	0.60
5:S:207:LEU:HA	5:S:209(E):ASN:ND2	2.09	0.59
3:C:216:LYS:HB2	3:C:220:ASP:HB3	1.84	0.59
14:N:14:LEU:HD11	14:N:102:ALA:HB3	1.84	0.59
7:G:79:ASN:OD1	7:G:165:THR:HB	2.02	0.59
7:G:121:GLN:O	7:G:124:THR:HB	2.02	0.59
13:1:170:ASN:HD22	13:1:173:ARG:HH11	1.49	0.59
6:T:42:CYS:HB2	6:T:184:LEU:O	2.03	0.59
10:J:21:THR:HG21	10:X:167:PRO:HB3	1.85	0.59
11:K:111:TYR:CZ	11:K:121:LYS:HG3	2.37	0.59
2:P:202:THR:HG22	2:P:204:SER:H	1.68	0.59
9:I:165:ARG:NH2	12:Z:135:MET:CE	2.66	0.59
10:J:146:MET:HE2	10:J:150:GLU:HB3	1.84	0.58
3:Q:55:THR:HG22	3:Q:56:LEU:HD22	1.84	0.58
2:P:169:THR:O	2:P:173:GLN:HB2	2.03	0.58
5:E:132:TYR:O	5:E:153:PRO:HB3	2.04	0.58
5:S:114:HIS:HB3	6:T:86:ARG:NH2	2.18	0.58
10:X:6:ILE:HD11	10:X:142:TYR:CE1	2.39	0.58
6:F:37:SER:HB3	6:F:50:VAL:HG23	1.86	0.58
6:T:95:GLU:HG3	6:T:115:ARG:HH11	1.67	0.58
13:1:69:ASN:HB3	13:1:72:ALA:HB2	1.84	0.58
6:F:13:SER:HB2	7:G:130:ARG:HB3	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:S:132:TYR:O	5:S:153:PRO:HB3	2.04	0.57
14:2:146:MET:HE2	14:2:150:GLU:HB3	1.86	0.57
2:B:97:GLN:NE2	9:I:64:ASN:HD22	2.01	0.57
6:F:36:THR:HB	6:F:168:GLY:H	1.69	0.57
2:B:112:LEU:HD23	2:B:112:LEU:C	2.29	0.57
1:O:60:MET:HE3	1:O:63:THR:HG21	1.86	0.57
3:C:206:GLY:HA3	3:C:209:ASN:CB	2.34	0.57
5:E:73:HIS:HE1	5:E:107:LEU:O	1.87	0.57
13:1:69:ASN:ND2	13:1:72:ALA:CA	2.66	0.57
4:D:12:VAL:HA	4:D:23:GLN:HG3	1.87	0.57
6:F:95:GLU:CG	6:F:115:ARG:HD2	2.34	0.57
4:R:162:ALA:HB1	4:R:176:LEU:HD22	1.87	0.57
6:T:13:SER:HB2	7:U:130:ARG:HB3	1.86	0.57
1:A:203:GLU:CD	1:A:203:GLU:H	2.13	0.57
5:E:12:THR:HG21	5:E:124:THR:HA	1.85	0.57
1:A:130:ARG:NH2	7:G:124:THR:CG2	2.59	0.57
3:C:160:TRP:CZ2	4:D:59:LEU:HD23	2.39	0.56
5:E:109:VAL:HG12	5:E:149:LEU:HD22	1.87	0.56
3:C:206:GLY:HA3	3:C:209:ASN:HB3	1.86	0.56
2:B:185:LYS:HD3	2:B:186:VAL:N	2.19	0.56
6:T:9:ASP:HB2	6:T:26:TYR:HE2	1.70	0.56
6:T:12:ASN:C	6:T:14:VAL:H	2.13	0.56
10:X:48:GLU:HB3	10:X:96:GLN:HB2	1.87	0.56
5:S:143:LYS:HE3	13:1:82:TYR:OH	2.06	0.56
6:T:170:GLN:CD	6:T:170:GLN:N	2.54	0.56
1:A:124:THR:CG2	2:B:130:ARG:HH21	2.18	0.56
2:B:15:PHE:H	3:C:23:GLN:HE22	1.51	0.56
6:T:35:THR:CG2	6:T:51:GLU:O	2.53	0.56
5:E:86:ARG:O	5:E:90:ASN:HB2	2.06	0.56
6:T:192:GLN:HE21	6:T:195:LYS:HE3	1.70	0.56
4:D:215:ILE:HG22	4:D:221:PHE:CD2	2.40	0.56
13:M:170:ASN:ND2	13:M:173:ARG:HH11	2.04	0.56
12:Z:-2:ASN:HA	12:Z:21:ILE:O	2.05	0.56
3:Q:160:TRP:CZ2	4:R:59:LEU:HD23	2.41	0.56
14:N:157:HIS:CD2	14:N:187(J):LEU:HD13	2.41	0.56
8:H:172:ASN:HD22	8:H:193:THR:HA	1.71	0.55
5:S:209(B):THR:H	5:S:209(E):ASN:HB2	1.71	0.55
6:T:12:ASN:O	6:T:14:VAL:N	2.40	0.55
10:X:24:ILE:HG12	10:X:24:ILE:O	2.06	0.55
3:C:57:LYS:O	3:C:58:LEU:CB	2.55	0.55
10:J:34:THR:HG21	10:J:176:LYS:NZ	2.21	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:71:ASN:ND2	2:P:72:ASP:H	2.04	0.55
9:W:110:ILE:HD12	9:W:125:ILE:HG12	1.87	0.55
10:X:161:GLU:OE2	10:X:161:GLU:HA	2.06	0.55
7:U:96:ALA:CA	7:U:107:MET:HE2	2.22	0.55
11:K:4:LEU:CD1	11:K:159:ILE:CD1	2.85	0.55
13:1:130:SER:HB3	13:1:132:THR:O	2.07	0.54
14:N:176:VAL:HG12	14:N:178:LEU:HD13	1.88	0.54
2:P:181:LYS:O	2:P:184:MET:HG3	2.08	0.54
10:X:7:ARG:O	10:X:7:ARG:HG3	2.06	0.54
9:I:2:ILE:HG21	9:I:130:ALA:HB3	1.88	0.54
12:L:166:HIS:HD2	12:L:168:GLN:H	1.56	0.54
14:N:36:ARG:HG3	14:N:42:TRP:CE2	2.43	0.54
1:A:121:GLN:O	1:A:124:THR:HB	2.08	0.54
5:E:207:LEU:HD23	5:E:207:LEU:H	1.73	0.54
5:S:97:ASN:ND2	12:Z:61:ASN:HD21	2.00	0.54
6:T:12:ASN:C	6:T:12:ASN:OD1	2.50	0.54
6:T:120:VAL:HG21	6:T:151:LEU:HD21	1.89	0.54
12:L:-2:ASN:HA	12:L:21:ILE:O	2.07	0.53
7:G:184(G):GLU:HG2	7:G:188:LYS:HB2	1.91	0.53
8:H:80:LEU:HD12	8:H:113:ILE:HD11	1.91	0.53
12:Z:-6:PRO:O	13:1:95:ARG:NH1	2.39	0.53
13:1:71:LEU:C	13:1:73:ASP:H	2.16	0.53
8:V:62:ASN:HB3	8:V:82:MET:HE1	1.91	0.53
7:G:49:ILE:HD11	7:G:193:ALA:HB3	1.91	0.53
10:J:4:LEU:HD21	10:J:134:THR:HG21	1.91	0.53
4:R:67:ILE:HG22	4:R:221:PHE:HZ	1.74	0.53
5:S:227:GLU:CD	5:S:227:GLU:H	2.16	0.53
12:Z:40:ASN:HD21	12:Z:183:GLY:HA2	1.73	0.53
1:A:8:TYR:HE2	6:F:127:ASN:OD1	1.92	0.53
12:L:40:ASN:ND2	12:L:183:GLY:HA2	2.22	0.53
12:L:135:MET:CE	9:W:165:ARG:NH2	2.67	0.53
6:T:186:ALA:O	6:T:190:VAL:HG23	2.09	0.53
5:E:54:ASN:ND2	5:E:56:ASP:O	2.42	0.53
14:N:161:GLN:HE21	14:2:136:GLY:CA	2.06	0.53
6:F:43:ASN:N	6:F:43:ASN:HD22	2.07	0.53
14:N:67:THR:HA	14:N:72:GLY:O	2.08	0.53
8:V:105:ASP:HB2	8:V:105(A):PRO:HD2	1.91	0.53
6:T:192:GLN:NE2	6:T:195:LYS:HE2	2.24	0.52
10:X:6:ILE:HD11	10:X:142:TYR:CD1	2.44	0.52
11:Y:196:PHE:HZ	11:Y:209:VAL:HG21	1.74	0.52
8:V:172:ASN:HB3	8:V:192:LEU:O	2.08	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:1:73:ASP:HA	13:1:77:ALA:HB2	1.91	0.52
4:R:186:LEU:O	4:R:190:GLU:HG3	2.09	0.52
4:R:215:ILE:HG22	4:R:221:PHE:HD2	1.75	0.52
9:W:113:PHE:HA	9:W:118:CYS:O	2.10	0.52
12:Z:134:ILE:HG22	12:Z:138:LEU:HD22	1.91	0.52
13:M:118:LEU:HG	13:M:133:LEU:HD12	1.92	0.52
7:G:224:LEU:HB3	7:G:228:ASN:HB2	1.91	0.52
6:T:7:GLY:C	6:T:9:ASP:H	2.18	0.52
6:F:158:TRP:CZ3	7:G:64:VAL:HA	2.45	0.52
1:A:86:ARG:HH21	7:G:118:ASN:HD22	1.58	0.52
9:W:166:ASP:OD2	9:W:168:LEU:N	2.41	0.52
10:X:24:ILE:HD13	11:Y:132:THR:HG21	1.91	0.52
8:H:197:ARG:HH21	9:I:139:GLU:HG3	1.75	0.52
7:U:152:ASP:HB2	7:U:153:PRO:CD	2.40	0.52
5:S:134:VAL:O	5:S:153:PRO:HG3	2.11	0.51
14:2:4:MET:HB3	14:2:126:ILE:HG22	1.92	0.51
3:C:40:VAL:HG12	3:C:162:ALA:HB1	1.93	0.51
5:E:107:LEU:HD11	5:E:111:ARG:HG2	1.92	0.51
11:K:174:ASN:HD21	11:K:189:ASN:ND2	2.03	0.51
12:L:9:GLU:O	12:L:107:LYS:HA	2.11	0.51
5:E:31:ILE:HD11	5:E:153:PRO:HD3	1.91	0.51
7:G:87:ASN:C	7:G:87:ASN:ND2	2.69	0.51
11:K:200:LYS:HG3	11:K:206:PHE:HB2	1.93	0.51
16:K:302:3SD:H28	17:K:303:MES:H81	1.91	0.51
2:P:107:ILE:HD11	2:P:111:ILE:HG22	1.92	0.51
2:P:112:LEU:C	2:P:112:LEU:HD23	2.35	0.51
12:L:19:ARG:NE	12:L:171:ASP:OD2	2.39	0.51
6:T:52:LYS:HG2	6:T:66:LYS:HD3	1.92	0.51
6:T:126:TYR:HB2	6:T:129:VAL:HG22	1.92	0.51
7:U:79:ASN:OD1	7:U:165:THR:HB	2.10	0.51
13:1:170:ASN:HD22	13:1:173:ARG:NH1	2.08	0.51
2:B:163:ILE:HG13	2:B:164:SER:N	2.26	0.51
6:T:187:ARG:HH11	6:T:187:ARG:HG3	1.72	0.51
8:V:50:ALA:HB2	9:W:118:CYS:HB2	1.93	0.51
7:U:87:ASN:C	7:U:87:ASN:ND2	2.68	0.51
1:A:112:LEU:O	1:A:116:VAL:HG23	2.11	0.51
5:E:207:LEU:H	5:E:207:LEU:CD2	2.24	0.51
7:G:151:THR:HG22	7:G:157:TYR:CB	2.40	0.51
9:I:182:ASP:OD1	9:I:182:ASP:N	2.40	0.51
2:B:41:MET:HB2	2:B:148:LEU:HD22	1.93	0.50
6:F:31:VAL:HG11	6:F:135:SER:HB2	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:N:14:LEU:O	14:N:175:MET:HA	2.11	0.50
5:E:111:ARG:HG2	5:E:111:ARG:HH11	1.74	0.50
7:G:49:ILE:HD13	7:G:193:ALA:HB1	1.94	0.50
2:P:78:VAL:HG22	2:P:136:PHE:CE2	2.47	0.50
1:A:233:LEU:O	1:A:236:LEU:HB2	2.11	0.50
2:B:69:LYS:HG3	2:B:221:GLN:OE1	2.11	0.50
14:2:14:LEU:HD23	14:2:44:CYS:SG	2.52	0.50
12:Z:9:GLU:O	12:Z:107:LYS:HA	2.12	0.50
3:Q:156:ILE:HD12	4:R:83:ALA:HB2	1.94	0.50
8:V:105:ASP:HB2	8:V:105(A):PRO:CD	2.41	0.50
2:P:97:GLN:NE2	9:W:64:ASN:HD22	2.07	0.50
6:F:203:GLU:HA	6:F:206:LYS:HB3	1.94	0.49
6:T:176:LEU:HB3	7:U:58:LEU:HD21	1.93	0.49
6:F:187:ARG:HH11	6:F:187:ARG:HG2	1.76	0.49
7:G:233:LEU:O	7:G:236:ILE:HG13	2.12	0.49
2:B:52:ARG:HH22	2:B:63(A):SER:HB3	1.77	0.49
6:F:38:ILE:HG22	6:F:164:ALA:HB2	1.94	0.49
12:L:7:ALA:HB2	12:L:110:VAL:HG23	1.94	0.49
2:P:126:HIS:HB3	3:Q:129:VAL:HG12	1.95	0.49
5:S:226:GLY:O	5:S:229:VAL:HG22	2.13	0.49
2:B:215:ILE:HG12	2:B:221:GLN:HG2	1.95	0.49
6:F:127:ASN:C	6:F:127:ASN:HD22	2.20	0.49
7:G:49:ILE:CD1	7:G:193:ALA:HB3	2.42	0.49
3:Q:168:ASN:O	3:Q:172:VAL:HG12	2.13	0.49
11:K:86:LEU:C	11:K:86:LEU:HD13	2.38	0.48
1:O:39:GLY:HA2	1:O:47:VAL:O	2.12	0.48
3:Q:71:ASP:HA	10:X:68:ILE:HD13	1.94	0.48
7:G:105:TYR:OH	8:H:66:HIS:HE1	1.95	0.48
2:P:15:PHE:H	3:Q:23:GLN:HE22	1.60	0.48
2:P:152:ASN:HB2	2:P:153:PRO:HD2	1.95	0.48
3:Q:163:GLN:HE21	3:Q:164:THR:N	2.03	0.48
7:G:59:LEU:O	7:G:61:PRO:HD3	2.13	0.48
4:R:179:GLU:HB3	4:R:192:LEU:HD21	1.95	0.48
5:S:198:SER:C	5:S:200:SER:H	2.21	0.48
7:U:38:LEU:C	7:U:38:LEU:HD12	2.38	0.48
11:Y:114:ASP:OD1	11:Y:116:ASP:HB2	2.14	0.48
6:F:12:ASN:C	6:F:14:VAL:H	2.21	0.48
6:T:95:GLU:HG2	6:T:115:ARG:CB	2.41	0.48
11:K:87:VAL:CG1	11:K:115:SER:HA	2.43	0.48
6:T:9:ASP:HB2	6:T:26:TYR:CE2	2.49	0.48
5:S:12:THR:HG21	5:S:124:THR:HA	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:U:77:VAL:HG12	7:U:137:THR:HB	1.95	0.48
13:1:150:VAL:HG23	13:1:150:VAL:O	2.13	0.48
8:H:124:TYR:HB2	8:H:138:LEU:HD13	1.94	0.48
13:M:147:ARG:HH11	8:V:165:ASN:ND2	2.09	0.48
5:E:100:SER:O	5:E:104:ASN:HA	2.14	0.48
5:S:139:ILE:HD12	5:S:215:VAL:HG12	1.95	0.48
6:T:127:ASN:C	6:T:127:ASN:HD22	2.21	0.48
8:V:172:ASN:HD22	8:V:193:THR:HA	1.79	0.48
6:F:35:THR:CG2	6:F:51:GLU:O	2.56	0.47
5:S:52:LYS:HD2	5:S:63:TYR:O	2.14	0.47
13:1:118:LEU:HG	13:1:133:LEU:HD12	1.96	0.47
14:2:36:ARG:HG3	14:2:42:TRP:CE2	2.49	0.47
13:M:88:ALA:HA	13:M:121:VAL:HG21	1.96	0.47
13:M:120:TYR:O	13:M:127:THR:HA	2.13	0.47
7:U:39:ALA:HB2	7:U:48:VAL:HG12	1.97	0.47
12:L:-7:ASN:ND2	12:L:-5:TYR:H	2.12	0.47
2:P:146:TYR:OH	2:P:216(A):LYS:HB2	2.14	0.47
9:W:2:ILE:HG21	9:W:130:ALA:HB3	1.97	0.47
13:1:6:LYS:HB3	13:1:11:VAL:HG12	1.96	0.47
12:L:135:MET:HE3	9:W:165:ARG:HH21	1.75	0.47
1:O:118:LYS:O	1:O:122:GLU:HG3	2.14	0.47
5:S:86:ARG:O	5:S:90:ASN:HB2	2.14	0.47
5:S:160:LEU:HD13	5:S:163:THR:HB	1.96	0.47
8:V:197:ARG:NH2	9:W:139:GLU:HG3	2.28	0.47
14:2:55:ILE:O	14:2:59:VAL:HG23	2.15	0.47
2:P:76:VAL:HG12	2:P:138:TYR:CD2	2.50	0.47
13:1:84:PHE:CZ	13:1:119:ARG:HG2	2.48	0.47
13:1:71:LEU:C	13:1:73:ASP:N	2.69	0.47
6:F:18:ASP:OD2	6:F:18:ASP:N	2.47	0.47
11:K:197:TRP:CD1	9:W:190:LYS:HE3	2.50	0.47
2:P:78:VAL:HG22	2:P:136:PHE:HE2	1.78	0.47
6:T:237:GLN:HA	6:T:237:GLN:NE2	2.30	0.47
9:W:29:ASN:HB3	9:W:171:TRP:CE3	2.50	0.47
12:Z:-7:ASN:HD22	12:Z:-6:PRO:HD2	1.79	0.47
13:1:66:ALA:HA	13:1:72:ALA:CB	2.44	0.47
4:R:194:LEU:HD12	4:R:207:LEU:HD11	1.95	0.47
13:1:152:ARG:HG3	13:1:152:ARG:NH1	2.14	0.47
11:Y:4:LEU:HD13	11:Y:159:ILE:HD11	1.96	0.47
11:Y:156:LYS:HD3	11:Y:195:LEU:HD11	1.96	0.47
12:Z:112:SER:HB3	12:Z:125:ARG:HG2	1.97	0.47
6:F:42:CYS:HB2	6:F:184:LEU:O	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:113:ILE:HA	10:J:118:THR:O	2.15	0.47
2:B:185:LYS:HD3	2:B:187:ASP:H	1.81	0.46
6:F:210:LEU:HD21	6:F:212:ILE:HD11	1.96	0.46
7:U:107:MET:HE3	7:U:112:LEU:HD13	1.97	0.46
8:V:126:SER:O	8:V:127:LEU:HD23	2.16	0.46
4:R:52:LYS:HE3	4:R:211:GLN:HB2	1.97	0.46
10:X:113:ILE:HA	10:X:118:THR:O	2.16	0.46
13:1:120:TYR:O	13:1:127:THR:HA	2.16	0.46
14:2:149:GLU:H	14:2:149:GLU:HG3	1.56	0.46
7:U:49:ILE:HD13	7:U:193:ALA:HB1	1.98	0.46
10:X:12:VAL:HG23	10:X:108:PRO:HB2	1.97	0.46
1:A:81:MET:HE1	7:G:21:LEU:HD11	1.97	0.46
6:F:150:MET:O	6:F:157:TYR:HA	2.15	0.46
5:S:188:GLU:OE1	5:S:191:LYS:HD2	2.16	0.46
6:T:169:ARG:HB3	6:T:169:ARG:HE	1.68	0.46
10:X:2:ILE:HG13	10:X:130:SER:OG	2.14	0.46
12:Z:113:PHE:CD2	12:Z:119:TYR:HB3	2.50	0.46
2:P:138:TYR:HB2	2:P:149:TYR:HB2	1.97	0.46
4:R:215:ILE:HG13	4:R:215:ILE:O	2.16	0.46
11:Y:87:VAL:CG1	11:Y:115:SER:HA	2.46	0.46
1:A:13:THR:HG22	1:A:21:LEU:HD22	1.98	0.46
2:B:166:GLY:O	2:B:169:THR:HG23	2.15	0.46
11:K:6:PHE:HA	11:K:123:ASP:O	2.15	0.46
11:K:210:ILE:HB	9:W:30:LYS:HE3	1.96	0.46
2:P:152:ASN:HB2	2:P:153:PRO:CD	2.46	0.46
3:Q:216:LYS:HB2	3:Q:220:ASP:HB3	1.97	0.46
4:D:161:ASN:HB3	4:D:180:TRP:CE2	2.51	0.46
7:G:39:ALA:HB2	7:G:48:VAL:HG12	1.97	0.46
7:U:168:LYS:HD2	7:U:201:LEU:HD22	1.98	0.46
7:U:233:LEU:O	7:U:236:ILE:HG13	2.16	0.46
8:H:144:GLN:O	8:H:145:ASP:HB2	2.15	0.45
13:1:73:ASP:O	13:1:73:ASP:CG	2.58	0.45
6:F:126:TYR:HE1	7:G:129:MET:SD	2.40	0.45
7:G:215:ALA:HB2	7:G:221:PHE:HD2	1.81	0.45
8:H:3:ILE:HG13	8:H:100:ILE:HD12	1.98	0.45
1:O:97:HIS:HD2	8:V:61:SER:OG	1.98	0.45
2:P:147:GLN:HG2	3:Q:62(A):ILE:HG21	1.98	0.45
3:Q:169:SER:HA	3:Q:172:VAL:HG13	1.97	0.45
4:R:85:ALA:O	4:R:89:ILE:HG12	2.17	0.45
10:X:120:VAL:HG13	10:X:122:LEU:HG	1.97	0.45
10:J:2:ILE:HB	10:J:17:SER:HB3	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:N:32:ASP:OD1	14:N:186:ARG:NH2	2.50	0.45
1:O:78:TYR:HB3	1:O:85:TYR:CD1	2.52	0.45
4:R:209:GLU:HG3	4:R:226:ASN:HB3	1.98	0.45
6:T:126:TYR:HE1	7:U:129:MET:SD	2.39	0.45
2:B:150:THR:O	2:B:157:TYR:HA	2.16	0.45
7:G:78:VAL:HG11	7:G:85:ALA:CB	2.46	0.45
10:J:166:MET:HE2	10:J:166:MET:HB3	1.89	0.45
7:U:192:PHE:CD1	7:U:192:PHE:C	2.94	0.45
4:D:90:GLU:OE1	11:K:69:ARG:HD2	2.17	0.45
6:F:11:SER:HB2	6:F:14:VAL:HG23	1.98	0.45
2:P:45:GLY:HA2	2:P:146:TYR:CE1	2.52	0.45
6:T:79:SER:OG	6:T:165:THR:HG23	2.17	0.45
7:G:151:THR:HG22	7:G:157:TYR:HB2	1.98	0.45
3:Q:97:GLN:HG3	10:X:65:LEU:HB2	1.97	0.45
5:S:207:LEU:HD23	5:S:207:LEU:H	1.81	0.45
8:V:172:ASN:ND2	8:V:193:THR:HG22	2.32	0.45
4:D:45:GLY:HA2	4:D:146:TYR:CE1	2.52	0.45
1:O:20:LYS:HA	1:O:20:LYS:HD3	1.78	0.45
13:1:120:TYR:HE1	13:1:135:THR:HG22	1.81	0.45
10:J:7:ARG:HG3	10:J:7:ARG:O	2.16	0.45
7:U:151:THR:HG22	7:U:157:TYR:HB2	1.99	0.45
8:V:3:ILE:HD11	8:V:127:LEU:HB2	1.99	0.45
10:X:44:SER:OG	10:X:100:LEU:HB2	2.17	0.45
5:E:92:LEU:HD11	5:E:112:ALA:HB1	1.98	0.45
6:F:203:GLU:C	6:F:205:ASN:H	2.24	0.45
1:O:152:ASP:HB3	1:O:153:PRO:HD2	1.99	0.45
7:U:47:VAL:HG12	7:U:49:ILE:HD12	1.99	0.45
7:U:49:ILE:HD13	7:U:193:ALA:CB	2.48	0.45
13:1:0:THR:HG23	13:1:1:SER:H	1.80	0.45
14:2:14:LEU:O	14:2:175:MET:HA	2.16	0.45
3:C:17:PRO:HA	4:D:26:TYR:CD1	2.51	0.44
5:E:103:PHE:HE2	13:M:61:LEU:HD21	1.82	0.44
1:O:150:GLN:O	1:O:157:TYR:HA	2.17	0.44
10:X:90(A):ILE:HD12	10:X:90(A):ILE:HA	1.81	0.44
13:1:39:ASN:H	13:1:39:ASN:HD22	1.65	0.44
12:L:137:PHE:CE1	12:L:141:GLN:HG3	2.52	0.44
13:M:119:ARG:HH11	13:M:129:SER:HB2	1.82	0.44
4:R:51:GLU:HG3	4:R:201:MET:HE3	1.99	0.44
4:R:163:LYS:HG3	4:R:164:ALA:N	2.32	0.44
5:S:173:LYS:O	5:S:177:GLU:HB2	2.16	0.44
9:W:143:GLU:HG3	9:W:146:LEU:HD21	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:1:120:TYR:CE1	13:1:135:THR:HG22	2.52	0.44
7:G:152:ASP:HB2	7:G:153:PRO:CD	2.47	0.44
9:I:48:LEU:HG	9:I:50:THR:HG22	2.00	0.44
10:J:59:ILE:O	10:J:63:ILE:HG12	2.18	0.44
11:K:63:CYS:SG	11:K:74:ILE:HG21	2.58	0.44
7:U:180(A):ILE:CD1	7:U:184:ASN:HB2	2.48	0.44
1:A:118:LYS:O	1:A:122:GLU:HG3	2.17	0.44
12:L:114:ASP:OD2	12:L:114:ASP:C	2.60	0.44
6:T:22:PHE:HD1	6:T:22:PHE:HA	1.76	0.44
1:A:97:HIS:CD2	8:H:61:SER:OG	2.69	0.44
3:C:17:PRO:HA	4:D:26:TYR:CE1	2.53	0.44
4:D:192:LEU:O	4:D:196:ILE:HG13	2.18	0.44
2:P:60:GLU:O	2:P:63(A):SER:HB2	2.17	0.44
5:S:227:GLU:CD	5:S:227:GLU:N	2.76	0.44
10:J:12:VAL:HG23	10:J:108:PRO:HB2	2.00	0.44
6:T:43:ASN:HD22	6:T:44:ASP:H	1.65	0.44
11:Y:31:VAL:HG21	16:Y:302:3SD:H25	2.00	0.44
13:1:88:ALA:HA	13:1:121:VAL:HG21	2.00	0.44
3:Q:150:GLN:HE21	3:Q:160:TRP:NE1	2.16	0.44
5:S:11:ASP:OD1	5:S:13:VAL:HG12	2.17	0.44
5:S:209(B):THR:N	5:S:209(E):ASN:HB2	2.32	0.44
6:T:13:SER:O	7:U:130:ARG:HB3	2.16	0.44
12:Z:51:ASP:OD1	12:Z:95:TYR:HA	2.17	0.44
14:2:32:ASP:OD1	14:2:186:ARG:NH2	2.51	0.44
7:G:151:THR:HG22	7:G:157:TYR:HB3	1.99	0.44
9:I:33:LYS:O	9:I:44:GLY:HA2	2.17	0.44
10:J:137:LEU:HD21	11:Y:140:SER:OG	2.18	0.44
13:M:39:ASN:N	13:M:39:ASN:HD22	2.16	0.44
6:T:43:ASN:HD22	6:T:44:ASP:N	2.16	0.44
3:C:228:GLU:O	3:C:232:TYR:HD1	2.01	0.44
13:1:152:ARG:CG	13:1:152:ARG:NH1	2.76	0.44
1:A:78:TYR:HB3	1:A:85:TYR:CD1	2.52	0.43
4:D:97:VAL:HG11	11:K:65:LEU:HD22	2.00	0.43
5:E:31:ILE:HD11	5:E:153:PRO:CD	2.48	0.43
12:Z:129:ALA:HB1	12:Z:166:HIS:CE1	2.53	0.43
14:2:34:LEU:HD13	14:2:176:VAL:HG23	2.00	0.43
5:E:179:THR:O	5:E:180:LEU:C	2.61	0.43
8:H:165:ASN:HD22	13:1:147:ARG:HH11	1.65	0.43
12:L:144(A):LYS:HB3	12:L:144(A):LYS:HE3	1.81	0.43
2:P:116:LEU:HD23	2:P:116:LEU:HA	1.83	0.43
3:C:35:THR:HB	3:C:51:GLU:HG3	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:R:194:LEU:HD22	4:R:212:LEU:HD11	2.00	0.43
7:U:150:LYS:O	7:U:157:TYR:HA	2.17	0.43
6:F:35:THR:CG2	6:F:36:THR:N	2.81	0.43
7:G:192:PHE:CD1	7:G:192:PHE:C	2.95	0.43
8:H:172:ASN:ND2	8:H:193:THR:HA	2.34	0.43
3:Q:36:CYS:H	3:Q:51:GLU:HG2	1.83	0.43
3:Q:57:LYS:HD2	3:Q:58:LEU:N	2.33	0.43
2:B:37:ALA:O	2:B:164:SER:HA	2.19	0.43
11:K:87:VAL:HG13	11:K:115:SER:HA	2.00	0.43
2:B:125:GLN:HG3	3:C:130:ARG:HG2	2.01	0.43
10:J:34:THR:HG21	10:J:176:LYS:HZ3	1.83	0.43
5:S:74:MET:HE2	5:S:109:VAL:HA	2.00	0.43
5:S:76:LEU:HA	5:S:137:LEU:O	2.19	0.43
4:D:75:GLY:HA3	4:D:221:PHE:CE2	2.54	0.43
13:M:7:TYR:CE2	13:M:161:VAL:HG22	2.54	0.43
14:N:8:PHE:HB2	14:N:146:MET:O	2.19	0.43
4:D:194:LEU:HD22	4:D:212:LEU:HD11	2.00	0.43
9:I:156:SER:O	9:I:160:LEU:HD22	2.19	0.43
5:S:75:GLY:HA3	5:S:221:PHE:CE2	2.54	0.43
9:W:11:CYS:HA	9:W:104:ILE:HD11	2.00	0.43
13:1:71:LEU:O	13:1:73:ASP:N	2.52	0.43
13:1:141:MET:C	13:1:144:PRO:HD2	2.44	0.43
4:D:67:ILE:HG22	4:D:221:PHE:HZ	1.82	0.43
4:D:85:ALA:O	4:D:89:ILE:HG12	2.18	0.43
6:F:187:ARG:HG2	6:F:187:ARG:NH1	2.34	0.43
10:J:140:HIS:HE1	11:Y:203:GLU:OE1	2.01	0.43
3:C:215:VAL:HB	3:C:221:ILE:HG12	2.01	0.43
5:E:160:LEU:HD13	5:E:163:THR:HB	2.01	0.43
2:P:69:LYS:CG	2:P:221:GLN:OE1	2.66	0.43
7:U:123:TYR:CE1	7:U:129:MET:HE3	2.54	0.43
7:U:152:ASP:HB2	7:U:153:PRO:HD2	1.98	0.43
9:W:55:LEU:HD11	9:W:97:VAL:HG21	2.00	0.43
13:M:16:ASP:HA	13:M:186:PHE:CB	2.49	0.42
13:M:39:ASN:HD22	13:M:39:ASN:H	1.66	0.42
13:M:152:ARG:HH11	13:M:152:ARG:CG	2.29	0.42
8:V:109:HIS:HB3	8:V:111:PHE:CE2	2.54	0.42
1:A:58:LEU:HD12	7:G:173:THR:HG23	2.00	0.42
2:B:149:TYR:CZ	3:C:62(A):ILE:HD12	2.55	0.42
2:B:152:ASN:HB2	2:B:153:PRO:CD	2.48	0.42
2:P:21:LEU:O	2:P:22:TYR:C	2.62	0.42
2:P:97:GLN:NE2	9:W:61:TYR:HA	2.33	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Q:71:ASP:OD1	3:Q:100:ARG:NH1	2.52	0.42
7:U:48:VAL:HG13	7:U:139:VAL:HG11	2.01	0.42
10:X:129:TYR:O	10:X:132:PHE:HB2	2.19	0.42
4:D:38:ILE:HD12	4:D:197:LEU:HG	2.00	0.42
3:C:206:GLY:HA3	3:C:209:ASN:HB2	2.00	0.42
6:F:24:VAL:HG11	6:F:154:SER:HB3	2.01	0.42
3:Q:140:GLY:HA2	3:Q:215:VAL:HG21	2.01	0.42
14:2:15:GLY:HA2	14:2:174:ARG:O	2.19	0.42
5:E:160:LEU:HD23	6:F:59:LEU:HA	1.99	0.42
7:G:172:ILE:H	7:G:172:ILE:HG13	1.71	0.42
11:K:5:ALA:HA	11:K:13:ILE:O	2.20	0.42
13:M:178:ARG:NH1	8:V:139:GLU:OE1	2.38	0.42
1:O:221:PHE:CD2	1:O:221:PHE:C	2.97	0.42
3:C:97:GLN:NE2	3:C:97:GLN:HA	2.35	0.42
5:S:111:ARG:HH11	5:S:111:ARG:HG2	1.84	0.42
8:V:112:SER:HB3	8:V:125:LEU:HD13	2.01	0.42
8:V:128:GLY:O	8:V:131:SER:HB2	2.19	0.42
11:Y:37:ILE:HB	11:Y:41:LEU:HB3	2.02	0.42
12:L:8:GLY:HA3	12:L:11:PHE:CE2	2.55	0.42
14:N:161:GLN:HE22	14:2:139:ASP:HB3	1.85	0.42
1:O:158:PHE:HD1	1:O:160:TRP:HE1	1.68	0.42
3:Q:215:VAL:HB	3:Q:221:ILE:HG12	2.02	0.42
5:S:15:PHE:H	6:T:23:GLN:NE2	2.12	0.42
8:V:128:GLY:O	8:V:131:SER:CB	2.67	0.42
2:B:234:VAL:HG22	2:B:239:THR:HA	2.02	0.42
4:D:40:ILE:CD1	4:D:193:VAL:HG23	2.47	0.42
10:J:44:SER:OG	10:J:100:LEU:HB2	2.20	0.42
6:T:210:LEU:HD21	6:T:212:ILE:HD11	2.01	0.42
10:X:112:GLN:HE22	10:X:126:ALA:H	1.68	0.42
1:A:41:LYS:HG3	1:A:46:VAL:HG22	2.02	0.42
2:B:152:ASN:HB2	2:B:153:PRO:HD2	2.02	0.42
12:L:2:THR:HG23	12:L:127:GLY:O	2.20	0.42
4:R:46:VAL:HG11	4:R:139:ALA:HB1	2.01	0.42
6:T:18:ASP:OD1	6:T:20:ARG:NH1	2.46	0.42
9:W:55:LEU:HD23	9:W:55:LEU:HA	1.91	0.42
10:X:3:ILE:HD11	10:X:127:HIS:HD2	1.84	0.42
11:Y:20:ALA:HA	16:Y:302:3SD:O19	2.20	0.42
12:Z:90:LYS:HD3	12:Z:95:TYR:CZ	2.55	0.42
1:A:67:VAL:HG11	1:A:213:ALA:CB	2.50	0.41
1:A:111:LEU:HD23	1:A:111:LEU:HA	1.95	0.41
3:C:57:LYS:CD	3:C:58:LEU:H	2.16	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:134:VAL:O	5:E:153:PRO:HG3	2.20	0.41
1:O:13:THR:O	2:P:130:ARG:HD3	2.20	0.41
7:U:96:ALA:CA	7:U:107:MET:CE	2.93	0.41
3:C:172:VAL:HG23	3:C:196:SER:HB2	2.01	0.41
5:E:226:GLY:O	5:E:229:VAL:HG22	2.20	0.41
11:K:114:ASP:OD1	11:K:114:ASP:C	2.63	0.41
3:C:237:GLU:HA	3:C:240:LYS:HB2	2.01	0.41
6:F:39:GLY:HA2	6:F:47:VAL:O	2.19	0.41
7:G:96:ALA:CA	7:G:107:MET:CE	2.93	0.41
8:H:3:ILE:HD11	8:H:127:LEU:HB2	2.01	0.41
11:K:112:TYR:O	11:K:119:ARG:HA	2.20	0.41
10:X:113:ILE:HG12	10:X:119:LYS:HG3	2.01	0.41
12:Z:113:PHE:CD1	12:Z:113:PHE:N	2.87	0.41
12:Z:146:LEU:HD22	12:Z:150:GLU:HG2	2.02	0.41
13:1:141:MET:HE1	13:1:178:ARG:HG3	2.03	0.41
8:H:223:ASP:OD2	8:H:223:ASP:N	2.54	0.41
12:L:153:LYS:HG2	8:V:201:GLN:HG3	2.02	0.41
1:O:67:VAL:HG11	1:O:213:ALA:HB3	2.03	0.41
3:Q:17:PRO:HA	4:R:26:TYR:CD1	2.55	0.41
6:T:18:ASP:OD1	6:T:20:ARG:HD3	2.20	0.41
9:W:55:LEU:CD1	9:W:97:VAL:HG21	2.50	0.41
11:Y:19:ARG:HH21	11:Y:29:GLN:HE22	1.68	0.41
6:F:95:GLU:HG3	6:F:115:ARG:HD2	2.03	0.41
6:F:127:ASN:C	6:F:127:ASN:ND2	2.79	0.41
10:J:3:ILE:HD13	10:J:3:ILE:HA	1.94	0.41
10:J:36:GLN:HG3	10:J:184:ILE:CD1	2.51	0.41
11:K:196:PHE:CE1	9:W:193:GLN:HG3	2.55	0.41
5:S:92:LEU:HD11	5:S:112:ALA:HB1	2.02	0.41
7:U:65:SER:HA	7:U:211:GLU:OE2	2.21	0.41
13:1:87:LEU:O	13:1:91:MET:HG2	2.20	0.41
2:B:163:ILE:HG13	2:B:164:SER:H	1.85	0.41
8:H:165:ASN:ND2	13:1:147:ARG:HH11	2.19	0.41
9:I:28:SER:CB	10:J:120:VAL:HG21	2.50	0.41
14:N:4:MET:HB3	14:N:126:ILE:HG22	2.02	0.41
7:U:59:LEU:O	7:U:61:PRO:HD3	2.20	0.41
11:Y:100:MET:SD	11:Y:125:PHE:HB2	2.61	0.41
12:Z:135:MET:N	12:Z:136:PRO:CD	2.83	0.41
2:B:44:ASP:OD2	2:B:44:ASP:N	2.54	0.41
6:F:170:GLN:H	6:F:170:GLN:CD	2.28	0.41
7:G:152:ASP:HB2	7:G:153:PRO:HD2	2.01	0.41
11:K:7:ARG:HG3	11:K:12:ILE:HG12	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:110:VAL:HG12	13:M:111:GLN:O	2.20	0.41
7:U:69:CYS:O	7:U:93:LYS:HE2	2.21	0.41
10:X:112:GLN:NE2	10:X:126:ALA:H	2.19	0.41
12:Z:112:SER:CB	12:Z:125:ARG:HG2	2.51	0.41
14:2:38:HIS:O	14:2:39:ASP:C	2.63	0.41
6:F:121:GLN:HE21	6:F:121:GLN:HB3	1.66	0.41
6:F:126:TYR:HB2	6:F:129:VAL:CG2	2.51	0.41
9:I:174:VAL:HG21	9:I:186:LYS:HE2	2.02	0.41
10:J:48:GLU:HB3	10:J:96:GLN:HB2	2.03	0.41
2:P:144(A):TYR:HB2	2:P:147:GLN:NE2	2.36	0.41
5:E:207(B):THR:H	5:E:209(E):ASN:HB2	1.84	0.41
6:F:166:GLY:O	6:F:169:ARG:HB3	2.21	0.41
1:O:11:SER:OG	2:P:129:LEU:HA	2.21	0.41
4:R:90:GLU:OE2	11:Y:69:ARG:NH1	2.54	0.41
5:S:13:VAL:HG21	6:T:128:SER:O	2.21	0.41
8:V:38:SER:O	8:V:39:PRO:C	2.63	0.41
10:X:52:THR:CG2	10:X:53:VAL:N	2.83	0.41
13:1:142:ALA:O	13:1:143:ASN:C	2.59	0.41
1:O:33:GLN:H	1:O:33:GLN:HG2	1.69	0.41
1:O:217(K):GLY:HA3	8:V:186:TYR:HB3	2.04	0.41
3:Q:53:ARG:HD3	3:Q:55:THR:OG1	2.20	0.41
11:Y:114:ASP:OD1	11:Y:114:ASP:C	2.64	0.41
13:1:121:VAL:HA	13:1:126:VAL:O	2.22	0.41
3:C:57:LYS:CD	3:C:58:LEU:N	2.80	0.40
11:K:99:THR:HB	11:K:113:VAL:O	2.22	0.40
13:M:6:LYS:HB3	13:M:11:VAL:HG12	2.03	0.40
13:M:141:MET:HE1	13:M:178:ARG:HG3	2.03	0.40
2:P:149:TYR:CZ	3:Q:62(A):ILE:HD12	2.56	0.40
6:T:7:GLY:O	7:U:11:HIS:CE1	2.74	0.40
6:T:143:LYS:HE3	6:T:143:LYS:HB3	1.93	0.40
14:2:36:ARG:HG3	14:2:42:TRP:CZ2	2.57	0.40
4:D:173:GLN:HE21	5:E:56:ASP:CG	2.29	0.40
5:E:198:SER:C	5:E:200:SER:H	2.30	0.40
3:Q:84:ASP:CG	3:Q:130:ARG:HH22	2.29	0.40
13:1:69:ASN:HA	13:1:70:PRO:HD2	1.97	0.40
3:C:84:ASP:CG	3:C:130:ARG:HH22	2.29	0.40
5:E:75:GLY:HA3	5:E:221:PHE:CE2	2.56	0.40
11:K:4:LEU:HD12	11:K:159:ILE:CD1	2.51	0.40
1:O:8:TYR:HE2	6:T:127:ASN:OD1	2.05	0.40
1:O:217(G):LEU:HD13	1:O:218:GLY:HA2	2.03	0.40
10:X:4:LEU:HD23	10:X:126:ALA:HB2	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:1:69:ASN:HD21	13:1:72:ALA:HA	1.82	0.40
2:B:46:ILE:HD11	2:B:146:TYR:HB3	2.01	0.40
5:E:68:ILE:HB	5:E:76:LEU:CD2	2.51	0.40
6:T:180(E):GLU:H	6:T:180(E):GLU:HG3	1.32	0.40
9:I:94:PRO:HB3	9:I:116:ILE:HG22	2.04	0.40
13:M:178:ARG:HD3	8:V:139:GLU:OE1	2.22	0.40
2:P:215:ILE:HG12	2:P:221:GLN:HG2	2.03	0.40
7:U:161:LYS:HG2	7:U:180(B):ASP:HB2	2.03	0.40
11:Y:87:VAL:HG13	11:Y:115:SER:HA	2.03	0.40
11:Y:200:LYS:HG3	11:Y:206:PHE:HB2	2.03	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	244/250 (98%)	239 (98%)	4 (2%)	1 (0%)	30	45
1	O	244/250 (98%)	232 (95%)	10 (4%)	2 (1%)	16	27
2	B	233/235 (99%)	218 (94%)	12 (5%)	3 (1%)	9	16
2	P	233/235 (99%)	217 (93%)	12 (5%)	4 (2%)	7	12
3	C	236/241 (98%)	227 (96%)	5 (2%)	4 (2%)	7	12
3	Q	236/241 (98%)	226 (96%)	7 (3%)	3 (1%)	9	16
4	D	224/260 (86%)	215 (96%)	8 (4%)	1 (0%)	30	45
4	R	225/260 (86%)	216 (96%)	8 (4%)	1 (0%)	30	45
5	E	228/233 (98%)	214 (94%)	12 (5%)	2 (1%)	14	24
5	S	228/233 (98%)	211 (92%)	14 (6%)	3 (1%)	9	16
6	F	240/242 (99%)	228 (95%)	11 (5%)	1 (0%)	30	45
6	T	240/242 (99%)	225 (94%)	12 (5%)	3 (1%)	9	16

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
7	G	238/243 (98%)	225 (94%)	13 (6%)	0	100	100
7	U	238/243 (98%)	229 (96%)	9 (4%)	0	100	100
8	H	220/222 (99%)	209 (95%)	11 (5%)	0	100	100
8	V	220/222 (99%)	210 (96%)	10 (4%)	0	100	100
9	I	202/204 (99%)	196 (97%)	6 (3%)	0	100	100
9	W	202/204 (99%)	192 (95%)	10 (5%)	0	100	100
10	J	196/198 (99%)	188 (96%)	7 (4%)	1 (0%)	24	39
10	X	196/198 (99%)	188 (96%)	7 (4%)	1 (0%)	24	39
11	K	210/212 (99%)	204 (97%)	5 (2%)	1 (0%)	24	39
11	Y	210/212 (99%)	201 (96%)	9 (4%)	0	100	100
12	L	220/222 (99%)	214 (97%)	6 (3%)	0	100	100
12	Z	220/222 (99%)	217 (99%)	3 (1%)	0	100	100
13	1	231/233 (99%)	221 (96%)	8 (4%)	2 (1%)	14	24
13	M	231/233 (99%)	221 (96%)	9 (4%)	1 (0%)	30	45
14	2	194/196 (99%)	186 (96%)	8 (4%)	0	100	100
14	N	194/196 (99%)	189 (97%)	5 (3%)	0	100	100
All	All	6233/6382 (98%)	5958 (96%)	241 (4%)	34 (0%)	24	39

All (34) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	58	LEU
4	D	180(E)	SER
11	K	180	GLU
2	P	218(C)	ASP
3	Q	58	LEU
3	Q	203	THR
6	T	13	SER
2	B	54	VAL
2	B	218(C)	ASP
6	F	13	SER
13	M	1	SER
1	O	167	LYS
5	S	199	GLN
5	S	202	ARG
1	A	167	LYS

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Mol	Chain	Res	Type
3	C	183	PRO
3	C	203	THR
5	E	203	ASP
5	E	217	LYS
1	O	53	LYS
2	P	54	VAL
2	P	218(D)	GLY
3	Q	183	PRO
6	T	8	TYR
3	C	55	THR
2	P	62	ASP
4	R	180(D)	SER
10	X	8	VAL
10	J	8	VAL
6	T	206	LYS
13	1	72	ALA
5	S	186	PRO
2	B	218(D)	GLY
13	1	220	GLY

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	205/209 (98%)	199 (97%)	6 (3%)	37	58
1	O	205/209 (98%)	189 (92%)	16 (8%)	11	20
2	B	194/195 (100%)	176 (91%)	18 (9%)	8	13
2	P	194/195 (100%)	181 (93%)	13 (7%)	15	25
3	C	210/213 (99%)	193 (92%)	17 (8%)	11	18
3	Q	210/213 (99%)	194 (92%)	16 (8%)	12	21
4	D	186/215 (86%)	172 (92%)	14 (8%)	12	21
4	R	186/215 (86%)	173 (93%)	13 (7%)	14	24
5	E	187/191 (98%)	167 (89%)	20 (11%)	6	9

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	S	187/191 (98%)	169 (90%)	18 (10%)	8	12
6	F	200/200 (100%)	178 (89%)	22 (11%)	6	9
6	T	200/200 (100%)	182 (91%)	18 (9%)	9	14
7	G	205/207 (99%)	192 (94%)	13 (6%)	16	29
7	U	205/207 (99%)	194 (95%)	11 (5%)	20	35
8	H	181/181 (100%)	171 (94%)	10 (6%)	19	33
8	V	181/181 (100%)	169 (93%)	12 (7%)	15	26
9	I	172/172 (100%)	161 (94%)	11 (6%)	16	28
9	W	172/172 (100%)	165 (96%)	7 (4%)	27	46
10	J	174/175 (99%)	162 (93%)	12 (7%)	14	24
10	X	174/175 (99%)	157 (90%)	17 (10%)	7	11
11	K	169/169 (100%)	153 (90%)	16 (10%)	8	13
11	Y	169/169 (100%)	159 (94%)	10 (6%)	18	30
12	L	185/185 (100%)	175 (95%)	10 (5%)	20	35
12	Z	185/185 (100%)	175 (95%)	10 (5%)	20	35
13	1	199/199 (100%)	189 (95%)	10 (5%)	22	37
13	M	199/199 (100%)	191 (96%)	8 (4%)	28	47
14	2	162/162 (100%)	151 (93%)	11 (7%)	14	25
14	N	162/162 (100%)	150 (93%)	12 (7%)	13	21
All	All	5258/5346 (98%)	4887 (93%)	371 (7%)	13	23

All (371) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	62	GLU
1	A	87	VAL
1	A	124	THR
1	A	158	PHE
1	A	212	LEU
1	A	222	ARG
2	B	58	LEU
2	B	61	GLN
2	B	63	THR
2	B	63(A)	SER
2	B	65	GLU

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Mol	Chain	Res	Type
2	B	67	LEU
2	B	71	ASN
2	B	91	THR
2	B	104	ASN
2	B	124	THR
2	B	150	THR
2	B	185	LYS
2	B	192	LEU
2	B	202	THR
2	B	216	ARG
2	B	216(A)	LYS
2	B	232	ILE
2	B	239	THR
3	C	18	ASP
3	C	25	GLU
3	C	55	THR
3	C	57	LYS
3	C	66	LYS
3	C	87	ILE
3	C	112	LEU
3	C	150	GLN
3	C	156	ILE
3	C	170	LYS
3	C	172	VAL
3	C	174	GLU
3	C	178	LYS
3	C	185	THR
3	C	209	ASN
3	C	215	VAL
3	C	226	SER
4	D	27	SER
4	D	28	LEU
4	D	48	LEU
4	D	52	LYS
4	D	59	LEU
4	D	110	GLU
4	D	119	LEU
4	D	170	GLU
4	D	177	LEU
4	D	191	LEU
4	D	192	LEU
4	D	194	LEU

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Mol	Chain	Res	Type
4	D	215	ILE
4	D	237	LEU
5	E	12	THR
5	E	13	VAL
5	E	28	LEU
5	E	32	LYS
5	E	58	LEU
5	E	76	LEU
5	E	78	LEU
5	E	90	ASN
5	E	97	ASN
5	E	111	ARG
5	E	149	LEU
5	E	189	LEU
5	E	198	SER
5	E	207	LEU
5	E	207(B)	THR
5	E	208(C)	VAL
5	E	219	THR
5	E	222	THR
5	E	227	GLU
5	E	231	LYS
6	F	9	ASP
6	F	11	SER
6	F	18	ASP
6	F	35	THR
6	F	43	ASN
6	F	59	LEU
6	F	72	ARG
6	F	98	SER
6	F	121	GLN
6	F	127	ASN
6	F	129	VAL
6	F	135	SER
6	F	136	THR
6	F	167	LYS
6	F	169	ARG
6	F	171	SER
6	F	176	LEU
6	F	187	ARG
6	F	192	GLN
6	F	203	GLU

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Mol	Chain	Res	Type
6	F	205	ASN
6	F	240	ILE
7	G	29	LYS
7	G	38	LEU
7	G	72	ARG
7	G	87	ASN
7	G	119	LEU
7	G	124	THR
7	G	171	GLU
7	G	197	MET
7	G	203	THR
7	G	204	GLU
7	G	217	LYS
7	G	232	ARG
7	G	233	LEU
8	H	7	LYS
8	H	34	LEU
8	H	55	VAL
8	H	56	THR
8	H	63	ILE
8	H	68	LEU
8	H	101	VAL
8	H	113	ILE
8	H	144	GLN
8	H	223	ASP
9	I	-8	SER
9	I	4	VAL
9	I	29	ASN
9	I	104	ILE
9	I	122(A)	LYS
9	I	159	LEU
9	I	160	LEU
9	I	171	TRP
9	I	174	VAL
9	I	181	LYS
9	I	182	ASP
10	J	6	ILE
10	J	34	THR
10	J	52	THR
10	J	68	ILE
10	J	70	GLU
10	J	90	SER

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Mol	Chain	Res	Type
10	J	90(A)	ILE
10	J	90(B)	ARG
10	J	130	SER
10	J	155	LEU
10	J	157	LEU
10	J	166	MET
11	K	4	LEU
11	K	7	ARG
11	K	9	GLN
11	K	31	VAL
11	K	35	ILE
11	K	41	LEU
11	K	65	LEU
11	K	69	ARG
11	K	73	ARG
11	K	87	VAL
11	K	91	LYS
11	K	99	THR
11	K	121	LYS
11	K	143	LYS
11	K	175	LEU
11	K	201	GLU
12	L	-9	GLN
12	L	4	LEU
12	L	14	LEU
12	L	25	SER
12	L	40	ASN
12	L	58	ARG
12	L	99	THR
12	L	118	SER
12	L	123	GLN
12	L	138	LEU
13	M	39	ASN
13	M	61	LEU
13	M	64	GLU
13	M	95	ARG
13	M	152	ARG
13	M	185	ASN
13	M	195	THR
13	M	217	LYS
14	N	10	ASP
14	N	20	THR

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Mol	Chain	Res	Type
14	N	65	LEU
14	N	84	LYS
14	N	105	ASP
14	N	105(A)	ASP
14	N	105(B)	LYS
14	N	115	LEU
14	N	119	VAL
14	N	132	THR
14	N	149	GLU
14	N	178	LEU
1	O	32	LYS
1	O	33	GLN
1	O	54	SER
1	O	62	GLU
1	O	64	LEU
1	O	65	SER
1	O	87	VAL
1	O	110	LYS
1	O	124	THR
1	O	158	PHE
1	O	165	ILE
1	O	170	VAL
1	O	212	LEU
1	O	222	ARG
1	O	223	LYS
1	O	236	LEU
2	P	55	THR
2	P	57	THR
2	P	58	LEU
2	P	90	ASN
2	P	91	THR
2	P	150	THR
2	P	156	ASN
2	P	170	SER
2	P	181	LYS
2	P	185	LYS
2	P	192	LEU
2	P	202	THR
2	P	203	ASP
3	Q	18	ASP
3	Q	35	THR
3	Q	40	VAL

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Mol	Chain	Res	Type
3	Q	57	LYS
3	Q	61	THR
3	Q	63	THR
3	Q	75	VAL
3	Q	156	ILE
3	Q	163	GLN
3	Q	172	VAL
3	Q	185	THR
3	Q	201	VAL
3	Q	208	LYS
3	Q	209	ASN
3	Q	215	VAL
3	Q	240	LYS
4	R	28	LEU
4	R	48	LEU
4	R	59	LEU
4	R	76	CYS
4	R	119	LEU
4	R	177	LEU
4	R	184	LEU
4	R	191	LEU
4	R	192	LEU
4	R	194	LEU
4	R	207	LEU
4	R	215	ILE
4	R	237	LEU
5	S	11	ASP
5	S	12	THR
5	S	13	VAL
5	S	32	LYS
5	S	33	GLN
5	S	43	ASN
5	S	58	LEU
5	S	76	LEU
5	S	111	ARG
5	S	168	ARG
5	S	189	LEU
5	S	198	SER
5	S	199	GLN
5	S	211	SER
5	S	219	THR
5	S	222	THR

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Mol	Chain	Res	Type
5	S	227	GLU
5	S	231	LYS
6	T	12	ASN
6	T	20	ARG
6	T	22	PHE
6	T	35	THR
6	T	36	THR
6	T	43	ASN
6	T	72	ARG
6	T	98	SER
6	T	127	ASN
6	T	169	ARG
6	T	170	GLN
6	T	171	SER
6	T	176	LEU
6	T	187	ARG
6	T	192	GLN
6	T	199	LEU
6	T	203	GLU
6	T	205	ASN
7	U	29	LYS
7	U	38	LEU
7	U	43	LYS
7	U	49	ILE
7	U	76	MET
7	U	87	ASN
7	U	119	LEU
7	U	204	GLU
7	U	232	ARG
7	U	233	LEU
7	U	239	GLN
8	V	13	VAL
8	V	30	ASN
8	V	34	LEU
8	V	55	VAL
8	V	56	THR
8	V	63	ILE
8	V	68	LEU
8	V	84	LYS
8	V	113	ILE
8	V	121	VAL
8	V	144	GLN

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Mol	Chain	Res	Type
8	V	221	ILE
9	W	-8	SER
9	W	29	ASN
9	W	122(A)	LYS
9	W	160	LEU
9	W	171	TRP
9	W	181	LYS
9	W	182	ASP
10	X	2	ILE
10	X	6	ILE
10	X	9	GLN
10	X	24	ILE
10	X	34	THR
10	X	35	ARG
10	X	52	THR
10	X	68	ILE
10	X	70	GLU
10	X	90	SER
10	X	90(A)	ILE
10	X	90(B)	ARG
10	X	120	VAL
10	X	137	LEU
10	X	157	LEU
10	X	166	MET
10	X	191	GLN
11	Y	4	LEU
11	Y	31	VAL
11	Y	41	LEU
11	Y	65	LEU
11	Y	69	ARG
11	Y	87	VAL
11	Y	145	ASP
11	Y	146	LEU
11	Y	208	ASN
11	Y	210	ILE
12	Z	-9	GLN
12	Z	2	THR
12	Z	4	LEU
12	Z	14	LEU
12	Z	25	SER
12	Z	40	ASN
12	Z	106	GLU

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Mol	Chain	Res	Type
12	Z	106(A)	ASP
12	Z	118	SER
12	Z	138	LEU
13	1	-8	THR
13	1	39	ASN
13	1	61	LEU
13	1	95	ARG
13	1	152	ARG
13	1	161	VAL
13	1	195	THR
13	1	203	LEU
13	1	204	GLN
13	1	217	LYS
14	2	20	THR
14	2	22	THR
14	2	36	ARG
14	2	78	THR
14	2	105	ASP
14	2	105(A)	ASP
14	2	105(B)	LYS
14	2	119	VAL
14	2	132	THR
14	2	149	GLU
14	2	178	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (188) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	97	HIS
2	B	23	GLN
2	B	71	ASN
2	B	97	GLN
2	B	121	GLN
2	B	125	GLN
2	B	156	ASN
2	B	177	GLN
3	C	20	HIS
3	C	23	GLN
3	C	120	GLN
3	C	121	GLN
3	C	125	GLN
3	C	163	GLN

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Mol	Chain	Res	Type
3	C	168	ASN
3	C	235	GLN
4	D	23	GLN
4	D	108	ASN
4	D	114	GLN
4	D	141	HIS
4	D	199	GLN
4	D	226	ASN
5	E	64	GLN
5	E	73	HIS
5	E	97	ASN
5	E	104	ASN
5	E	121	GLN
5	E	125	GLN
5	E	170	GLN
5	E	185	ASN
5	E	209(E)	ASN
6	F	12	ASN
6	F	23	GLN
6	F	43	ASN
6	F	90	ASN
6	F	121	GLN
6	F	127	ASN
7	G	11	HIS
7	G	34(A)	ASN
7	G	87	ASN
7	G	118	ASN
7	G	121	GLN
7	G	125	GLN
7	G	169	GLN
7	G	170	GLN
7	G	178	ASN
7	G	184	ASN
8	H	30	ASN
8	H	57	GLN
8	H	66	HIS
8	H	144	GLN
8	H	165	ASN
8	H	172	ASN
8	H	190	ASN
8	H	201	GLN
9	I	23	GLN

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Mol	Chain	Res	Type
9	I	29	ASN
9	I	81	GLN
9	I	157	GLN
9	I	193	GLN
10	J	36	GLN
10	J	54	GLN
10	J	62	ASN
10	J	77	GLN
10	J	85	GLN
10	J	112	GLN
10	J	140	HIS
10	J	186	GLN
11	K	9	GLN
11	K	85	ASN
11	K	174	ASN
11	K	189	ASN
11	K	207	ASN
12	L	-7	ASN
12	L	27	ASN
12	L	40	ASN
12	L	67	HIS
12	L	70(A)	ASN
12	L	82	ASN
12	L	123	GLN
12	L	166	HIS
13	M	-7	GLN
13	M	39	ASN
13	M	93	GLN
13	M	99	ASN
13	M	111	GLN
13	M	162	GLN
13	M	170	ASN
13	M	202	ASN
14	N	69	GLN
14	N	141	ASN
14	N	145	ASN
14	N	157	HIS
14	N	161	GLN
1	O	97	HIS
1	O	191	HIS
2	P	23	GLN
2	P	71	ASN

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Mol	Chain	Res	Type
2	P	97	GLN
2	P	121	GLN
2	P	125	GLN
2	P	156	ASN
2	P	177	GLN
2	P	218	ASN
3	Q	23	GLN
3	Q	44	ASN
3	Q	121	GLN
3	Q	125	GLN
3	Q	150	GLN
3	Q	163	GLN
3	Q	179	ASN
3	Q	235	GLN
3	Q	243	GLN
4	R	23	GLN
4	R	108	ASN
4	R	147	GLN
4	R	150	HIS
4	R	199	GLN
4	R	218	GLN
4	R	226	ASN
5	S	73	HIS
5	S	104	ASN
5	S	121	GLN
5	S	123	ASN
5	S	125	GLN
5	S	156	ASN
5	S	209(E)	ASN
6	T	23	GLN
6	T	43	ASN
6	T	90	ASN
6	T	121	GLN
6	T	127	ASN
6	T	147	HIS
6	T	192	GLN
6	T	237	GLN
7	U	11	HIS
7	U	87	ASN
7	U	118	ASN
7	U	121	GLN
7	U	125	GLN

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Mol	Chain	Res	Type
7	U	178	ASN
7	U	180(C)	HIS
8	V	30	ASN
8	V	35	HIS
8	V	66	HIS
8	V	86	HIS
8	V	144	GLN
8	V	165	ASN
8	V	172	ASN
8	V	190	ASN
9	W	81	GLN
10	X	54	GLN
10	X	77	GLN
10	X	85	GLN
10	X	106	ASN
10	X	112	GLN
10	X	127	HIS
10	X	186	GLN
11	Y	9	GLN
11	Y	85	ASN
11	Y	141	ASN
11	Y	174	ASN
11	Y	207	ASN
12	Z	-9	GLN
12	Z	-7	ASN
12	Z	40	ASN
12	Z	61	ASN
12	Z	67	HIS
12	Z	70(A)	ASN
12	Z	140	ASN
12	Z	141	GLN
12	Z	143	ASN
12	Z	144(B)	ASN
12	Z	144(C)	GLN
12	Z	166	HIS
13	1	9	ASN
13	1	39	ASN
13	1	69	ASN
13	1	93	GLN
13	1	99	ASN
13	1	162	GLN
13	1	170	ASN

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Mol	Chain	Res	Type
13	1	185	ASN
13	1	204	GLN
14	2	69	GLN
14	2	141	ASN
14	2	157	HIS
14	2	161	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 24 ligands modelled in this entry, 20 are monoatomic - leaving 4 for Mogul analysis.

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	$\# Z > 2$
16	3SD	K	302	-	44,44,44	0.83	3 (6%)	59,60,60	1.57	7 (11%)
16	3SD	Y	302	-	44,44,44	0.89	2 (4%)	59,60,60	1.58	6 (10%)
17	MES	Y	303	-	12,12,12	2.37	1 (8%)	15,16,16	1.24	1 (6%)
17	MES	K	303	-	12,12,12	2.09	1 (8%)	15,16,16	1.43	2 (13%)

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
16	3SD	K	302	-	-	0/40/40/40	0/3/3/3
16	3SD	Y	302	-	-	4/40/40/40	0/3/3/3
17	MES	Y	303	-	-	0/6/14/14	0/1/1/1
17	MES	K	303	-	-	0/6/14/14	0/1/1/1

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	Y	303	MES	C8-S	-7.92	1.66	1.77
17	K	303	MES	C8-S	-6.90	1.67	1.77
16	Y	302	3SD	C4-C3	-2.89	1.34	1.41
16	K	302	3SD	C4-C3	-2.69	1.34	1.41
16	Y	302	3SD	C3-C41	2.37	1.53	1.48
16	K	302	3SD	C3-C41	2.35	1.53	1.48
16	K	302	3SD	O1-C5	2.18	1.38	1.35

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	Y	302	3SD	O1-C5-C6	7.06	125.61	115.89
16	K	302	3SD	O1-C5-C6	6.50	124.83	115.89
16	Y	302	3SD	C6-C5-C4	-5.59	124.39	134.05
16	K	302	3SD	C6-C5-C4	-5.22	125.04	134.05
16	Y	302	3SD	C5-O1-N2	-3.63	104.77	108.47
17	K	303	MES	O3S-S-C8	3.61	113.07	106.00
16	K	302	3SD	C5-O1-N2	-3.10	105.31	108.47
16	K	302	3SD	C9-C8-C10	-2.91	103.70	110.57
16	Y	302	3SD	C4-C3-C41	-2.87	122.87	127.35
17	Y	303	MES	O3S-S-C8	2.74	111.36	106.00
16	K	302	3SD	C4-C3-C41	-2.70	123.13	127.35
16	Y	302	3SD	C3-C4-C5	2.57	108.38	105.23
17	K	303	MES	O1S-S-C8	2.56	110.60	106.73
16	K	302	3SD	C9-C33-N34	-2.45	112.20	115.97
16	Y	302	3SD	C9-C8-C10	-2.20	105.38	110.57
16	K	302	3SD	C37-C36-N34	-2.07	110.65	113.90

There are no chirality outliers.

All (4) torsion outliers are listed below:

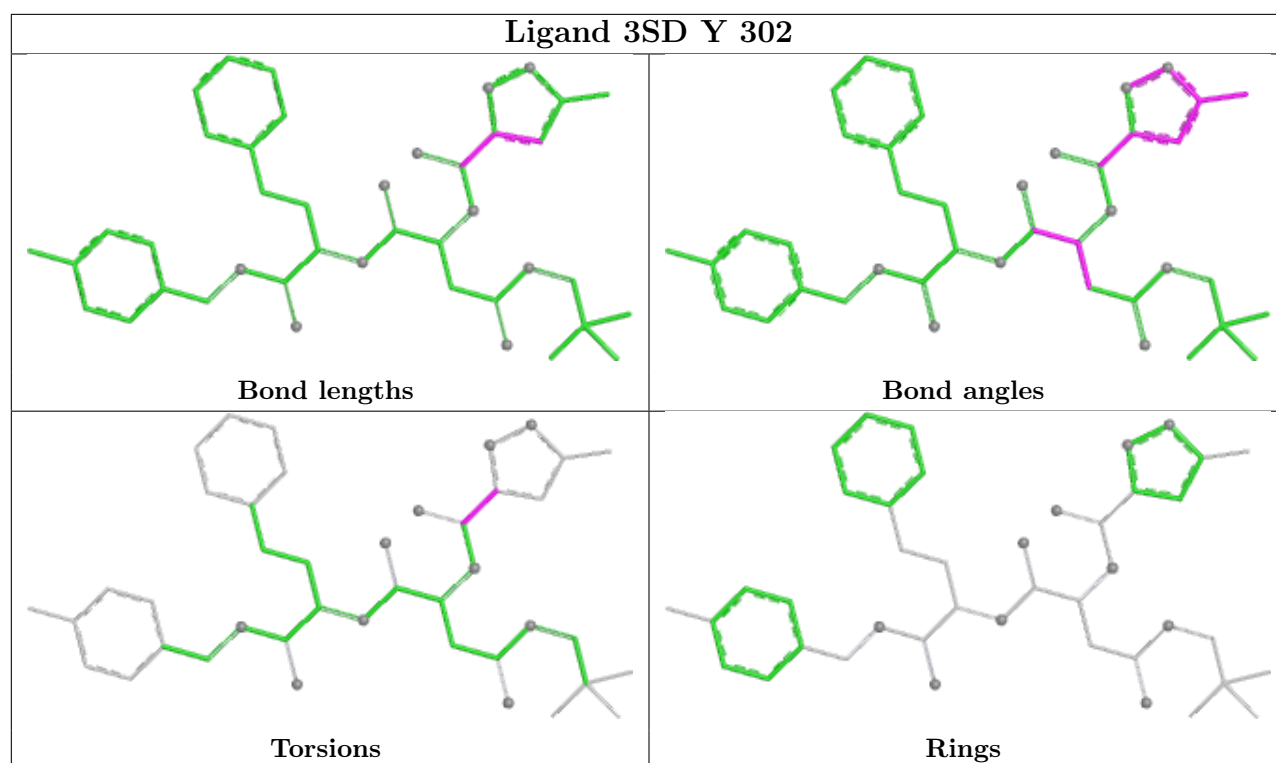
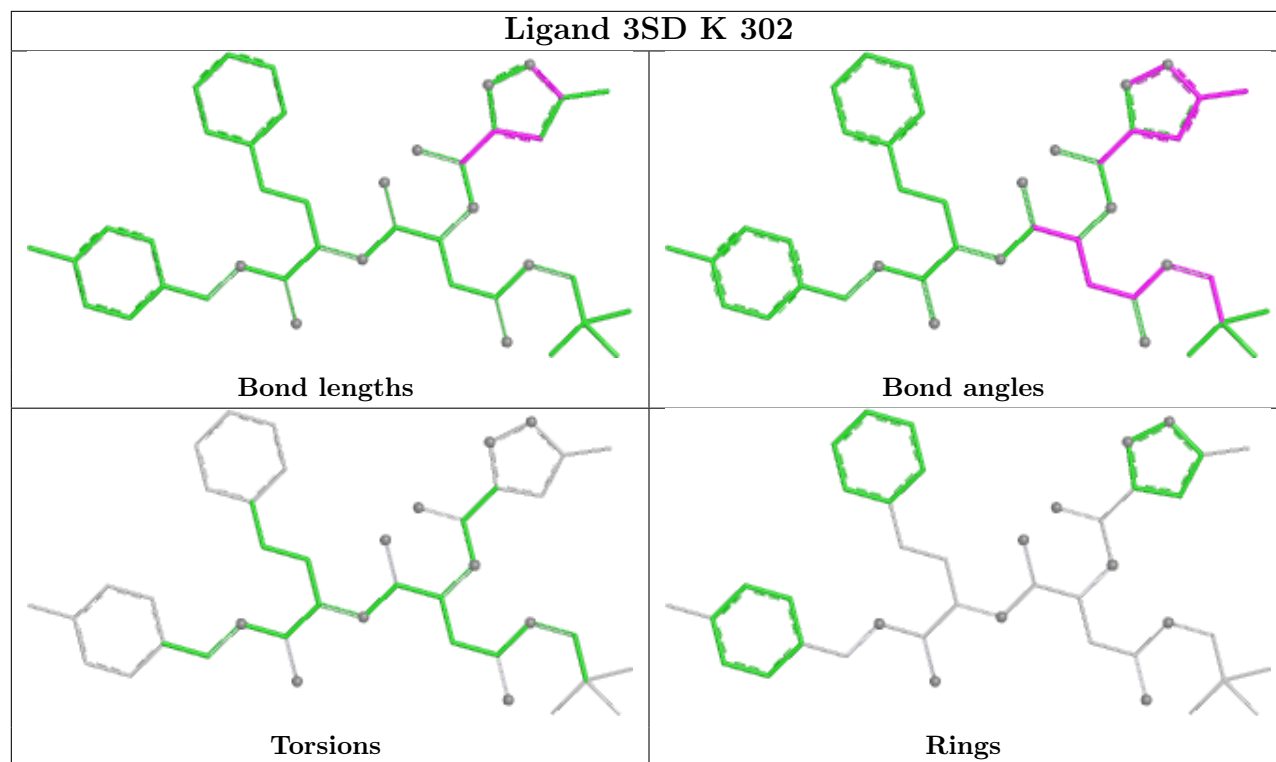
Mol	Chain	Res	Type	Atoms
16	Y	302	3SD	C4-C3-C41-N7
16	Y	302	3SD	N2-C3-C41-N7
16	Y	302	3SD	C4-C3-C41-O42
16	Y	302	3SD	N2-C3-C41-O42

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
16	K	302	3SD	1	0
16	Y	302	3SD	2	0
17	K	303	MES	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	246/250 (98%)	-0.02	5 (2%) 65 59	31, 43, 64, 89	0
1	O	246/250 (98%)	0.19	5 (2%) 65 59	31, 50, 74, 94	0
2	B	235/235 (100%)	0.47	17 (7%) 21 16	26, 51, 82, 90	0
2	P	235/235 (100%)	0.49	20 (8%) 16 12	27, 51, 85, 94	0
3	C	238/241 (98%)	0.68	34 (14%) 6 5	31, 59, 103, 118	0
3	Q	238/241 (98%)	1.08	47 (19%) 3 2	34, 63, 111, 127	0
4	D	228/260 (87%)	0.31	12 (5%) 32 25	28, 51, 73, 95	0
4	R	229/260 (88%)	0.45	12 (5%) 33 25	29, 53, 77, 102	0
5	E	230/233 (98%)	0.40	8 (3%) 47 38	37, 52, 78, 92	0
5	S	230/233 (98%)	0.69	27 (11%) 9 7	34, 54, 89, 99	0
6	F	242/242 (100%)	0.37	13 (5%) 31 25	29, 49, 85, 109	0
6	T	242/242 (100%)	0.41	15 (6%) 26 20	29, 48, 76, 109	0
7	G	240/243 (98%)	-0.04	7 (2%) 53 46	28, 42, 68, 99	0
7	U	240/243 (98%)	-0.10	8 (3%) 49 40	26, 42, 63, 85	0
8	H	222/222 (100%)	-0.15	1 (0%) 87 85	27, 37, 56, 85	0
8	V	222/222 (100%)	-0.09	4 (1%) 67 63	29, 41, 59, 87	0
9	I	204/204 (100%)	-0.27	2 (0%) 79 76	25, 37, 53, 61	0
9	W	204/204 (100%)	-0.19	2 (0%) 79 76	28, 38, 56, 62	0
10	J	198/198 (100%)	0.03	9 (4%) 38 31	28, 41, 57, 114	0
10	X	198/198 (100%)	0.07	8 (4%) 42 34	30, 42, 55, 115	0
11	K	212/212 (100%)	-0.22	2 (0%) 81 78	26, 37, 54, 63	0
11	Y	212/212 (100%)	-0.21	2 (0%) 81 78	29, 39, 57, 61	0
12	L	222/222 (100%)	-0.18	1 (0%) 87 85	27, 39, 58, 65	0
12	Z	222/222 (100%)	-0.26	1 (0%) 87 85	24, 38, 57, 65	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	1	233/233 (100%)	-0.30	4 (1%) 69 64	23, 35, 53, 62	0
13	M	233/233 (100%)	-0.19	6 (2%) 57 51	25, 39, 55, 61	0
14	2	196/196 (100%)	-0.31	3 (1%) 72 67	27, 35, 52, 69	0
14	N	196/196 (100%)	-0.30	1 (0%) 87 85	26, 36, 52, 64	0
All	All	6293/6382 (98%)	0.11	276 (4%) 39 31	23, 44, 80, 127	0

All (276) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
6	T	8	TYR	13.1
6	F	9	ASP	11.2
6	T	11	SER	10.8
6	T	10	LEU	10.7
6	T	9	ASP	10.5
6	F	10	LEU	10.4
3	Q	56	LEU	10.0
6	F	8	TYR	9.7
6	F	11	SER	9.1
6	F	12	ASN	8.9
10	J	-1	MET	8.3
10	X	-1	MET	8.3
2	B	217	ALA	8.0
3	Q	55	THR	7.8
3	C	55	THR	7.3
3	C	56	LEU	7.3
10	J	192	ALA	7.2
2	B	216(B)	GLY	6.6
2	P	217	ALA	6.4
2	P	54	VAL	6.2
2	B	218	ASN	6.1
4	R	123	PHE	6.0
6	T	7	GLY	5.9
13	M	-8	THR	5.7
5	S	7	ASN	5.6
6	F	7	GLY	5.5
13	1	72	ALA	5.5
3	C	208	LYS	5.3
3	Q	208	LYS	5.0
5	S	60	SER	5.0
3	Q	64	PRO	5.0
3	Q	58	LEU	5.0

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Mol	Chain	Res	Type	RSRZ
3	Q	57	LYS	4.9
3	C	207	ALA	4.9
6	T	12	ASN	4.9
1	O	236	LEU	4.8
7	G	9	ASP	4.8
10	X	192	ALA	4.7
2	B	239	THR	4.7
4	D	242	ALA	4.7
3	Q	207	ALA	4.6
2	B	13	THR	4.6
7	U	9	ASP	4.6
5	S	57	GLU	4.5
2	B	54	VAL	4.5
3	C	11	ALA	4.4
2	P	13	THR	4.3
6	F	13	SER	4.3
5	S	63	TYR	4.3
2	P	63	THR	4.2
3	Q	203	THR	4.2
4	D	243	ALA	4.2
3	C	57	LYS	4.2
3	Q	10	ARG	4.1
7	G	240	ASP	4.1
3	C	10	ARG	4.0
2	B	63	THR	3.9
4	R	243	ALA	3.9
7	G	237	ALA	3.9
3	Q	54	SER	3.8
6	T	240	ILE	3.8
5	E	7	ASN	3.8
4	D	244	GLU	3.7
5	E	206	SER	3.7
5	S	198	SER	3.7
5	S	51	LEU	3.7
6	F	204	ASP	3.7
10	J	191	GLN	3.7
10	J	193	GLN	3.6
7	U	199	ASP	3.6
14	2	149	GLU	3.6
5	S	58	LEU	3.6
10	J	168	MET	3.5
1	A	203	GLU	3.5

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Mol	Chain	Res	Type	RSRZ
4	D	241	GLU	3.5
5	S	59	SER	3.5
10	X	189	ASP	3.5
5	S	56	ASP	3.5
5	S	55	ALA	3.5
4	D	122	ARG	3.5
10	X	168	MET	3.4
11	K	210	ILE	3.4
2	B	216(A)	LYS	3.4
3	Q	240	LYS	3.4
2	B	127	GLY	3.4
3	C	240	LYS	3.3
3	Q	63	THR	3.3
7	U	240	ASP	3.3
5	E	203	ASP	3.3
2	B	22	TYR	3.3
2	P	218	ASN	3.3
6	F	240	ILE	3.3
2	P	239	THR	3.3
4	R	244	GLU	3.3
5	S	8	TYR	3.3
10	J	189	ASP	3.3
2	P	220	TYR	3.2
3	C	206	GLY	3.2
3	Q	206	GLY	3.2
4	R	158	TYR	3.2
3	Q	66	LYS	3.2
10	X	191	GLN	3.1
9	W	121	GLU	3.1
2	P	216(B)	GLY	3.1
3	Q	186	VAL	3.1
3	C	64	PRO	3.1
2	P	232	ILE	3.1
3	Q	40	VAL	3.1
5	S	207	LEU	3.1
13	1	-8	THR	3.1
1	O	56	SER	3.1
2	B	62	ASP	3.0
4	R	241	GLU	3.0
13	M	60	ASP	3.0
3	Q	233	VAL	3.0
3	C	12	LEU	3.0

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Mol	Chain	Res	Type	RSRZ
10	X	193	GLN	3.0
6	T	13	SER	3.0
3	Q	217	PRO	3.0
3	Q	65	SER	2.9
1	A	235	ALA	2.9
2	B	60	GLU	2.9
4	R	12	VAL	2.9
5	S	203	ASP	2.9
6	F	205	ASN	2.8
3	Q	180(C)	LYS	2.8
3	Q	232	TYR	2.8
13	M	38	ASP	2.8
9	W	-8	SER	2.8
4	R	237	LEU	2.8
4	R	170	GLU	2.8
10	J	190	PHE	2.8
7	G	236	ILE	2.8
3	Q	196	SER	2.8
2	B	238	ILE	2.7
3	C	203	THR	2.7
7	U	239	GLN	2.7
3	Q	62(A)	ILE	2.7
3	Q	53	ARG	2.7
1	O	8	TYR	2.7
3	Q	61	THR	2.7
1	A	236	LEU	2.7
5	S	52	LYS	2.7
8	V	223	ASP	2.7
6	T	199	LEU	2.6
6	T	206	LYS	2.6
5	S	12	THR	2.6
5	E	207	LEU	2.6
9	I	121	GLU	2.6
3	Q	209	ASN	2.6
4	D	22	PHE	2.6
5	S	64	GLN	2.6
3	C	58	LEU	2.6
3	Q	241	GLN	2.6
7	G	239	GLN	2.6
2	P	218(D)	GLY	2.6
3	Q	184	ALA	2.6
5	E	209(E)	ASN	2.6

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Mol	Chain	Res	Type	RSRZ
10	X	190	PHE	2.6
2	B	64	THR	2.5
2	P	64	THR	2.5
5	S	206	SER	2.5
3	Q	237	GLU	2.5
2	P	55	THR	2.5
4	D	238	LYS	2.5
3	Q	44	ASN	2.5
4	D	170	GLU	2.5
2	B	220	TYR	2.5
3	C	233	VAL	2.5
3	Q	59	GLN	2.5
3	C	54	SER	2.5
14	N	149	GLU	2.5
3	C	232	TYR	2.5
2	B	61	GLN	2.5
5	S	127	ALA	2.5
5	S	53	ARG	2.4
3	Q	198	LEU	2.4
11	Y	211	GLY	2.4
9	I	122(A)	LYS	2.4
2	P	238	ILE	2.4
6	T	127	ASN	2.4
4	R	231	GLU	2.4
3	Q	238	GLN	2.4
3	C	52	ARG	2.4
3	C	63	THR	2.4
4	R	178	ASN	2.4
7	U	218	ASP	2.4
14	2	187(I)	GLN	2.4
3	C	224	LEU	2.3
5	S	233	ILE	2.3
3	C	16	SER	2.3
5	S	65	LYS	2.3
6	T	206(C)	LYS	2.3
10	J	10	ASP	2.3
12	L	17	ASP	2.3
3	C	211	GLU	2.3
1	A	9	SER	2.3
3	C	241	GLN	2.3
4	D	237	LEU	2.3
13	M	224	ILE	2.3

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Mol	Chain	Res	Type	RSRZ
2	P	216(A)	LYS	2.3
5	S	32	LYS	2.3
12	Z	144(R)	LYS	2.3
3	C	18	ASP	2.3
8	V	145	ASP	2.3
3	C	53	ARG	2.3
3	Q	62	ARG	2.3
8	V	197	ARG	2.3
3	Q	202	GLN	2.3
3	C	229	ILE	2.3
4	R	238	LYS	2.3
6	T	63	LYS	2.2
3	C	238	GLN	2.2
13	1	38	ASP	2.2
14	2	187(J)	LEU	2.2
6	T	22	PHE	2.2
3	Q	185	THR	2.2
1	A	8	TYR	2.2
3	Q	180	TYR	2.2
5	S	13	VAL	2.2
3	Q	229	ILE	2.2
3	C	235	GLN	2.2
3	C	243	GLN	2.2
2	P	185	LYS	2.2
3	Q	200	VAL	2.2
3	Q	215	VAL	2.2
8	V	221	ILE	2.2
7	U	237	ALA	2.2
4	D	231	GLU	2.2
5	S	204	GLU	2.2
3	Q	189	CYS	2.2
3	Q	144(B)	ASP	2.2
3	Q	222	VAL	2.2
11	K	73	ARG	2.1
3	C	222	VAL	2.1
5	E	198	SER	2.1
13	M	206	GLU	2.1
2	P	187	ASP	2.1
6	T	207	ASP	2.1
7	U	236	ILE	2.1
4	D	175	GLU	2.1
7	U	184(H)	GLU	2.1

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Mol	Chain	Res	Type	RSRZ
8	H	197	ARG	2.1
13	1	28	ASN	2.1
2	P	143	ASP	2.1
6	F	207	ASP	2.1
1	O	9	SER	2.1
2	P	63(A)	SER	2.1
3	C	65	SER	2.1
3	C	227	GLU	2.1
4	R	242	ALA	2.1
5	E	204	GLU	2.1
10	J	49	ALA	2.1
2	P	235	LYS	2.1
3	Q	183	PRO	2.1
3	Q	243	GLN	2.1
5	E	199	GLN	2.1
5	S	180(F)	ILE	2.1
10	X	10	ASP	2.0
3	Q	188	GLU	2.0
5	S	33	GLN	2.0
6	F	127	ASN	2.0
3	C	14	ILE	2.0
3	C	236	ILE	2.0
3	Q	212	ILE	2.0
5	S	175	TYR	2.0
7	G	128	TYR	2.0
3	C	239	GLU	2.0
7	G	227	GLU	2.0
2	B	181	LYS	2.0
1	O	65	SER	2.0
4	D	13	SER	2.0
13	M	112	SER	2.0
6	F	184	LEU	2.0
11	Y	210	ILE	2.0
2	P	219(E)	VAL	2.0

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

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

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

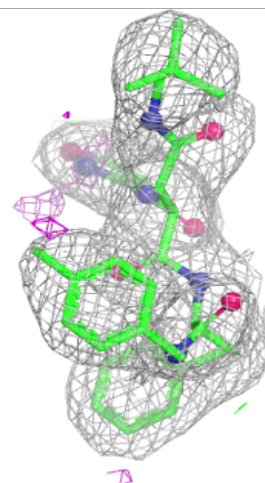
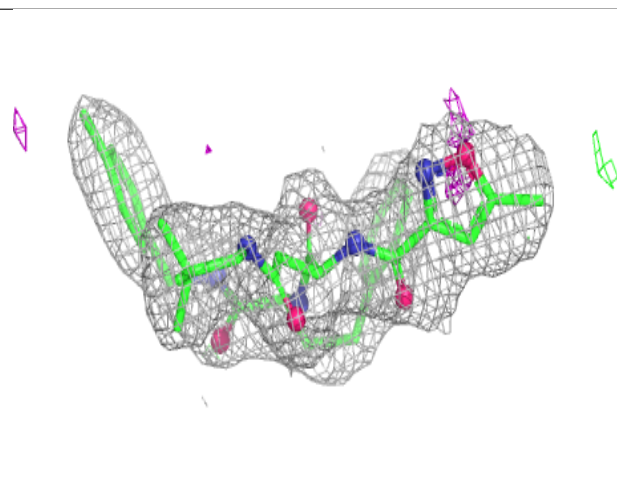
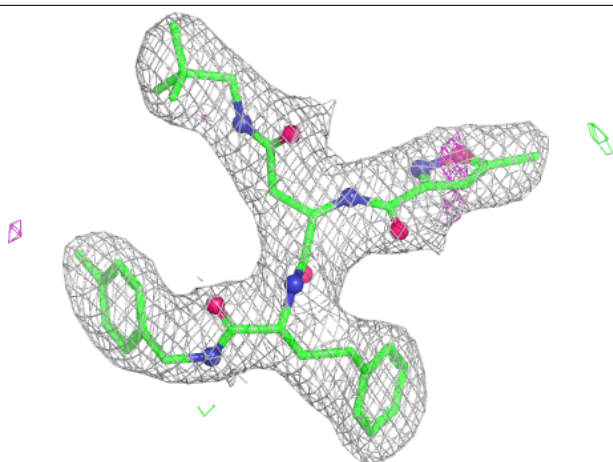
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
15	MG	T	301	1/1	0.59	0.25	69,69,69,69	0
15	MG	W	201	1/1	0.67	0.19	53,53,53,53	0
15	MG	Z	201	1/1	0.73	0.19	65,65,65,65	0
15	MG	F	301	1/1	0.81	0.10	74,74,74,74	0
15	MG	L	201	1/1	0.83	0.15	52,52,52,52	0
15	MG	I	201	1/1	0.86	0.15	46,46,46,46	0
15	MG	Z	202	1/1	0.87	0.12	49,49,49,49	0
15	MG	F	302	1/1	0.88	0.27	120,120,120,120	0
15	MG	T	302	1/1	0.90	0.23	110,110,110,110	0
15	MG	W	202	1/1	0.92	0.13	50,50,50,50	0
15	MG	L	202	1/1	0.93	0.10	46,46,46,46	0
15	MG	Y	301	1/1	0.94	0.06	53,53,53,53	0
15	MG	H	301	1/1	0.94	0.07	47,47,47,47	0
15	MG	G	9001	1/1	0.94	0.06	45,45,45,45	0
16	3SD	K	302	42/42	0.94	0.10	28,35,49,50	0
16	3SD	Y	302	42/42	0.94	0.10	37,39,48,50	0
15	MG	I	202	1/1	0.95	0.20	50,50,50,50	0
17	MES	K	303	12/12	0.95	0.12	55,57,58,58	0
15	MG	U	301	1/1	0.96	0.04	38,38,38,38	0
15	MG	K	301	1/1	0.96	0.06	50,50,50,50	0
15	MG	2	201	1/1	0.96	0.07	30,30,30,30	0
15	MG	V	301	1/1	0.97	0.07	42,42,42,42	0
17	MES	Y	303	12/12	0.97	0.08	57,61,64,64	0
15	MG	N	201	1/1	0.98	0.06	41,41,41,41	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

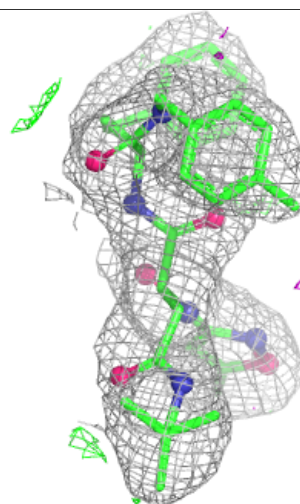
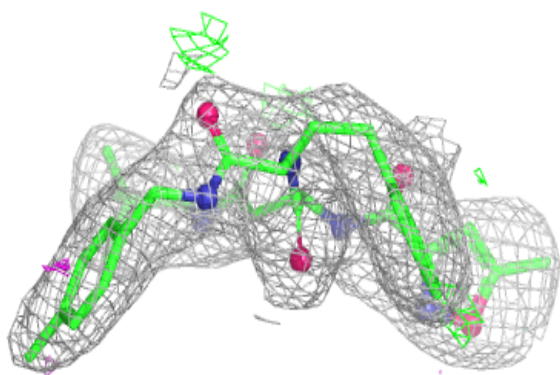
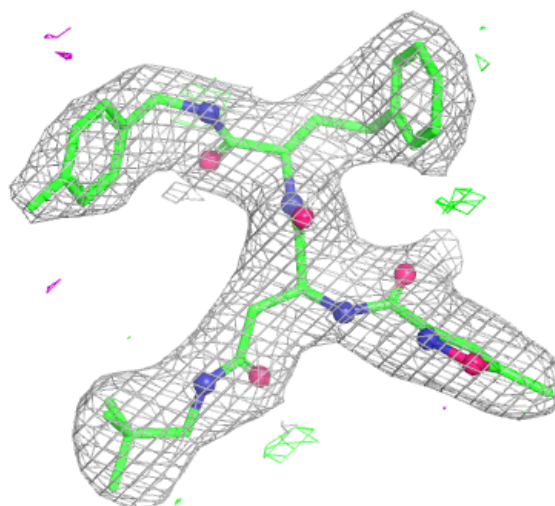
Electron density around 3SD K 302:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around 3SD Y 302:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers [i](#)

There are no such residues in this entry.