



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 7, 2026 – 03:33 AM UTC

PDB ID : 3MG7 / pdb_00003mg7
Title : Structure of yeast 20S open-gate proteasome with Compound 8
Authors : Sintchak, M.D.
Deposited on : 2010-04-05
Resolution : 2.78 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

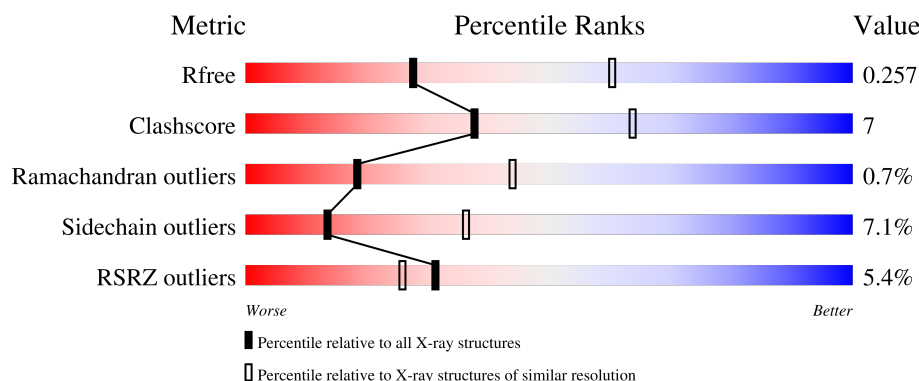
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.78 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	5248 (2.80-2.76)
Clashscore	190562	5693 (2.80-2.76)
Ramachandran outliers	187476	5590 (2.80-2.76)
Sidechain outliers	187428	5592 (2.80-2.76)
RSRZ outliers	180081	5251 (2.80-2.76)

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	4% 80% 18% .
1	O	250	6% 79% 19% .
2	B	245	8% 74% 19% .
2	P	245	9% 75% 19% .
3	C	243	14% 83% 15% ..

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Mol	Chain	Length	Quality of chain
3	Q	243	
4	D	250	
4	R	250	
5	E	234	
5	S	234	
6	F	248	
6	T	248	
7	G	252	
7	U	252	
8	H	222	
8	V	222	
9	I	205	
9	W	205	
10	J	198	
10	X	198	
11	K	212	
11	Y	212	
12	L	241	
12	Z	241	
13	1	266	
13	M	266	
14	2	196	
14	N	196	

2 Entry composition

There are 18 unique types of molecules in this entry. The entry contains 49424 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	250	Total	C	N	O	S	0	0	0
			1915	1219	315	377	4			
1	O	250	Total	C	N	O	S	0	0	0
			1915	1219	315	377	4			

- 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
			1829	1158	303	365	3			
2	P	235	Total	C	N	O	S	0	0	0
			1829	1158	303	365	3			

- Molecule 3 is a protein called Proteasome component PRE6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	241	Total	C	N	O	S	0	0	0
			1891	1181	331	375	4			
3	Q	241	Total	C	N	O	S	0	0	0
			1891	1181	331	375	4			

- Molecule 4 is a protein called Proteasome component PUP2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	242	Total	C	N	O	S	0	0	0
			1862	1162	314	379	7			
4	R	242	Total	C	N	O	S	0	0	0
			1862	1162	314	379	7			

- Molecule 5 is a protein called Proteasome component PRE5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	233	Total	C	N	O	S	0	0	0
			1795	1129	312	350	4			
5	S	233	Total	C	N	O	S	0	0	0
			1795	1129	312	350	4			

- Molecule 6 is a protein called Proteasome component C1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	237	Total	C	N	O	S	0	0	0
			1848	1175	323	346	4			
6	T	237	Total	C	N	O	S	0	0	0
			1848	1175	323	346	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	G	243	Total	C	N	O	S	0	0	0
			1921	1221	322	370	8			
7	U	243	Total	C	N	O	S	0	0	0
			1921	1221	322	370	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
			1585	1005	269	305	6			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	X	198	Total	C	N	O	S	0	0	0
			1585	1005	269	305	6			

- 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).

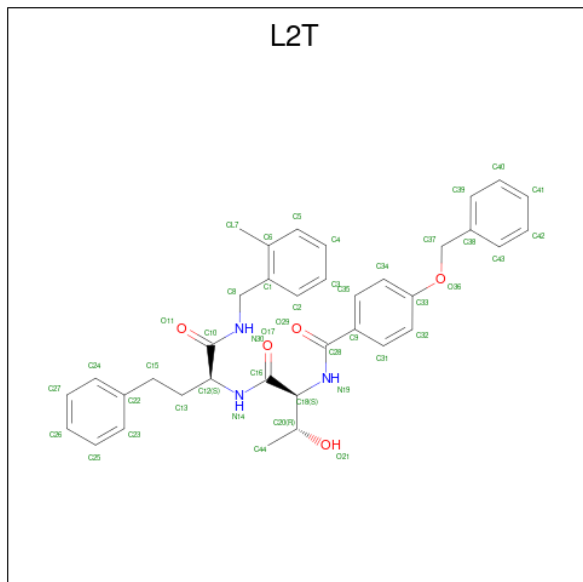
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
15	F	2	Total	Mg	0	0
			2	2		
15	G	1	Total	Mg	0	0
			1	1		

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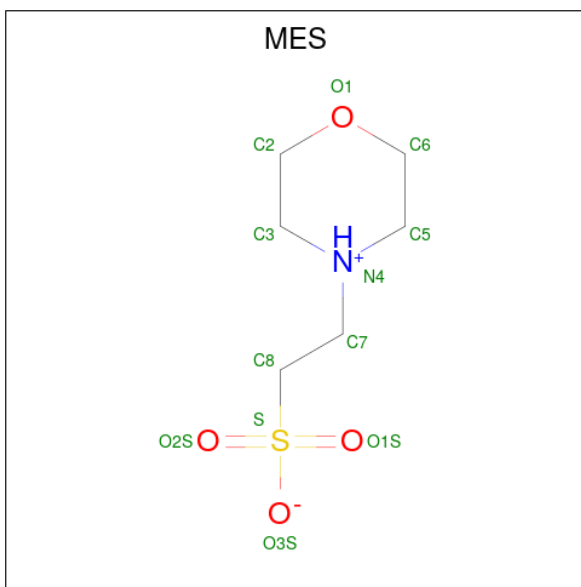
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
15	H	1	Total	Mg	0	0
			1	1		
15	I	2	Total	Mg	0	0
			2	2		
15	K	1	Total	Mg	0	0
			1	1		
15	L	2	Total	Mg	0	0
			2	2		
15	N	1	Total	Mg	0	0
			1	1		

- Molecule 16 is 4-(benzyloxy)-N-[(1S,2R)-2-hydroxy-1-({(1S)-1-[(2-methylbenzyl)carbamoyl]-3-phenylpropyl}carbamoyl)propyl]benzamide (CCD ID: L2T) (formula: C₃₆H₃₉N₃O₅).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
16	K	1	Total	C	N	O	0	0
			44	36	3	5		
16	Y	1	Total	C	N	O	0	0
			44	36	3	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		
17	Y	1	Total	C	N	O	S	0	0
			12	6	1	4	1		

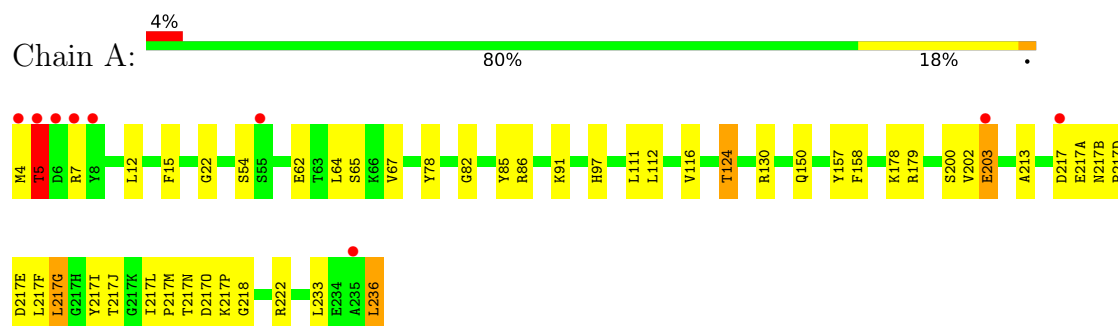
- Molecule 18 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
18	L	2	Total	O	0	0
			2	2		
18	Z	2	Total	O	0	0
			2	2		

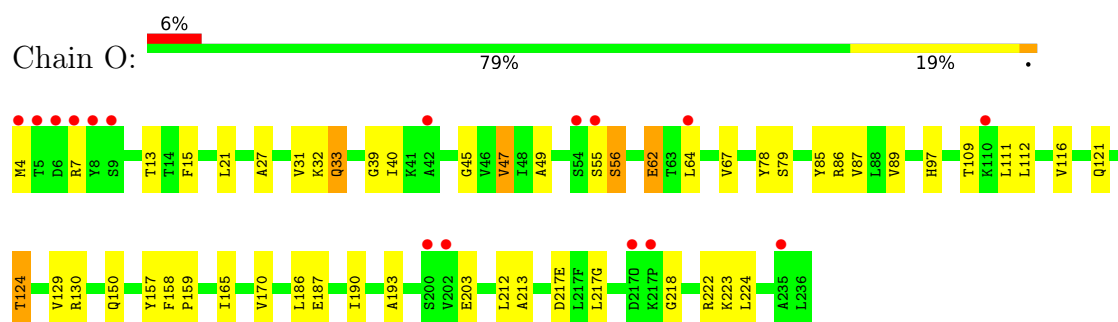
3 Residue-property plots [i](#)

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.

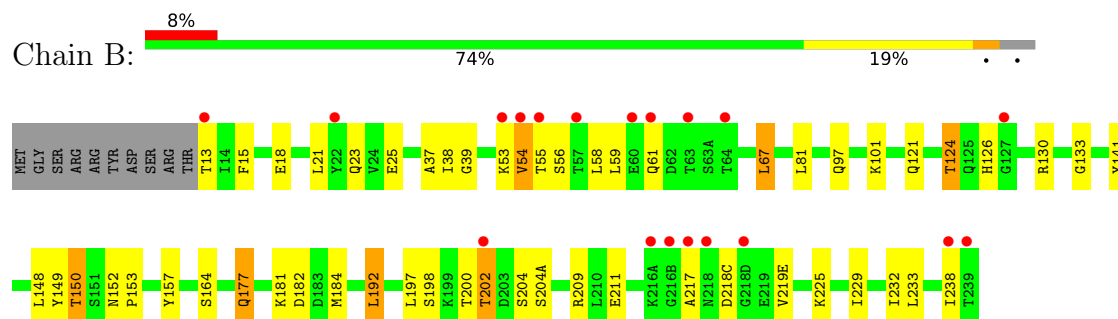
- Molecule 1: Proteasome component Y7



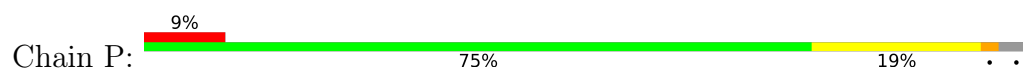
- Molecule 1: Proteasome component Y7

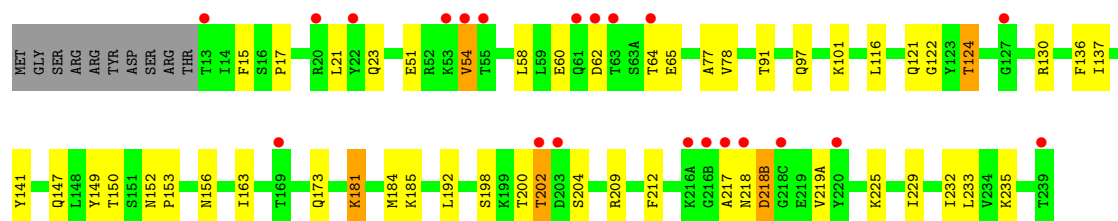


- Molecule 2: Proteasome component Y13

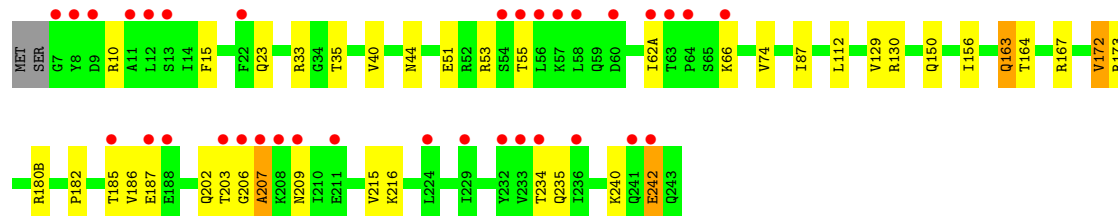
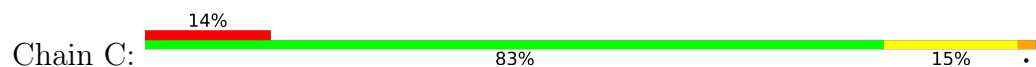


- Molecule 2: Proteasome component Y13

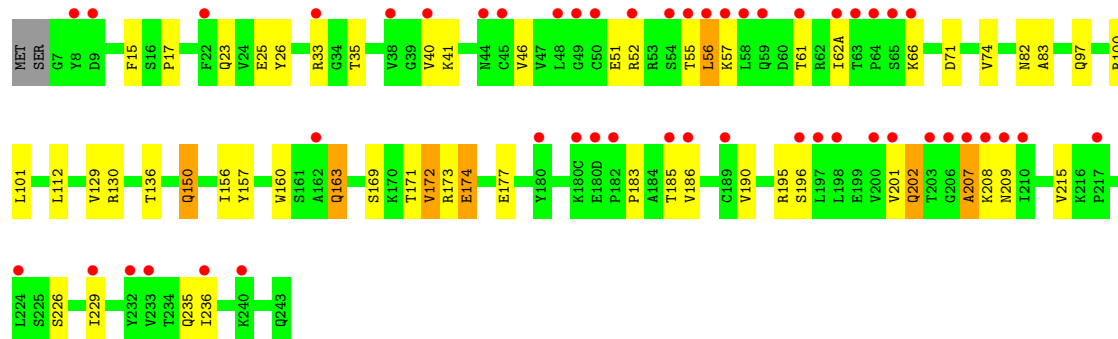
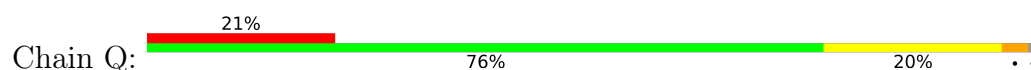




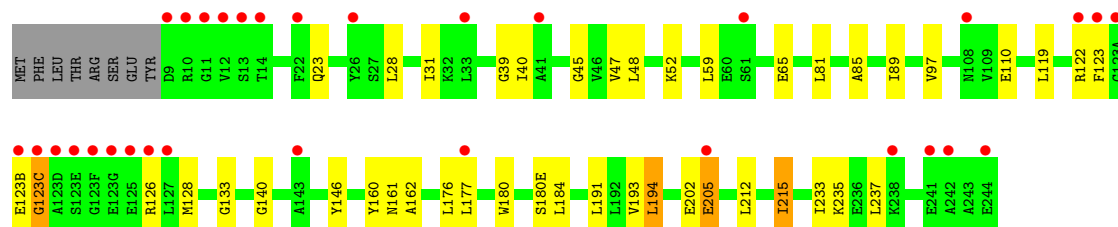
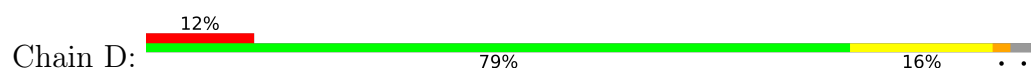
• Molecule 3: Proteasome component PRE6



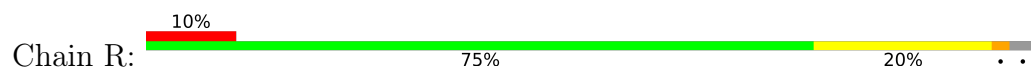
• Molecule 3: Proteasome component PRE6

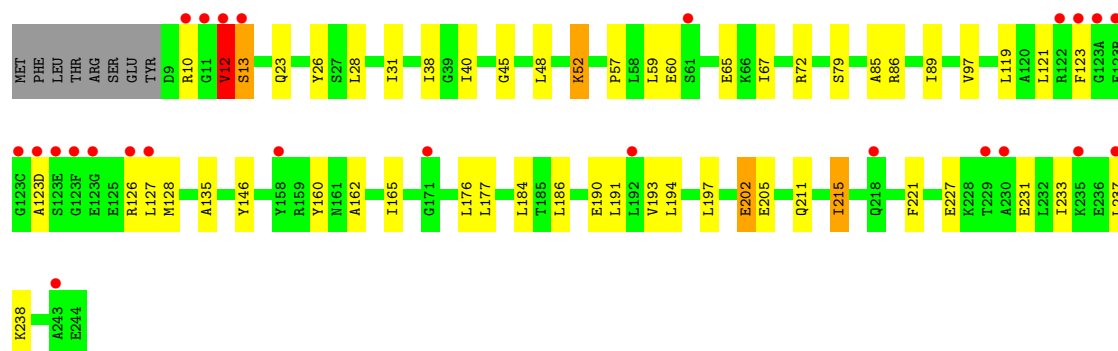


• Molecule 4: Proteasome component PUP2

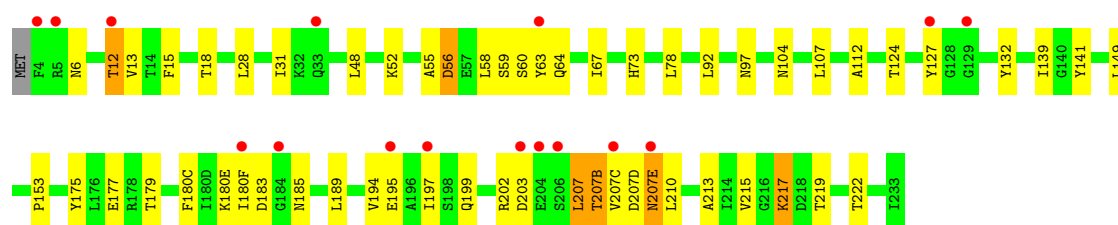
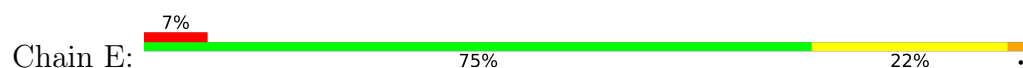


• Molecule 4: Proteasome component PUP2

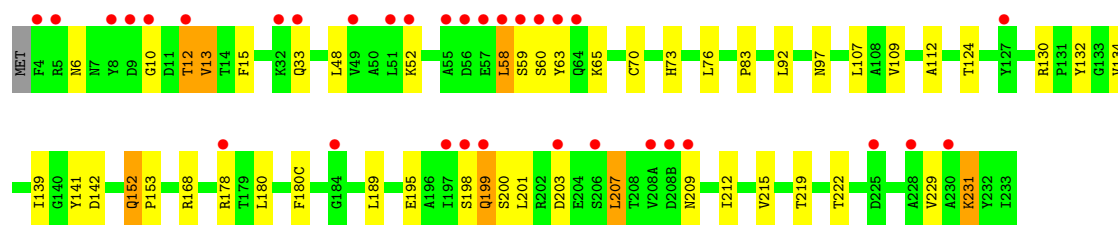
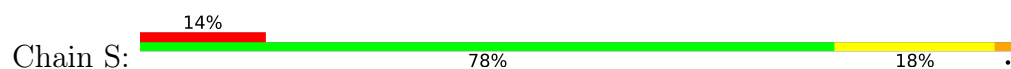




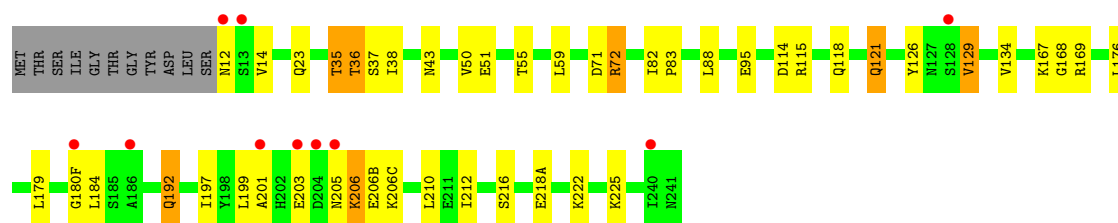
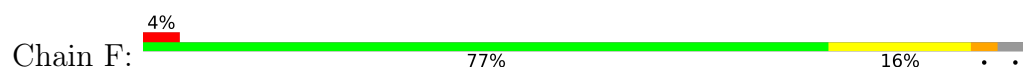
• Molecule 5: Proteasome component PRE5



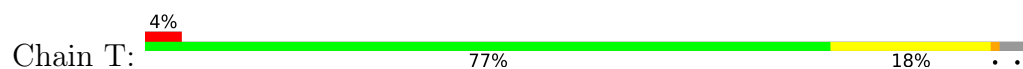
• Molecule 5: Proteasome component PRE5

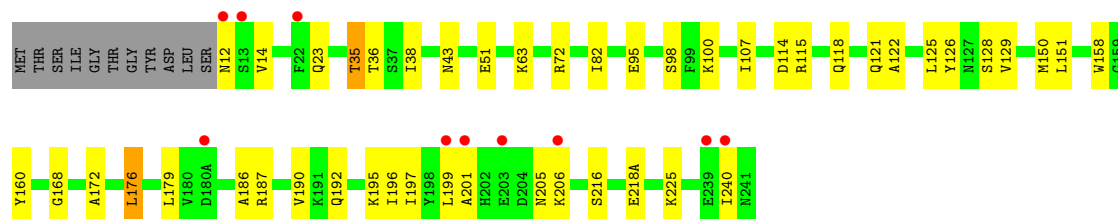


• Molecule 6: Proteasome component C1

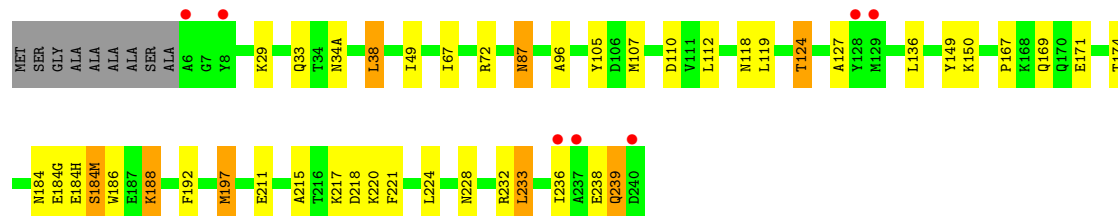
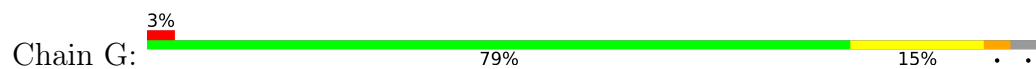


• Molecule 6: Proteasome component C1

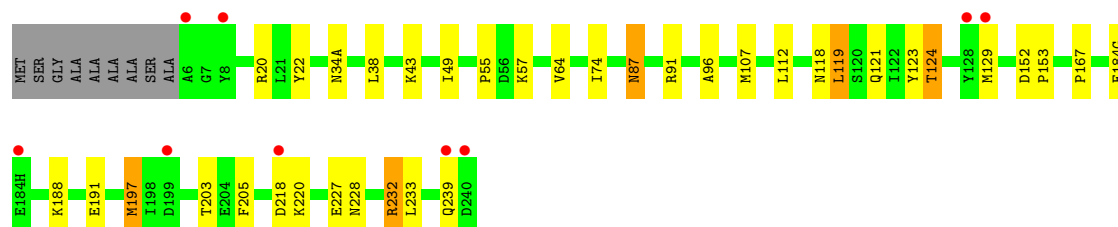
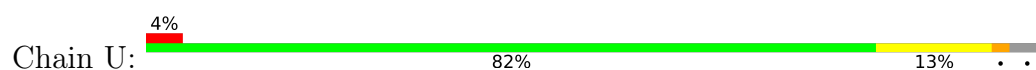




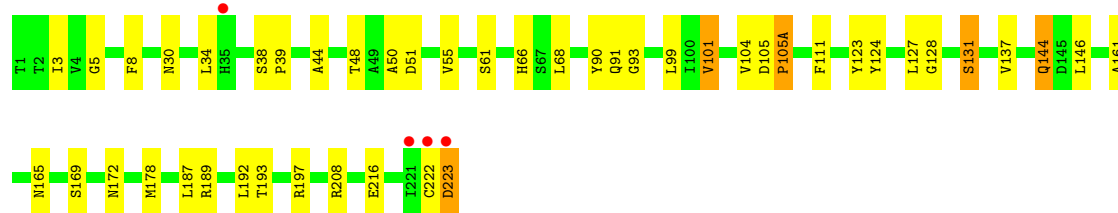
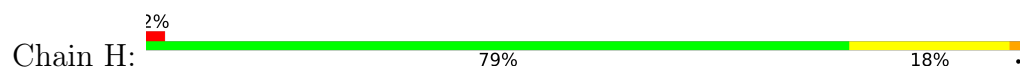
• Molecule 7: Proteasome component C7-alpha



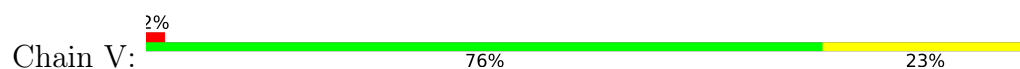
• Molecule 7: Proteasome component C7-alpha



• Molecule 8: Proteasome component PUP1

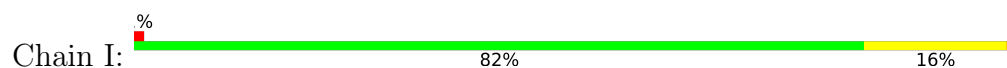


• Molecule 8: Proteasome component PUP1

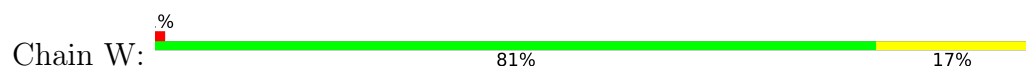




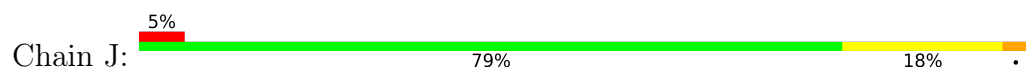
• Molecule 9: Proteasome component PUP3



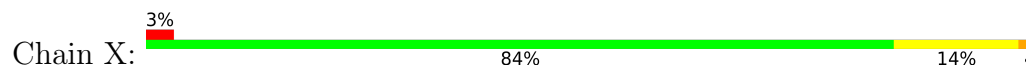
• Molecule 9: Proteasome component PUP3



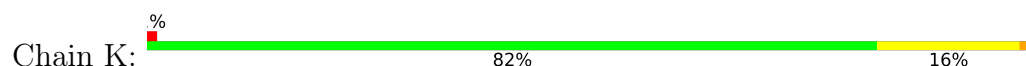
• Molecule 10: Proteasome component C11

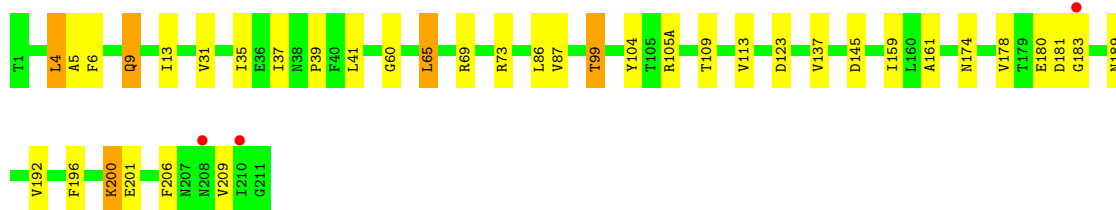


• Molecule 10: Proteasome component C11



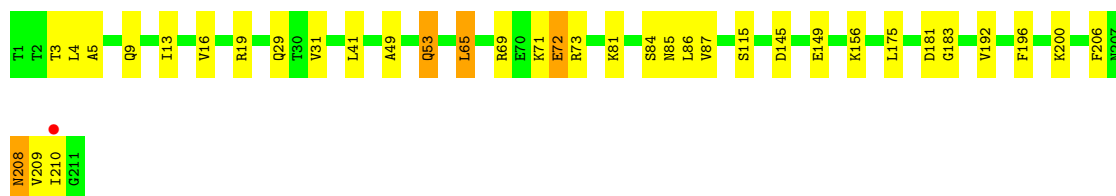
• Molecule 11: Proteasome component PRE2





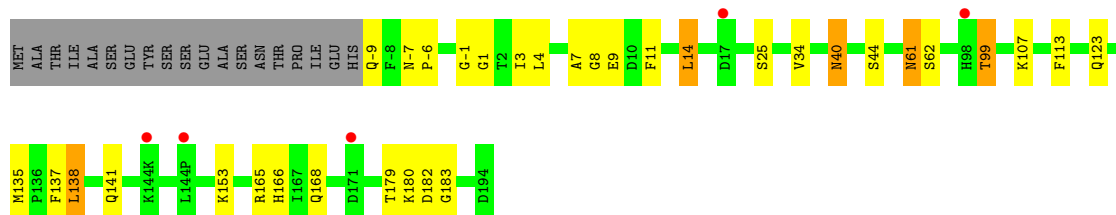
• Molecule 11: Proteasome component PRE2

Chain Y: 83% 15% •



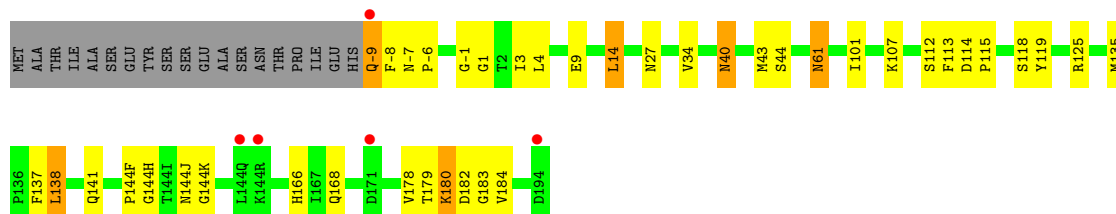
• Molecule 12: Proteasome component C5

Chain L: 78% 12% 8% •



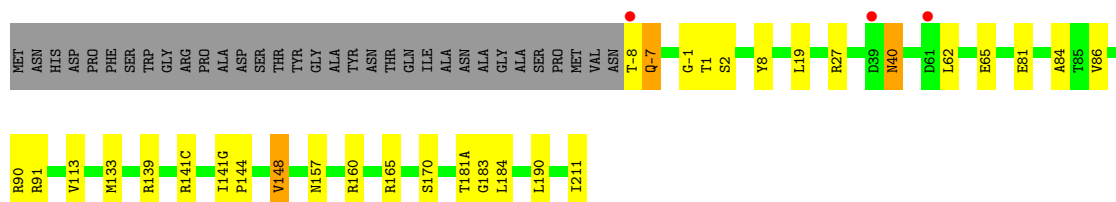
• Molecule 12: Proteasome component C5

Chain Z: 75% 15% 8% •

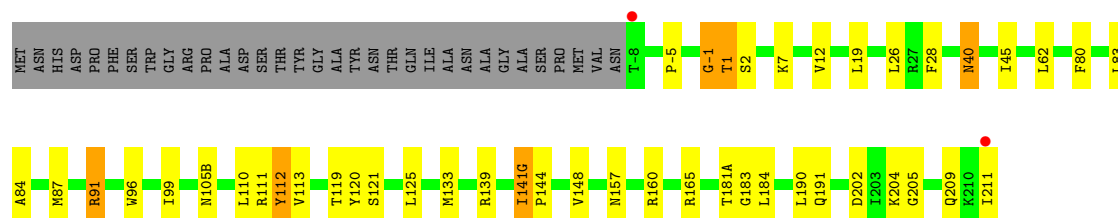


• Molecule 13: Proteasome component PRE4

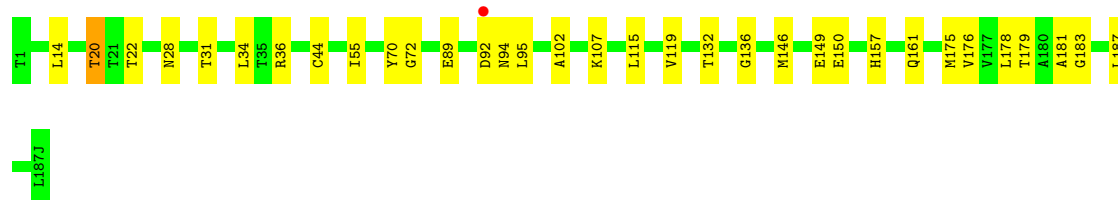
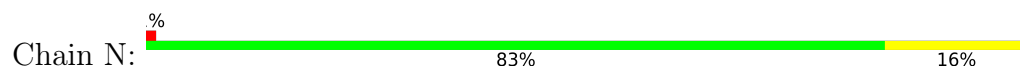
Chain M: 76% 11% 12% •



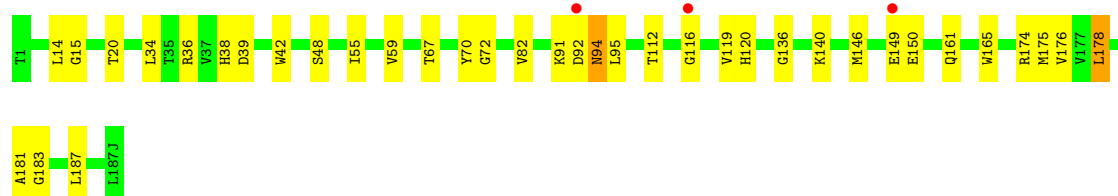
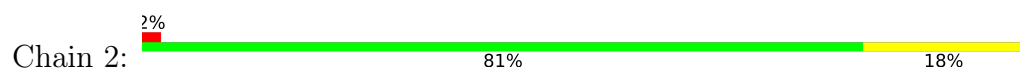
- Molecule 13: Proteasome component PRE4



- 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	136.02Å 300.38Å 145.81Å 90.00° 113.73° 90.00°	Depositor
Resolution (Å)	48.68 – 2.78 48.68 – 2.78	Depositor EDS
% Data completeness (in resolution range)	95.8 (48.68-2.78) 95.8 (48.68-2.78)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.96 (at 2.77Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.217 , 0.259 0.217 , 0.257	Depositor DCC
R_{free} test set	5191 reflections (2.02%)	wwPDB-VP
Wilson B-factor (Å ²)	58.1	Xtriage
Anisotropy	0.051	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 25.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.53$, $\langle L^2 \rangle = 0.37$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	49424	wwPDB-VP
Average B, all atoms (Å ²)	58.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.48% 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: L2T, MES, 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	0.51	0/1951	0.81	0/2639
1	O	0.52	0/1951	0.82	0/2639
2	B	0.53	0/1857	0.83	1/2513 (0.0%)
2	P	0.51	0/1857	0.82	0/2513
3	C	0.51	0/1918	0.85	0/2591
3	Q	0.53	0/1918	0.85	0/2591
4	D	0.51	0/1883	0.82	0/2529
4	R	0.50	0/1884	0.83	1/2532 (0.0%)
5	E	0.48	0/1819	0.82	1/2451 (0.0%)
5	S	0.49	0/1821	0.85	2/2457 (0.1%)
6	F	0.53	0/1885	0.83	0/2540
6	T	0.55	1/1886 (0.1%)	0.85	1/2543 (0.0%)
7	G	0.54	0/1956	0.83	0/2643
7	U	0.53	0/1958	0.83	0/2649
8	H	0.52	0/1714	0.81	0/2320
8	V	0.52	0/1714	0.79	0/2320
9	I	0.53	0/1608	0.83	0/2165
9	W	1.25	1/1609 (0.1%)	1.02	1/2168 (0.0%)
10	J	0.54	0/1611	0.82	0/2167
10	X	0.54	0/1611	0.80	0/2167
11	K	0.52	0/1680	0.83	0/2271
11	Y	0.51	0/1680	0.80	0/2271
12	L	0.51	0/1793	0.76	0/2414
12	Z	0.52	0/1793	0.79	0/2414
13	1	1.03	1/1853 (0.1%)	1.07	4/2507 (0.2%)
13	M	0.51	0/1852	0.83	2/2504 (0.1%)
14	2	0.53	0/1538	0.82	0/2078
14	N	0.55	0/1538	0.80	0/2078
All	All	0.58	3/50138 (0.0%)	0.84	13/67674 (0.0%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	W	-1	GLY	C-N	45.56	2.00	1.33
13	1	-1	GLY	C-N	38.19	1.87	1.33
6	T	82	ILE	CA-CB	5.89	1.57	1.54

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	1	-1	GLY	O-C-N	-31.21	82.12	122.70
9	W	-1	GLY	O-C-N	-27.46	95.40	122.86
13	1	-1	GLY	CA-C-N	7.43	135.74	121.54
13	1	-1	GLY	C-N-CA	7.43	135.74	121.54
4	R	233	ILE	N-CA-C	6.74	116.83	110.30
5	E	202	ARG	N-CA-C	-5.80	106.04	113.23
13	M	27	ARG	N-CA-C	5.78	117.38	111.14
13	1	141(G)	ILE	CB-CA-C	-5.57	108.44	114.35
13	M	2	SER	N-CA-C	5.45	117.33	110.24
2	B	238	ILE	N-CA-C	-5.36	107.90	113.10
6	T	107	ILE	N-CA-C	5.34	114.18	108.95
5	S	152	GLN	CA-C-N	5.22	124.93	119.82
5	S	152	GLN	C-N-CA	5.22	124.93	119.82

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1915	0	1925	24	0
1	O	1915	0	1925	35	0
2	B	1829	0	1828	33	0
2	P	1829	0	1828	31	0
3	C	1891	0	1899	24	0
3	Q	1891	0	1899	36	0
4	D	1862	0	1832	26	0
4	R	1862	0	1833	29	0
5	E	1795	0	1793	29	0
5	S	1795	0	1795	29	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	F	1848	0	1842	25	0
6	T	1848	0	1843	30	0
7	G	1921	0	1907	31	0
7	U	1921	0	1909	25	0
8	H	1685	0	1686	30	0
8	V	1685	0	1686	36	0
9	I	1581	0	1574	32	0
9	W	1581	0	1574	27	0
10	J	1585	0	1591	30	0
10	X	1585	0	1591	17	0
11	K	1644	0	1594	22	0
11	Y	1644	0	1594	19	0
12	L	1757	0	1712	24	0
12	Z	1757	0	1712	32	0
13	1	1824	0	1833	33	0
13	M	1824	0	1833	23	0
14	2	1512	0	1478	26	0
14	N	1512	0	1478	23	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
16	K	44	0	39	4	0
16	Y	44	0	39	1	0
17	K	12	0	13	1	0
17	Y	12	0	13	1	0
18	L	2	0	0	0	0
18	Z	2	0	0	0	0
All	All	49424	0	49098	685	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 (685) 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)
16:K:213:L2T:C6	16:K:213:L2T:CL7	1.75	1.60
13:1:-1:GLY:C	13:1:1:THR:H1	1.33	1.34

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:1:-1:GLY:C	13:1:1:THR:N	1.87	1.32
9:W:-1:GLY:C	9:W:1:GLY:H1	1.40	1.29
11:K:181:ASP:C	11:K:183:GLY:HA2	1.64	1.21
9:W:-1:GLY:C	9:W:1:GLY:N	2.00	1.17
14:N:92:ASP:C	14:N:94:ASN:N	2.04	1.15
9:I:-1:GLY:C	9:I:1:GLY:N	2.05	1.13
13:M:-1:GLY:C	13:M:1:THR:H1	1.57	1.13
7:G:218:ASP:C	7:G:220:LYS:N	2.10	1.08
12:Z:-1:GLY:O	12:Z:1:GLY:HA3	1.56	1.05
9:W:36:HIS:C	9:W:38:TYR:N	2.16	1.03
9:I:36:HIS:C	9:I:38:TYR:N	2.17	1.02
13:M:141(G):ILE:C	13:M:144:PRO:N	2.18	1.01
9:I:-1:GLY:C	9:I:1:GLY:H1	1.67	1.00
8:H:91:GLN:C	8:H:93:GLY:N	2.20	1.00
13:M:-1:GLY:C	13:M:1:THR:N	2.19	0.99
14:N:70:TYR:C	14:N:72:GLY:N	2.21	0.98
7:G:96:ALA:HA	7:G:107:MET:HE2	1.46	0.96
13:M:157:ASN:HD22	13:M:160:ARG:HH11	1.10	0.96
6:T:95:GLU:HG2	6:T:115:ARG:HB3	1.46	0.95
2:B:200:THR:C	2:B:202:THR:N	2.25	0.95
8:H:187:LEU:C	8:H:189:ARG:N	2.23	0.95
13:1:141(G):ILE:C	13:1:144:PRO:N	2.27	0.93
2:P:200:THR:O	2:P:202:THR:N	2.02	0.93
6:T:192:GLN:NE2	6:T:195:LYS:HE3	1.86	0.89
2:B:126:HIS:HB3	3:C:129:VAL:HG12	1.52	0.89
1:O:7:ARG:HG3	6:T:128:SER:HB3	1.55	0.88
14:2:70:TYR:C	14:2:72:GLY:N	2.31	0.88
4:D:123(C):GLY:HA2	4:D:126:ARG:H	1.37	0.87
3:Q:163:GLN:HE21	3:Q:163:GLN:HA	1.40	0.87
9:I:-1:GLY:C	9:I:1:GLY:H3	1.76	0.87
13:1:-1:GLY:C	13:1:1:THR:H2	1.77	0.86
8:V:187:LEU:C	8:V:189:ARG:N	2.33	0.86
1:A:130:ARG:HH21	7:G:124:THR:CG2	1.91	0.84
10:X:166:MET:HE3	10:X:168:MET:HE1	1.60	0.84
7:U:96:ALA:HA	7:U:107:MET:HE2	1.59	0.82
12:Z:179:THR:HG1	12:Z:182:ASP:N	1.78	0.82
7:U:107:MET:HE3	7:U:112:LEU:HD13	1.58	0.82
3:C:163:GLN:NE2	3:C:164:THR:H	1.78	0.81
6:F:168:GLY:HA3	6:F:201:ALA:HB1	1.61	0.81
13:M:141(C):ARG:HG3	13:M:141(C):ARG:HH11	1.46	0.80
3:C:163:GLN:HE21	3:C:164:THR:H	1.27	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:15:PHE:H	6:F:23:GLN:HE22	1.30	0.80
5:E:97:ASN:HD21	12:L:61:ASN:HD21	1.32	0.77
3:Q:15:PHE:H	4:R:23:GLN:HE22	1.31	0.77
1:A:130:ARG:HH21	7:G:124:THR:HG22	1.48	0.77
12:Z:166:HIS:HD2	12:Z:168:GLN:H	1.31	0.77
7:G:184(M):SER:HA	7:G:186:TRP:N	1.99	0.76
11:K:181:ASP:C	11:K:183:GLY:CA	2.54	0.76
12:Z:-7:ASN:HD22	12:Z:-6:PRO:HD2	1.49	0.76
12:L:-7:ASN:HD22	12:L:-6:PRO:HD2	1.49	0.75
6:F:95:GLU:HG2	6:F:115:ARG:HB3	1.69	0.75
14:N:181:ALA:O	14:N:183:GLY:CA	2.35	0.75
2:B:181:LYS:O	2:B:184:MET:HG3	1.87	0.74
13:1:157:ASN:HD22	13:1:160:ARG:HH11	1.35	0.74
8:H:128:GLY:O	8:H:131:SER:HB3	1.88	0.74
10:J:181:ASP:C	10:J:183:GLY:N	2.46	0.74
6:F:35:THR:HG21	6:F:51:GLU:O	1.88	0.73
7:U:191:GLU:HG3	7:U:232:ARG:HG3	1.69	0.73
13:M:157:ASN:HD22	13:M:160:ARG:NH1	1.84	0.73
9:W:-1:GLY:C	9:W:1:GLY:H3	1.95	0.73
7:U:218:ASP:C	7:U:220:LYS:N	2.46	0.73
13:1:181(A):THR:O	13:1:183:GLY:N	2.22	0.72
4:R:123(D):ALA:HB3	4:R:126:ARG:HG3	1.71	0.72
2:P:124:THR:HG22	3:Q:130:ARG:HH21	1.54	0.72
1:O:130:ARG:HH21	7:U:124:THR:HG22	1.53	0.72
9:W:179:LYS:C	9:W:181:LYS:N	2.47	0.72
1:O:130:ARG:HH21	7:U:124:THR:CG2	2.03	0.72
1:A:15:PHE:H	2:B:23:GLN:HE22	1.38	0.71
13:M:40:ASN:H	13:M:40:ASN:HD22	1.37	0.71
14:N:92:ASP:O	14:N:94:ASN:N	2.24	0.71
14:N:161:GLN:HE21	14:2:136:GLY:HA2	1.55	0.71
6:T:199:LEU:C	6:T:201:ALA:N	2.48	0.71
1:O:124:THR:CG2	2:P:130:ARG:HH21	2.04	0.71
8:V:30:ASN:O	8:V:189:ARG:NH2	2.23	0.70
7:G:67:ILE:HD12	7:G:211:GLU:HG2	1.72	0.70
1:A:200:SER:O	1:A:202:VAL:HA	1.91	0.70
4:D:180(E):SER:C	4:D:184:LEU:N	2.50	0.70
6:T:192:GLN:HE21	6:T:195:LYS:HE3	1.55	0.70
13:M:157:ASN:ND2	13:M:160:ARG:HH11	1.89	0.70
5:S:52:LYS:HB2	5:S:63:TYR:HB3	1.73	0.70
9:I:179:LYS:C	9:I:181:LYS:N	2.50	0.70
5:S:207:LEU:HA	5:S:209:ASN:HD22	1.58	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:W:36:HIS:CA	9:W:38:TYR:N	2.55	0.69
13:1:-1:GLY:O	13:1:1:THR:N	2.09	0.69
5:S:92:LEU:HD11	5:S:112:ALA:HB1	1.75	0.69
1:A:86:ARG:HE	7:G:118:ASN:HD21	1.41	0.68
12:Z:-1:GLY:O	12:Z:1:GLY:CA	2.40	0.68
5:E:12:THR:HG21	5:E:124:THR:HA	1.76	0.68
3:Q:201:VAL:O	3:Q:202:GLN:HB2	1.93	0.68
5:E:132:TYR:O	5:E:153:PRO:HB3	1.93	0.68
7:U:87:ASN:C	7:U:87:ASN:HD22	2.02	0.68
9:W:110:ILE:HD12	9:W:125:ILE:HG12	1.76	0.68
5:S:13:VAL:HG21	6:T:128:SER:O	1.94	0.68
14:2:176:VAL:HG12	14:2:178:LEU:HD13	1.76	0.68
11:Y:208:ASN:H	11:Y:208:ASN:HD22	1.42	0.67
12:L:4:LEU:CD1	12:L:138:LEU:HD21	2.24	0.67
12:L:4:LEU:HD13	12:L:138:LEU:HD21	1.77	0.67
8:V:187:LEU:O	8:V:189:ARG:N	2.26	0.67
3:C:163:GLN:HE21	3:C:164:THR:N	1.92	0.67
14:2:92:ASP:O	14:2:94:ASN:N	2.28	0.66
3:C:15:PHE:H	4:D:23:GLN:HE22	1.40	0.66
9:I:36:HIS:CA	9:I:38:TYR:N	2.59	0.65
5:S:132:TYR:O	5:S:153:PRO:HB3	1.95	0.65
7:U:107:MET:CE	7:U:112:LEU:HD13	2.27	0.65
5:E:73:HIS:HE1	5:E:107:LEU:O	1.80	0.65
2:P:202:THR:HG22	2:P:204:SER:H	1.59	0.65
5:E:60:SER:C	5:E:63:TYR:N	2.55	0.64
10:X:-1:MET:HG3	10:X:1:ASP:H1	1.62	0.64
6:F:95:GLU:HG3	6:F:115:ARG:HH11	1.63	0.64
5:S:97:ASN:HD21	12:Z:61:ASN:HD21	1.46	0.64
13:1:157:ASN:HD22	13:1:160:ARG:NH1	1.96	0.64
12:L:180:LYS:C	12:L:182:ASP:N	2.56	0.64
9:I:179:LYS:O	9:I:181:LYS:N	2.31	0.64
12:L:14:LEU:HD13	12:L:34:VAL:HG13	1.80	0.63
1:O:97:HIS:HD2	8:V:61:SER:OG	1.81	0.63
5:E:207(B):THR:H	5:E:207(E):ASN:HD22	1.45	0.63
9:W:179:LYS:O	9:W:181:LYS:N	2.32	0.63
10:X:2:ILE:HG12	10:X:130:SER:HB3	1.81	0.63
8:V:91:GLN:O	8:V:93:GLY:HA3	1.99	0.63
1:A:67:VAL:HG11	1:A:213:ALA:HB2	1.80	0.63
4:D:233:ILE:C	4:D:235:LYS:N	2.56	0.63
3:Q:33:ARG:HB2	3:Q:33:ARG:HH11	1.64	0.63
14:2:34:LEU:HD13	14:2:176:VAL:HG23	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:15:PHE:H	3:C:23:GLN:HE22	1.45	0.63
13:M:181(A):THR:O	13:M:183:GLY:N	2.32	0.62
6:T:12:ASN:C	6:T:14:VAL:H	2.07	0.62
5:E:180(E):LYS:O	5:E:183:ASP:N	2.33	0.62
14:N:55:ILE:HD11	14:N:95:LEU:HD13	1.81	0.62
10:J:143:ARG:O	10:J:146:MET:HG3	2.00	0.62
5:S:73:HIS:HE1	5:S:107:LEU:O	1.82	0.62
4:D:180(E):SER:O	4:D:184:LEU:N	2.32	0.62
12:L:166:HIS:HD2	12:L:168:GLN:H	1.48	0.62
4:D:202:GLU:C	4:D:205:GLU:N	2.58	0.61
4:R:12:VAL:HG23	4:R:13:SER:H	1.64	0.61
6:T:95:GLU:HG3	6:T:115:ARG:HH11	1.65	0.61
13:M:40:ASN:HD22	13:M:40:ASN:N	1.96	0.61
10:X:181:ASP:C	10:X:183:GLY:N	2.58	0.61
14:N:181:ALA:O	14:N:183:GLY:N	2.33	0.61
7:G:34(A):ASN:HD22	7:G:167:PRO:HG2	1.64	0.61
1:O:86:ARG:HE	7:U:118:ASN:HD21	1.47	0.61
3:Q:171:THR:O	3:Q:174:GLU:HB3	1.98	0.61
6:T:179:LEU:HD11	6:T:192:GLN:HG2	1.83	0.61
14:2:181:ALA:C	14:2:183:GLY:N	2.59	0.61
2:P:121:GLN:O	2:P:124:THR:HB	1.98	0.61
12:L:40:ASN:HD21	12:L:183:GLY:HA2	1.65	0.60
13:1:40:ASN:H	13:1:40:ASN:HD22	1.49	0.60
2:P:15:PHE:H	3:Q:23:GLN:HE22	1.49	0.60
3:C:163:GLN:HE21	3:C:163:GLN:HA	1.66	0.60
9:W:36:HIS:HA	9:W:38:TYR:N	2.16	0.60
14:N:14:LEU:HD11	14:N:102:ALA:HB3	1.83	0.60
1:O:212:LEU:HD22	1:O:224:LEU:HD12	1.83	0.60
1:A:7:ARG:HD2	5:E:127:TYR:CD2	2.37	0.60
13:M:139:ARG:HH11	8:V:165:ASN:HD22	1.50	0.60
1:O:124:THR:HG22	2:P:130:ARG:HH21	1.65	0.60
10:X:-1:MET:HG3	10:X:1:ASP:N	2.16	0.60
10:X:113:ILE:HG12	10:X:119:LYS:HG3	1.83	0.60
5:E:55:ALA:O	5:E:56:ASP:HB2	2.01	0.60
1:O:7:ARG:HG3	6:T:128:SER:CB	2.31	0.60
12:Z:40:ASN:HD21	12:Z:183:GLY:HA2	1.66	0.60
5:S:12:THR:HG21	5:S:124:THR:HA	1.84	0.59
13:1:181(A):THR:C	13:1:183:GLY:N	2.59	0.59
4:D:122:ARG:HA	4:D:126:ARG:HD3	1.84	0.59
9:I:10:ASP:HB3	9:I:181:LYS:HE2	1.84	0.59
14:2:92:ASP:C	14:2:94:ASN:N	2.60	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:S:15:PHE:H	6:T:23:GLN:HE22	1.48	0.59
5:E:180(F):ILE:C	5:E:183:ASP:N	2.61	0.59
6:T:122:ALA:HA	6:T:125:LEU:HD12	1.83	0.59
12:L:99:THR:HG23	12:L:113:PHE:HB2	1.85	0.59
4:R:10:ARG:HD2	5:S:10:GLY:HA2	1.84	0.59
14:N:136:GLY:HA2	14:2:161:GLN:HE21	1.68	0.58
6:T:95:GLU:HG2	6:T:115:ARG:CB	2.27	0.58
10:J:12:VAL:HG23	10:J:108:PRO:HB2	1.83	0.58
10:J:48:GLU:HB3	10:J:96:GLN:HB2	1.84	0.58
13:M:-1:GLY:O	13:M:1:THR:N	2.28	0.58
8:V:172:ASN:HB3	8:V:192:LEU:O	2.03	0.58
3:C:53:ARG:HG3	3:C:167:ARG:HH12	1.69	0.58
7:G:184(M):SER:CA	7:G:186:TRP:N	2.66	0.58
3:Q:71:ASP:OD1	3:Q:100:ARG:NH1	2.35	0.58
16:K:213:L2T:CL7	16:K:213:L2T:C5	2.72	0.58
1:O:32:LYS:HE2	1:O:32:LYS:HA	1.86	0.58
11:Y:49:ALA:O	11:Y:53:GLN:HB2	2.03	0.58
12:Z:144(H):GLY:C	12:Z:144(J):ASN:H	2.12	0.58
6:F:179:LEU:HD11	6:F:192:GLN:HG2	1.86	0.57
5:S:52:LYS:HB2	5:S:63:TYR:CB	2.33	0.57
7:U:87:ASN:C	7:U:87:ASN:ND2	2.61	0.57
4:D:202:GLU:O	4:D:205:GLU:N	2.37	0.57
10:J:179:ASP:O	10:J:183:GLY:N	2.38	0.57
10:X:181:ASP:O	10:X:183:GLY:HA3	2.04	0.57
12:Z:180:LYS:O	12:Z:182:ASP:HA	2.04	0.57
12:L:-1:GLY:O	12:L:1:GLY:HA3	2.04	0.57
8:V:50:ALA:HB2	9:W:118:CYS:HB2	1.86	0.57
5:S:134:VAL:O	5:S:153:PRO:HG3	2.05	0.57
2:B:101:LYS:NZ	10:J:85:GLN:NE2	2.52	0.56
13:M:-1:GLY:C	13:M:1:THR:H2	2.12	0.56
6:F:37:SER:HB3	6:F:50:VAL:HG23	1.87	0.56
10:J:6:ILE:HD11	10:J:8:VAL:HG13	1.86	0.56
14:N:161:GLN:NE2	14:2:136:GLY:HA2	2.20	0.56
8:V:20:SER:OG	8:V:28:ASP:HB3	2.05	0.56
13:M:211:ILE:HD11	14:2:36:ARG:HD2	1.87	0.56
14:N:181:ALA:O	14:N:183:GLY:HA3	2.06	0.56
7:U:152:ASP:HB2	7:U:153:PRO:CD	2.36	0.56
1:O:49:ALA:HB2	1:O:212:LEU:HG	1.88	0.56
2:B:54:VAL:HG13	2:B:209:ARG:HH22	1.71	0.56
8:H:50:ALA:HB2	9:I:118:CYS:HB2	1.87	0.56
9:I:36:HIS:HA	9:I:38:TYR:N	2.20	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:110:ILE:HD12	9:I:125:ILE:HG12	1.88	0.56
1:O:55:SER:O	1:O:56:SER:HB3	2.05	0.56
7:G:107:MET:HE3	7:G:112:LEU:HD13	1.88	0.55
12:L:165:ARG:NH2	8:V:29:LYS:HE2	2.20	0.55
2:B:124:THR:HG22	3:C:130:ARG:HH21	1.70	0.55
2:P:54:VAL:HA	2:P:209:ARG:HH12	1.72	0.55
2:B:38:ILE:HD12	2:B:197:LEU:HG	1.88	0.55
5:E:207:LEU:HA	5:E:207(E):ASN:HD22	1.72	0.55
2:P:51:GLU:OE2	2:P:202:THR:HG23	2.06	0.55
1:O:15:PHE:H	2:P:23:GLN:HE22	1.54	0.55
5:S:180:LEU:HA	5:S:180(C):PHE:CE2	2.42	0.55
1:A:124:THR:CG2	2:B:130:ARG:HH21	2.20	0.55
7:G:87:ASN:C	7:G:87:ASN:HD22	2.15	0.55
12:L:8:GLY:HA3	12:L:11:PHE:CE2	2.42	0.55
6:T:35:THR:HG21	6:T:51:GLU:O	2.06	0.54
1:O:121:GLN:O	1:O:124:THR:HB	2.07	0.54
16:K:213:L2T:CL7	16:K:213:L2T:C1	2.73	0.54
9:W:19:ARG:HD3	9:W:168:LEU:O	2.07	0.54
5:S:198:SER:HA	5:S:201:LEU:HD12	1.89	0.54
4:D:40:ILE:HD12	4:D:193:VAL:HG23	1.90	0.54
4:R:40:ILE:HD12	4:R:193:VAL:HG23	1.88	0.54
5:S:60:SER:HA	5:S:63:TYR:N	2.22	0.54
7:U:96:ALA:CA	7:U:107:MET:HE2	2.35	0.54
1:A:86:ARG:HE	7:G:118:ASN:ND2	2.06	0.54
4:D:97:VAL:HG21	11:K:65:LEU:HD13	1.89	0.54
4:R:13:SER:HB2	5:S:130:ARG:HD3	1.89	0.54
5:E:92:LEU:HD11	5:E:112:ALA:HB1	1.89	0.53
14:N:70:TYR:C	14:N:72:GLY:CA	2.81	0.53
9:I:2:ILE:HG21	9:I:130:ALA:HB3	1.91	0.53
8:V:105:ASP:HB2	8:V:105(A):PRO:HD2	1.91	0.53
10:J:17:SER:HB2	10:J:170:PHE:HB2	1.90	0.53
10:J:141:HIS:HB3	10:J:154:LEU:HD11	1.90	0.53
3:C:163:GLN:HE21	3:C:163:GLN:CA	2.22	0.53
11:K:181:ASP:O	11:K:183:GLY:HA2	2.06	0.53
12:L:180:LYS:O	12:L:182:ASP:N	2.42	0.53
1:A:124:THR:HG22	2:B:130:ARG:HH21	1.73	0.53
10:J:146:MET:HE2	10:J:150:GLU:HB3	1.91	0.53
8:V:80:LEU:HD12	8:V:113:ILE:HD11	1.90	0.52
1:O:86:ARG:HH21	7:U:118:ASN:ND2	2.06	0.52
4:D:123:PHE:HB3	4:D:128:MET:HE3	1.91	0.52
7:G:238:GLU:O	7:G:239:GLN:HB2	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:104:VAL:HG13	8:H:178:MET:HB3	1.90	0.52
2:P:97:GLN:NE2	9:W:61:TYR:HA	2.24	0.52
8:V:3:ILE:HD11	8:V:127:LEU:HB2	1.91	0.52
14:2:175:MET:HB2	14:2:187:LEU:HB2	1.92	0.52
5:E:52:LYS:HB3	5:E:63:TYR:HB3	1.92	0.52
14:N:176:VAL:HG12	14:N:178:LEU:HD13	1.90	0.52
12:Z:180:LYS:C	12:Z:182:ASP:N	2.68	0.52
1:A:233:LEU:HA	1:A:236:LEU:HB2	1.92	0.52
3:C:15:PHE:N	4:D:23:GLN:HE22	2.07	0.52
6:F:126:TYR:HB2	6:F:129:VAL:HG22	1.91	0.52
11:Y:181:ASP:O	11:Y:183:GLY:HA3	2.09	0.52
5:E:48:LEU:HB2	5:E:213:ALA:HB3	1.92	0.52
5:E:207:LEU:HD12	5:E:210:LEU:HD13	1.91	0.52
3:C:203:THR:HA	3:C:206:GLY:HA2	1.91	0.52
7:G:233:LEU:O	7:G:236:ILE:HG13	2.10	0.52
8:H:91:GLN:O	8:H:93:GLY:HA3	2.10	0.52
8:V:172:ASN:HD22	8:V:193:THR:HA	1.75	0.52
1:A:86:ARG:HH21	7:G:118:ASN:HD22	1.57	0.52
9:I:130:ALA:HB2	9:I:166:ASP:HB2	1.92	0.52
12:L:7:ALA:O	12:L:123:GLN:NE2	2.42	0.52
3:C:163:GLN:HE22	3:C:173:ARG:HE	1.57	0.51
11:Y:181:ASP:C	11:Y:183:GLY:N	2.68	0.51
5:E:194:VAL:O	5:E:197:ILE:HG22	2.11	0.51
3:C:242:GLU:CD	3:C:242:GLU:H	2.17	0.51
10:J:113:ILE:HG12	10:J:119:LYS:HG3	1.92	0.51
12:L:179:THR:HG1	12:L:182:ASP:N	2.09	0.51
4:D:160:TYR:CE2	5:E:59:SER:HB3	2.45	0.51
7:U:34(A):ASN:HD22	7:U:167:PRO:HG2	1.74	0.51
2:B:97:GLN:HE22	9:I:64:ASN:HD22	1.58	0.51
5:E:141:TYR:CE2	5:E:217:LYS:HA	2.46	0.51
6:F:199:LEU:C	6:F:201:ALA:N	2.68	0.51
14:N:149:GLU:CD	14:N:149:GLU:H	2.18	0.51
5:E:104:ASN:HB2	13:M:81:GLU:HG2	1.93	0.51
14:N:146:MET:HE2	14:N:150:GLU:HB3	1.92	0.51
7:U:184(G):GLU:HG2	7:U:188:LYS:HB3	1.91	0.51
14:2:14:LEU:O	14:2:175:MET:HA	2.11	0.51
5:E:67:ILE:HG21	5:E:213:ALA:HB2	1.93	0.51
6:T:192:GLN:HE22	6:T:195:LYS:HE3	1.72	0.51
3:Q:33:ARG:HB2	3:Q:33:ARG:NH1	2.25	0.50
4:R:121:LEU:HD21	5:S:83:PRO:HB3	1.92	0.50
4:R:227:GLU:H	4:R:227:GLU:CD	2.19	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:Z:-6:PRO:O	13:1:91:ARG:NH1	2.37	0.50
5:E:207(E):ASN:O	5:E:210:LEU:N	2.44	0.50
12:L:-7:ASN:HD22	12:L:-6:PRO:CD	2.20	0.50
6:F:180(F):GLY:O	6:F:184:LEU:N	2.45	0.50
6:F:216:SER:HB3	6:F:218(A):GLU:HB2	1.94	0.50
13:M:133:MET:HE1	13:M:165:ARG:HG3	1.92	0.50
4:R:85:ALA:O	4:R:89:ILE:HG12	2.12	0.50
14:2:38:HIS:HE1	14:2:67:THR:OG1	1.94	0.50
2:P:163:ILE:HA	2:P:173:GLN:HE22	1.76	0.50
3:Q:35:THR:HB	3:Q:51:GLU:HG3	1.93	0.50
8:V:105:ASP:HB2	8:V:105(A):PRO:CD	2.42	0.50
9:W:12:VAL:HG13	9:W:108:PRO:HB3	1.93	0.50
11:Y:196:PHE:HZ	11:Y:209:VAL:HG21	1.75	0.50
11:Y:200:LYS:HG3	11:Y:206:PHE:HB2	1.92	0.50
1:A:5:THR:HB	1:A:7:ARG:HH21	1.76	0.50
1:O:150:GLN:O	1:O:157:TYR:HA	2.12	0.50
11:K:137:VAL:HG21	11:K:161:ALA:HB2	1.94	0.50
1:A:67:VAL:HG11	1:A:213:ALA:CB	2.42	0.50
12:Z:178:VAL:HG22	12:Z:184:VAL:HG22	1.93	0.50
3:C:164:THR:HG21	3:C:172:VAL:HG22	1.94	0.50
12:Z:27:ASN:HB3	13:1:120:TYR:CE1	2.47	0.50
8:H:90:TYR:O	8:H:91:GLN:C	2.54	0.49
4:R:186:LEU:O	4:R:190:GLU:HG3	2.12	0.49
1:A:217(G):LEU:HD13	1:A:218:GLY:HA2	1.93	0.49
11:K:4:LEU:HD12	11:K:159:ILE:CD1	2.43	0.49
7:U:184(G):GLU:HG2	7:U:188:LYS:CB	2.42	0.49
3:C:35:THR:HB	3:C:51:GLU:HG3	1.94	0.49
4:R:215:ILE:O	4:R:215:ILE:HG13	2.12	0.49
6:T:114:ASP:O	6:T:118:GLN:HG2	2.12	0.49
14:2:112:THR:HG22	14:2:120:HIS:HB2	1.94	0.49
8:H:48:THR:HB	8:H:51:ASP:HB2	1.93	0.49
13:M:-8:THR:O	13:M:-7:GLN:HB3	2.11	0.49
1:O:79:SER:HB2	1:O:165:ILE:HD12	1.93	0.49
2:P:21:LEU:HD13	2:P:124:THR:HG23	1.94	0.49
8:V:172:ASN:ND2	8:V:193:THR:HA	2.27	0.49
5:E:139:ILE:HD12	5:E:215:VAL:HG12	1.95	0.49
4:R:123:PHE:HA	4:R:128:MET:HB3	1.95	0.49
4:R:162:ALA:HB1	4:R:176:LEU:HD22	1.95	0.49
8:V:128:GLY:O	8:V:131:SER:HB2	2.12	0.49
13:1:141(G):ILE:C	13:1:144:PRO:CA	2.85	0.49
6:F:35:THR:CG2	6:F:51:GLU:O	2.58	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:196:PHE:HZ	11:K:209:VAL:HG21	1.77	0.49
7:G:215:ALA:HB2	7:G:221:PHE:HD2	1.78	0.49
10:J:-1:MET:HG3	10:J:1:ASP:N	2.28	0.49
5:S:52:LYS:CB	5:S:63:TYR:HB3	2.41	0.49
12:Z:4:LEU:CD1	12:Z:138:LEU:HD21	2.42	0.49
2:B:101:LYS:HZ1	10:J:85:GLN:NE2	2.10	0.49
14:N:136:GLY:HA2	14:2:161:GLN:NE2	2.26	0.49
10:J:2:ILE:HB	10:J:17:SER:HB3	1.95	0.49
10:J:141:HIS:HB3	10:J:154:LEU:CD1	2.41	0.49
1:O:86:ARG:HH21	7:U:118:ASN:HD22	1.61	0.49
2:B:37:ALA:O	2:B:164:SER:HA	2.13	0.49
9:I:181:LYS:HG2	9:I:182:ASP:OD1	2.13	0.49
8:H:105:ASP:HB2	8:H:105(A):PRO:HD2	1.95	0.48
9:I:165:ARG:NH2	12:Z:135:MET:HE3	2.28	0.48
11:K:86:LEU:C	11:K:86:LEU:HD13	2.39	0.48
14:N:14:LEU:O	14:N:175:MET:HA	2.13	0.48
7:U:121:GLN:O	7:U:124:THR:HB	2.13	0.48
11:K:4:LEU:HD12	11:K:159:ILE:HD11	1.95	0.48
2:P:152:ASN:HB2	2:P:153:PRO:HD2	1.95	0.48
4:R:97:VAL:HG21	11:Y:65:LEU:HD13	1.96	0.48
8:H:137:VAL:HG21	8:H:161:ALA:HB2	1.96	0.48
9:I:20:LEU:HB3	9:I:28:SER:HB3	1.96	0.48
4:D:45:GLY:HA2	4:D:146:TYR:CE1	2.48	0.48
10:J:141:HIS:CB	10:J:154:LEU:HD11	2.43	0.48
5:S:198:SER:C	5:S:200:SER:H	2.21	0.48
14:2:59:VAL:HG22	14:2:82:VAL:HG12	1.95	0.48
14:2:36:ARG:HG3	14:2:42:TRP:CE2	2.49	0.48
2:B:101:LYS:HG3	9:I:57:GLU:HB3	1.96	0.48
14:N:175:MET:HB2	14:N:187:LEU:HB2	1.94	0.48
9:W:2:ILE:HG21	9:W:130:ALA:HB3	1.94	0.48
13:1:-1:GLY:CA	13:1:1:THR:N	2.71	0.48
1:A:112:LEU:O	1:A:116:VAL:HG23	2.13	0.48
3:Q:169:SER:HA	3:Q:172:VAL:HG13	1.96	0.48
3:Q:186:VAL:O	3:Q:190:VAL:HG23	2.13	0.48
8:V:163:ILE:HG23	8:V:170:GLY:HA2	1.95	0.48
11:Y:86:LEU:C	11:Y:86:LEU:HD13	2.39	0.48
2:B:13:THR:O	3:C:130:ARG:HD3	2.14	0.47
3:C:15:PHE:H	4:D:23:GLN:NE2	2.10	0.47
10:J:90(A):ILE:HG12	10:J:116:LEU:HD23	1.95	0.47
14:N:157:HIS:HD2	14:2:140:LYS:NZ	2.12	0.47
8:V:90:TYR:O	8:V:91:GLN:C	2.57	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:137:PHE:CE1	12:L:141:GLN:HG3	2.49	0.47
14:N:20:THR:OG1	14:N:28:ASN:HB3	2.14	0.47
8:H:123:TYR:OH	13:1:202:ASP:HB2	2.14	0.47
9:I:122:ALA:HB3	9:I:125:ILE:HD11	1.97	0.47
11:K:6:PHE:HA	11:K:123:ASP:O	2.14	0.47
13:M:141(C):ARG:HH11	13:M:141(C):ARG:CG	2.21	0.47
1:O:13:THR:HG22	1:O:21:LEU:HD22	1.96	0.47
2:P:122:GLY:C	2:P:124:THR:H	2.23	0.47
9:W:87:LEU:HD11	9:W:99:PRO:HG2	1.96	0.47
11:Y:181:ASP:C	11:Y:183:GLY:HA3	2.38	0.47
4:R:67:ILE:HG22	4:R:221:PHE:HZ	1.78	0.47
6:T:172:ALA:O	6:T:176:LEU:HD22	2.14	0.47
11:K:4:LEU:CD1	11:K:159:ILE:HD11	2.45	0.47
14:N:34:LEU:HD13	14:N:176:VAL:HG23	1.97	0.47
3:C:163:GLN:NE2	3:C:163:GLN:HA	2.29	0.47
8:V:91:GLN:O	8:V:93:GLY:CA	2.62	0.47
8:V:91:GLN:C	8:V:93:GLY:N	2.72	0.47
5:E:31:ILE:HD11	5:E:153:PRO:CD	2.44	0.47
1:O:67:VAL:HG11	1:O:213:ALA:CB	2.45	0.47
3:Q:207:ALA:C	3:Q:209:ASN:H	2.23	0.47
6:T:158:TRP:CZ3	7:U:64:VAL:HA	2.50	0.47
7:U:20:ARG:HH21	7:U:22:TYR:HE1	1.60	0.47
8:V:35:HIS:CB	8:V:56:THR:HG21	2.45	0.47
13:1:110:LEU:HG	13:1:125:LEU:HD12	1.96	0.47
9:I:9:LYS:HD2	9:I:145:ASN:HB3	1.97	0.47
10:J:-1:MET:HA	10:J:1:ASP:H2	1.80	0.47
7:G:192:PHE:CD1	7:G:192:PHE:C	2.93	0.47
1:O:45:GLY:HA3	1:O:186:LEU:HD13	1.96	0.47
2:B:67:LEU:HD22	2:B:211:GLU:HB3	1.97	0.47
2:B:124:THR:CG2	3:C:130:ARG:HH21	2.28	0.47
2:P:181:LYS:O	2:P:184:MET:HG3	2.15	0.47
13:1:157:ASN:ND2	13:1:160:ARG:HH11	2.09	0.47
2:B:152:ASN:HB2	2:B:153:PRO:CD	2.46	0.46
4:D:161:ASN:HB3	4:D:180:TRP:CE2	2.50	0.46
7:G:184(M):SER:C	7:G:186:TRP:N	2.73	0.46
4:R:45:GLY:HA2	4:R:146:TYR:CE1	2.50	0.46
12:Z:43:MET:HG3	12:Z:101:ILE:HG22	1.97	0.46
8:H:197:ARG:HH21	9:I:139:GLU:HG3	1.80	0.46
1:A:12:LEU:HD11	7:G:127:ALA:HB2	1.97	0.46
11:K:99:THR:HG22	11:K:113:VAL:HB	1.97	0.46
12:L:3:ILE:HG21	12:L:44:SER:OG	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:Z:180:LYS:O	12:Z:182:ASP:CA	2.63	0.46
14:2:38:HIS:O	14:2:39:ASP:C	2.58	0.46
14:2:161:GLN:NE2	14:2:165:TRP:HE1	2.13	0.46
8:H:101:VAL:HG13	8:H:111:PHE:HB2	1.97	0.46
8:H:208:ARG:O	12:Z:144(F):PRO:HB3	2.15	0.46
3:Q:17:PRO:HA	4:R:26:TYR:CD1	2.49	0.46
10:J:15:ALA:HB2	10:J:155:LEU:HD11	1.97	0.46
1:O:217(G):LEU:HD13	1:O:218:GLY:HA2	1.98	0.46
7:U:123:TYR:CE1	7:U:129:MET:HE2	2.51	0.46
5:E:207:LEU:HA	5:E:207(E):ASN:ND2	2.31	0.46
9:W:6:MET:HE3	9:W:155:ILE:HA	1.97	0.46
11:Y:156:LYS:HB2	11:Y:175:LEU:HD11	1.98	0.46
8:V:3:ILE:O	8:V:126:SER:HA	2.16	0.46
14:2:55:ILE:HD11	14:2:95:LEU:HD13	1.98	0.46
14:2:146:MET:HE2	14:2:150:GLU:HB3	1.97	0.46
3:C:207:ALA:C	3:C:209:ASN:H	2.23	0.46
6:F:203:GLU:O	6:F:206:LYS:HG3	2.15	0.46
11:K:174:ASN:ND2	11:K:189:ASN:HD22	2.14	0.46
11:K:200:LYS:HG3	11:K:206:PHE:HB2	1.98	0.46
6:T:206:LYS:HE3	6:T:206:LYS:HB2	1.74	0.46
2:B:150:THR:O	2:B:157:TYR:HA	2.15	0.46
9:I:104:ILE:HD12	9:I:178:ILE:HG22	1.98	0.46
10:J:129:TYR:HB3	10:X:24:ILE:HD11	1.98	0.46
8:V:126:SER:O	8:V:127:LEU:HD23	2.16	0.46
3:C:186:VAL:HG21	3:C:216:LYS:HE2	1.97	0.45
4:D:194:LEU:HD22	4:D:212:LEU:HD11	1.97	0.45
10:J:113:ILE:HA	10:J:118:THR:O	2.16	0.45
1:O:159:PRO:HB2	2:P:60:GLU:HB3	1.98	0.45
3:Q:163:GLN:HE22	3:Q:173:ARG:HE	1.64	0.45
3:Q:172:VAL:HG23	3:Q:196:SER:HB2	1.97	0.45
3:Q:52:ARG:HB2	3:Q:209:ASN:HD22	1.82	0.45
1:A:130:ARG:NH2	7:G:124:THR:HG22	2.24	0.45
2:B:141:TYR:CD1	2:B:219(E):VAL:HG21	2.51	0.45
7:G:38:LEU:HD23	7:G:197:MET:HE3	1.98	0.45
16:K:213:L2T:H24	17:K:214:MES:H82	1.99	0.45
9:W:12:VAL:HG23	9:W:178:ILE:HB	1.98	0.45
10:X:161:GLU:OE2	10:X:161:GLU:HA	2.16	0.45
13:1:83:LEU:O	13:1:87:MET:HG2	2.16	0.45
13:1:205:GLY:HA3	13:1:209:GLN:HB3	1.97	0.45
10:J:24:ILE:HG12	10:J:24:ILE:O	2.16	0.45
13:M:165:ARG:NH1	8:V:139:GLU:OE1	2.45	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:Z:-9:GLN:HE21	12:Z:-8:PHE:H	1.64	0.45
8:H:44:ALA:O	8:H:99:LEU:HA	2.16	0.45
8:H:216:GLU:HG3	9:I:187:ARG:HG2	1.98	0.45
10:J:-1:MET:HA	10:J:1:ASP:N	2.31	0.45
2:P:17:PRO:HA	3:Q:26:TYR:CE1	2.52	0.45
2:P:152:ASN:HB2	2:P:153:PRO:CD	2.46	0.45
6:T:168:GLY:HA3	6:T:201:ALA:HB1	1.98	0.45
2:B:202:THR:HG22	2:B:204:SER:H	1.81	0.45
6:F:82:ILE:HB	6:F:83:PRO:HD3	1.98	0.45
11:K:37:ILE:HB	11:K:41:LEU:HB3	1.98	0.45
8:V:35:HIS:HB2	8:V:56:THR:HG21	1.99	0.45
13:1:19:LEU:HD12	13:1:28:PHE:O	2.17	0.45
9:W:107:LYS:HA	9:W:108:PRO:HD3	1.85	0.45
14:2:181:ALA:O	14:2:183:GLY:HA3	2.17	0.45
4:D:162:ALA:HB1	4:D:176:LEU:HD22	1.98	0.45
8:H:3:ILE:HD11	8:H:127:LEU:HB2	1.99	0.45
11:K:5:ALA:HA	11:K:13:ILE:O	2.16	0.45
1:O:112:LEU:O	1:O:116:VAL:HG23	2.17	0.45
4:D:140:GLY:HA2	4:D:215:ILE:HG12	1.98	0.45
6:F:71:ASP:OD2	6:F:72:ARG:N	2.48	0.45
2:P:121:GLN:HG3	3:Q:83:ALA:HB1	1.99	0.45
3:Q:195:ARG:HG3	3:Q:236:ILE:HD13	1.97	0.45
4:R:31:ILE:HD13	4:R:135:ALA:HB2	1.99	0.45
14:2:15:GLY:HA2	14:2:174:ARG:O	2.16	0.45
10:X:32:ASP:OD2	10:X:34:THR:HG22	2.17	0.45
12:Z:14:LEU:HD13	12:Z:34:VAL:HG13	1.99	0.45
9:I:36:HIS:O	9:I:38:TYR:N	2.50	0.44
11:K:37:ILE:HG23	11:K:60:GLY:HA2	1.98	0.44
5:S:73:HIS:HB2	5:S:141:TYR:O	2.17	0.44
11:Y:71:LYS:O	11:Y:72:GLU:HB2	2.16	0.44
14:2:91:LYS:HE2	14:2:116:GLY:O	2.16	0.44
1:A:130:ARG:NH2	7:G:124:THR:CG2	2.72	0.44
7:G:184(M):SER:C	7:G:188:LYS:H	2.25	0.44
9:I:99:PRO:HB2	9:I:113:PHE:HD2	1.81	0.44
12:Z:3:ILE:HG21	12:Z:44:SER:OG	2.16	0.44
13:1:7:LYS:HB3	13:1:12:VAL:HG12	1.99	0.44
13:1:80:PHE:CZ	13:1:111:ARG:HG2	2.52	0.44
2:B:121:GLN:O	2:B:124:THR:HB	2.18	0.44
2:B:229:ILE:O	2:B:233:LEU:HB2	2.18	0.44
8:H:30:ASN:O	8:H:189:ARG:NH2	2.51	0.44
11:K:196:PHE:CZ	11:K:209:VAL:HG21	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:R:79:SER:HB3	4:R:165:ILE:HD12	1.98	0.44
1:A:97:HIS:HD2	8:H:61:SER:OG	2.00	0.44
2:B:55:THR:HB	2:B:56:SER:H	1.65	0.44
1:O:86:ARG:HE	7:U:118:ASN:ND2	2.13	0.44
8:V:41:ILE:HG12	8:V:76:VAL:HG22	2.00	0.44
8:V:63:ILE:HG23	8:V:74:PRO:HB3	1.98	0.44
12:Z:113:PHE:CD1	12:Z:113:PHE:N	2.84	0.44
12:Z:27:ASN:HB3	13:1:120:TYR:CZ	2.53	0.44
12:Z:113:PHE:CD2	12:Z:119:TYR:HB3	2.52	0.44
13:1:111:ARG:HH11	13:1:121:SER:HB2	1.83	0.44
2:B:81:LEU:HD23	2:B:133:GLY:HA3	2.00	0.44
7:G:87:ASN:C	7:G:87:ASN:ND2	2.76	0.44
1:O:40:ILE:HD12	1:O:193:ALA:HB2	2.00	0.44
7:G:224:LEU:HB3	7:G:228:ASN:HB2	1.98	0.44
13:M:84:ALA:HA	13:M:113:VAL:HG21	2.00	0.44
7:U:74:ILE:HD11	7:U:107:MET:O	2.18	0.44
8:V:91:GLN:O	8:V:93:GLY:N	2.51	0.44
1:A:150:GLN:O	1:A:157:TYR:HA	2.18	0.44
5:E:180(F):ILE:O	5:E:183:ASP:HA	2.18	0.44
6:F:167:LYS:HG2	6:F:205:ASN:HD21	1.83	0.44
8:H:223:ASP:N	8:H:223:ASP:OD2	2.50	0.44
3:Q:97:GLN:HG3	10:X:65:LEU:HB2	1.99	0.44
3:Q:201:VAL:O	3:Q:202:GLN:CB	2.62	0.44
5:S:109:VAL:HG23	5:S:142:ASP:OD1	2.18	0.44
6:T:35:THR:CG2	6:T:51:GLU:O	2.66	0.44
8:H:8:PHE:HB2	8:H:146:LEU:O	2.18	0.43
11:Y:5:ALA:HA	11:Y:13:ILE:O	2.18	0.43
13:1:112:TYR:O	13:1:119:THR:HA	2.18	0.43
6:F:179:LEU:CD1	6:F:192:GLN:HG2	2.48	0.43
3:Q:55:THR:O	3:Q:56:LEU:HD13	2.18	0.43
8:V:84:LYS:HG3	8:V:85:GLN:N	2.33	0.43
5:E:180(C):PHE:HA	5:E:180(F):ILE:HG13	2.01	0.43
8:H:187:LEU:O	8:H:189:ARG:N	2.48	0.43
12:L:135:MET:HE3	9:W:165:ARG:NH2	2.33	0.43
2:P:229:ILE:O	2:P:233:LEU:HB2	2.18	0.43
3:Q:226:SER:HA	3:Q:229:ILE:HD12	2.00	0.43
7:U:197:MET:HG2	7:U:205:PHE:CE1	2.53	0.43
12:Z:137:PHE:CE1	12:Z:141:GLN:HG3	2.53	0.43
1:A:130:ARG:HH21	7:G:124:THR:HG23	1.77	0.43
8:H:38:SER:HB2	8:H:39:PRO:HD2	2.01	0.43
12:L:153:LYS:HG2	8:V:201:GLN:HG3	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:78:VAL:HG22	2:P:136:PHE:HE2	1.83	0.43
12:Z:-1:GLY:C	12:Z:1:GLY:CA	2.90	0.43
13:1:19:LEU:HD21	13:1:26:LEU:HD22	2.00	0.43
2:B:101:LYS:HZ2	10:J:85:GLN:HE21	1.66	0.43
6:F:95:GLU:HG2	6:F:115:ARG:CB	2.45	0.43
4:R:38:ILE:HD12	4:R:197:LEU:HG	1.99	0.43
8:H:5:GLY:O	8:H:124:TYR:HA	2.18	0.43
8:H:91:GLN:C	8:H:93:GLY:CA	2.89	0.43
1:O:39:GLY:HA2	1:O:47:VAL:O	2.19	0.43
12:Z:-7:ASN:HD22	12:Z:-6:PRO:CD	2.24	0.43
12:Z:9:GLU:O	12:Z:107:LYS:HA	2.19	0.43
7:G:238:GLU:O	7:G:239:GLN:CB	2.67	0.43
9:W:104:ILE:HD12	9:W:178:ILE:HG22	2.01	0.43
13:1:105(B):ASN:C	13:1:105(B):ASN:OD1	2.61	0.43
6:T:216:SER:HB3	6:T:218(A):GLU:HB2	2.01	0.43
8:V:128:GLY:O	8:V:131:SER:CB	2.67	0.43
2:B:184:MET:HE1	2:B:192:LEU:HD12	2.01	0.43
9:I:114:ASP:OD2	9:I:114:ASP:C	2.62	0.43
14:N:14:LEU:HD23	14:N:44:CYS:SG	2.59	0.43
6:F:121:GLN:HE21	6:F:121:GLN:HB3	1.67	0.42
2:B:177:GLN:HE21	2:B:177:GLN:HB2	1.53	0.42
8:H:172:ASN:ND2	8:H:193:THR:HA	2.34	0.42
3:Q:163:GLN:HE21	3:Q:163:GLN:CA	2.16	0.42
8:H:165:ASN:HD22	13:1:139:ARG:HH11	1.68	0.42
1:O:97:HIS:HD2	8:V:61:SER:HG	1.68	0.42
7:G:107:MET:CE	7:G:112:LEU:HD13	2.49	0.42
7:G:136:LEU:O	7:G:150:LYS:HA	2.19	0.42
10:J:2:ILE:HD13	10:J:162:LEU:HD13	2.01	0.42
1:O:111:LEU:HD21	9:W:69:LYS:HB3	2.00	0.42
5:S:48:LEU:HG	5:S:139:ILE:HG12	2.02	0.42
5:S:139:ILE:HD12	5:S:215:VAL:HG12	2.01	0.42
5:S:212:ILE:HD12	5:S:229:VAL:HG12	2.01	0.42
6:T:186:ALA:O	6:T:190:VAL:HG23	2.19	0.42
9:W:-1:GLY:C	9:W:1:GLY:CA	2.86	0.42
13:1:-5:PRO:HD3	13:1:96:TRP:CE2	2.54	0.42
10:J:90(A):ILE:HA	10:J:94:PRO:HB3	2.02	0.42
12:L:9:GLU:O	12:L:107:LYS:HA	2.18	0.42
2:P:116:LEU:HD23	2:P:116:LEU:HA	1.93	0.42
13:1:45:ILE:HG12	13:1:99:ILE:HG12	2.00	0.42
5:E:15:PHE:H	6:F:23:GLN:NE2	2.06	0.42
9:I:194:ASP:HB3	11:Y:192:VAL:HG11	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Q:41:LYS:HA	3:Q:46:VAL:HA	2.02	0.42
13:M:8:TYR:CE2	13:M:148:VAL:HG22	2.54	0.42
2:P:200:THR:C	2:P:202:THR:N	2.75	0.42
2:P:218:ASN:O	2:P:218(B):ASP:HB2	2.18	0.42
11:Y:3:THR:HG22	11:Y:16:VAL:HG12	2.02	0.42
13:1:84:ALA:HA	13:1:113:VAL:HG21	2.02	0.42
13:1:133:MET:HE1	13:1:165:ARG:HG3	2.01	0.42
4:D:123(C):GLY:HA2	4:D:126:ARG:N	2.19	0.42
9:I:99:PRO:HB2	9:I:113:PHE:CD2	2.55	0.42
11:K:104:TYR:OH	11:K:105(A):ARG:NH1	2.53	0.42
2:P:147:GLN:HG2	3:Q:62(A):ILE:HG21	2.01	0.42
4:R:227:GLU:CD	4:R:227:GLU:N	2.78	0.42
9:W:107:LYS:HE2	9:W:107:LYS:HB3	1.74	0.42
4:D:85:ALA:O	4:D:89:ILE:HG12	2.20	0.42
8:H:144:GLN:HE21	8:H:144:GLN:HB2	1.67	0.42
10:J:2:ILE:HD12	10:J:170:PHE:CG	2.55	0.42
1:O:27:ALA:O	1:O:31:VAL:HG23	2.19	0.42
3:Q:57:LYS:HD2	3:Q:57:LYS:HA	1.75	0.42
6:T:12:ASN:ND2	6:T:126:TYR:O	2.46	0.42
9:W:113:PHE:HA	9:W:118:CYS:O	2.20	0.42
1:A:82:GLY:O	1:A:85:TYR:HB3	2.20	0.41
2:B:21:LEU:O	2:B:25:GLU:HG2	2.20	0.41
4:R:215:ILE:HG22	4:R:221:PHE:HD2	1.85	0.41
6:F:12:ASN:C	6:F:14:VAL:H	2.28	0.41
1:O:217(E):ASP:OD1	1:O:217(E):ASP:N	2.49	0.41
2:P:17:PRO:HA	3:Q:26:TYR:CD1	2.55	0.41
2:P:141:TYR:CD1	2:P:219(A):VAL:HG21	2.55	0.41
10:X:103:GLY:HA2	10:X:178:VAL:HG11	2.02	0.41
4:D:28:LEU:HA	4:D:31:ILE:HD12	2.02	0.41
13:M:19:LEU:HB2	13:M:170:SER:HB2	2.03	0.41
3:Q:150:GLN:HE21	3:Q:160:TRP:HE1	1.68	0.41
11:Y:208:ASN:H	11:Y:208:ASN:ND2	2.12	0.41
16:Y:212:L2T:H24	17:Y:213:MES:H71	2.01	0.41
12:Z:113:PHE:HA	12:Z:118:SER:O	2.20	0.41
10:J:138:LEU:O	10:J:142:TYR:HB3	2.21	0.41
2:P:147:GLN:HB3	2:P:149:TYR:CE2	2.55	0.41
6:T:179:LEU:HD21	6:T:192:GLN:HG2	2.01	0.41
14:2:36:ARG:HG3	14:2:42:TRP:NE1	2.35	0.41
6:F:38:ILE:HG12	6:F:197:ILE:HD11	2.02	0.41
10:J:35:ARG:HA	10:J:35:ARG:HD3	1.87	0.41
6:T:176:LEU:HD13	6:T:196:ILE:HD13	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:Y:19:ARG:HH21	11:Y:29:GLN:HE22	1.67	0.41
5:S:152:GLN:HA	5:S:153:PRO:HD3	1.94	0.41
2:B:39:GLY:C	2:B:148:LEU:HD21	2.46	0.41
4:D:97:VAL:HG11	11:K:65:LEU:HD22	2.03	0.41
6:F:36:THR:HB	6:F:168:GLY:H	1.85	0.41
7:G:105:TYR:OH	8:H:66:HIS:HE1	2.02	0.41
5:S:70:CYS:SG	5:S:92:LEU:HD23	2.60	0.41
5:S:231:LYS:HE3	5:S:231:LYS:HB2	1.95	0.41
6:T:38:ILE:HG12	6:T:197:ILE:HD11	2.01	0.41
8:V:152:ILE:HD11	8:V:177:VAL:HG21	2.02	0.41
11:Y:181:ASP:C	11:Y:183:GLY:CA	2.93	0.41
2:B:149:TYR:OH	3:C:62(A):ILE:HB	2.21	0.41
4:D:123:PHE:O	4:D:126:ARG:HD2	2.19	0.41
11:K:39:PRO:O	11:K:183:GLY:N	2.53	0.41
12:L:14:LEU:HD23	12:L:14:LEU:HA	1.92	0.41
4:R:52:LYS:HE3	4:R:211:GLN:HB2	2.02	0.41
9:W:186:LYS:HE2	9:W:188:TYR:CE1	2.55	0.41
11:Y:85:ASN:HD22	11:Y:85:ASN:HA	1.64	0.41
12:Z:114:ASP:HB2	12:Z:115:PRO:CD	2.51	0.41
4:D:39:GLY:HA2	4:D:47:VAL:O	2.21	0.41
5:E:175:TYR:HB2	5:E:199:GLN:HG2	2.03	0.41
10:J:181:ASP:O	10:J:183:GLY:HA3	2.20	0.41
1:O:33:GLN:H	1:O:33:GLN:HG2	1.64	0.41
2:P:77:ALA:HB3	2:P:137:ILE:HB	2.03	0.41
3:Q:101:LEU:HD13	10:X:61:ALA:HB2	2.02	0.41
3:Q:177:GLU:HG2	4:R:57:PRO:HG2	2.03	0.41
4:R:162:ALA:HB3	5:S:58:LEU:HD23	2.02	0.41
6:T:150:MET:HB3	6:T:160:TYR:CE1	2.56	0.41
10:X:113:ILE:HA	10:X:118:THR:O	2.21	0.41
6:F:210:LEU:HD21	6:F:212:ILE:HD11	2.03	0.41
9:I:130:ALA:HB2	9:I:166:ASP:CB	2.51	0.41
6:T:12:ASN:C	6:T:14:VAL:N	2.73	0.41
9:W:33:LYS:O	9:W:44:GLY:HA2	2.21	0.41
10:X:179:ASP:O	10:X:183:GLY:N	2.53	0.41
12:Z:144(H):GLY:C	12:Z:144(J):ASN:N	2.78	0.41
2:B:152:ASN:HB2	2:B:153:PRO:HD2	2.02	0.40
13:M:86:VAL:O	13:M:90:ARG:HG2	2.21	0.40
3:Q:157:TYR:OH	4:R:86:ARG:NH2	2.54	0.40
4:R:160:TYR:CE2	5:S:59:SER:HB3	2.56	0.40
10:X:57:GLU:OE1	11:Y:81:LYS:NZ	2.54	0.40
14:N:179:THR:O	14:N:183:GLY:N	2.54	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:78:TYR:HB3	1:O:85:TYR:CD1	2.56	0.40
1:O:187:GLU:HA	1:O:190:ILE:HD12	2.03	0.40
7:U:91:ARG:CZ	7:U:119:LEU:HD21	2.50	0.40
13:1:40:ASN:HD22	13:1:40:ASN:N	2.11	0.40
8:H:172:ASN:HD22	8:H:193:THR:HA	1.86	0.40
3:Q:52:ARG:HB2	3:Q:209:ASN:HA	2.03	0.40
4:R:202:GLU:O	4:R:205:GLU:N	2.55	0.40
8:V:34:LEU:HD22	8:V:174:ASP:HB3	2.03	0.40
8:V:206:PHE:HA	8:V:207:PRO:HD2	1.95	0.40
1:A:78:TYR:HB3	1:A:85:TYR:CD1	2.57	0.40
3:C:180(B):ARG:O	3:C:182:PRO:HD3	2.21	0.40
4:D:81:LEU:HD12	4:D:133:GLY:HA3	2.04	0.40
6:F:114:ASP:O	6:F:118:GLN:HG2	2.22	0.40
9:I:1:GLY:O	9:I:1:GLY:N	2.44	0.40
12:L:4:LEU:HD11	12:L:138:LEU:HD21	2.02	0.40
12:L:180:LYS:O	12:L:182:ASP:CA	2.69	0.40
4:R:202:GLU:C	4:R:205:GLU:N	2.80	0.40
10:X:181:ASP:O	10:X:183:GLY:CA	2.70	0.40
12:Z:112:SER:HB3	12:Z:125:ARG:HG2	2.03	0.40
7:G:110:ASP:HB3	7:G:149:TYR:CZ	2.57	0.40
9:I:159:LEU:HD23	9:I:159:LEU:C	2.47	0.40
9:I:166:ASP:HB3	9:I:169:SER:HB2	2.03	0.40
11:K:192:VAL:HG11	9:W:194:ASP:HB3	2.04	0.40
1:O:62:GLU:CD	1:O:62:GLU:H	2.29	0.40
2:P:156:ASN:OD1	3:Q:82:ASN:HB2	2.21	0.40
3:Q:136:THR:O	3:Q:150:GLN:HA	2.22	0.40
6:T:179:LEU:HD11	6:T:192:GLN:CG	2.50	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	246/250 (98%)	234 (95%)	9 (4%)	3 (1%)	10	30
1	O	246/250 (98%)	235 (96%)	10 (4%)	1 (0%)	30	57
2	B	231/245 (94%)	216 (94%)	10 (4%)	5 (2%)	5	17
2	P	231/245 (94%)	218 (94%)	8 (4%)	5 (2%)	5	17
3	C	235/243 (97%)	229 (97%)	5 (2%)	1 (0%)	30	57
3	Q	235/243 (97%)	228 (97%)	3 (1%)	4 (2%)	7	22
4	D	232/250 (93%)	219 (94%)	11 (5%)	2 (1%)	14	37
4	R	234/250 (94%)	216 (92%)	17 (7%)	1 (0%)	30	57
5	E	223/234 (95%)	211 (95%)	8 (4%)	4 (2%)	6	21
5	S	227/234 (97%)	211 (93%)	12 (5%)	4 (2%)	6	21
6	F	231/248 (93%)	217 (94%)	14 (6%)	0	100	100
6	T	233/248 (94%)	222 (95%)	10 (4%)	1 (0%)	30	57
7	G	235/252 (93%)	224 (95%)	10 (4%)	1 (0%)	30	57
7	U	239/252 (95%)	234 (98%)	3 (1%)	2 (1%)	16	40
8	H	216/222 (97%)	207 (96%)	8 (4%)	1 (0%)	24	52
8	V	216/222 (97%)	205 (95%)	11 (5%)	0	100	100
9	I	196/205 (96%)	188 (96%)	8 (4%)	0	100	100
9	W	198/205 (97%)	190 (96%)	8 (4%)	0	100	100
10	J	193/198 (98%)	183 (95%)	8 (4%)	2 (1%)	12	35
10	X	193/198 (98%)	184 (95%)	6 (3%)	3 (2%)	7	23
11	K	208/212 (98%)	202 (97%)	5 (2%)	1 (0%)	24	52
11	Y	208/212 (98%)	198 (95%)	9 (4%)	1 (0%)	24	52
12	L	216/241 (90%)	212 (98%)	4 (2%)	0	100	100
12	Z	216/241 (90%)	208 (96%)	7 (3%)	1 (0%)	24	52
13	1	227/266 (85%)	217 (96%)	9 (4%)	1 (0%)	30	57
13	M	225/266 (85%)	215 (96%)	9 (4%)	1 (0%)	30	57
14	2	188/196 (96%)	181 (96%)	7 (4%)	0	100	100
14	N	188/196 (96%)	181 (96%)	7 (4%)	0	100	100
All	All	6166/6524 (94%)	5885 (95%)	236 (4%)	45 (1%)	18	44

All (45) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	54	VAL
5	E	6	ASN
5	E	203	ASP
5	E	217	LYS
7	G	239	GLN
2	P	54	VAL
2	P	218(B)	ASP
3	Q	202	GLN
5	S	203	ASP
13	1	1	THR
1	A	5	THR
2	B	204(A)	SER
2	B	217	ALA
5	E	56	ASP
13	M	-7	GLN
2	P	217	ALA
3	Q	207	ALA
3	Q	208	LYS
5	S	199	GLN
7	U	239	GLN
11	Y	72	GLU
2	B	218(C)	ASP
3	C	207	ALA
11	K	9	GLN
2	P	62	ASP
5	S	6	ASN
10	X	189	ASP
1	A	203	GLU
4	D	123(B)	GLU
10	J	49	ALA
2	P	65	GLU
6	T	205	ASN
12	Z	144(K)	GLY
4	D	123(C)	GLY
5	S	231	LYS
7	U	55	PRO
2	B	182	ASP
1	O	56	SER
1	A	22	GLY
3	Q	183	PRO
8	H	105(A)	PRO
10	J	8	VAL
10	X	8	VAL

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Mol	Chain	Res	Type
10	X	187	VAL
4	R	12	VAL

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	209/209 (100%)	180 (86%)	29 (14%)	3	11
1	O	209/209 (100%)	194 (93%)	15 (7%)	13	35
2	B	195/204 (96%)	181 (93%)	14 (7%)	13	35
2	P	195/204 (96%)	180 (92%)	15 (8%)	12	33
3	C	213/215 (99%)	192 (90%)	21 (10%)	7	22
3	Q	213/215 (99%)	197 (92%)	16 (8%)	12	34
4	D	198/206 (96%)	186 (94%)	12 (6%)	17	43
4	R	198/206 (96%)	178 (90%)	20 (10%)	7	21
5	E	192/193 (100%)	172 (90%)	20 (10%)	7	20
5	S	192/193 (100%)	178 (93%)	14 (7%)	13	35
6	F	196/205 (96%)	178 (91%)	18 (9%)	8	25
6	T	196/205 (96%)	182 (93%)	14 (7%)	13	36
7	G	207/210 (99%)	187 (90%)	20 (10%)	8	23
7	U	207/210 (99%)	194 (94%)	13 (6%)	16	41
8	H	181/181 (100%)	171 (94%)	10 (6%)	19	47
8	V	181/181 (100%)	168 (93%)	13 (7%)	13	35
9	I	172/173 (99%)	166 (96%)	6 (4%)	32	64
9	W	172/173 (99%)	163 (95%)	9 (5%)	21	50
10	J	175/175 (100%)	164 (94%)	11 (6%)	16	41
10	X	175/175 (100%)	164 (94%)	11 (6%)	16	41
11	K	169/169 (100%)	154 (91%)	15 (9%)	9	26
11	Y	169/169 (100%)	154 (91%)	15 (9%)	9	26

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
12	L	185/201 (92%)	177 (96%)	8 (4%)	26	57
12	Z	185/201 (92%)	179 (97%)	6 (3%)	34	67
13	1	199/224 (89%)	188 (94%)	11 (6%)	19	47
13	M	199/224 (89%)	192 (96%)	7 (4%)	32	64
14	2	162/162 (100%)	156 (96%)	6 (4%)	30	62
14	N	162/162 (100%)	153 (94%)	9 (6%)	19	46
All	All	5306/5454 (97%)	4928 (93%)	378 (7%)	13	36

All (378) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	MET
1	A	5	THR
1	A	54	SER
1	A	62	GLU
1	A	64	LEU
1	A	65	SER
1	A	91	LYS
1	A	111	LEU
1	A	124	THR
1	A	158	PHE
1	A	178	LYS
1	A	179	ARG
1	A	203	GLU
1	A	217	ASP
1	A	217(A)	GLU
1	A	217(B)	ASN
1	A	217(D)	PRO
1	A	217(E)	ASP
1	A	217(F)	LEU
1	A	217(G)	LEU
1	A	217(I)	TYR
1	A	217(J)	THR
1	A	217(L)	ILE
1	A	217(M)	PRO
1	A	217(N)	THR
1	A	217(O)	ASP
1	A	217(P)	LYS
1	A	222	ARG
1	A	236	LEU

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Mol	Chain	Res	Type
2	B	18	GLU
2	B	53	LYS
2	B	58	LEU
2	B	59	LEU
2	B	61	GLN
2	B	67	LEU
2	B	124	THR
2	B	150	THR
2	B	177	GLN
2	B	192	LEU
2	B	198	SER
2	B	202	THR
2	B	225	LYS
2	B	232	ILE
3	C	10	ARG
3	C	33	ARG
3	C	40	VAL
3	C	44	ASN
3	C	55	THR
3	C	66	LYS
3	C	74	VAL
3	C	87	ILE
3	C	112	LEU
3	C	150	GLN
3	C	156	ILE
3	C	163	GLN
3	C	172	VAL
3	C	185	THR
3	C	187	GLU
3	C	202	GLN
3	C	215	VAL
3	C	234	THR
3	C	235	GLN
3	C	240	LYS
3	C	242	GLU
4	D	48	LEU
4	D	52	LYS
4	D	59	LEU
4	D	65	GLU
4	D	110	GLU
4	D	119	LEU
4	D	177	LEU

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Mol	Chain	Res	Type
4	D	191	LEU
4	D	194	LEU
4	D	205	GLU
4	D	215	ILE
4	D	237	LEU
5	E	12	THR
5	E	13	VAL
5	E	18	THR
5	E	28	LEU
5	E	58	LEU
5	E	64	GLN
5	E	78	LEU
5	E	149	LEU
5	E	177	GLU
5	E	179	THR
5	E	185	ASN
5	E	189	LEU
5	E	195	GLU
5	E	207	LEU
5	E	207(B)	THR
5	E	207(C)	VAL
5	E	207(D)	ASP
5	E	207(E)	ASN
5	E	219	THR
5	E	222	THR
6	F	35	THR
6	F	36	THR
6	F	43	ASN
6	F	55	THR
6	F	59	LEU
6	F	72	ARG
6	F	88	LEU
6	F	121	GLN
6	F	129	VAL
6	F	134	VAL
6	F	169	ARG
6	F	176	LEU
6	F	192	GLN
6	F	206	LYS
6	F	206(B)	GLU
6	F	206(C)	LYS
6	F	222	LYS

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Mol	Chain	Res	Type
6	F	225	LYS
7	G	29	LYS
7	G	33	GLN
7	G	38	LEU
7	G	49	ILE
7	G	72	ARG
7	G	87	ASN
7	G	119	LEU
7	G	124	THR
7	G	169	GLN
7	G	171	GLU
7	G	174	THR
7	G	184	ASN
7	G	184(G)	GLU
7	G	184(H)	GLU
7	G	184(M)	SER
7	G	188	LYS
7	G	197	MET
7	G	217	LYS
7	G	232	ARG
7	G	233	LEU
8	H	34	LEU
8	H	55	VAL
8	H	68	LEU
8	H	101	VAL
8	H	131	SER
8	H	144	GLN
8	H	169	SER
8	H	192	LEU
8	H	222	CYS
8	H	223	ASP
9	I	4	VAL
9	I	9	LYS
9	I	20	LEU
9	I	160	LEU
9	I	174	VAL
9	I	181	LYS
10	J	6	ILE
10	J	9	GLN
10	J	24	ILE
10	J	34	THR
10	J	35	ARG

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Mol	Chain	Res	Type
10	J	48	GLU
10	J	52	THR
10	J	68	ILE
10	J	70	GLU
10	J	155	LEU
10	J	191	GLN
11	K	4	LEU
11	K	9	GLN
11	K	31	VAL
11	K	35	ILE
11	K	65	LEU
11	K	69	ARG
11	K	73	ARG
11	K	87	VAL
11	K	99	THR
11	K	109	THR
11	K	145	ASP
11	K	178	VAL
11	K	180	GLU
11	K	200	LYS
11	K	201	GLU
12	L	-9	GLN
12	L	14	LEU
12	L	25	SER
12	L	40	ASN
12	L	61	ASN
12	L	62	SER
12	L	99	THR
12	L	138	LEU
13	M	40	ASN
13	M	62	LEU
13	M	65	GLU
13	M	91	ARG
13	M	148	VAL
13	M	184	LEU
13	M	190	LEU
14	N	20	THR
14	N	22	THR
14	N	31	THR
14	N	36	ARG
14	N	89	GLU
14	N	107	LYS

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Mol	Chain	Res	Type
14	N	115	LEU
14	N	119	VAL
14	N	132	THR
1	O	4	MET
1	O	33	GLN
1	O	47	VAL
1	O	62	GLU
1	O	64	LEU
1	O	87	VAL
1	O	89	VAL
1	O	109	THR
1	O	124	THR
1	O	129	VAL
1	O	158	PHE
1	O	170	VAL
1	O	203	GLU
1	O	222	ARG
1	O	223	LYS
2	P	58	LEU
2	P	64	THR
2	P	91	THR
2	P	101	LYS
2	P	124	THR
2	P	150	THR
2	P	181	LYS
2	P	185	LYS
2	P	192	LEU
2	P	198	SER
2	P	202	THR
2	P	212	PHE
2	P	225	LYS
2	P	232	ILE
2	P	235	LYS
3	Q	25	GLU
3	Q	40	VAL
3	Q	56	LEU
3	Q	61	THR
3	Q	66	LYS
3	Q	74	VAL
3	Q	112	LEU
3	Q	129	VAL
3	Q	150	GLN

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Mol	Chain	Res	Type
3	Q	156	ILE
3	Q	163	GLN
3	Q	172	VAL
3	Q	174	GLU
3	Q	185	THR
3	Q	215	VAL
3	Q	235	GLN
4	R	12	VAL
4	R	13	SER
4	R	28	LEU
4	R	48	LEU
4	R	52	LYS
4	R	59	LEU
4	R	60	GLU
4	R	65	GLU
4	R	72	ARG
4	R	119	LEU
4	R	127	LEU
4	R	177	LEU
4	R	184	LEU
4	R	191	LEU
4	R	194	LEU
4	R	202	GLU
4	R	215	ILE
4	R	231	GLU
4	R	237	LEU
4	R	238	LYS
5	S	12	THR
5	S	13	VAL
5	S	33	GLN
5	S	58	LEU
5	S	65	LYS
5	S	76	LEU
5	S	168	ARG
5	S	178	ARG
5	S	189	LEU
5	S	195	GLU
5	S	199	GLN
5	S	207	LEU
5	S	219	THR
5	S	222	THR
6	T	35	THR

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Mol	Chain	Res	Type
6	T	36	THR
6	T	43	ASN
6	T	63	LYS
6	T	72	ARG
6	T	98	SER
6	T	100	LYS
6	T	121	GLN
6	T	129	VAL
6	T	151	LEU
6	T	176	LEU
6	T	187	ARG
6	T	225	LYS
6	T	240	ILE
7	U	38	LEU
7	U	43	LYS
7	U	49	ILE
7	U	57	LYS
7	U	87	ASN
7	U	119	LEU
7	U	124	THR
7	U	197	MET
7	U	203	THR
7	U	227	GLU
7	U	228	ASN
7	U	232	ARG
7	U	233	LEU
8	V	13	VAL
8	V	34	LEU
8	V	55	VAL
8	V	68	LEU
8	V	101	VAL
8	V	144	GLN
8	V	149	GLU
8	V	192	LEU
8	V	196	VAL
8	V	197	ARG
8	V	218	ILE
8	V	221	ILE
8	V	222	CYS
9	W	-7	ASP
9	W	-4	SER
9	W	32	GLU

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Mol	Chain	Res	Type
9	W	107	LYS
9	W	121	GLU
9	W	160	LEU
9	W	171	TRP
9	W	174	VAL
9	W	181	LYS
10	X	-1	MET
10	X	6	ILE
10	X	24	ILE
10	X	34	THR
10	X	35	ARG
10	X	48	GLU
10	X	52	THR
10	X	68	ILE
10	X	157	LEU
10	X	168	MET
10	X	191	GLN
11	Y	4	LEU
11	Y	9	GLN
11	Y	31	VAL
11	Y	41	LEU
11	Y	53	GLN
11	Y	65	LEU
11	Y	69	ARG
11	Y	73	ARG
11	Y	84	SER
11	Y	87	VAL
11	Y	115	SER
11	Y	145	ASP
11	Y	149	GLU
11	Y	208	ASN
11	Y	210	ILE
12	Z	-9	GLN
12	Z	14	LEU
12	Z	40	ASN
12	Z	61	ASN
12	Z	138	LEU
12	Z	180	LYS
13	1	2	SER
13	1	40	ASN
13	1	62	LEU
13	1	91	ARG

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Mol	Chain	Res	Type
13	1	112	TYR
13	1	148	VAL
13	1	184	LEU
13	1	190	LEU
13	1	191	GLN
13	1	204	LYS
13	1	211	ILE
14	2	20	THR
14	2	48	SER
14	2	94	ASN
14	2	119	VAL
14	2	149	GLU
14	2	178	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (190) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	97	HIS
1	A	227	GLN
2	B	23	GLN
2	B	95	HIS
2	B	97	GLN
2	B	121	GLN
2	B	125	GLN
2	B	156	ASN
2	B	168	ASN
2	B	177	GLN
2	B	227	GLN
3	C	23	GLN
3	C	44	ASN
3	C	82	ASN
3	C	125	GLN
3	C	150	GLN
3	C	163	GLN
3	C	168	ASN
3	C	235	GLN
4	D	23	GLN
4	D	108	ASN
4	D	114	GLN
4	D	161	ASN
4	D	199	GLN
4	D	211	GLN

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Mol	Chain	Res	Type
4	D	218	GLN
4	D	226	ASN
5	E	6	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	207(E)	ASN
6	F	23	GLN
6	F	43	ASN
6	F	90	ASN
6	F	121	GLN
6	F	205	ASN
7	G	33	GLN
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	178	ASN
8	H	22	GLN
8	H	30	ASN
8	H	66	HIS
8	H	144	GLN
8	H	165	ASN
8	H	172	ASN
8	H	190	ASN
9	I	29	ASN
9	I	56	ASN
10	J	9	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	141	HIS
10	J	186	GLN
11	K	85	ASN

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Mol	Chain	Res	Type
11	K	141	ASN
11	K	174	ASN
11	K	207	ASN
12	L	-7	ASN
12	L	40	ASN
12	L	67	HIS
12	L	70	HIS
12	L	70(A)	ASN
12	L	140	ASN
12	L	143	ASN
12	L	144(B)	ASN
12	L	144(I)	ASN
12	L	166	HIS
13	M	10	ASN
13	M	40	ASN
13	M	89	GLN
13	M	149	GLN
13	M	157	ASN
13	M	172	ASN
14	N	38	HIS
14	N	69	GLN
14	N	94	ASN
14	N	141	ASN
14	N	157	HIS
14	N	161	GLN
1	O	97	HIS
1	O	191	HIS
2	P	23	GLN
2	P	97	GLN
2	P	121	GLN
2	P	125	GLN
2	P	147	GLN
2	P	173	GLN
2	P	177	GLN
2	P	221	GLN
3	Q	23	GLN
3	Q	82	ASN
3	Q	97	GLN
3	Q	121	GLN
3	Q	150	GLN
3	Q	163	GLN
3	Q	209	ASN

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Mol	Chain	Res	Type
3	Q	235	GLN
4	R	23	GLN
4	R	99	HIS
4	R	108	ASN
4	R	147	GLN
4	R	161	ASN
4	R	199	GLN
4	R	211	GLN
4	R	226	ASN
5	S	73	HIS
5	S	104	ASN
5	S	121	GLN
5	S	125	GLN
5	S	156	ASN
5	S	170	GLN
5	S	185	ASN
5	S	209	ASN
6	T	23	GLN
6	T	43	ASN
6	T	90	ASN
6	T	121	GLN
6	T	192	GLN
6	T	205	ASN
6	T	218(C)	ASN
7	U	33	GLN
7	U	34(A)	ASN
7	U	87	ASN
7	U	118	ASN
7	U	121	GLN
7	U	125	GLN
7	U	169	GLN
7	U	178	ASN
7	U	182	HIS
7	U	184	ASN
8	V	30	ASN
8	V	66	HIS
8	V	165	ASN
8	V	172	ASN
9	W	56	ASN
9	W	64	ASN
9	W	145	ASN
10	X	36	GLN

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Mol	Chain	Res	Type
10	X	54	GLN
10	X	62	ASN
10	X	77	GLN
10	X	112	GLN
10	X	141	HIS
10	X	160	GLN
10	X	191	GLN
10	X	193	GLN
11	Y	9	GLN
11	Y	85	ASN
11	Y	141	ASN
11	Y	174	ASN
11	Y	207	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	123	GLN
12	Z	140	ASN
12	Z	141	GLN
12	Z	144(B)	ASN
12	Z	144(J)	ASN
12	Z	166	HIS
13	1	-7	GLN
13	1	40	ASN
13	1	89	GLN
13	1	93	ASN
13	1	149	GLN
13	1	157	ASN
13	1	172	ASN
13	1	191	GLN
14	2	38	HIS
14	2	62	HIS
14	2	69	GLN
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 14 ligands modelled in this entry, 10 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	Y	213	-	12,12,12	2.24	1 (8%)	15,16,16	1.28	2 (13%)
17	MES	K	214	-	12,12,12	2.07	1 (8%)	15,16,16	1.28	1 (6%)
16	L2T	Y	212	-	47,47,47	1.98	2 (4%)	61,62,62	0.82	1 (1%)
16	L2T	K	213	-	47,47,47	2.07	2 (4%)	61,62,62	0.83	1 (1%)

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	Y	213	-	-	1/6/14/14	0/1/1/1
17	MES	K	214	-	-	5/6/14/14	0/1/1/1
16	L2T	Y	212	-	-	6/39/39/39	0/4/4/4
16	L2T	K	213	-	-	2/39/39/39	0/4/4/4

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	K	213	L2T	CL7-C6	12.85	1.75	1.51
16	Y	212	L2T	CL7-C6	12.15	1.73	1.51
17	Y	213	MES	C8-S	-7.37	1.67	1.77
17	K	214	MES	C8-S	-6.72	1.68	1.77
16	K	213	L2T	C37-C38	-4.75	1.39	1.50
16	Y	212	L2T	C37-C38	-4.19	1.40	1.50

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	Y	212	L2T	O36-C37-C38	3.34	118.96	109.16
17	K	214	MES	O3S-S-C8	2.98	111.83	106.00
17	Y	213	MES	O3S-S-C8	2.60	111.09	106.00
17	Y	213	MES	O2S-S-C8	2.39	110.34	106.73
16	K	213	L2T	O36-C37-C38	2.31	115.95	109.16

There are no chirality outliers.

All (14) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
17	K	214	MES	C8-C7-N4-C3
17	K	214	MES	C8-C7-N4-C5
17	K	214	MES	C7-C8-S-O1S
17	K	214	MES	C7-C8-S-O2S
17	K	214	MES	C7-C8-S-O3S
16	Y	212	L2T	N19-C28-C9-C31
17	Y	213	MES	N4-C7-C8-S
16	Y	212	L2T	O29-C28-C9-C31
16	Y	212	L2T	C34-C33-O36-C37
16	Y	212	L2T	C32-C33-O36-C37
16	Y	212	L2T	N19-C28-C9-C35
16	Y	212	L2T	O29-C28-C9-C35
16	K	213	L2T	O29-C28-C9-C31
16	K	213	L2T	N19-C28-C9-C31

There are no ring outliers.

4 monomers are involved in 5 short contacts:

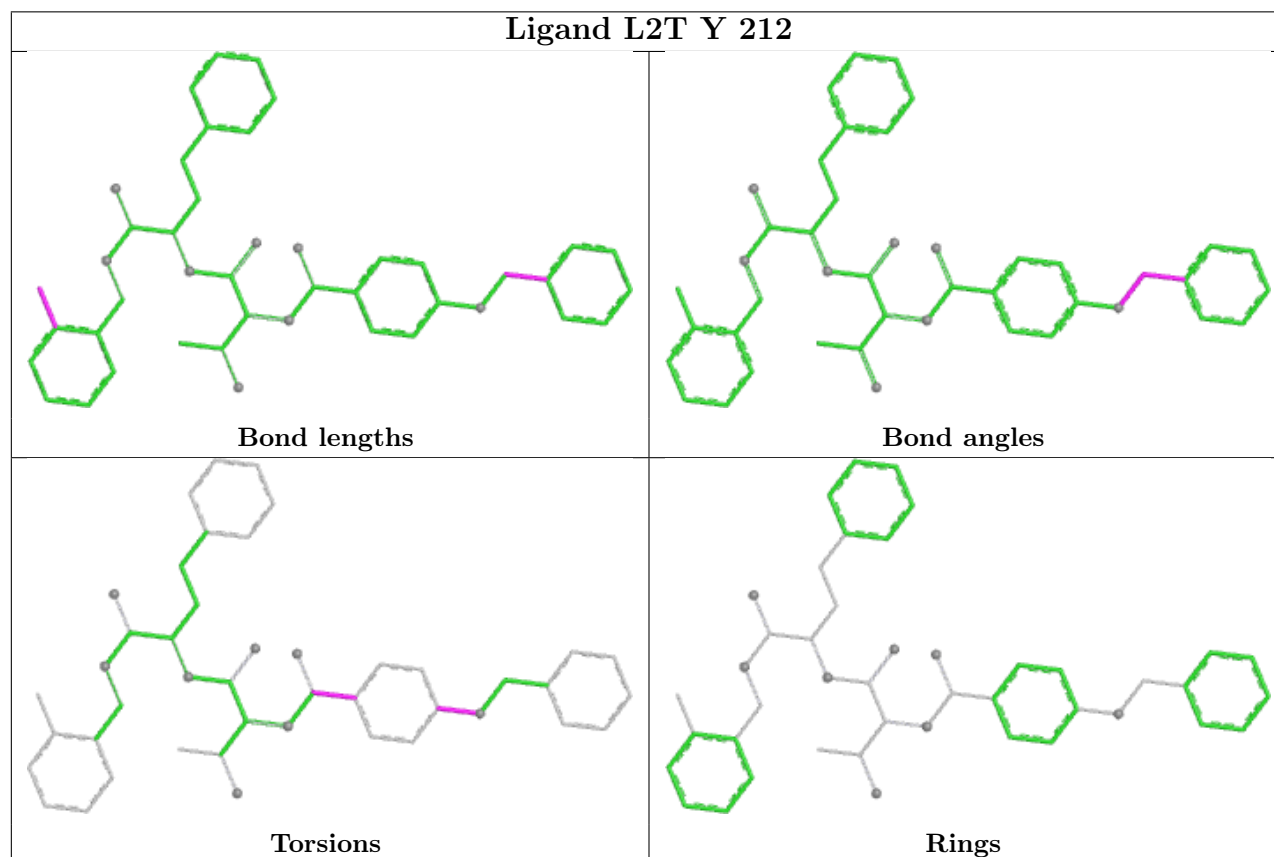
Mol	Chain	Res	Type	Clashes	Symm-Clashes
17	Y	213	MES	1	0

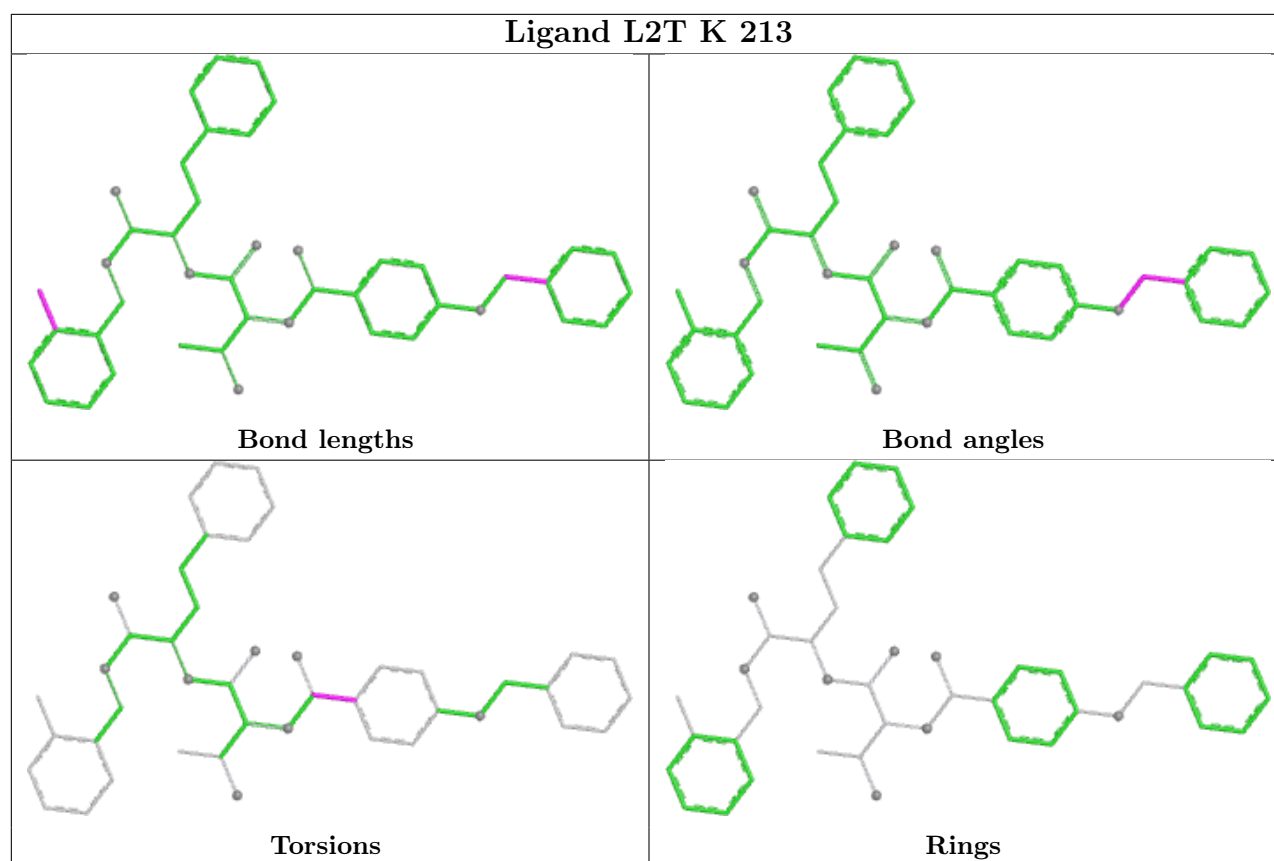
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
17	K	214	MES	1	0
16	Y	212	L2T	1	0
16	K	213	L2T	4	0

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 [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
4	D	4
5	E	4
4	R	3
13	M	3
14	N	3
7	G	3
14	2	3
13	1	3
9	I	3
9	W	3
3	C	2
10	J	2

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Mol	Chain	Number of breaks
10	X	2
3	Q	2
5	S	2
6	F	2
12	Z	2
12	L	2
8	V	2
8	H	2
11	K	1
1	A	1
1	O	1
2	P	1
11	Y	1
6	T	1
7	U	1
2	B	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	D	123(G):GLU	C	125:GLU	N	4.65
1	C	203:THR	C	206:GLY	N	4.56
1	R	123(G):GLU	C	125:GLU	N	4.48
1	J	-1:MET	C	1:ASP	N	4.02
1	X	-1:MET	C	1:ASP	N	3.71
1	Q	180(D):GLU	C	182:PRO	N	3.30
1	S	204:GLU	C	206:SER	N	3.24
1	M	181(A):THR	C	183:GLY	N	3.20
1	K	181:ASP	C	183:GLY	N	3.19
1	Q	203:THR	C	206:GLY	N	3.18
1	E	204:GLU	C	206:SER	N	3.11
1	C	180(D):GLU	C	182:PRO	N	3.08
1	F	180(F):GLY	C	184:LEU	N	3.02
1	S	60:SER	C	63:TYR	N	3.01
1	A	200:SER	C	202:VAL	N	3.00
1	N	181:ALA	C	183:GLY	N	3.00
1	O	200:SER	C	202:VAL	N	3.00
1	E	207(E):ASN	C	210:LEU	N	2.96
1	R	233:ILE	C	235:LYS	N	2.96
1	Z	-1:GLY	C	1:GLY	N	2.87
1	G	180(D):ILE	C	184:ASN	N	2.83
1	L	-1:GLY	C	1:GLY	N	2.83
1	R	202:GLU	C	205:GLU	N	2.80

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	P	200:THR	C	202:THR	N	2.75
1	G	184(M):SER	C	186:TRP	N	2.73
1	V	91:GLN	C	93:GLY	N	2.72
1	F	199:LEU	C	201:ALA	N	2.68
1	Y	181:ASP	C	183:GLY	N	2.68
1	Z	180:LYS	C	182:ASP	N	2.68
1	E	180(F):ILE	C	183:ASP	N	2.61
1	2	92:ASP	C	94:ASN	N	2.60
1	1	181(A):THR	C	183:GLY	N	2.59
1	2	181:ALA	C	183:GLY	N	2.59
1	D	202:GLU	C	205:GLU	N	2.58
1	X	181:ASP	C	183:GLY	N	2.58
1	D	233:ILE	C	235:LYS	N	2.56
1	L	180:LYS	C	182:ASP	N	2.56
1	E	60:SER	C	63:TYR	N	2.55
1	D	180(E):SER	C	184:LEU	N	2.50
1	I	179:LYS	C	181:LYS	N	2.50
1	T	199:LEU	C	201:ALA	N	2.48
1	W	179:LYS	C	181:LYS	N	2.47
1	J	181:ASP	C	183:GLY	N	2.46
1	U	218:ASP	C	220:LYS	N	2.46
1	V	187:LEU	C	189:ARG	N	2.33
1	2	70:TYR	C	72:GLY	N	2.31
1	1	141(G):ILE	C	144:PRO	N	2.27
1	B	200:THR	C	202:THR	N	2.25
1	H	187:LEU	C	189:ARG	N	2.23
1	N	70:TYR	C	72:GLY	N	2.21
1	H	91:GLN	C	93:GLY	N	2.20
1	M	-1:GLY	C	1:THR	N	2.19
1	M	141(G):ILE	C	144:PRO	N	2.18
1	I	36:HIS	C	38:TYR	N	2.17
1	W	36:HIS	C	38:TYR	N	2.16
1	G	218:ASP	C	220:LYS	N	2.10
1	I	-1:GLY	C	1:GLY	N	2.05
1	N	92:ASP	C	94:ASN	N	2.04
1	W	-1:GLY	C	1:GLY	N	2.00
1	1	-1:GLY	C	1:THR	N	1.87

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	250/250 (100%)	0.32	9 (3%) 46 39	37, 54, 80, 110	0
1	O	250/250 (100%)	0.52	16 (6%) 25 20	41, 62, 88, 115	0
2	B	235/245 (95%)	0.59	19 (8%) 18 14	41, 60, 92, 106	0
2	P	235/245 (95%)	0.60	21 (8%) 15 12	39, 63, 97, 108	0
3	C	241/243 (99%)	0.89	34 (14%) 6 5	43, 69, 110, 125	0
3	Q	241/243 (99%)	1.22	50 (20%) 2 2	45, 74, 121, 140	0
4	D	242/250 (96%)	0.81	31 (12%) 7 6	40, 65, 101, 122	0
4	R	242/250 (96%)	0.78	25 (10%) 12 9	41, 65, 101, 129	0
5	E	233/234 (99%)	0.65	16 (6%) 23 18	48, 63, 91, 111	0
5	S	233/234 (99%)	0.85	33 (14%) 6 5	46, 64, 97, 125	0
6	F	237/248 (95%)	0.32	10 (4%) 40 34	39, 57, 95, 107	0
6	T	237/248 (95%)	0.34	10 (4%) 40 34	38, 58, 85, 109	0
7	G	243/252 (96%)	0.21	7 (2%) 53 46	36, 51, 80, 111	0
7	U	243/252 (96%)	0.19	9 (3%) 45 38	35, 51, 73, 101	0
8	H	222/222 (100%)	0.09	4 (1%) 67 60	34, 48, 65, 99	0
8	V	222/222 (100%)	0.18	5 (2%) 61 53	39, 52, 72, 107	0
9	I	204/205 (99%)	0.08	3 (1%) 72 65	36, 48, 66, 82	0
9	W	204/205 (99%)	0.12	2 (0%) 79 74	35, 51, 69, 86	0
10	J	198/198 (100%)	0.26	10 (5%) 33 27	38, 51, 68, 127	0
10	X	198/198 (100%)	0.28	5 (2%) 58 50	39, 53, 68, 125	0
11	K	212/212 (100%)	0.09	3 (1%) 73 67	36, 50, 69, 88	0
11	Y	212/212 (100%)	0.06	1 (0%) 87 83	36, 51, 70, 77	0
12	L	222/241 (92%)	0.13	5 (2%) 61 53	36, 51, 71, 82	0
12	Z	222/241 (92%)	0.12	5 (2%) 61 53	34, 50, 72, 83	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å ²)	Q<0.9
13	1	233/266 (87%)	-0.03	2 (0%)	81 76	34, 48, 63, 67	0
13	M	233/266 (87%)	0.10	3 (1%)	75 69	36, 51, 65, 71	0
14	2	196/196 (100%)	-0.04	3 (1%)	72 65	34, 46, 64, 79	0
14	N	196/196 (100%)	-0.08	1 (0%)	87 83	37, 45, 60, 76	0
All	All	6336/6524 (97%)	0.36	342 (5%)	31 26	34, 54, 91, 140	0

All (342) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	Q	56	LEU	9.7
2	B	217	ALA	8.8
10	X	-1	MET	8.5
10	J	-1	MET	7.7
4	D	123(B)	GLU	6.9
13	M	-8	THR	6.9
4	R	123(E)	SER	6.8
5	S	4	PHE	6.8
3	Q	55	THR	6.7
6	F	12	ASN	6.6
4	D	127	LEU	6.4
1	O	4	MET	6.3
4	R	123(D)	ALA	6.2
6	T	12	ASN	6.1
4	R	123(C)	GLY	6.0
11	K	208	ASN	5.9
3	C	11	ALA	5.9
13	1	-8	THR	5.8
3	C	56	LEU	5.8
6	F	180(F)	GLY	5.6
4	R	127	LEU	5.3
3	Q	64	PRO	5.3
4	D	123(D)	ALA	5.2
2	P	217	ALA	5.2
11	K	210	ILE	5.2
4	D	12	VAL	5.2
10	J	192	ALA	5.1
4	R	123(F)	GLY	5.1
1	A	203	GLU	5.1
5	E	4	PHE	5.0
3	C	207	ALA	5.0
4	D	123(C)	GLY	5.0

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Mol	Chain	Res	Type	RSRZ
4	D	123(E)	SER	4.9
10	J	191	GLN	4.9
10	X	192	ALA	4.9
2	B	218	ASN	4.7
2	B	239	THR	4.6
3	C	9	ASP	4.6
3	Q	58	LEU	4.5
2	P	63	THR	4.5
2	P	54	VAL	4.5
1	A	4	MET	4.5
3	Q	57	LYS	4.4
4	D	123(G)	GLU	4.4
3	C	8	TYR	4.3
2	B	54	VAL	4.3
4	D	123(A)	GLY	4.2
1	O	5	THR	4.2
3	C	206	GLY	4.2
7	U	199	ASP	4.1
2	P	239	THR	4.1
10	X	191	GLN	4.1
4	R	123(A)	GLY	4.1
2	P	216(B)	GLY	4.1
4	R	123(B)	GLU	4.1
1	O	217(O)	ASP	4.1
2	B	216(B)	GLY	4.0
4	D	123(F)	GLY	4.0
7	U	240	ASP	4.0
6	T	13	SER	3.9
3	C	12	LEU	3.9
3	Q	54	SER	3.9
3	C	57	LYS	3.9
3	Q	236	ILE	3.8
6	T	240	ILE	3.8
5	S	198	SER	3.8
3	C	7	GLY	3.8
1	O	202	VAL	3.8
3	Q	206	GLY	3.8
3	Q	208	LYS	3.8
1	A	5	THR	3.7
3	Q	210	ILE	3.7
10	J	168	MET	3.7
6	T	199	LEU	3.7

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Mol	Chain	Res	Type	RSRZ
3	Q	62(A)	ILE	3.7
3	Q	207	ALA	3.7
4	D	10	ARG	3.7
4	D	241	GLU	3.7
4	R	123(G)	GLU	3.7
1	A	8	TYR	3.7
3	Q	59	GLN	3.7
2	P	218	ASN	3.6
4	D	11	GLY	3.6
7	U	6	ALA	3.6
4	D	242	ALA	3.6
6	F	13	SER	3.6
4	D	22	PHE	3.5
3	Q	63	THR	3.5
3	Q	203	THR	3.5
3	C	208	LYS	3.5
7	G	240	ASP	3.5
3	C	203	THR	3.4
5	S	57	GLU	3.4
2	B	22	TYR	3.4
3	Q	40	VAL	3.4
5	E	207(C)	VAL	3.4
5	E	207(E)	ASN	3.4
3	Q	240	LYS	3.3
1	O	7	ARG	3.3
8	V	223	ASP	3.3
10	J	49	ALA	3.3
3	C	62(A)	ILE	3.3
2	B	13	THR	3.3
5	S	58	LEU	3.3
6	T	203	GLU	3.3
3	Q	200	VAL	3.3
5	E	5	ARG	3.2
3	Q	201	VAL	3.2
5	S	208(A)	VAL	3.2
4	R	12	VAL	3.2
1	O	6	ASP	3.2
4	D	9	ASP	3.2
5	S	230	ALA	3.2
5	S	63	TYR	3.2
10	J	190	PHE	3.2
2	B	63	THR	3.1

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Mol	Chain	Res	Type	RSRZ
5	S	55	ALA	3.1
4	D	13	SER	3.1
3	C	58	LEU	3.1
6	F	201	ALA	3.1
5	S	206	SER	3.1
5	S	5	ARG	3.1
5	S	32	LYS	3.1
4	R	10	ARG	3.1
5	S	199	GLN	3.1
3	Q	65	SER	3.1
4	D	205	GLU	3.0
5	S	56	ASP	3.0
6	T	22	PHE	3.0
1	A	7	ARG	3.0
2	B	218(D)	GLY	3.0
3	Q	182	PRO	3.0
6	F	205	ASN	3.0
3	Q	232	TYR	3.0
3	Q	229	ILE	3.0
7	G	6	ALA	2.9
9	W	181	LYS	2.9
4	R	126	ARG	2.9
11	Y	210	ILE	2.9
3	Q	66	LYS	2.9
4	R	13	SER	2.9
6	F	128	SER	2.9
14	N	92	ASP	2.9
11	K	183	GLY	2.9
4	R	123	PHE	2.9
6	F	203	GLU	2.9
5	E	206	SER	2.9
12	L	171	ASP	2.9
3	Q	198	LEU	2.9
3	Q	233	VAL	2.9
4	R	122	ARG	2.8
1	O	9	SER	2.8
3	Q	209	ASN	2.8
5	S	209	ASN	2.8
4	D	126	ARG	2.8
2	B	238	ILE	2.8
7	G	237	ALA	2.8
3	Q	185	THR	2.8

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Mol	Chain	Res	Type	RSRZ
3	C	211	GLU	2.8
7	U	218	ASP	2.8
1	O	217(P)	LYS	2.7
3	Q	186	VAL	2.7
3	C	209	ASN	2.7
2	B	64	THR	2.7
2	B	61	GLN	2.7
4	D	125	GLU	2.7
2	P	62	ASP	2.7
8	V	221	ILE	2.7
12	Z	144(R)	LYS	2.7
3	Q	9	ASP	2.7
10	J	193	GLN	2.6
12	Z	-9	GLN	2.6
5	S	127	TYR	2.6
1	O	42	ALA	2.6
3	C	55	THR	2.6
14	2	92	ASP	2.6
2	P	64	THR	2.6
3	Q	61	THR	2.6
12	L	144(K)	LYS	2.6
4	D	123	PHE	2.6
3	C	13	SER	2.6
5	S	12	THR	2.6
1	A	6	ASP	2.6
7	G	129	MET	2.6
7	G	236	ILE	2.6
8	H	222	CYS	2.6
5	E	203	ASP	2.5
3	C	229	ILE	2.5
1	O	64	LEU	2.5
12	Z	144(Q)	LEU	2.5
3	Q	8	TYR	2.5
3	Q	22	PHE	2.5
2	B	55	THR	2.5
2	P	13	THR	2.5
5	S	203	ASP	2.5
6	F	204	ASP	2.5
2	P	53	LYS	2.5
3	C	66	LYS	2.5
14	2	116	GLY	2.5
3	Q	38	VAL	2.5

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Mol	Chain	Res	Type	RSRZ
3	Q	44	ASN	2.5
3	Q	180(C)	LYS	2.5
8	H	221	ILE	2.5
8	H	223	ASP	2.5
3	Q	217	PRO	2.5
2	P	169	THR	2.5
5	E	180(F)	ILE	2.5
5	S	51	LEU	2.5
6	F	240	ILE	2.5
3	C	60	ASP	2.5
2	P	218(C)	GLY	2.5
4	R	158	TYR	2.5
5	E	129	GLY	2.5
4	D	143	ALA	2.5
3	C	185	THR	2.4
5	S	178	ARG	2.4
2	B	216(A)	LYS	2.4
3	C	22	PHE	2.4
3	C	63	THR	2.4
4	D	244	GLU	2.4
5	E	195	GLU	2.4
8	V	197	ARG	2.4
8	V	222	CYS	2.4
2	P	216(A)	LYS	2.4
8	V	182	LYS	2.4
9	I	181	LYS	2.4
3	C	233	VAL	2.4
3	C	224	LEU	2.4
3	C	242	GLU	2.4
3	Q	196	SER	2.4
10	X	188	ASP	2.4
3	Q	50	CYS	2.4
2	P	61	GLN	2.4
1	A	235	ALA	2.4
7	G	128	TYR	2.3
3	C	187	GLU	2.3
1	A	55	SER	2.3
10	J	10	ASP	2.3
4	R	218	GLN	2.3
1	O	235	ALA	2.3
4	D	26	TYR	2.3
2	P	55	THR	2.3

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Mol	Chain	Res	Type	RSRZ
1	O	110	LYS	2.3
2	B	53	LYS	2.3
12	L	17	ASP	2.3
5	S	49	VAL	2.3
13	1	211	ILE	2.3
3	C	232	TYR	2.3
3	Q	180	TYR	2.3
7	U	8	TYR	2.3
1	O	200	SER	2.3
5	S	9	ASP	2.3
12	Z	171	ASP	2.3
13	M	61	ASP	2.3
3	Q	33	ARG	2.3
4	R	230	ALA	2.3
10	X	49	ALA	2.3
2	P	220	TYR	2.3
7	G	8	TYR	2.3
1	O	55	SER	2.3
4	D	122	ARG	2.3
2	P	127	GLY	2.3
4	R	11	GLY	2.3
12	L	144(P)	LEU	2.3
4	D	41	ALA	2.2
5	S	228	ALA	2.2
2	B	57	THR	2.2
14	2	149	GLU	2.2
3	C	54	SER	2.2
2	B	127	GLY	2.2
5	S	10	GLY	2.2
3	Q	189	CYS	2.2
3	C	234	THR	2.2
7	U	128	TYR	2.2
7	U	239	GLN	2.2
5	E	184	GLY	2.2
5	S	59	SER	2.2
6	T	180(A)	ASP	2.2
3	Q	180(D)	GLU	2.2
5	E	12	THR	2.2
5	E	204	GLU	2.2
4	D	33	LEU	2.2
4	D	177	LEU	2.2
4	R	235	LYS	2.2

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Mol	Chain	Res	Type	RSRZ
5	S	52	LYS	2.2
7	U	129	MET	2.2
10	J	187	VAL	2.2
2	P	202	THR	2.2
4	R	229	THR	2.2
1	O	8	TYR	2.2
5	E	63	TYR	2.2
5	S	33	GLN	2.2
5	S	225	ASP	2.2
12	Z	194	ASP	2.2
6	T	201	ALA	2.1
2	P	22	TYR	2.1
3	C	241	GLN	2.1
5	S	208(B)	ASP	2.1
12	L	98	HIS	2.1
1	O	54	SER	2.1
4	R	243	ALA	2.1
3	Q	52	ARG	2.1
9	I	122(A)	LYS	2.1
3	Q	48	LEU	2.1
3	Q	224	LEU	2.1
1	A	217	ASP	2.1
5	S	197	ILE	2.1
13	M	39	ASP	2.1
4	R	61	SER	2.1
3	C	188	GLU	2.1
7	U	184(H)	GLU	2.1
2	B	202	THR	2.1
4	D	238	LYS	2.1
6	T	206	LYS	2.1
3	C	64	PRO	2.1
4	R	192	LEU	2.1
4	R	171	GLY	2.1
5	S	8	TYR	2.1
3	C	236	ILE	2.1
9	I	182	ASP	2.1
6	T	239	GLU	2.1
9	W	122(A)	LYS	2.1
4	D	14	THR	2.1
4	R	237	LEU	2.1
4	D	108	ASN	2.1
8	H	35	HIS	2.1

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Mol	Chain	Res	Type	RSRZ
2	B	60	GLU	2.0
2	P	20	ARG	2.0
4	D	61	SER	2.0
5	S	60	SER	2.0
6	F	186	ALA	2.0
3	Q	197	LEU	2.0
5	E	33	GLN	2.0
5	S	64	GLN	2.0
3	Q	45	CYS	2.0
2	P	203	ASP	2.0
3	Q	162	ALA	2.0
3	Q	49	GLY	2.0
5	E	197	ILE	2.0
5	S	184	GLY	2.0
10	J	24	ILE	2.0
5	E	127	TYR	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
15	MG	I	195	1/1	0.66	0.35	72,72,72,72	0
15	MG	L	195	1/1	0.70	0.24	66,66,66,66	0
15	MG	I	196	1/1	0.76	0.20	68,68,68,68	0
17	MES	K	214	12/12	0.85	0.22	90,90,90,90	0
15	MG	L	196	1/1	0.86	0.11	52,52,52,52	0
15	MG	F	242	1/1	0.86	0.19	74,74,74,74	0
15	MG	K	212	1/1	0.88	0.15	55,55,55,55	0

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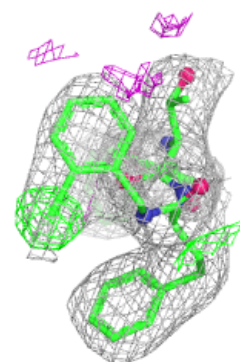
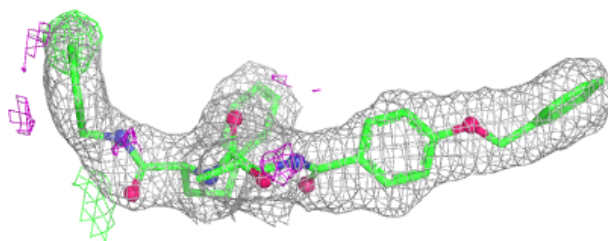
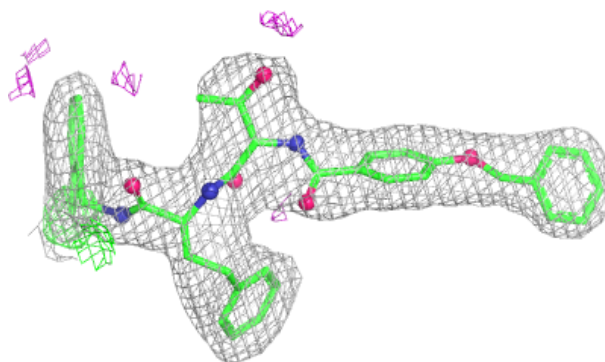
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
17	MES	Y	213	12/12	0.89	0.18	97,98,98,98	0
15	MG	G	241	1/1	0.90	0.09	54,54,54,54	0
15	MG	F	243	1/1	0.91	0.21	118,118,118,118	0
15	MG	H	224	1/1	0.92	0.08	57,57,57,57	0
16	L2T	K	213	44/44	0.93	0.10	45,47,55,55	1
16	L2T	Y	212	44/44	0.93	0.11	49,51,56,57	1
15	MG	N	188	1/1	0.94	0.09	50,50,50,50	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.

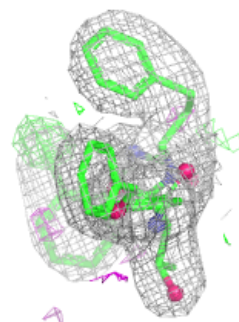
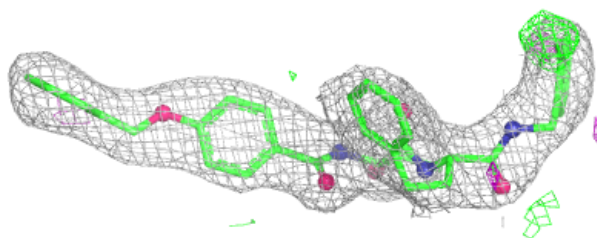
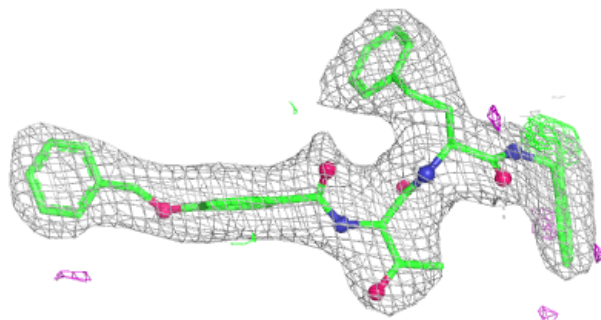
Electron density around L2T K 213:

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 L2T Y 212:

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



6.5 Other polymers ⓘ

There are no such residues in this entry.