



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 16, 2020 – 05:06 pm BST

PDB ID : 3SDI
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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

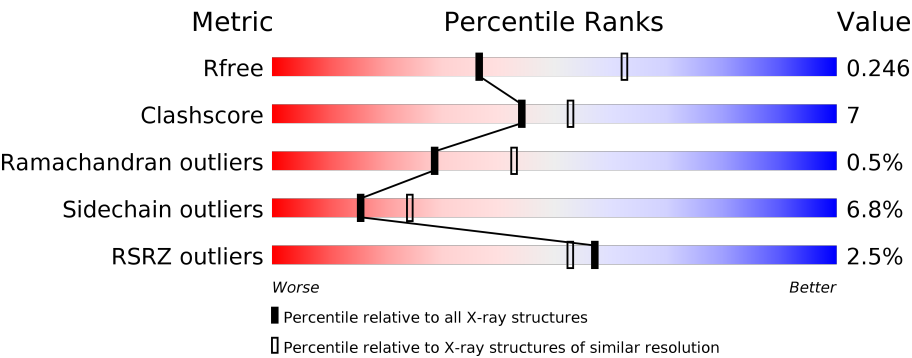
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.65 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.



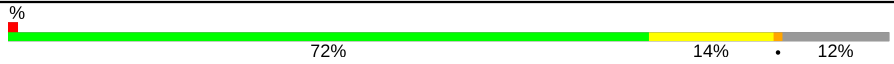



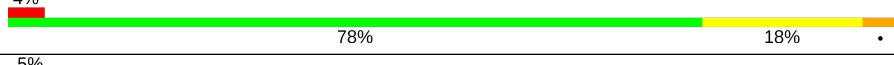
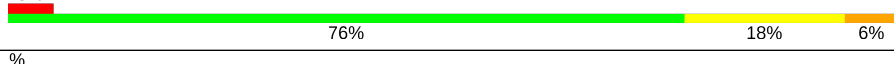
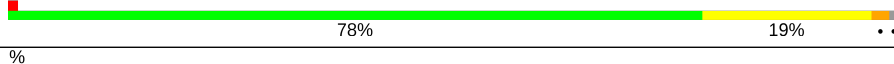

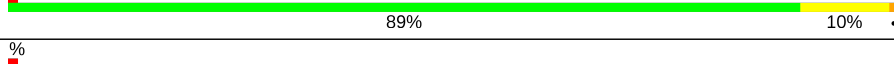

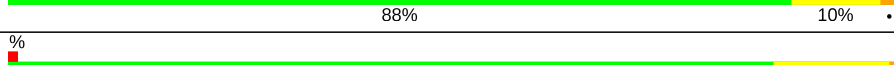
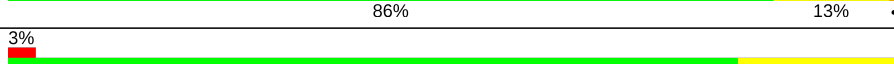

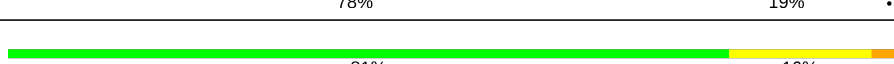

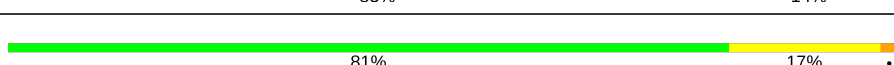
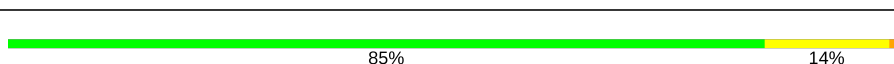
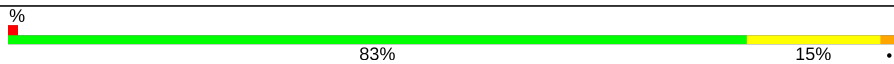
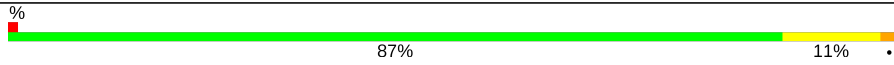


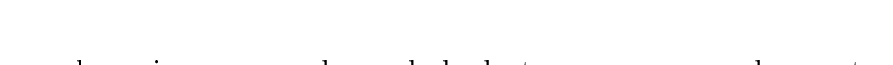
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1332 (2.68-2.64)
Clashscore	141614	1374 (2.68-2.64)
Ramachandran outliers	138981	1349 (2.68-2.64)
Sidechain outliers	138945	1349 (2.68-2.64)
RSRZ outliers	127900	1318 (2.68-2.64)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria 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	<div><div>2%</div><div><div></div><div>86%</div><div>12%</div><div></div></div><div></div></div>
1	O	250	<div><div>2%</div><div><div></div><div>84%</div><div>14%</div><div></div></div><div></div></div>
2	B	235	<div><div>6%</div><div><div></div><div>76%</div><div>21%</div><div></div></div><div></div></div>
2	P	235	<div><div>4%</div><div><div></div><div>75%</div><div>23%</div><div></div></div><div></div></div>
3	C	241	<div><div>7%</div><div><div></div><div>80%</div><div>16%</div><div></div></div><div></div></div>
3	Q	241	<div><div>10%</div><div><div></div><div>82%</div><div>14%</div><div></div></div><div></div></div>

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Mol	Chain	Length	Quality of chain
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	

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
15	MG	F	302	-	-	-	X

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			

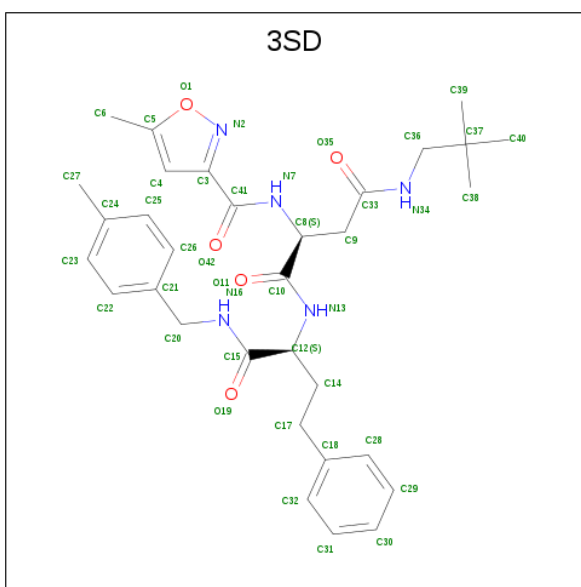
- Molecule 14 is a protein called Proteasome component PRE3.

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 (three-letter code: MG) (formula: Mg).

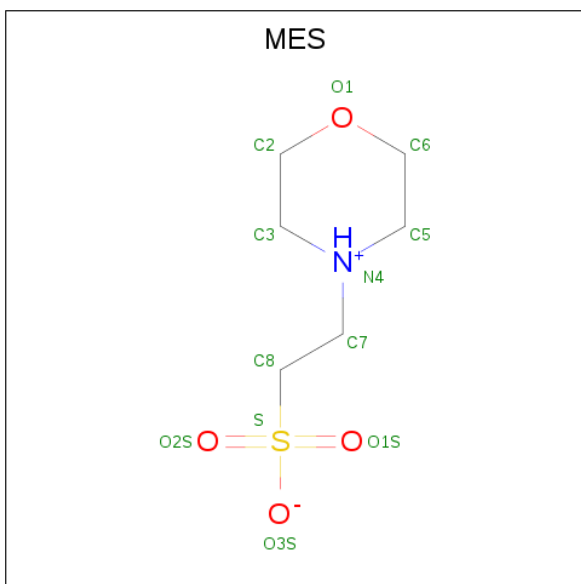
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
15	G	1	Total 1 Mg 1	0	0
15	K	1	Total 1 Mg 1	0	0
15	H	1	Total 1 Mg 1	0	0
15	I	2	Total 2 Mg 2	0	0
15	V	1	Total 1 Mg 1	0	0
15	W	2	Total 2 Mg 2	0	0
15	Z	2	Total 2 Mg 2	0	0
15	T	2	Total 2 Mg 2	0	0
15	N	1	Total 1 Mg 1	0	0
15	U	1	Total 1 Mg 1	0	0
15	2	1	Total 1 Mg 1	0	0
15	Y	1	Total 1 Mg 1	0	0
15	L	2	Total 2 Mg 2	0	0
15	F	2	Total 2 Mg 2	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 (three-letter code: 3SD) (formula: C₃₂H₄₁N₅O₅).



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

- Molecule 17 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (three-letter code: MES) (formula: $\text{C}_6\text{H}_{13}\text{NO}_4\text{S}$).



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		

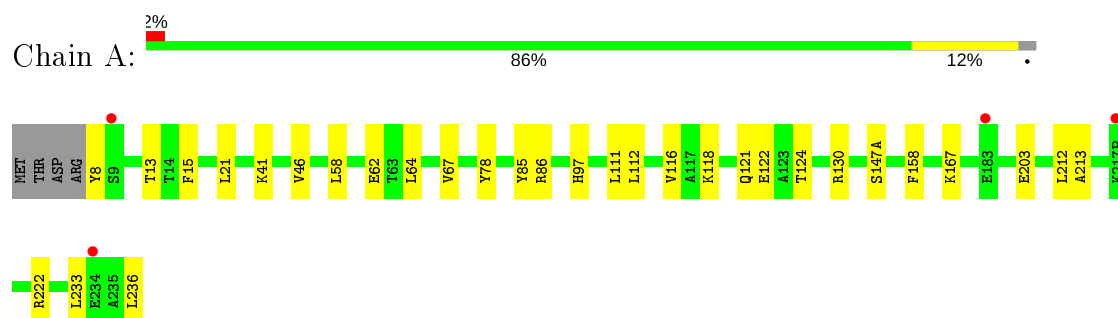
- Molecule 18 is water.

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

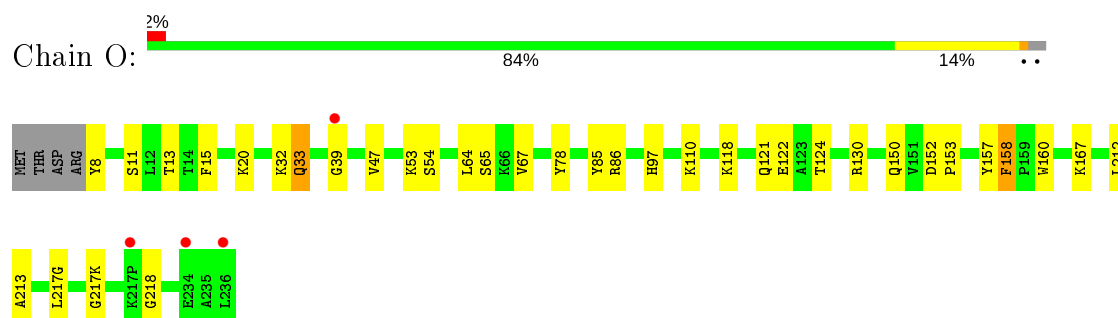
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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.

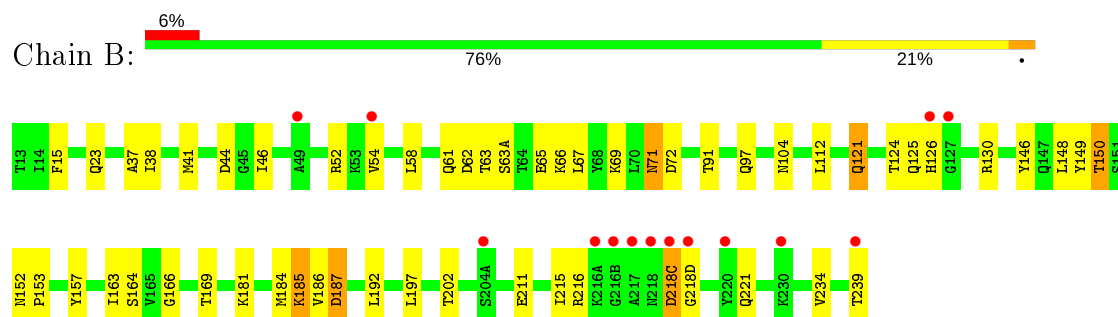
- Molecule 1: Proteasome component Y7



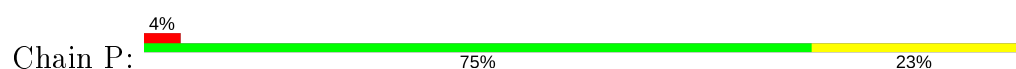
- Molecule 1: Proteasome component Y7

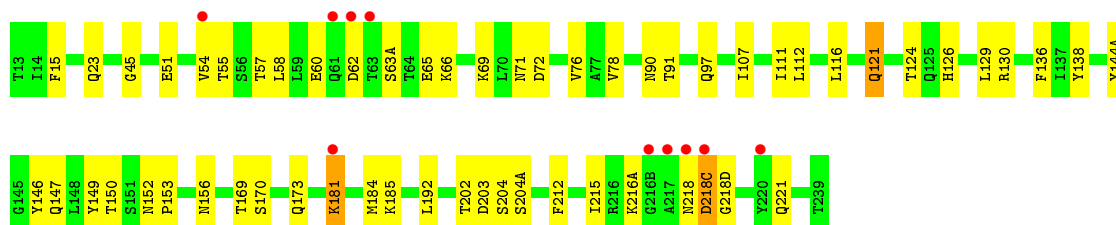


- Molecule 2: Proteasome component Y13

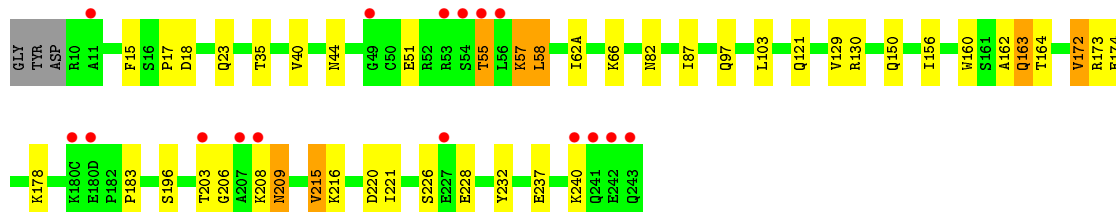
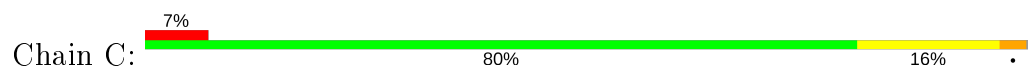


- Molecule 2: Proteasome component Y13

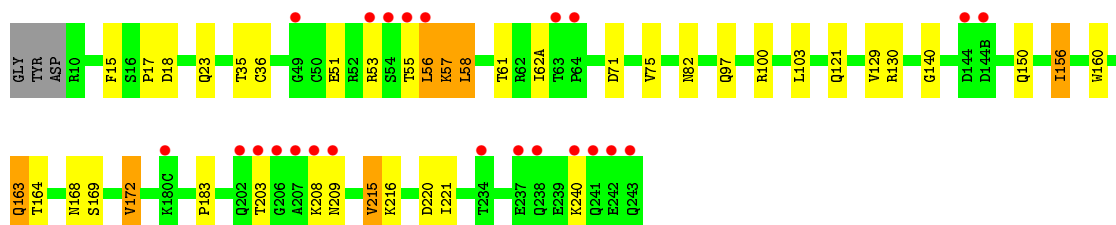
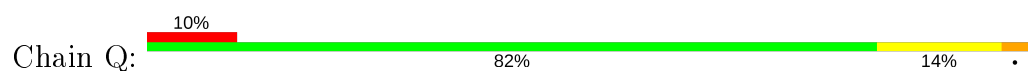




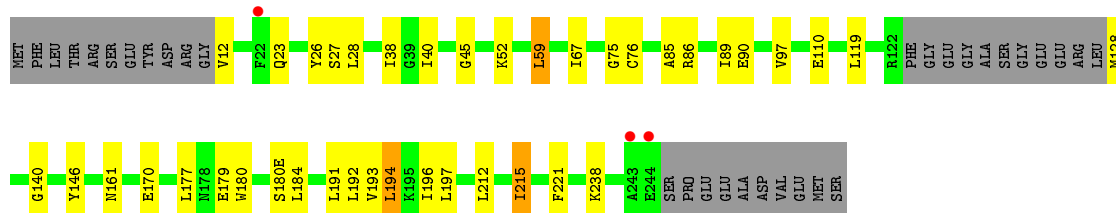
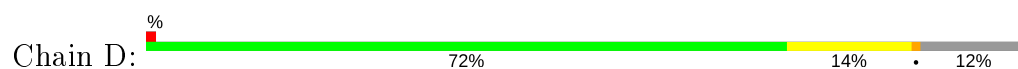
• Molecule 3: Proteasome component PRE6



• Molecule 3: Proteasome component PRE6

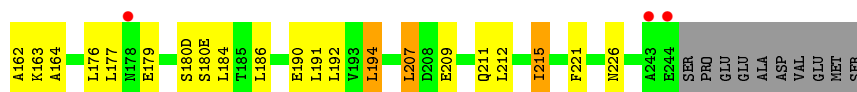


• Molecule 4: Proteasome component PUP2

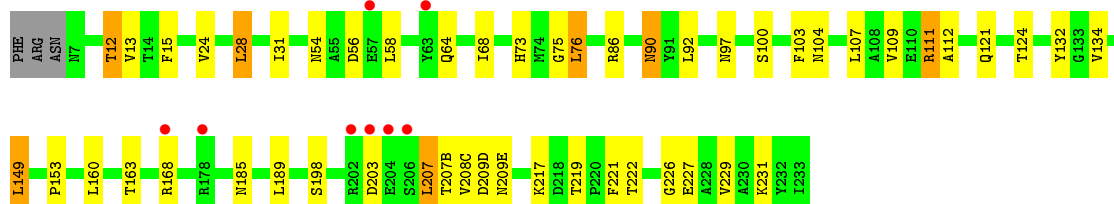
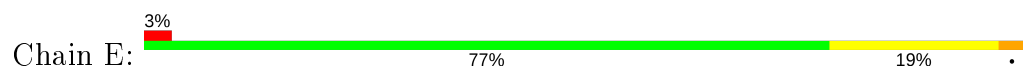


• Molecule 4: Proteasome component PUP2

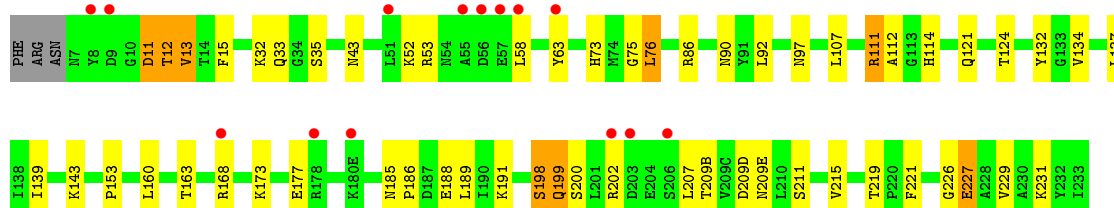
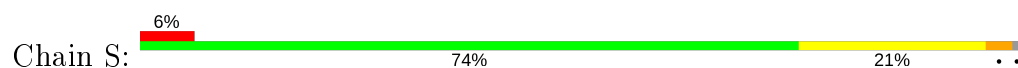




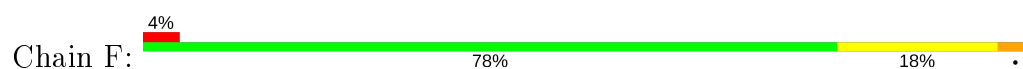
• Molecule 5: Proteasome component PRE5



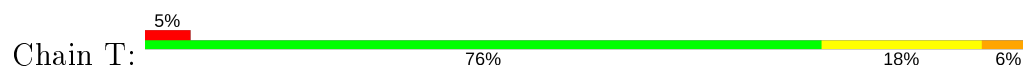
• Molecule 5: Proteasome component PRE5



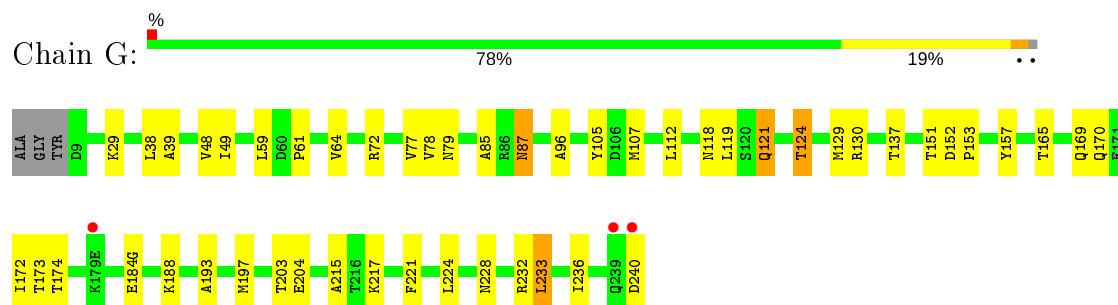
• Molecule 6: Proteasome component C1



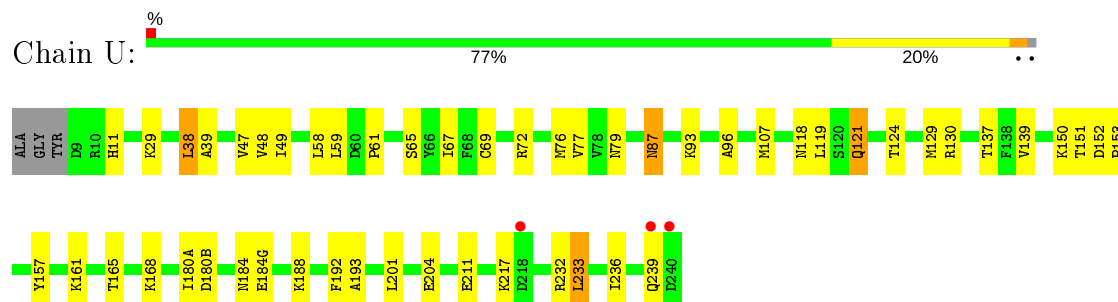
• Molecule 6: Proteasome component C1



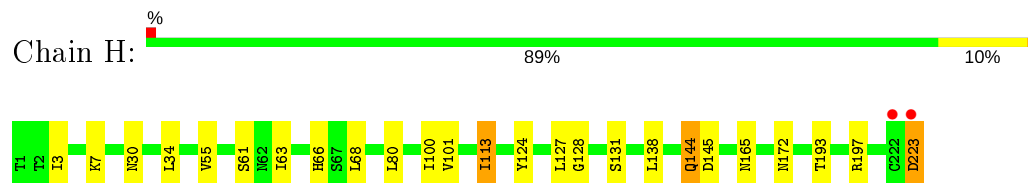
• Molecule 7: Proteasome component C7-alpha



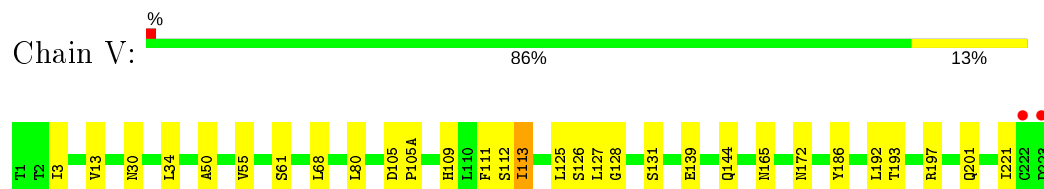
- Molecule 7: Proteasome component C7-alpha



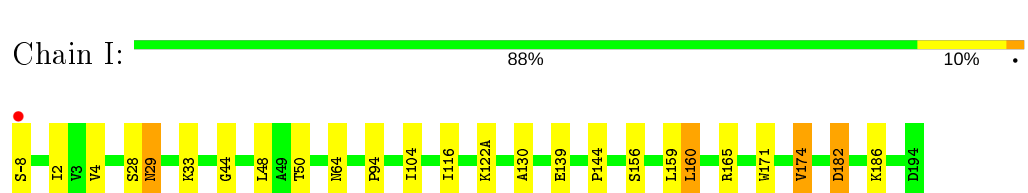
- Molecule 8: Proteasome component PUP1



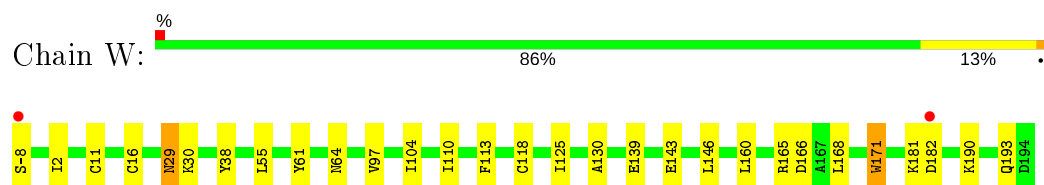
- Molecule 8: Proteasome component PUP1



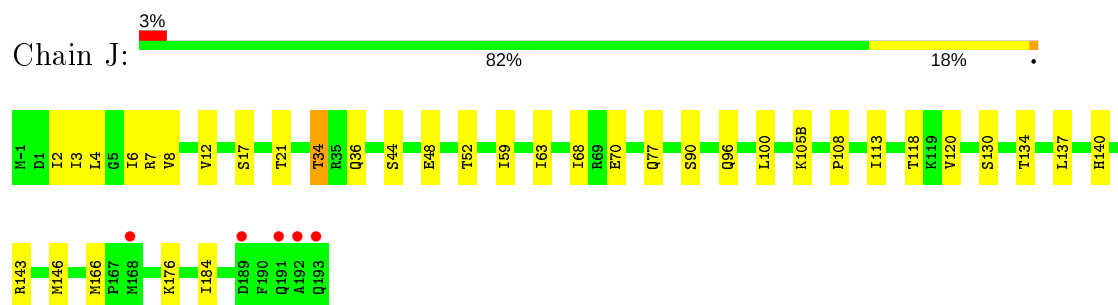
- Molecule 9: Proteasome component PUP3



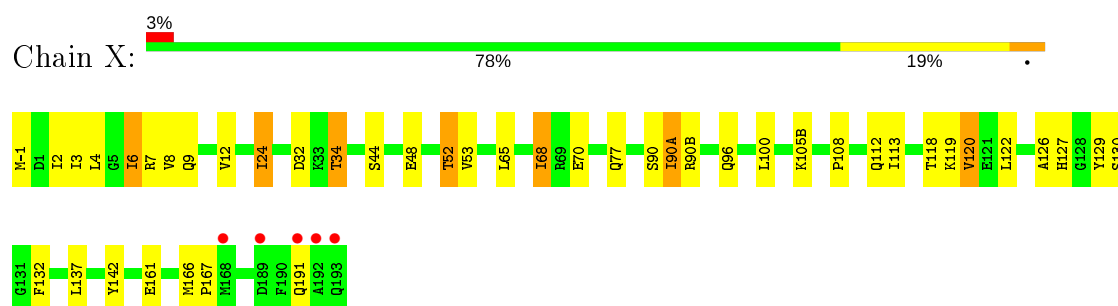
- Molecule 9: Proteasome component PUP3



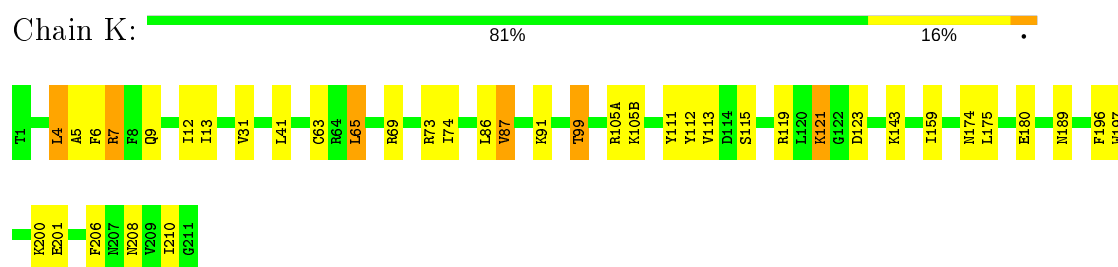
- Molecule 10: Proteasome component C11



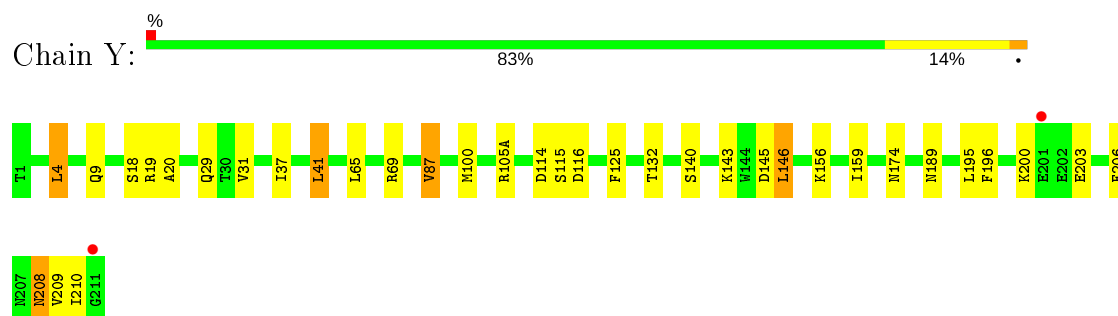
- Molecule 10: Proteasome component C11



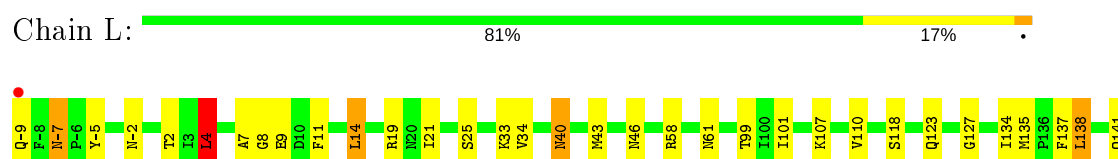
- Molecule 11: Proteasome component PRE2



- Molecule 11: Proteasome component PRE2



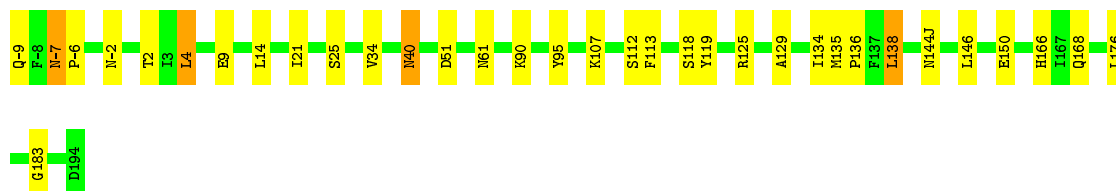
- Molecule 12: Proteasome component C5





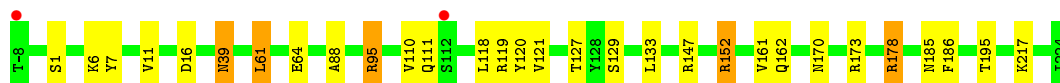
- Molecule 12: Proteasome component C5

Chain Z: 85% 14%



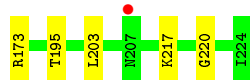
- Molecule 13: Proteasome component PRE4

Chain M: 87% 11%



- Molecule 13: Proteasome component PRE4

Chain 1: 83% 15%



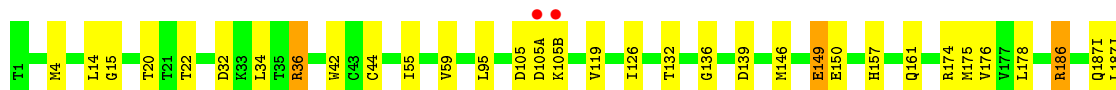
- Molecule 14: Proteasome component PRE3

Chain N: 86% 13%



- Molecule 14: Proteasome component PRE3

Chain 2: 83% 15%



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 29.95 – 2.65	Depositor EDS
% Data completeness (in resolution range)	95.4 (30.00-2.65) 95.5 (29.95-2.65)	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)	0.32 , 28.9	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: 3SD, MG, MES

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	0.50	0/1918	0.60	0/2597
1	O	0.49	0/1918	0.59	0/2597
2	B	0.46	0/1856	0.61	0/2513
2	P	0.48	0/1856	0.61	0/2513
3	C	0.46	0/1889	0.59	1/2557 (0.0%)
3	Q	0.47	0/1889	0.61	2/2557 (0.1%)
4	D	0.51	0/1770	0.66	1/2387 (0.0%)
4	R	0.47	0/1775	0.63	2/2394 (0.1%)
5	E	0.49	0/1781	0.61	0/2407
5	S	0.47	0/1781	0.60	0/2407
6	F	0.50	0/1926	0.59	0/2599
6	T	0.54	1/1926 (0.1%)	0.63	0/2599
7	G	0.52	0/1934	0.60	0/2618
7	U	0.52	0/1934	0.62	0/2618
8	H	0.51	0/1716	0.64	0/2326
8	V	0.49	0/1716	0.61	0/2326
9	I	0.58	0/1611	0.63	0/2174
9	W	0.64	1/1611 (0.1%)	0.63	0/2174
10	J	0.52	0/1610	0.66	0/2170
10	X	0.54	0/1610	0.68	2/2170 (0.1%)
11	K	0.51	0/1681	0.65	0/2274
11	Y	0.49	0/1681	0.63	0/2274
12	L	0.56	0/1795	0.63	1/2420 (0.0%)
12	Z	0.56	0/1795	0.62	1/2420 (0.0%)
13	1	0.60	0/1855	0.76	1/2514 (0.0%)
13	M	0.63	0/1855	0.70	1/2514 (0.0%)
14	2	0.59	0/1541	0.63	0/2087
14	N	0.62	0/1541	0.61	0/2087
All	All	0.53	2/49771 (0.0%)	0.63	12/67293 (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 (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	W	38	TYR	CD1-CE1	-5.17	1.31	1.39
6	T	7	GLY	N-CA	5.01	1.53	1.46

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	1	74	ALA	O-C-N	-16.84	95.75	122.70
4	D	128	MET	N-CA-C	-7.50	90.76	111.00
10	X	-1	MET	O-C-N	-6.45	112.38	122.70
10	X	-1	MET	C-N-CA	6.29	137.43	121.70
4	R	59	LEU	CA-CB-CG	6.21	129.59	115.30
3	Q	56	LEU	CA-CB-CG	5.68	128.37	115.30
3	Q	103	LEU	CA-CB-CG	5.57	128.12	115.30
12	Z	4	LEU	CA-CB-CG	5.53	128.01	115.30
4	R	128	MET	N-CA-C	-5.25	96.82	111.00
12	L	4	LEU	CA-CB-CG	5.16	127.17	115.30
13	M	95	ARG	NE-CZ-NH1	5.16	122.88	120.30
3	C	103	LEU	CA-CB-CG	5.12	127.09	115.30

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	24	0
1	O	1881	0	1893	26	0
2	B	1827	0	1824	36	0
2	P	1827	0	1824	39	0
3	C	1861	0	1873	31	0
3	Q	1861	0	1873	25	0
4	D	1747	0	1718	22	0
4	R	1752	0	1720	18	0
5	E	1755	0	1761	27	0
5	S	1755	0	1761	34	0
6	F	1886	0	1876	36	0
6	T	1886	0	1875	50	0
7	G	1897	0	1891	44	0
7	U	1897	0	1891	42	0
8	H	1685	0	1688	15	0
8	V	1685	0	1688	22	0
9	I	1581	0	1574	15	0
9	W	1581	0	1574	24	0
10	J	1582	0	1583	17	0
10	X	1582	0	1582	24	0
11	K	1644	0	1595	24	0
11	Y	1644	0	1595	21	0
12	L	1757	0	1711	23	0
12	Z	1757	0	1711	24	0
13	1	1824	0	1832	35	0
13	M	1824	0	1832	20	0
14	2	1512	0	1481	21	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	48708	641	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 (641) 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:G:96:ALA:HA	7:G:107:MET:HE2	1.31	1.06
7:U:96:ALA:HA	7:U:107:MET:HE2	1.36	1.04
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
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
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:T:170:GLN:CD	6:T:170:GLN:H	1.80	0.84
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
14:2:157:HIS:HD2	14:2:187(J):LEU:HD13	1.47	0.79
2:B:181:LYS:O	2:B:184:MET:HG3	1.83	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: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:CG	6:T:187:ARG:HH11	1.99	0.75
7:U:96:ALA:HA	7:U:107:MET:CE	2.16	0.75
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:126:HIS:HB3	3:C:129:VAL:HG12	1.71	0.72
2:B:124:THR:HG22	3:C:130:ARG:HH21	1.52	0.72
14:2:157:HIS:CD2	14:2:187(J):LEU:HD13	2.25	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
7:G:96:ALA:HA	7:G:107:MET:CE	2.14	0.69
2:P:97:GLN:HE22	9:W:64:ASN:HD22	1.38	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:HH11	13:M:152:ARG:HG3	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
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
13:1:152:ARG:HH11	13:1:152:ARG:CG	2.10	0.64
2:B:124:THR:CG2	3:C:130:ARG:HH21	2.11	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
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
14:2:176:VAL:HG12	14:2:178:LEU:HD13	1.82	0.61
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
14:2:55:ILE:HD11	14:2:95:LEU:HD13	1.82	0.60
2:P:65:GLU:HG3	2:P:66:LYS:HG3	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
1:A:97:HIS:HD2	8:H:61:SER:OG	1.84	0.60
6:T:187:ARG:HG2	6:T:187:ARG:HH11	1.66	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
13:1:170:ASN:HD22	13:1:173:ARG:HH11	1.49	0.59
7:G:121:GLN:O	7:G:124:THR:HB	2.02	0.59
7:G:79:ASN:OD1	7:G:165:THR:HB	2.02	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
5:E:227:GLU:CD	5:E:227:GLU:H	2.06	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
13:1:69:ASN:HB3	13:1:72:ALA:HB2	1.84	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
6:F:13:SER:HB2	7:G:130:ARG:HB3	1.86	0.58
5:S:132:TYR:O	5:S:153:PRO:HB3	2.04	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
7:G:87:ASN:C	7:G:87:ASN:HD22	2.08	0.57
13:1:69:ASN:ND2	13:1:72:ALA:CA	2.66	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
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
12:L:135:MET:CE	9:W:165:ARG:NH2	2.67	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
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
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
7:U:87:ASN:C	7:U:87:ASN:HD22	2.08	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:T:12:ASN:O	6:T:14:VAL:N	2.40	0.55
6:T:170:GLN:N	6:T:170:GLN:CD	2.54	0.55
10:X:24:ILE:O	10:X:24:ILE:HG12	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
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:HA	10:X:161:GLU:OE2	2.06	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:HG3	10:X:7:ARG:O	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
6:T:120:VAL:HG21	6:T:151:LEU:HD21	1.89	0.54
5:S:97:ASN:ND2	12:Z:61:ASN:HD21	2.00	0.54
9:I:165:ARG:NH2	12:Z:135:MET:HE3	2.23	0.53
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
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
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
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
2:B:112:LEU:HD23	2:B:112:LEU:C	2.29	0.53
6:F:43:ASN:HD22	6:F:43:ASN:N	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

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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
8:V:172:ASN:HB3	8:V:192:LEU:O	2.08	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
1:A:203:GLU:CD	1:A:203:GLU:H	2.13	0.52
7:G:224:LEU:HB3	7:G:228:ASN:HB2	1.91	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
14:2:4:MET:HB3	14:2:126:ILE:HG22	1.92	0.51
5:S:134:VAL:O	5:S:153:PRO:HG3	2.11	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
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
13:1:170:ASN:HD22	13:1:173:ARG:NH1	2.08	0.51
12:L:19:ARG:NE	12:L:171:ASP:OD2	2.39	0.51
6:T:126:TYR:HB2	6:T:129:VAL:HG22	1.92	0.51
6:T:52:LYS:HG2	6:T:66:LYS:HD3	1.92	0.51
7:U:79:ASN:OD1	7:U:165:THR:HB	2.10	0.51
2:B:163:ILE:HG13	2:B:164:SER:N	2.26	0.51
6:T:187:ARG:HG3	6:T:187:ARG:HH11	1.72	0.51
8:V:50:ALA:HB2	9:W:118:CYS:HB2	1.93	0.51
6:T:12:ASN:C	6:T:14:VAL:H	2.13	0.51
1:A:112:LEU:O	1:A:116:VAL:HG23	2.11	0.51
5:E:207:LEU:CD2	5:E:207:LEU:H	2.24	0.51
7:G:151:THR:HG22	7:G:157:TYR:CB	2.40	0.51
9:I:182:ASP:N	9:I:182:ASP:OD1	2.40	0.51
12:L:135:MET:HE2	9:W:165:ARG:NH2	2.26	0.50
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
14:2:14:LEU:HD23	14:2:44:CYS:SG	2.52	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
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:HG2	6:F:187:ARG:HH11	1.76	0.49
7:G:233:LEU:O	7:G:236:ILE:HG13	2.12	0.49
12:L:135:MET:HE3	9:W:165:ARG:NH2	2.28	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
13:1:71:LEU:C	13:1:73:ASP:H	2.16	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
6:T:12:ASN:C	6:T:12:ASN:OD1	2.50	0.49
2:B:215:ILE:HG12	2:B:221:GLN:HG2	1.95	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
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: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
2:P:15:PHE:H	3:Q:23:GLN:HE22	1.60	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
7:U:96:ALA:CA	7:U:107:MET:HE2	2.25	0.48
11:Y:114:ASP:OD1	11:Y:116:ASP:HB2	2.14	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
13:1:150:VAL:HG23	13:1:150:VAL:O	2.13	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
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
8:V:172:ASN:HD22	8:V:193:THR:HA	1.79	0.48
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
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:M:120:TYR:O	13:M:127:THR:HA	2.13	0.47
13:M:88:ALA:HA	13:M:121:VAL:HG21	1.96	0.47
7:U:39:ALA:HB2	7:U:48:VAL:HG12	1.97	0.47
13:1:6:LYS:HB3	13:1:11:VAL:HG12	1.96	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
5:S:227:GLU:H	5:S:227:GLU:CD	2.16	0.47
9:W:2:ILE:HG21	9:W:130:ALA:HB3	1.97	0.47
14:2:55:ILE:O	14:2:59:VAL:HG23	2.15	0.47
1:O:118:LYS:O	1:O:122:GLU:HG3	2.14	0.47
5:S:160:LEU:HD13	5:S:163:THR:HB	1.96	0.47
5:S:86:ARG:O	5:S:90:ASN:HB2	2.14	0.47
6:T:7:GLY:C	6:T:9:ASP:H	2.18	0.47
8:V:197:ARG:NH2	9:W:139:GLU:HG3	2.28	0.47
11:Y:18:SER:OG	11:Y:29:GLN:O	2.32	0.47
13:1:84:PHE:CZ	13:1:119:ARG:HG2	2.48	0.47
2:P:76:VAL:HG12	2:P:138:TYR:CD2	2.50	0.47
2:P:78:VAL:HG22	2:P:136:PHE:HE2	1.78	0.47
9:W:29:ASN:HB3	9:W:171:TRP:CE3	2.50	0.47
11:K:197:TRP:CD1	9:W:190:LYS:HE3	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
6:F:18:ASP:OD2	6:F:18:ASP:N	2.47	0.47
6:T:237:GLN:HA	6:T:237:GLN:NE2	2.30	0.47
13:1:152:ARG:HG3	13:1:152:ARG:NH1	2.14	0.47
4:R:194:LEU:HD12	4:R:207:LEU:HD11	1.95	0.47
11:Y:156:LYS:HD3	11:Y:195:LEU:HD11	1.96	0.47
11:Y:4:LEU:HD13	11:Y:159:ILE: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
10:J:113:ILE:HA	10:J:118:THR:O	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:87:ASN:ND2	7:G:87:ASN:C	2.69	0.46
7:U:87:ASN:C	7:U:87:ASN:ND2	2.68	0.46
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
8:H:144:GLN:O	8:H:145:ASP:HB2	2.15	0.46
2:P:112:LEU:HD23	2:P:112:LEU:C	2.35	0.46
8:V:126:SER:O	8:V:127:LEU:HD23	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
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
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
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:HE	6:T:169:ARG:HB3	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
13:1:71:LEU:C	13:1:73:ASP:N	2.69	0.46
2:P:138:TYR:HB2	2:P:149:TYR:HB2	1.97	0.46
4:R:215:ILE:O	4:R:215:ILE:HG13	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
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
11:K:210:ILE:HB	9:W:30:LYS:HE3	1.96	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
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
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
1:O:97:HIS:HD2	8:V:61:SER:OG	1.98	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
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
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
3:Q:97:GLN:HG3	10:X:65:LEU:HB2	1.97	0.45
13:1:120:TYR:HE1	13:1:135:THR:HG22	1.81	0.45
4:D:45:GLY:HA2	4:D:146:TYR:CE1	2.52	0.45
9:I:165:ARG:NH2	12:Z:135:MET:HE2	2.32	0.45
1:O:20:LYS:HA	1:O:20:LYS:HD3	1.78	0.45
4:R:163:LYS:HG3	4:R:164:ALA:N	2.32	0.45
10:J:7:ARG:O	10:J:7:ARG:HG3	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
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
5:E:92:LEU:HD11	5:E:112:ALA:HB1	1.98	0.45
1:O:152:ASP:HB3	1:O:153:PRO:HD2	1.99	0.45
7:U:49:ILE:HD13	7:U:193:ALA:CB	2.48	0.45
7:U:47:VAL:HG12	7:U:49:ILE:HD12	1.99	0.45
13:1:39:ASN:H	13:1:39:ASN:HD22	1.65	0.44
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
13:1:120:TYR:CE1	13:1:135:THR:HG22	2.52	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
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
6:F:127:ASN:HD22	6:F:127:ASN:C	2.20	0.44
6:T:22:PHE:HA	6:T:22:PHE:HD1	1.76	0.44
4:D:192:LEU:O	4:D:196:ILE:HG13	2.18	0.44
3:C:17:PRO:HA	4:D:26:TYR:CE1	2.53	0.44
1:A:97:HIS:CD2	8:H:61:SER:OG	2.69	0.44
2:P:60:GLU:O	2:P:63(A):SER:HB2	2.17	0.44
13:1:88:ALA:HA	13:1:121:VAL:HG21	2.00	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
14:2:32:ASP:OD1	14:2:186:ARG:NH2	2.51	0.44
11:K:86:LEU:C	11:K:86:LEU:HD13	2.38	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
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
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
10:J:137:LEU:HD21	11:Y:140:SER:OG	2.18	0.44
13:1:152:ARG:NH1	13:1:152:ARG:CG	2.76	0.44
3:C:228:GLU:O	3:C:232:TYR:HD1	2.01	0.44
6:T:127:ASN:HD22	6:T:127:ASN:C	2.21	0.44
14:2:34:LEU:HD13	14:2:176:VAL:HG23	2.00	0.43
1:A:78:TYR:HB3	1:A:85:TYR:CD1	2.52	0.43
5:E:31:ILE:HD11	5:E:153:PRO:CD	2.48	0.43
4:D:97:VAL:HG11	11:K:65:LEU:HD22	2.00	0.43
7:U:38:LEU:HD12	7:U:38:LEU:C	2.38	0.43
12:Z:129:ALA:HB1	12:Z:166:HIS:CE1	2.53	0.43
6:F:12:ASN:C	6:F:14:VAL:H	2.21	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
5:S:198:SER:C	5:S:200:SER:H	2.21	0.43
3:C:35:THR:HB	3:C:51:GLU:HG3	2.00	0.43
4:R:194:LEU:HD22	4:R:212:LEU:HD11	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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
7:U:96:ALA:CA	7:U:107:MET:CE	2.93	0.43
13:I:71:LEU:O	13:I:73:ASP:N	2.52	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
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:NH1	6:F:187:ARG:HG2	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: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:152:ARG:CG	13:M:152:ARG:HH11	2.29	0.42
13:M:16:ASP:HA	13:M:186:PHE:CB	2.49	0.42
13:M:39:ASN:H	13:M:39:ASN:HD22	1.66	0.42
8:V:109:HIS:HB3	8:V:111:PHE:CE2	2.54	0.42
2:B:152:ASN:HB2	2:B:153:PRO:CD	2.48	0.42
2:B:149:TYR:CZ	3:C:62(A):ILE:HD12	2.55	0.42
1:A:58:LEU:HD12	7:G:173:THR:HG23	2.00	0.42
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
2:P:97:GLN:NE2	9:W:61:TYR:HA	2.33	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
14:2:15:GLY:HA2	14:2:174:ARG:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
5:E:160:LEU:HD23	6:F:59:LEU:HA	1.99	0.42
7:G:107:MET:HE1	7:G:112:LEU:HD13	2.01	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
3:C:97:GLN:HA	3:C:97:GLN:NE2	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:HA	9:W:55:LEU:HD23	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
13:1:73:ASP:CG	13:1:73:ASP:O	2.58	0.41
1:A:111:LEU:HA	1:A:111:LEU:HD23	1.95	0.41
1:A:67:VAL:HG11	1:A:213:ALA:CB	2.50	0.41
3:C:57:LYS:CD	3:C:58:LEU:H	2.16	0.41
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
8:H:223:ASP:OD2	8:H:223:ASP:N	2.54	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
12:L:153:LYS:HG2	8:V:201:GLN:HG3	2.02	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
13:1:87:LEU:O	13:1:91:MET:HG2	2.20	0.41
6:F:95:GLU:HG3	6:F:115:ARG:HD2	2.03	0.41
10:J:36:GLN:HG3	10:J:184:ILE:CD1	2.51	0.41
10:J:3:ILE:HD13	10:J:3:ILE:HA	1.94	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
8:H:165:ASN:ND2	13:1:147:ARG:HH11	2.19	0.41
2:B:163:ILE:HG13	2:B:164:SER:H	1.85	0.41
7:G:96:ALA:CA	7:G:107:MET:HE2	2.23	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:N	2:B:44:ASP:OD2	2.54	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
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
14:2:146:MET:HE3	14:2:150:GLU:HB3	2.03	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
10:X:52:THR:CG2	10:X:53:VAL:N	2.83	0.41
5:E:207(B):THR:H	5:E:209(E):ASN:HB2	1.84	0.41
5:S:13:VAL:HG21	6:T:128:SER:O	2.21	0.41
4:R:90:GLU:OE2	11:Y:69:ARG:NH1	2.54	0.41
13:1:121:VAL:HA	13:1:126:VAL:O	2.22	0.41
1:O:217(K):GLY:HA3	8:V:186:TYR:HB3	2.04	0.41
1:O:33:GLN:HG2	1:O:33:GLN:H	1.69	0.41
2:P:218:ASN:O	2:P:218(C):ASP:HB2	2.22	0.41
3:Q:53:ARG:HD3	3:Q:55:THR:OG1	2.20	0.41
5:S:13:VAL:HG13	5:S:13:VAL:O	2.21	0.41
14:2:36:ARG:HG3	14:2:42:TRP:CZ2	2.57	0.40
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
2:P:149:TYR:CZ	3:Q:62(A):ILE:HD12	2.56	0.40
6:T:143:LYS:HE3	6:T:143:LYS:HB3	1.93	0.40
6:T:7:GLY:O	7:U:11:HIS:CE1	2.74	0.40
13:1:69:ASN:HA	13:1:70:PRO:HD2	1.97	0.40
7:U:192:PHE:C	7:U:192:PHE:CD1	2.94	0.40
13:1:69:ASN:HD21	13:1:72:ALA:HA	1.82	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:217(G):LEU:HD13	1:O:218:GLY:HA2	2.03	0.40
1:O:8:TYR:HE2	6:T:127:ASN:OD1	2.05	0.40
10:X:4:LEU:HD23	10:X:126:ALA:HB2	2.02	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
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
13:M:178:ARG:HD3	8:V:139:GLU:OE1	2.22	0.40
11:Y:200:LYS:HG3	11:Y:206:PHE:HB2	2.03	0.40
11:Y:87:VAL:HG13	11:Y:115:SER:HA	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	244/250 (98%)	239 (98%)	4 (2%)	1 (0%)	34	48
1	O	244/250 (98%)	232 (95%)	10 (4%)	2 (1%)	19	29
2	B	233/235 (99%)	218 (94%)	12 (5%)	3 (1%)	12	18
2	P	233/235 (99%)	217 (93%)	12 (5%)	4 (2%)	9	13
3	C	236/241 (98%)	227 (96%)	5 (2%)	4 (2%)	9	13
3	Q	236/241 (98%)	226 (96%)	7 (3%)	3 (1%)	12	18
4	D	224/260 (86%)	215 (96%)	8 (4%)	1 (0%)	34	48
4	R	225/260 (86%)	216 (96%)	8 (4%)	1 (0%)	34	48
5	E	228/233 (98%)	214 (94%)	12 (5%)	2 (1%)	17	26
5	S	228/233 (98%)	211 (92%)	14 (6%)	3 (1%)	12	18
6	F	240/242 (99%)	228 (95%)	11 (5%)	1 (0%)	34	48
6	T	240/242 (99%)	225 (94%)	12 (5%)	3 (1%)	12	18
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%)	29	43
10	X	196/198 (99%)	188 (96%)	7 (4%)	1 (0%)	29	43
11	K	210/212 (99%)	204 (97%)	5 (2%)	1 (0%)	29	43
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%)	17	26

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
13	M	231/233 (99%)	221 (96%)	9 (4%)	1 (0%)	34	48
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%)	29	43

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
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

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Mol	Chain	Res	Type
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%)	42	60
1	O	205/209 (98%)	197 (96%)	8 (4%)	32	48
2	B	194/195 (100%)	179 (92%)	15 (8%)	13	20
2	P	194/195 (100%)	179 (92%)	15 (8%)	13	20
3	C	210/213 (99%)	192 (91%)	18 (9%)	10	15
3	Q	210/213 (99%)	195 (93%)	15 (7%)	14	22
4	D	186/215 (86%)	171 (92%)	15 (8%)	11	17
4	R	186/215 (86%)	173 (93%)	13 (7%)	15	23
5	E	187/191 (98%)	167 (89%)	20 (11%)	6	9
5	S	187/191 (98%)	167 (89%)	20 (11%)	6	9
6	F	200/200 (100%)	179 (90%)	21 (10%)	7	10
6	T	200/200 (100%)	179 (90%)	21 (10%)	7	10
7	G	205/207 (99%)	190 (93%)	15 (7%)	14	21
7	U	205/207 (99%)	193 (94%)	12 (6%)	19	30
8	H	181/181 (100%)	171 (94%)	10 (6%)	21	33
8	V	181/181 (100%)	173 (96%)	8 (4%)	28	43
9	I	172/172 (100%)	161 (94%)	11 (6%)	17	27
9	W	172/172 (100%)	165 (96%)	7 (4%)	30	46
10	J	174/175 (99%)	164 (94%)	10 (6%)	20	31
10	X	174/175 (99%)	158 (91%)	16 (9%)	9	13
11	K	169/169 (100%)	153 (90%)	16 (10%)	8	12
11	Y	169/169 (100%)	159 (94%)	10 (6%)	19	30
12	L	185/185 (100%)	172 (93%)	13 (7%)	15	23

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
12	Z	185/185 (100%)	176 (95%)	9 (5%)	25	38
13	1	199/199 (100%)	191 (96%)	8 (4%)	31	47
13	M	199/199 (100%)	189 (95%)	10 (5%)	24	38
14	2	162/162 (100%)	151 (93%)	11 (7%)	16	24
14	N	162/162 (100%)	155 (96%)	7 (4%)	29	44
All	All	5258/5346 (98%)	4898 (93%)	360 (7%)	16	24

All (360) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	62	GLU
1	A	64	LEU
1	A	147(A)	SER
1	A	158	PHE
1	A	212	LEU
1	A	222	ARG
2	B	58	LEU
2	B	61	GLN
2	B	62	ASP
2	B	63	THR
2	B	71	ASN
2	B	91	THR
2	B	104	ASN
2	B	121	GLN
2	B	150	THR
2	B	185	LYS
2	B	187	ASP
2	B	192	LEU
2	B	202	THR
2	B	216	ARG
2	B	218(C)	ASP
3	C	18	ASP
3	C	44	ASN
3	C	55	THR
3	C	57	LYS
3	C	66	LYS
3	C	82	ASN
3	C	87	ILE
3	C	121	GLN
3	C	150	GLN

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Mol	Chain	Res	Type
3	C	156	ILE
3	C	163	GLN
3	C	172	VAL
3	C	174	GLU
3	C	178	LYS
3	C	208	LYS
3	C	209	ASN
3	C	215	VAL
3	C	226	SER
4	D	27	SER
4	D	28	LEU
4	D	52	LYS
4	D	59	LEU
4	D	76	CYS
4	D	86	ARG
4	D	110	GLU
4	D	119	LEU
4	D	170	GLU
4	D	177	LEU
4	D	184	LEU
4	D	191	LEU
4	D	194	LEU
4	D	215	ILE
4	D	238	LYS
5	E	12	THR
5	E	13	VAL
5	E	28	LEU
5	E	58	LEU
5	E	64	GLN
5	E	76	LEU
5	E	90	ASN
5	E	111	ARG
5	E	121	GLN
5	E	149	LEU
5	E	168	ARG
5	E	185	ASN
5	E	189	LEU
5	E	198	SER
5	E	207	LEU
5	E	208(C)	VAL
5	E	209(D)	ASP
5	E	219	THR

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Mol	Chain	Res	Type
5	E	222	THR
5	E	231	LYS
6	F	9	ASP
6	F	18	ASP
6	F	43	ASN
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	180(E)	GLU
6	F	187	ARG
6	F	192	GLN
6	F	203	GLU
6	F	205	ASN
6	F	206(B)	GLU
6	F	214	TRP
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	121	GLN
7	G	124	THR
7	G	169	GLN
7	G	197	MET
7	G	203	THR
7	G	204	GLU
7	G	217	LYS
7	G	232	ARG
7	G	233	LEU
7	G	240	ASP
8	H	7	LYS
8	H	30	ASN
8	H	34	LEU
8	H	55	VAL

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Mol	Chain	Res	Type
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	144	PRO
9	I	159	LEU
9	I	160	LEU
9	I	171	TRP
9	I	174	VAL
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	77	GLN
10	J	90	SER
10	J	105(B)	LYS
10	J	130	SER
10	J	166	MET
11	K	4	LEU
11	K	7	ARG
11	K	9	GLN
11	K	31	VAL
11	K	41	LEU
11	K	65	LEU
11	K	73	ARG
11	K	87	VAL
11	K	91	LYS
11	K	99	THR
11	K	105(A)	ARG
11	K	105(B)	LYS
11	K	121	LYS
11	K	143	LYS
11	K	175	LEU

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Mol	Chain	Res	Type
11	K	201	GLU
12	L	-9	GLN
12	L	-7	ASN
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
12	L	144(K)	LYS
12	L	144(P)	LEU
13	M	39	ASN
13	M	61	LEU
13	M	64	GLU
13	M	95	ARG
13	M	152	ARG
13	M	162	GLN
13	M	178	ARG
13	M	185	ASN
13	M	195	THR
13	M	217	LYS
14	N	20	THR
14	N	105	ASP
14	N	105(A)	ASP
14	N	105(B)	LYS
14	N	119	VAL
14	N	149	GLU
14	N	178	LEU
1	O	32	LYS
1	O	33	GLN
1	O	54	SER
1	O	64	LEU
1	O	65	SER
1	O	110	LYS
1	O	158	PHE
1	O	212	LEU
2	P	55	THR
2	P	57	THR
2	P	58	LEU

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Mol	Chain	Res	Type
2	P	90	ASN
2	P	91	THR
2	P	121	GLN
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	203	ASP
2	P	204(A)	SER
2	P	212	PHE
3	Q	18	ASP
3	Q	35	THR
3	Q	57	LYS
3	Q	61	THR
3	Q	75	VAL
3	Q	82	ASN
3	Q	121	GLN
3	Q	150	GLN
3	Q	156	ILE
3	Q	163	GLN
3	Q	172	VAL
3	Q	208	LYS
3	Q	209	ASN
3	Q	215	VAL
3	Q	240	LYS
4	R	48	LEU
4	R	59	LEU
4	R	62	ASP
4	R	76	CYS
4	R	86	ARG
4	R	119	LEU
4	R	177	LEU
4	R	180(E)	SER
4	R	184	LEU
4	R	191	LEU
4	R	194	LEU
4	R	207	LEU
4	R	215	ILE
5	S	11	ASP
5	S	12	THR

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Mol	Chain	Res	Type
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	121	GLN
5	S	168	ARG
5	S	185	ASN
5	S	189	LEU
5	S	198	SER
5	S	199	GLN
5	S	209(D)	ASP
5	S	211	SER
5	S	219	THR
5	S	227	GLU
5	S	231	LYS
6	T	20	ARG
6	T	22	PHE
6	T	36	THR
6	T	43	ASN
6	T	98	SER
6	T	121	GLN
6	T	127	ASN
6	T	135	SER
6	T	143	LYS
6	T	169	ARG
6	T	170	GLN
6	T	171	SER
6	T	176	LEU
6	T	180(E)	GLU
6	T	187	ARG
6	T	192	GLN
6	T	203	GLU
6	T	205	ASN
6	T	206(B)	GLU
6	T	206(C)	LYS
6	T	214	TRP
7	U	29	LYS
7	U	38	LEU
7	U	72	ARG

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Mol	Chain	Res	Type
7	U	76	MET
7	U	87	ASN
7	U	119	LEU
7	U	121	GLN
7	U	204	GLU
7	U	217	LYS
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	68	LEU
8	V	113	ILE
8	V	144	GLN
8	V	221	ILE
9	W	-8	SER
9	W	16	CYS
9	W	29	ASN
9	W	160	LEU
9	W	171	TRP
9	W	181	LYS
9	W	182	ASP
10	X	6	ILE
10	X	9	GLN
10	X	24	ILE
10	X	34	THR
10	X	52	THR
10	X	68	ILE
10	X	70	GLU
10	X	77	GLN
10	X	90	SER
10	X	90(A)	ILE
10	X	90(B)	ARG
10	X	105(B)	LYS
10	X	120	VAL
10	X	137	LEU
10	X	166	MET
10	X	191	GLN
11	Y	4	LEU
11	Y	9	GLN

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Mol	Chain	Res	Type
11	Y	41	LEU
11	Y	65	LEU
11	Y	87	VAL
11	Y	105(A)	ARG
11	Y	145	ASP
11	Y	146	LEU
11	Y	208	ASN
11	Y	210	ILE
12	Z	-9	GLN
12	Z	-7	ASN
12	Z	2	THR
12	Z	14	LEU
12	Z	25	SER
12	Z	40	ASN
12	Z	118	SER
12	Z	138	LEU
12	Z	144(J)	ASN
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	217	LYS
14	2	20	THR
14	2	22	THR
14	2	36	ARG
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	186	ARG
14	2	187(I)	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (166) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	97	HIS
2	B	23	GLN

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Mol	Chain	Res	Type
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	82	ASN
3	C	97	GLN
3	C	121	GLN
3	C	125	GLN
3	C	150	GLN
3	C	163	GLN
3	C	209	ASN
4	D	23	GLN
4	D	108	ASN
4	D	141	HIS
4	D	199	GLN
4	D	226	ASN
5	E	73	HIS
5	E	97	ASN
5	E	121	GLN
5	E	125	GLN
5	E	185	ASN
5	E	199	GLN
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
6	F	192	GLN
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

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Mol	Chain	Res	Type
7	G	178	ASN
7	G	184	ASN
8	H	66	HIS
8	H	144	GLN
8	H	165	ASN
8	H	172	ASN
10	J	54	GLN
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	131	GLN
11	K	174	ASN
11	K	208	ASN
12	L	-7	ASN
12	L	40	ASN
12	L	67	HIS
12	L	70(A)	ASN
12	L	123	GLN
12	L	144(B)	ASN
12	L	166	HIS
13	M	9	ASN
13	M	39	ASN
13	M	93	GLN
13	M	162	GLN
13	M	170	ASN
13	M	204	GLN
14	N	145	ASN
14	N	157	HIS
14	N	161	GLN
1	O	97	HIS
2	P	23	GLN
2	P	71	ASN
2	P	97	GLN
2	P	121	GLN
2	P	125	GLN
2	P	156	ASN
2	P	177	GLN
2	P	218	ASN

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Mol	Chain	Res	Type
3	Q	23	GLN
3	Q	82	ASN
3	Q	121	GLN
3	Q	125	GLN
3	Q	150	GLN
3	Q	163	GLN
3	Q	179	ASN
3	Q	243	GLN
4	R	23	GLN
4	R	108	ASN
4	R	147	GLN
4	R	199	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	185	ASN
5	S	199	GLN
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	34(A)	ASN
7	U	87	ASN
7	U	118	ASN
7	U	121	GLN
7	U	125	GLN
7	U	170	GLN
7	U	178	ASN
7	U	180(C)	HIS
7	U	184	ASN
8	V	30	ASN
8	V	35	HIS
8	V	66	HIS

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Mol	Chain	Res	Type
8	V	86	HIS
8	V	144	GLN
8	V	165	ASN
8	V	172	ASN
8	V	190	ASN
9	W	81	GLN
9	W	145	ASN
10	X	54	GLN
10	X	77	GLN
10	X	85	GLN
10	X	112	GLN
10	X	127	HIS
10	X	186	GLN
11	Y	85	ASN
11	Y	141	ASN
11	Y	174	ASN
11	Y	208	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	144(B)	ASN
12	Z	144(J)	ASN
12	Z	166	HIS
13	1	9	ASN
13	1	39	ASN
13	1	69	ASN
13	1	93	GLN
13	1	162	GLN
13	1	170	ASN
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 carbohydrates 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$
17	MES	K	303	-	12,12,12	2.04	1 (8%)	14,16,16	1.74	3 (21%)
16	3SD	Y	302	-	42,44,44	1.17	3 (7%)	54,60,60	0.86	1 (1%)
16	3SD	K	302	-	42,44,44	1.07	3 (7%)	54,60,60	1.04	3 (5%)
17	MES	Y	303	-	12,12,12	2.32	1 (8%)	14,16,16	1.39	2 (14%)

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
17	MES	K	303	-	-	0/6/14/14	0/1/1/1
16	3SD	Y	302	-	-	1/37/40/40	0/3/3/3
16	3SD	K	302	-	-	0/37/40/40	0/3/3/3
17	MES	Y	303	-	-	0/6/14/14	0/1/1/1

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	Y	303	MES	C8-S	-7.76	1.66	1.77
17	K	303	MES	C8-S	-6.75	1.67	1.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	Y	302	3SD	C6-C5	4.20	1.53	1.48
16	Y	302	3SD	C4-C5	-4.16	1.33	1.39
16	K	302	3SD	C6-C5	3.98	1.53	1.48
16	K	302	3SD	C4-C5	-3.87	1.34	1.39
16	Y	302	3SD	C4-C3	-3.09	1.34	1.39
16	K	302	3SD	C4-C3	-2.82	1.34	1.39

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	K	303	MES	O3S-S-C8	4.52	113.07	105.77
17	Y	303	MES	O3S-S-C8	3.46	111.36	105.77
17	K	303	MES	O1S-S-C8	3.06	110.60	106.92
16	K	302	3SD	C9-C8-C10	-2.85	103.70	110.42
16	K	302	3SD	C9-C33-N34	-2.73	112.20	115.97
16	Y	302	3SD	C9-C8-C10	-2.14	105.38	110.42
16	K	302	3SD	C37-C36-N34	-2.07	110.65	113.90
17	Y	303	MES	O2S-S-C8	2.04	109.38	106.92
17	K	303	MES	O2S-S-C8	-2.03	104.47	106.92

There are no chirality outliers.

All (1) torsion outliers are listed below:

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

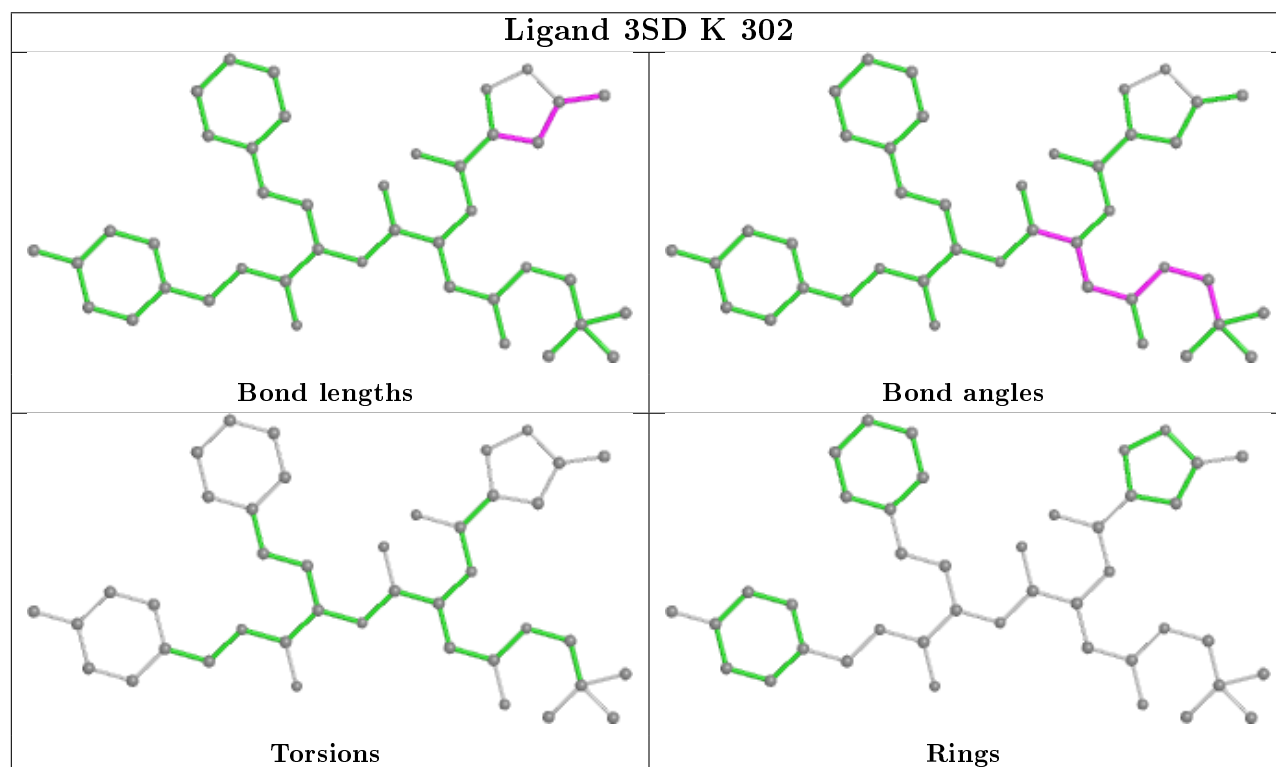
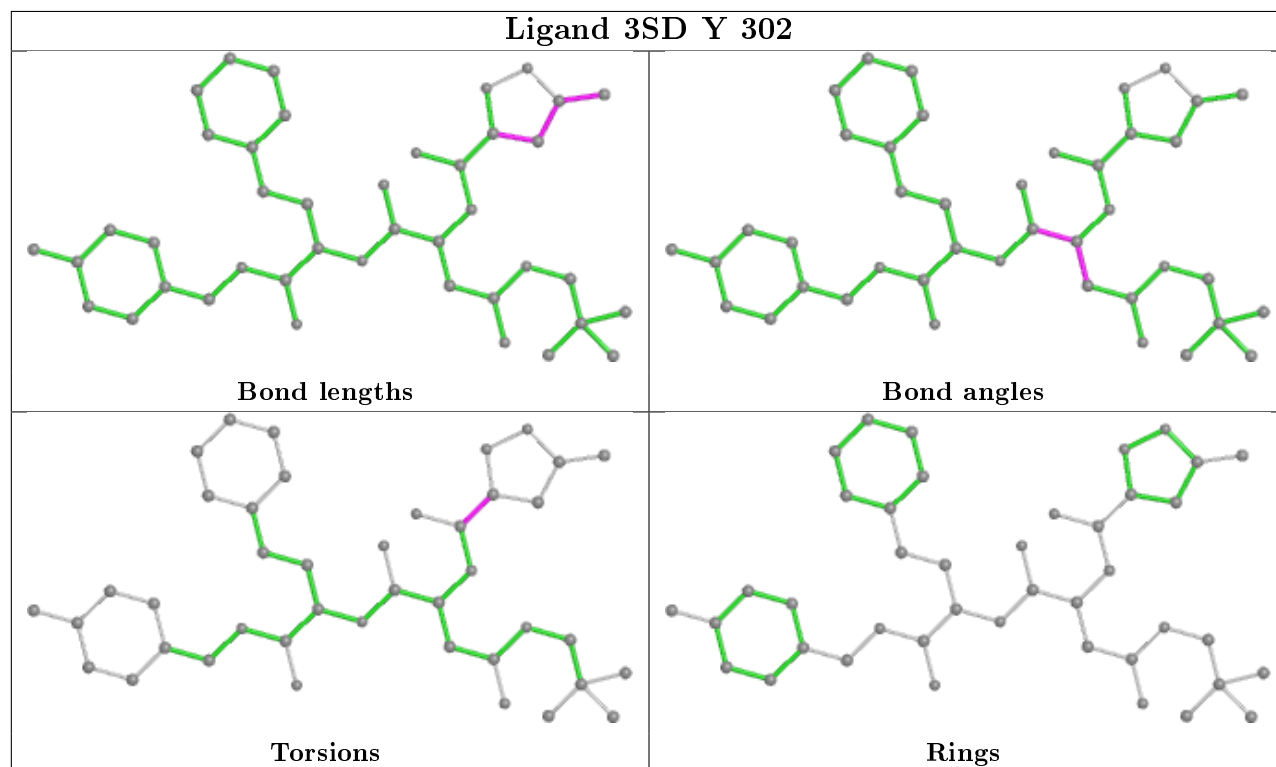
There are no ring outliers.

3 monomers are involved in 3 short contacts:

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

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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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%)	-0.29	4 (1%) 72 69	31, 43, 64, 89	0
1	O	246/250 (98%)	-0.08	4 (1%) 72 69	32, 50, 74, 94	0
2	B	235/235 (100%)	0.13	14 (5%) 21 18	26, 51, 82, 90	0
2	P	235/235 (100%)	0.14	10 (4%) 35 31	27, 51, 85, 94	0
3	C	238/241 (98%)	0.21	16 (6%) 17 14	31, 59, 103, 118	0
3	Q	238/241 (98%)	0.53	23 (9%) 7 6	34, 63, 111, 127	0
4	D	228/260 (87%)	-0.20	3 (1%) 77 75	28, 51, 73, 95	0
4	R	229/260 (88%)	-0.04	6 (2%) 56 52	29, 53, 77, 102	0
5	E	230/233 (98%)	-0.06	8 (3%) 44 40	37, 52, 78, 92	0
5	S	230/233 (98%)	0.18	14 (6%) 21 18	34, 54, 89, 99	0
6	F	242/242 (100%)	0.05	10 (4%) 37 33	29, 49, 85, 109	0
6	T	242/242 (100%)	0.20	11 (4%) 33 30	29, 48, 76, 109	0
7	G	240/243 (98%)	-0.26	3 (1%) 77 75	28, 42, 68, 99	0
7	U	240/243 (98%)	-0.38	3 (1%) 77 75	26, 42, 63, 85	0
8	H	222/222 (100%)	-0.33	2 (0%) 84 83	27, 37, 56, 85	0
8	V	222/222 (100%)	-0.30	2 (0%) 84 83	29, 41, 59, 87	0
9	I	204/204 (100%)	-0.42	1 (0%) 91 91	25, 37, 53, 61	0
9	W	204/204 (100%)	-0.37	2 (0%) 82 81	28, 38, 56, 62	0
10	J	198/198 (100%)	-0.14	5 (2%) 57 53	28, 41, 57, 114	0
10	X	198/198 (100%)	-0.16	5 (2%) 57 53	30, 42, 55, 115	0
11	K	212/212 (100%)	-0.33	0 100 100	26, 37, 54, 63	0
11	Y	212/212 (100%)	-0.30	2 (0%) 84 83	29, 39, 57, 61	0
12	L	222/222 (100%)	-0.40	1 (0%) 91 91	27, 39, 58, 65	0
12	Z	222/222 (100%)	-0.37	0 100 100	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%)	-0.36	3 (1%)	77	75	23, 35, 53, 62	0
13	M	233/233 (100%)	-0.40	2 (0%)	84	83	25, 39, 55, 61	0
14	2	196/196 (100%)	-0.34	2 (1%)	82	81	27, 35, 52, 69	0
14	N	196/196 (100%)	-0.39	0	100	100	26, 36, 52, 64	0
All	All	6293/6382 (98%)	-0.15	156 (2%)	57	53	23, 44, 80, 127	0

All (156) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
6	T	10	LEU	17.3
6	T	8	TYR	16.6
6	T	9	ASP	15.1
6	T	11	SER	13.2
6	F	9	ASP	12.6
6	F	10	LEU	10.3
2	B	217	ALA	9.3
2	B	216(B)	GLY	8.9
2	B	218	ASN	8.8
6	T	7	GLY	8.8
6	F	7	GLY	8.8
3	C	55	THR	8.3
10	J	192	ALA	8.3
6	F	8	TYR	8.2
2	P	217	ALA	7.6
6	F	11	SER	7.5
2	P	218	ASN	7.2
3	Q	207	ALA	7.1
7	G	240	ASP	6.7
3	Q	54	SER	6.6
3	Q	56	LEU	6.5
10	X	193	GLN	6.0
10	J	193	GLN	5.8
6	F	12	ASN	5.8
3	C	207	ALA	5.5
13	M	-8	THR	5.4
10	X	192	ALA	5.4
5	S	57	GLU	5.2
3	Q	55	THR	5.1
3	C	208	LYS	5.1
11	Y	211	GLY	4.8
10	X	191	GLN	4.8

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Mol	Chain	Res	Type	RSRZ
3	C	56	LEU	4.7
3	Q	243	GLN	4.6
3	C	11	ALA	4.5
2	P	54	VAL	4.5
2	B	239	THR	4.4
10	J	191	GLN	4.4
5	S	58	LEU	4.4
8	V	223	ASP	4.3
3	Q	242	GLU	4.3
3	Q	53	ARG	4.2
3	Q	203	THR	4.2
9	W	-8	SER	4.1
5	E	203	ASP	4.1
3	Q	241	GLN	4.0
3	Q	209	ASN	4.0
13	1	-8	THR	4.0
8	V	222	CYS	4.0
5	S	203	ASP	4.0
5	S	206	SER	4.0
5	S	63	TYR	3.9
2	B	218(C)	ASP	3.9
10	X	189	ASP	3.8
3	Q	240	LYS	3.8
2	B	127	GLY	3.8
2	P	63	THR	3.6
3	Q	208	LYS	3.6
5	S	8	TYR	3.6
6	F	204	ASP	3.5
1	O	236	LEU	3.5
2	B	216(A)	LYS	3.4
7	U	240	ASP	3.4
4	D	22	PHE	3.3
2	B	54	VAL	3.3
3	C	203	THR	3.2
9	I	-8	SER	3.2
8	H	222	CYS	3.2
4	R	244	GLU	3.1
5	S	178	ARG	3.1
6	T	12	ASN	3.1
10	J	168	MET	3.0
10	J	189	ASP	3.0
3	C	54	SER	3.0

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Mol	Chain	Res	Type	RSRZ
7	G	239	GLN	3.0
3	Q	238	GLN	2.9
3	Q	180(C)	LYS	2.9
3	Q	64	PRO	2.9
3	Q	63	THR	2.9
1	A	9	SER	2.9
3	Q	237	GLU	2.9
2	P	216(B)	GLY	2.9
6	T	180(E)	GLU	2.9
3	Q	206	GLY	2.8
13	1	72	ALA	2.8
3	C	180(C)	LYS	2.8
8	H	223	ASP	2.8
5	S	202	ARG	2.8
5	S	9	ASP	2.7
3	Q	234	THR	2.7
3	Q	144(B)	ASP	2.7
3	Q	202	GLN	2.7
4	R	178	ASN	2.7
14	2	105(B)	LYS	2.7
3	C	242	GLU	2.6
5	E	204	GLU	2.6
5	E	206	SER	2.6
5	E	57	GLU	2.6
1	O	217(P)	LYS	2.6
4	R	123	PHE	2.6
5	S	180(E)	LYS	2.6
3	C	227	GLU	2.6
6	F	206(B)	GLU	2.6
3	C	53	ARG	2.6
2	B	204(A)	SER	2.5
5	E	63	TYR	2.5
2	P	62	ASP	2.5
12	L	-9	GLN	2.5
2	B	220	TYR	2.5
4	D	244	GLU	2.5
7	U	218	ASP	2.5
2	P	220	TYR	2.5
2	P	181	LYS	2.4
5	S	55	ALA	2.4
13	M	112	SER	2.4
1	A	234	GLU	2.4

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Mol	Chain	Res	Type	RSRZ
6	F	205	ASN	2.4
5	S	51	LEU	2.4
6	T	206	LYS	2.4
1	A	183	GLU	2.4
6	T	241	ASN	2.4
7	U	239	GLN	2.3
6	F	241	ASN	2.3
4	R	57	PRO	2.3
3	Q	144	ASP	2.3
2	B	218(D)	GLY	2.3
3	C	49	GLY	2.3
3	Q	49	GLY	2.3
6	T	227	ASP	2.2
9	W	182	ASP	2.2
3	C	180(D)	GLU	2.2
2	P	218(C)	ASP	2.2
1	O	234	GLU	2.2
5	E	202	ARG	2.2
3	C	241	GLN	2.2
1	O	39	GLY	2.2
5	S	56	ASP	2.2
2	B	230	LYS	2.2
6	T	180(D)	PRO	2.2
14	2	105(A)	ASP	2.2
4	D	243	ALA	2.1
3	C	240	LYS	2.1
3	C	243	GLN	2.1
4	R	18	GLU	2.1
11	Y	201	GLU	2.1
2	B	126	HIS	2.1
4	R	243	ALA	2.1
2	P	61	GLN	2.1
1	A	217(P)	LYS	2.1
2	B	49	ALA	2.1
10	X	168	MET	2.1
5	S	168	ARG	2.1
13	1	207	ASN	2.1
7	G	179(E)	LYS	2.0
5	E	168	ARG	2.0
5	E	178	ARG	2.0

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

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.

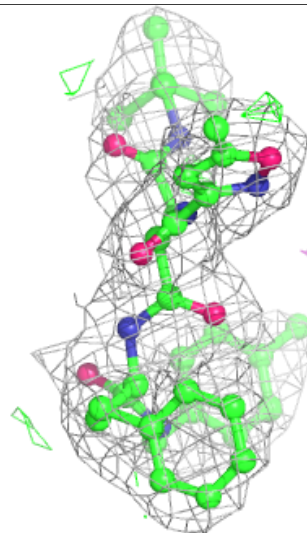
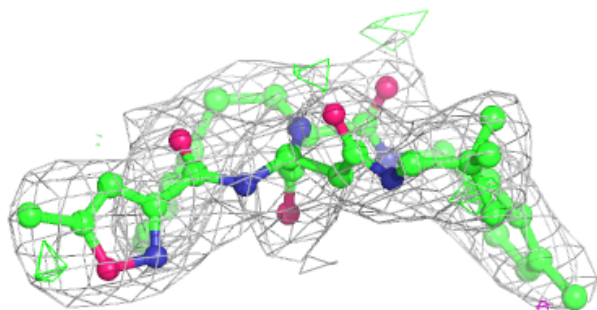
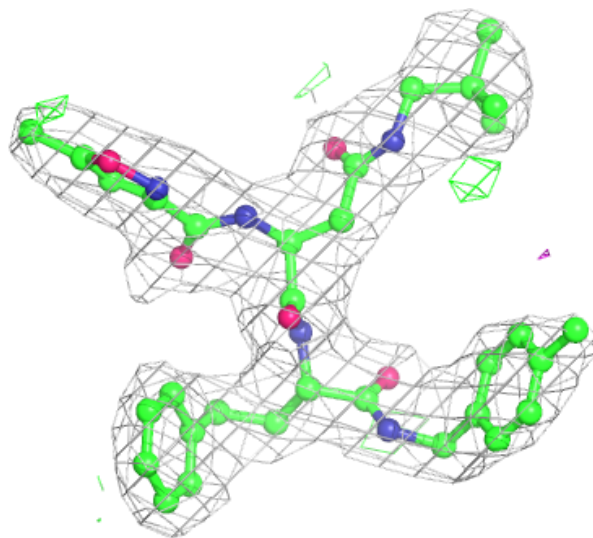
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
15	MG	L	201	1/1	0.59	0.11	52,52,52,52	0
15	MG	F	302	1/1	0.69	0.60	120,120,120,120	0
15	MG	Z	201	1/1	0.77	0.11	65,65,65,65	0
15	MG	W	201	1/1	0.77	0.14	53,53,53,53	0
15	MG	T	301	1/1	0.77	0.32	69,69,69,69	0
15	MG	F	301	1/1	0.84	0.79	74,74,74,74	0
15	MG	I	202	1/1	0.84	0.27	50,50,50,50	0
15	MG	I	201	1/1	0.86	0.10	46,46,46,46	0
15	MG	T	302	1/1	0.92	0.50	110,110,110,110	0
15	MG	Z	202	1/1	0.93	0.13	49,49,49,49	0
15	MG	U	301	1/1	0.93	0.07	38,38,38,38	0
15	MG	L	202	1/1	0.93	0.10	46,46,46,46	0
15	MG	W	202	1/1	0.94	0.14	50,50,50,50	0
16	3SD	Y	302	42/42	0.94	0.16	37,39,48,50	0
15	MG	N	201	1/1	0.95	0.14	41,41,41,41	0
15	MG	H	301	1/1	0.96	0.07	47,47,47,47	0
15	MG	G	9001	1/1	0.96	0.10	45,45,45,45	0
16	3SD	K	302	42/42	0.96	0.15	28,35,49,50	0
17	MES	K	303	12/12	0.96	0.18	55,57,58,58	0
15	MG	K	301	1/1	0.97	0.13	50,50,50,50	0
17	MES	Y	303	12/12	0.97	0.14	57,61,64,64	0
15	MG	V	301	1/1	0.97	0.08	42,42,42,42	0
15	MG	2	201	1/1	0.97	0.14	30,30,30,30	0
15	MG	Y	301	1/1	0.98	0.13	53,53,53,53	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.

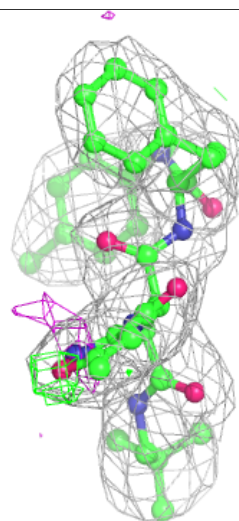
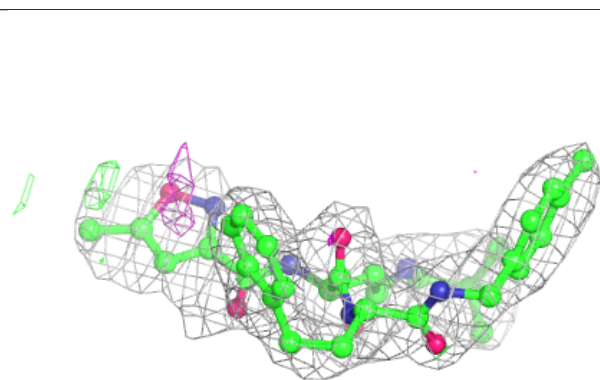
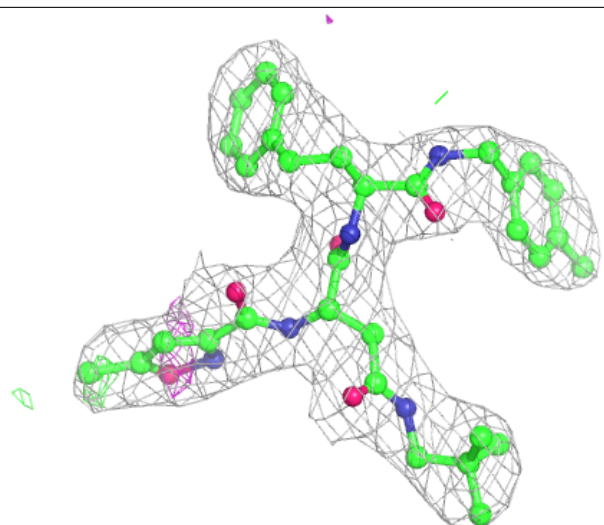
Electron density around 3SD Y 302:

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



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)



6.5 Other polymers [i](#)

There are no such residues in this entry.