



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 17, 2026 – 07:19 PM UTC

PDB ID : 3OEU / pdb_00003oeu
Title : Structure of yeast 20S open-gate proteasome with Compound 24
Authors : Sintchak, M.D.
Deposited on : 2010-08-13
Resolution : 2.60 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

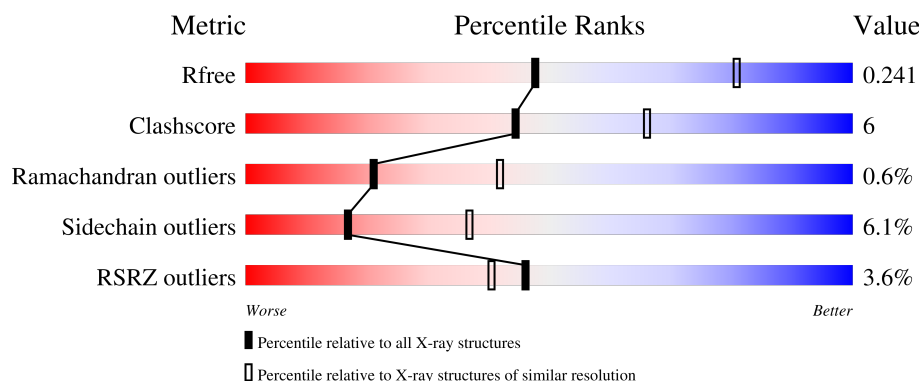
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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.



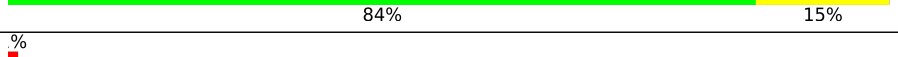
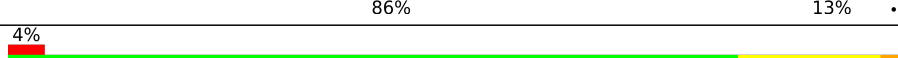
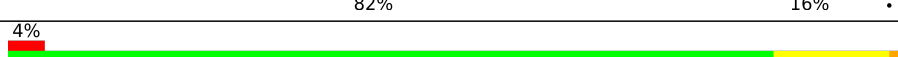
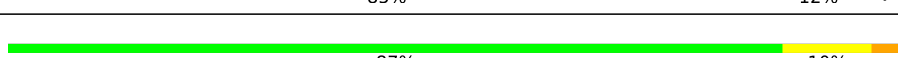
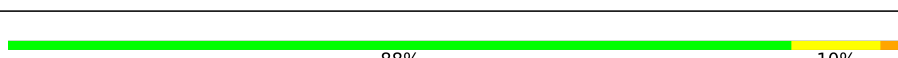
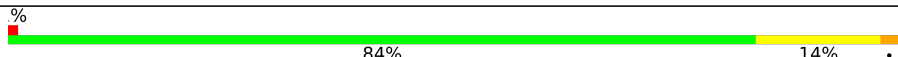
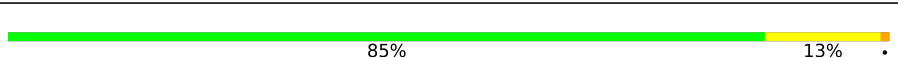
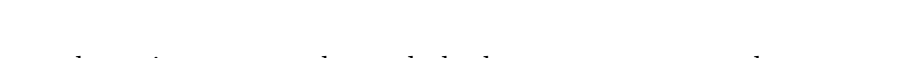
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (2.60-2.60)

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	3% 86% 13% .
1	O	250	4% 81% 16% .
2	B	235	6% 78% 19% .
2	P	235	6% 82% 16% .
3	C	241	9% 85% 15% .

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

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	242	-	-	-	X

2 Entry composition

There are 18 unique types of molecules in this entry. The entry contains 50340 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
			1861	1162	314	378	7			
4	R	236	Total	C	N	O	S	0	0	0
			1811	1134	305	365	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
			1788	1123	312	349	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
			1582	1003	269	305	5			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
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
			1511	954	250	300	7			

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

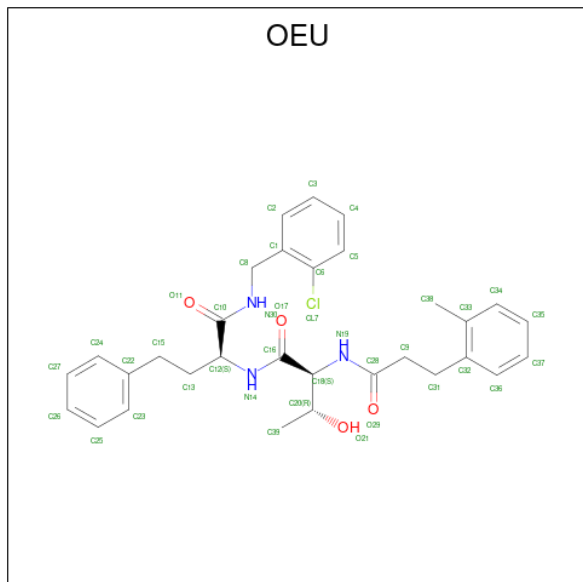
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
15	F	1	Total	Mg	0	0
			1	1		
15	G	1	Total	Mg	0	0
			1	1		

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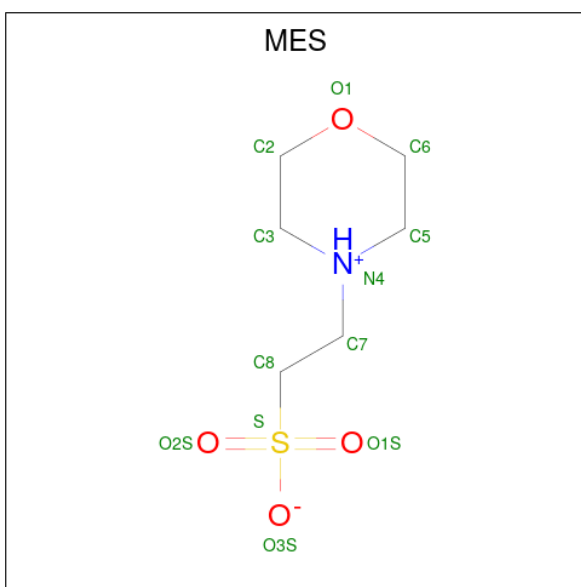
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
15	H	1	Total	Mg	0	0
			1	1		
15	I	2	Total	Mg	0	0
			2	2		
15	K	1	Total	Mg	0	0
			1	1		
15	L	2	Total	Mg	0	0
			2	2		
15	N	1	Total	Mg	0	0
			1	1		

- Molecule 16 is N-{(2S)-1-[(2-chlorobenzyl)amino]-1-oxo-4-phenylbutan-2-yl}-N 2 -[3-(2-methylphenyl)propanoyl]-L-threoninamide (CCD ID: OEU) (formula: $C_{31}H_{36}ClN_3O_4$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
16	K	1	Total 39	C 31	Cl 1	N 3	O 4	0	0
16	Y	1	Total 39	C 31	Cl 1	N 3	O 4	0	0

- Molecule 17 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (CCD ID: MES) (formula: $C_6H_{13}NO_4S$).



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	A	26	Total	O	0	0
			26	26		
18	B	31	Total	O	0	0
			31	31		
18	C	32	Total	O	0	0
			32	32		
18	D	35	Total	O	0	0
			35	35		
18	E	28	Total	O	0	0
			28	28		
18	F	32	Total	O	0	0
			32	32		
18	G	45	Total	O	0	0
			45	45		
18	H	44	Total	O	0	0
			44	44		
18	I	45	Total	O	0	0
			45	45		
18	J	40	Total	O	0	0
			40	40		

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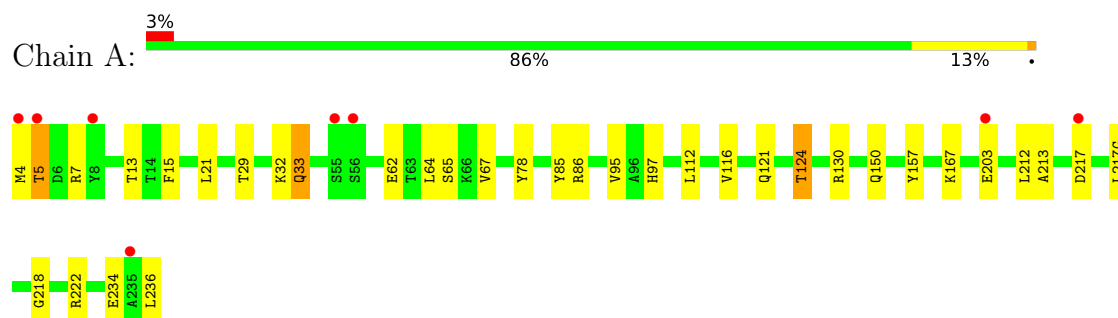
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
18	K	44	Total 44	O 44	0	0
18	L	42	Total 42	O 42	0	0
18	M	44	Total 44	O 44	0	0
18	N	38	Total 38	O 38	0	0
18	O	16	Total 16	O 16	0	0
18	P	26	Total 26	O 26	0	0
18	Q	19	Total 19	O 19	0	0
18	R	31	Total 31	O 31	0	0
18	S	22	Total 22	O 22	0	0
18	T	34	Total 34	O 34	0	0
18	U	48	Total 48	O 48	0	0
18	V	43	Total 43	O 43	0	0
18	W	39	Total 39	O 39	0	0
18	X	37	Total 37	O 37	0	0
18	Y	25	Total 25	O 25	0	0
18	Z	40	Total 40	O 40	0	0
18	1	49	Total 49	O 49	0	0
18	2	42	Total 42	O 42	0	0

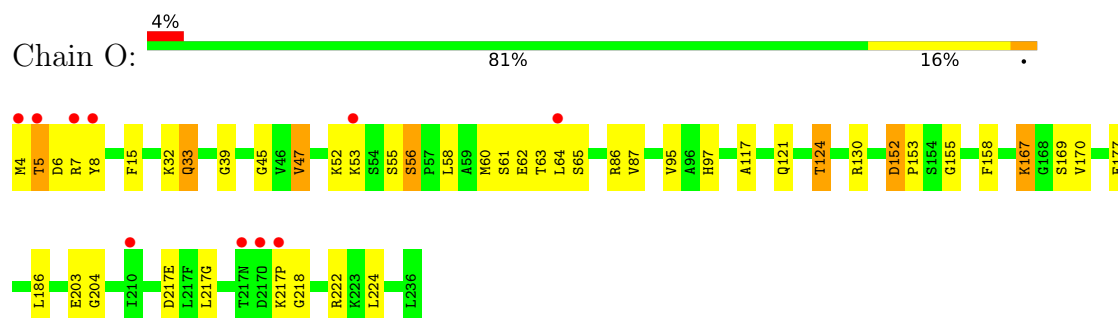
3 Residue-property plots [i](#)

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

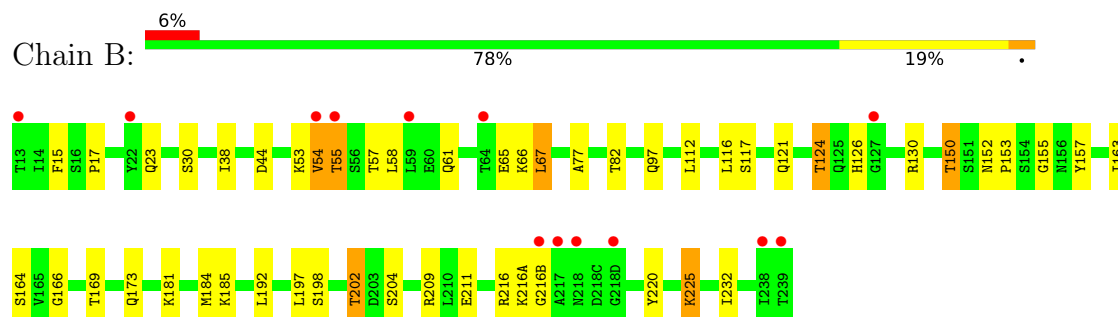
• Molecule 1: Proteasome component Y7



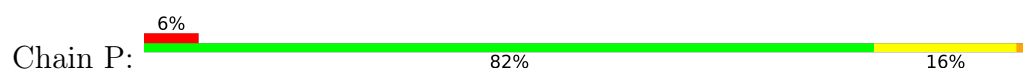
• Molecule 1: Proteasome component Y7

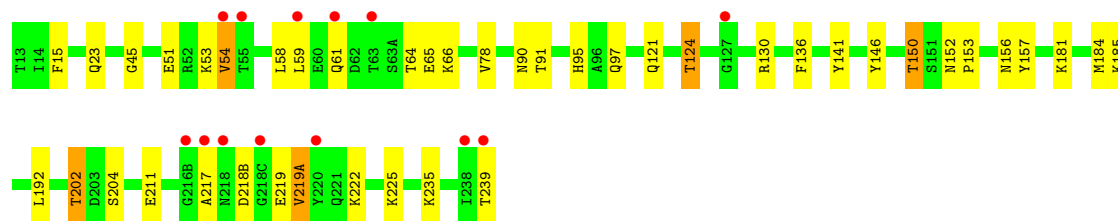


• Molecule 2: Proteasome component Y13

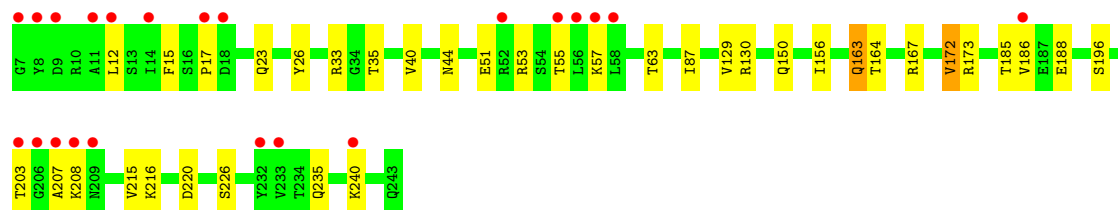
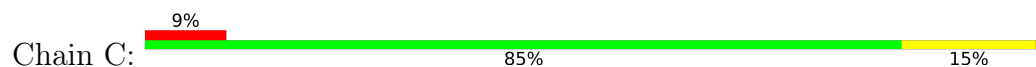


• Molecule 2: Proteasome component Y13

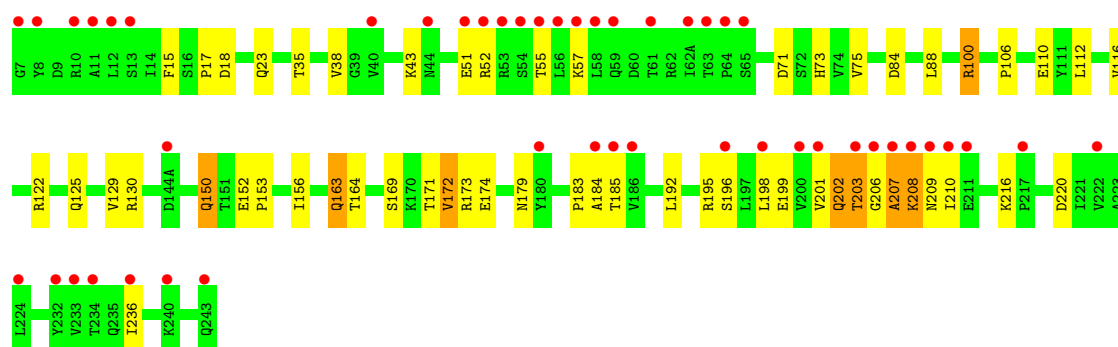
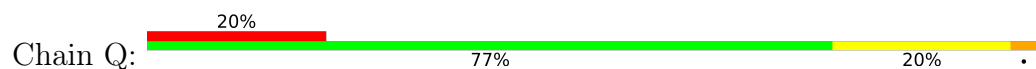




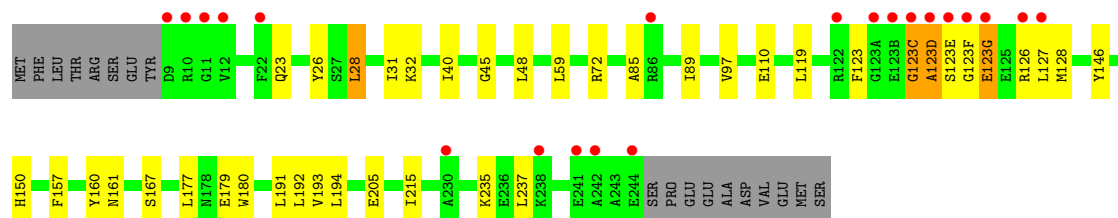
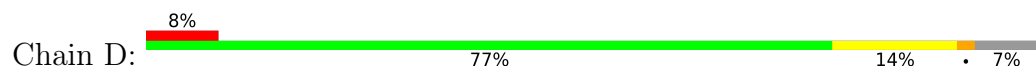
• Molecule 3: Proteasome component PRE6



• Molecule 3: Proteasome component PRE6

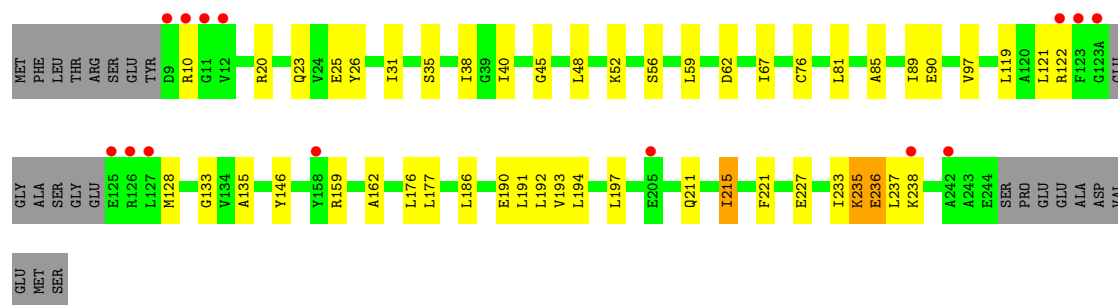


• Molecule 4: Proteasome component PUP2

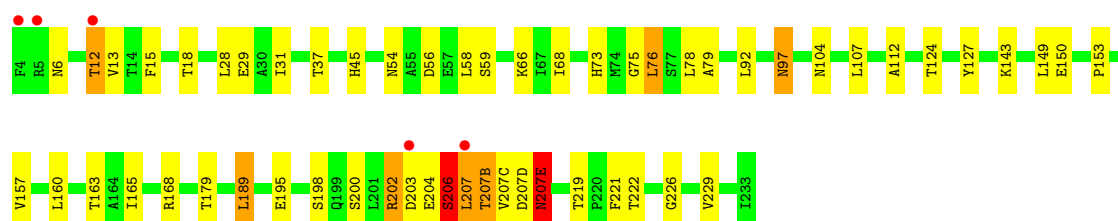
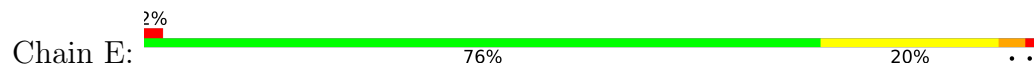


• Molecule 4: Proteasome component PUP2

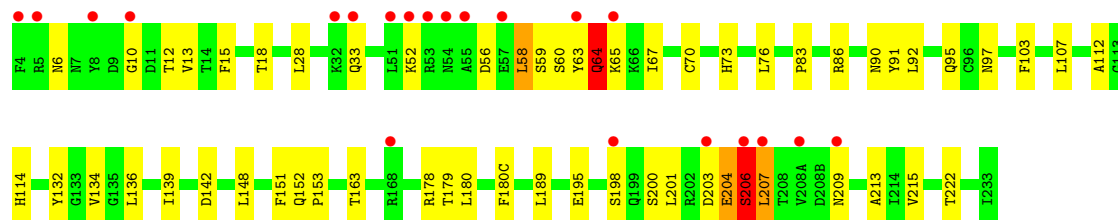




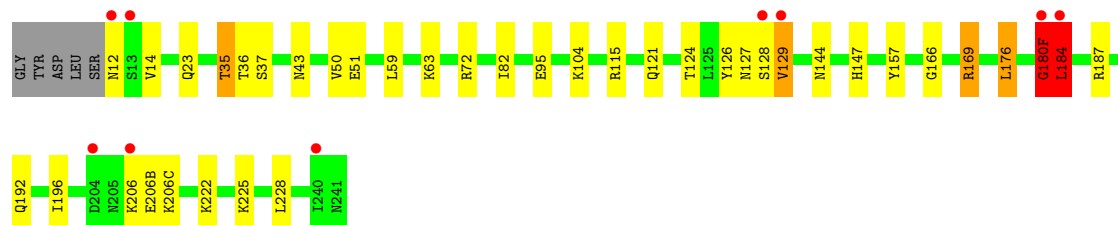
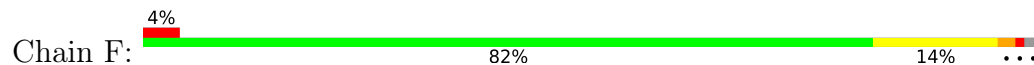
• Molecule 5: Proteasome component PRE5



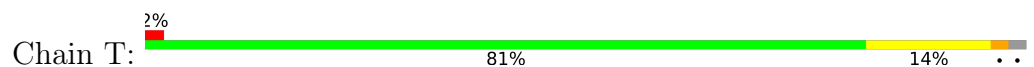
• Molecule 5: Proteasome component PRE5



• Molecule 6: Proteasome component C1

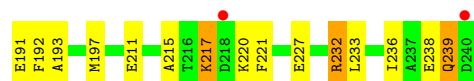
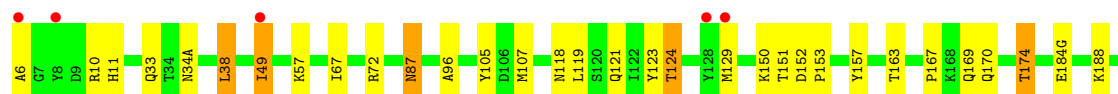
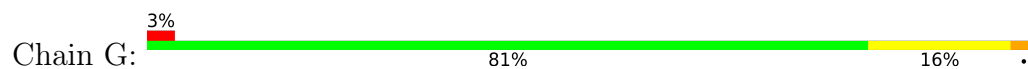


• Molecule 6: Proteasome component C1

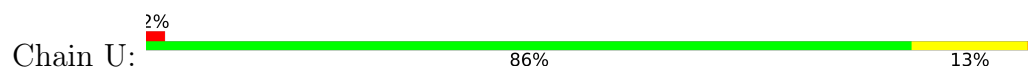




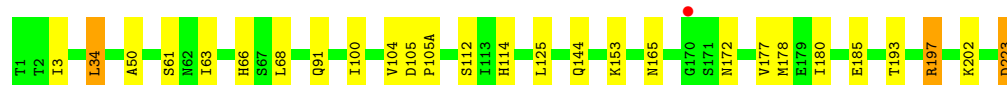
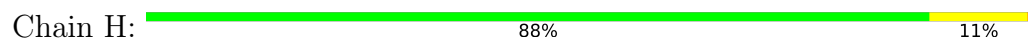
• Molecule 7: Proteasome component C7-alpha



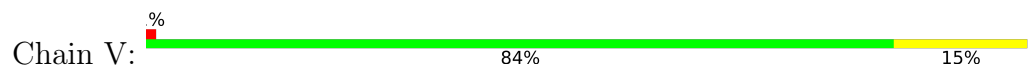
• Molecule 7: Proteasome component C7-alpha



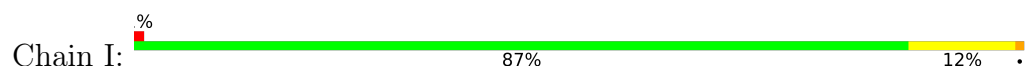
• Molecule 8: Proteasome component PUP1



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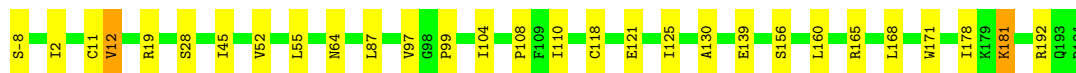


• Molecule 9: Proteasome component PUP3

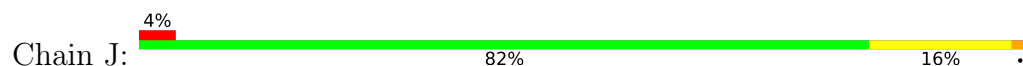




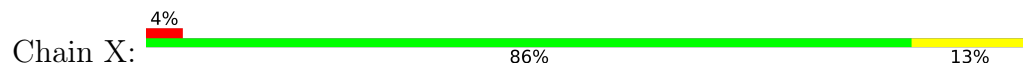
• Molecule 9: Proteasome component PUP3



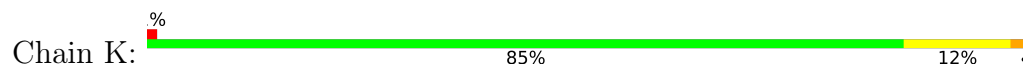
• Molecule 10: Proteasome component C11



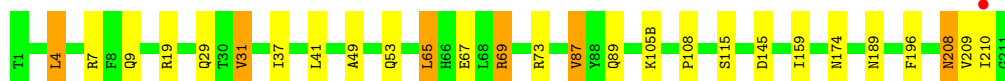
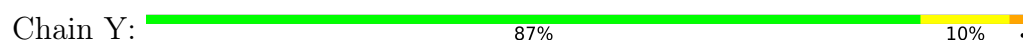
• Molecule 10: Proteasome component C11



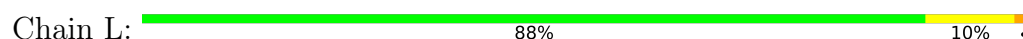
• Molecule 11: Proteasome component PRE2



• Molecule 11: Proteasome component PRE2

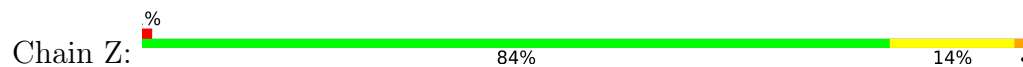


• Molecule 12: Proteasome component C5

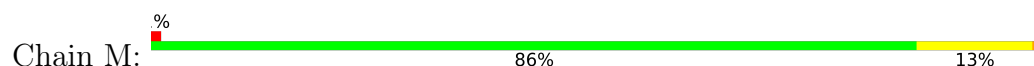




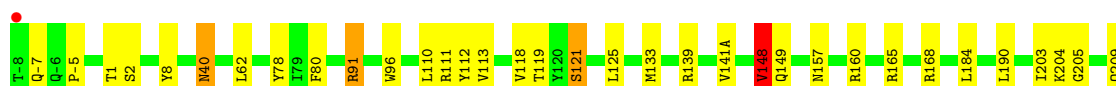
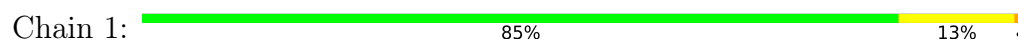
- Molecule 12: Proteasome component C5



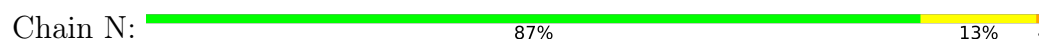
- Molecule 13: Proteasome component PRE4



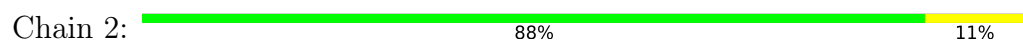
- Molecule 13: Proteasome component PRE4



- Molecule 14: Proteasome component PRE3



- Molecule 14: Proteasome component PRE3



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	136.77Å 299.67Å 145.30Å 90.00° 113.22° 90.00°	Depositor
Resolution (Å)	50.00 – 2.60 50.00 – 2.60	Depositor EDS
% Data completeness (in resolution range)	95.3 (50.00-2.60) 95.4 (50.00-2.60)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.62 (at 2.61Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.209 , 0.249 0.205 , 0.241	Depositor DCC
R_{free} test set	6321 reflections (2.02%)	wwPDB-VP
Wilson B-factor (Å ²)	52.8	Xtriage
Anisotropy	0.064	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 34.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	50340	wwPDB-VP
Average B, all atoms (Å ²)	54.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.22% 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: OEU, 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	0.51	0/1952	0.81	0/2642
1	O	0.50	0/1952	0.81	2/2642 (0.1%)
2	B	0.50	0/1858	0.83	0/2516
2	P	0.50	0/1858	0.81	0/2516
3	C	0.52	0/1920	1.06	2/2598 (0.1%)
3	Q	0.52	0/1920	0.84	1/2598 (0.0%)
4	D	0.69	2/1886 (0.1%)	0.80	0/2541
4	R	0.50	0/1835	0.82	1/2473 (0.0%)
5	E	0.57	3/1823 (0.2%)	0.80	1/2463 (0.0%)
5	S	0.63	3/1815 (0.2%)	0.82	2/2452 (0.1%)
6	F	0.68	4/1887 (0.2%)	0.85	4/2546 (0.2%)
6	T	0.51	0/1887	0.81	0/2546
7	G	0.54	0/1959	0.79	0/2652
7	U	0.53	1/1959 (0.1%)	0.82	1/2652 (0.0%)
8	H	0.55	0/1716	0.83	2/2326 (0.1%)
8	V	0.55	0/1716	0.79	0/2326
9	I	0.61	0/1611	0.82	1/2174 (0.0%)
9	W	0.62	0/1611	0.80	0/2174
10	J	0.53	0/1610	0.80	0/2170
10	X	0.53	0/1610	0.82	0/2170
11	K	0.68	2/1681 (0.1%)	0.87	5/2274 (0.2%)
11	Y	0.50	0/1681	0.80	0/2274
12	L	0.55	0/1795	0.78	0/2420
12	Z	0.56	0/1795	0.79	0/2420
13	1	0.54	0/1855	0.83	1/2514 (0.0%)
13	M	0.55	0/1855	0.80	1/2514 (0.0%)
14	2	0.66	0/1539	0.82	0/2083
14	N	0.64	0/1541	0.79	0/2087
All	All	0.57	15/50127 (0.0%)	0.82	24/67763 (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
4	D	0	1
5	E	0	1
5	S	0	1
6	F	0	1
11	K	0	1
All	All	0	5

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	123(G)	GLU	C-N	18.51	1.56	1.33
5	S	206	SER	N-CA	14.41	1.64	1.46
11	K	181	ASP	C-N	14.27	1.54	1.33
6	F	180(F)	GLY	C-N	13.54	1.52	1.33
11	K	183	GLY	N-CA	12.66	1.63	1.45
6	F	184	LEU	N-CA	8.84	1.57	1.46
5	E	206	SER	N-CA	8.17	1.56	1.46
6	F	180(F)	GLY	C-O	7.56	1.34	1.23
4	D	123(G)	GLU	C-O	7.37	1.33	1.24
6	F	82	ILE	CA-CB	6.00	1.57	1.54
7	U	82	ILE	CA-CB	5.45	1.57	1.53
5	S	204	GLU	C-O	5.28	1.29	1.23
5	E	207(E)	ASN	C-O	5.09	1.30	1.24
5	S	206	SER	CA-CB	5.08	1.62	1.53
5	E	206	SER	CA-CB	5.03	1.61	1.53

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	203	THR	O-C-N	24.53	155.22	122.59
3	C	203	THR	CA-C-O	-23.40	87.05	120.51
11	K	181	ASP	CA-C-N	-7.45	106.81	121.41
11	K	181	ASP	C-N-CA	-7.45	106.81	121.41
5	E	202	ARG	N-CA-C	-6.97	104.92	113.50
11	K	183	GLY	N-CA-C	6.85	129.42	113.18
13	M	2	SER	N-CA-C	6.53	118.73	110.24
8	H	91	GLN	N-CA-C	6.49	120.36	111.54
5	S	152	GLN	CA-C-N	6.11	125.80	119.82
5	S	152	GLN	C-N-CA	6.11	125.80	119.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	U	220	LYS	N-CA-C	6.05	118.36	108.55
8	H	180	ILE	N-CA-C	5.95	116.61	110.36
3	Q	125	GLN	N-CA-C	5.63	118.09	110.88
11	K	183	GLY	CA-C-N	-5.63	113.45	121.50
11	K	183	GLY	C-N-CA	-5.63	113.45	121.50
6	F	180(F)	GLY	CA-C-N	-5.37	111.28	121.54
6	F	180(F)	GLY	C-N-CA	-5.37	111.28	121.54
13	1	148	VAL	CB-CA-C	-5.33	105.06	112.04
1	O	152	ASP	CA-C-N	5.15	126.28	119.84
1	O	152	ASP	C-N-CA	5.15	126.28	119.84
6	F	63	LYS	N-CA-C	5.09	118.80	112.59
6	F	144	ASN	N-CA-C	5.09	116.55	110.44
4	R	236	GLU	N-CA-C	-5.07	108.84	114.62
9	I	-2	ASN	N-CA-C	5.00	119.51	113.41

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	D	123(G)	GLU	Mainchain
5	E	204	GLU	Peptide
6	F	180(F)	GLY	Mainchain
11	K	181	ASP	Peptide
5	S	204	GLU	Peptide

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	1926	24	0
1	O	1915	0	1926	30	0
2	B	1829	0	1829	35	0
2	P	1829	0	1829	25	0
3	C	1891	0	1899	19	0
3	Q	1891	0	1900	32	0
4	D	1861	0	1836	17	0
4	R	1811	0	1783	25	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	E	1795	0	1797	30	0
5	S	1788	0	1790	34	0
6	F	1848	0	1844	24	0
6	T	1848	0	1844	33	0
7	G	1921	0	1910	33	0
7	U	1921	0	1910	32	0
8	H	1685	0	1688	18	0
8	V	1685	0	1688	21	0
9	I	1581	0	1574	19	0
9	W	1581	0	1574	20	0
10	J	1582	0	1583	25	0
10	X	1582	0	1583	16	0
11	K	1644	0	1595	23	0
11	Y	1644	0	1595	18	0
12	L	1757	0	1711	16	0
12	Z	1757	0	1711	27	0
13	1	1824	0	1832	22	0
13	M	1824	0	1832	22	0
14	2	1511	0	1479	17	0
14	N	1512	0	1481	20	0
15	F	1	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	39	0	36	3	0
16	Y	39	0	36	1	0
17	K	12	0	13	0	0
17	Y	12	0	13	0	0
18	1	49	0	0	2	0
18	2	42	0	0	5	0
18	A	26	0	0	3	0
18	B	31	0	0	5	0
18	C	32	0	0	2	0
18	D	35	0	0	1	0
18	E	28	0	0	5	0
18	F	32	0	0	3	0
18	G	45	0	0	3	0
18	H	44	0	0	3	0
18	I	45	0	0	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
18	J	40	0	0	5	0
18	K	44	0	0	4	0
18	L	42	0	0	3	0
18	M	44	0	0	5	0
18	N	38	0	0	4	0
18	O	16	0	0	3	0
18	P	26	0	0	5	0
18	Q	19	0	0	1	0
18	R	31	0	0	2	0
18	S	22	0	0	1	0
18	T	34	0	0	5	0
18	U	48	0	0	2	0
18	V	43	0	0	3	0
18	W	39	0	0	3	0
18	X	37	0	0	1	0
18	Y	25	0	0	3	0
18	Z	40	0	0	5	0
All	All	50340	0	49047	586	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 6.

All (586) 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)
13:M:-7:GLN:HB3	18:M:784:HOH:O	1.41	1.18
7:U:96:ALA:HA	7:U:107:MET:HE2	1.32	1.12
7:G:96:ALA:HA	7:G:107:MET:HE2	1.32	1.10
5:E:66:LYS:HE3	18:E:600:HOH:O	1.52	1.08
6:T:192:GLN:HE22	6:T:195:LYS:HE3	1.19	1.08
5:S:209:ASN:HA	18:S:1083:HOH:O	1.56	1.04
14:N:136:GLY:HA2	14:2:161:GLN:HE21	1.24	1.00
1:A:130:ARG:HH21	7:G:124:THR:HG22	1.27	0.99
14:N:161:GLN:HE21	14:2:136:GLY:HA2	1.29	0.97
14:2:88:TYR:CG	14:2:88:TYR:CE1	2.48	0.97
7:G:96:ALA:HA	7:G:107:MET:CE	1.97	0.92
6:T:192:GLN:NE2	6:T:195:LYS:HE3	1.83	0.92
5:E:15:PHE:H	6:F:23:GLN:HE22	1.18	0.91
3:C:15:PHE:H	4:D:23:GLN:HE22	1.22	0.86
5:S:52:LYS:HB3	5:S:63:TYR:O	1.76	0.86
6:F:35:THR:HG21	6:F:51:GLU:O	1.77	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:S:97:ASN:HD21	12:Z:61:ASN:HD21	1.25	0.84
1:A:217:ASP:CB	18:A:237:HOH:O	2.25	0.84
2:B:65:GLU:HG3	2:B:66:LYS:HG3	1.60	0.84
1:A:217:ASP:HB2	18:A:237:HOH:O	1.77	0.84
1:O:86:ARG:HE	7:U:118:ASN:HD21	1.24	0.83
14:N:132:THR:HB	18:N:879:HOH:O	1.79	0.83
1:O:130:ARG:HH21	7:U:124:THR:HG22	1.42	0.83
1:O:15:PHE:H	2:P:23:GLN:HE22	1.26	0.83
5:S:207:LEU:HA	5:S:209:ASN:HD22	1.44	0.83
1:A:130:ARG:HH21	7:G:124:THR:CG2	1.92	0.82
13:1:157:ASN:HD22	13:1:160:ARG:HH11	1.26	0.81
1:O:124:THR:HG22	2:P:130:ARG:HH21	1.44	0.81
1:O:124:THR:CG2	2:P:130:ARG:HH21	1.95	0.80
7:G:38:LEU:HD23	7:G:197:MET:HE3	1.64	0.80
13:M:157:ASN:HD22	13:M:160:ARG:HH11	1.31	0.79
3:Q:15:PHE:H	4:R:23:GLN:HE22	1.31	0.79
6:F:95:GLU:HG2	6:F:115:ARG:HB3	1.64	0.78
2:P:90:ASN:HB2	18:P:409:HOH:O	1.84	0.78
7:U:96:ALA:CA	7:U:107:MET:HE2	2.14	0.77
9:I:-8:SER:HA	18:I:834:HOH:O	1.85	0.77
5:E:12:THR:HB	18:E:588:HOH:O	1.84	0.76
12:Z:4:LEU:HD11	12:Z:138:LEU:HD21	1.66	0.76
13:M:141(C):ARG:HG3	13:M:141(C):ARG:HH11	1.51	0.75
13:M:40:ASN:H	13:M:40:ASN:HD22	1.34	0.75
3:C:163:GLN:HE21	3:C:163:GLN:HA	1.52	0.74
6:T:35:THR:HG21	6:T:51:GLU:O	1.86	0.74
12:Z:166:HIS:HD2	12:Z:168:GLN:H	1.33	0.74
7:U:199:ASP:HB3	18:U:832:HOH:O	1.88	0.74
6:T:95:GLU:HG2	6:T:115:ARG:HB3	1.68	0.73
11:K:89:GLN:HG3	18:K:455:HOH:O	1.89	0.73
14:N:161:GLN:NE2	14:2:136:GLY:HA2	2.02	0.73
5:E:97:ASN:HD21	12:L:61:ASN:HD21	1.37	0.72
14:N:34:LEU:HD13	14:N:176:VAL:HG23	1.71	0.72
12:Z:40:ASN:HD21	12:Z:183:GLY:HA2	1.53	0.72
1:O:130:ARG:HH21	7:U:124:THR:CG2	2.01	0.72
7:U:96:ALA:HA	7:U:107:MET:CE	2.18	0.71
2:B:126:HIS:HB3	3:C:129:VAL:HG12	1.72	0.71
11:Y:174:ASN:HD21	11:Y:189:ASN:HD22	1.38	0.71
7:G:57:LYS:HB2	18:G:985:HOH:O	1.91	0.71
2:P:15:PHE:H	3:Q:23:GLN:HE22	1.39	0.70
14:N:146:MET:HE2	14:N:150:GLU:HB3	1.74	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:86:ARG:HE	7:G:118:ASN:HD21	1.39	0.70
14:2:146:MET:HE2	14:2:150:GLU:HB3	1.73	0.70
10:J:168:MET:HG3	18:J:224:HOH:O	1.91	0.69
4:R:121:LEU:HD21	5:S:83:PRO:HB3	1.73	0.69
10:J:90:SER:HG	10:J:95:TYR:H	1.40	0.69
11:K:31:VAL:HG11	16:K:213:OEU:C3	2.23	0.69
18:O:542:HOH:O	7:U:128:TYR:HB3	1.92	0.69
1:A:15:PHE:H	2:B:23:GLN:HE22	1.41	0.69
8:H:165:ASN:HD22	13:1:139:ARG:HH11	1.41	0.68
2:B:124:THR:HG22	3:C:130:ARG:HH21	1.56	0.68
11:K:174:ASN:HD21	11:K:189:ASN:HD22	1.40	0.68
13:M:-7:GLN:CB	18:M:784:HOH:O	2.16	0.68
5:S:73:HIS:HE1	5:S:107:LEU:O	1.75	0.68
2:B:97:GLN:HE22	9:I:64:ASN:HD22	1.39	0.68
5:E:37:THR:HB	18:E:600:HOH:O	1.93	0.67
9:I:10:ASP:HB3	9:I:181:LYS:HE2	1.76	0.67
13:M:139:ARG:HH11	8:V:165:ASN:HD22	1.39	0.67
3:Q:163:GLN:HE21	3:Q:163:GLN:HA	1.60	0.67
13:1:168:ARG:HD3	18:1:490:HOH:O	1.95	0.67
11:Y:208:ASN:H	11:Y:208:ASN:HD22	1.41	0.66
9:I:181:LYS:H	9:I:181:LYS:HD2	1.60	0.66
12:L:166:HIS:HD2	12:L:168:GLN:H	1.41	0.66
7:U:87:ASN:C	7:U:87:ASN:HD22	2.03	0.66
14:2:34:LEU:HD13	14:2:176:VAL:HG23	1.77	0.66
1:A:86:ARG:HE	7:G:118:ASN:ND2	1.93	0.66
6:F:95:GLU:HG3	6:F:115:ARG:HH11	1.60	0.65
3:Q:201:VAL:O	3:Q:202:GLN:HB2	1.96	0.65
4:D:97:VAL:HG21	11:K:65:LEU:HD13	1.79	0.65
8:V:80:LEU:HD12	8:V:113:ILE:HD11	1.77	0.65
1:A:124:THR:HG22	2:B:130:ARG:HH21	1.59	0.65
3:C:163:GLN:HE22	3:C:173:ARG:HE	1.41	0.65
5:S:15:PHE:H	6:T:23:GLN:HE22	1.43	0.65
1:O:86:ARG:HE	7:U:118:ASN:ND2	1.92	0.65
11:K:208:ASN:HB3	18:W:817:HOH:O	1.95	0.65
12:Z:4:LEU:CD1	12:Z:138:LEU:HD21	2.27	0.64
12:Z:-7:ASN:HD22	12:Z:-6:PRO:HD2	1.62	0.64
6:F:35:THR:CG2	6:F:51:GLU:O	2.44	0.64
7:U:121:GLN:O	7:U:124:THR:HB	1.97	0.64
12:Z:34:VAL:HG12	12:Z:176:LEU:HD22	1.79	0.64
2:B:54:VAL:HG22	2:B:209:ARG:HH12	1.63	0.64
5:E:73:HIS:HE1	5:E:107:LEU:O	1.80	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:T:179:LEU:HD11	6:T:192:GLN:HG3	1.80	0.63
2:B:38:ILE:HD12	2:B:197:LEU:HG	1.79	0.63
12:L:14:LEU:HD13	12:L:34:VAL:HG13	1.80	0.63
10:J:2:ILE:HD13	10:J:162:LEU:HD13	1.81	0.63
10:X:146:MET:HE2	10:X:150:GLU:HB3	1.80	0.63
10:J:12:VAL:HG23	10:J:108:PRO:HB2	1.80	0.62
11:K:210:ILE:HB	18:W:395:HOH:O	1.99	0.62
2:B:67:LEU:HD22	2:B:211:GLU:HB3	1.81	0.62
7:G:238:GLU:O	7:G:239:GLN:HB2	1.97	0.62
11:Y:174:ASN:ND2	11:Y:189:ASN:HD22	1.97	0.62
1:A:7:ARG:HD2	5:E:127:TYR:CD2	2.35	0.62
8:H:50:ALA:HB2	9:I:118:CYS:HB2	1.82	0.62
6:F:12:ASN:OD1	6:F:124:THR:HA	2.00	0.61
7:G:67:ILE:HD12	7:G:211:GLU:HG2	1.82	0.61
14:N:136:GLY:HA2	14:2:161:GLN:NE2	2.06	0.61
6:T:20:ARG:HH21	6:T:25:GLU:HG2	1.65	0.61
11:Y:196:PHE:HZ	11:Y:209:VAL:HG21	1.65	0.61
11:K:4:LEU:HD13	11:K:159:ILE:HD11	1.83	0.61
2:P:97:GLN:HE22	9:W:64:ASN:HD22	1.49	0.61
11:Y:89:GLN:HG3	18:Y:860:HOH:O	2.01	0.61
2:P:121:GLN:O	2:P:124:THR:HB	2.00	0.61
7:U:184(G):GLU:HG2	7:U:188:LYS:CB	2.31	0.61
10:J:105(B):LYS:HB2	18:J:797:HOH:O	2.00	0.60
6:T:12:ASN:C	6:T:14:VAL:H	2.09	0.60
4:R:38:ILE:HD12	4:R:197:LEU:HG	1.82	0.60
5:S:180:LEU:HA	5:S:180(C):PHE:CE2	2.36	0.60
13:1:8:TYR:CE2	13:1:148:VAL:HG13	2.36	0.60
5:E:12:THR:HG21	5:E:124:THR:HA	1.82	0.60
1:A:130:ARG:NH2	7:G:124:THR:HG22	2.08	0.60
1:A:217:ASP:HB3	18:A:237:HOH:O	1.96	0.60
7:U:184(G):GLU:HG2	7:U:188:LYS:HB3	1.83	0.60
4:D:40:ILE:HD12	4:D:193:VAL:HG23	1.83	0.60
7:G:170:GLN:HE21	7:G:174:THR:HG23	1.67	0.60
12:L:4:LEU:HD13	12:L:138:LEU:HD21	1.83	0.60
1:O:86:ARG:HH21	7:U:118:ASN:HD22	1.47	0.60
18:U:369:HOH:O	8:V:66:HIS:HD2	1.85	0.59
2:P:202:THR:HG22	2:P:204:SER:H	1.67	0.59
4:D:72:ARG:HG3	18:D:593:HOH:O	2.03	0.59
4:D:123(C):GLY:HA2	4:D:126:ARG:H	1.68	0.59
13:1:133:MET:HE1	13:1:165:ARG:HG3	1.83	0.59
1:O:55:SER:O	1:O:56:SER:HB3	2.01	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:124:THR:CG2	3:C:130:ARG:HH21	2.16	0.59
6:F:180(F):GLY:O	6:F:184:LEU:HB2	2.03	0.59
11:K:200:LYS:HE3	18:K:1048:HOH:O	2.03	0.59
6:F:147:HIS:HD2	18:F:441:HOH:O	1.85	0.58
4:R:81:LEU:HD12	4:R:133:GLY:HA3	1.85	0.58
1:A:124:THR:CG2	2:B:130:ARG:HH21	2.16	0.58
1:O:7:ARG:HG2	6:T:128:SER:HB3	1.85	0.58
1:O:65:SER:HA	18:O:757:HOH:O	2.04	0.58
3:Q:100:ARG:HH11	3:Q:106:PRO:HG3	1.67	0.58
14:2:176:VAL:HG12	14:2:178:LEU:HD13	1.84	0.58
4:D:179:GLU:HB3	4:D:192:LEU:HD21	1.85	0.58
7:G:96:ALA:CA	7:G:107:MET:CE	2.79	0.58
1:A:86:ARG:HH21	7:G:118:ASN:HD22	1.52	0.58
1:O:45:GLY:HA3	1:O:186:LEU:HD13	1.85	0.58
12:Z:166:HIS:HE1	18:Z:315:HOH:O	1.86	0.58
5:E:207:LEU:HD23	5:E:207:LEU:H	1.69	0.58
1:O:121:GLN:O	1:O:124:THR:HB	2.04	0.58
4:R:227:GLU:H	4:R:227:GLU:CD	2.12	0.58
6:F:180(F):GLY:O	6:F:184:LEU:CB	2.52	0.58
3:Q:206:GLY:HA2	3:Q:210:ILE:HD12	1.85	0.58
6:T:95:GLU:HG3	6:T:115:ARG:HH11	1.68	0.58
11:K:31:VAL:HG11	16:K:213:OEU:H3	1.85	0.57
12:L:185:ARG:HG2	18:L:759:HOH:O	2.02	0.57
1:A:7:ARG:HG2	6:F:128:SER:HB3	1.86	0.57
5:S:134:VAL:O	5:S:153:PRO:HG3	2.04	0.57
2:B:181:LYS:O	2:B:184:MET:HG3	2.04	0.57
8:H:105:ASP:HB2	8:H:105(A):PRO:HD2	1.86	0.57
13:M:40:ASN:HD22	13:M:40:ASN:N	1.98	0.57
6:T:35:THR:CG2	6:T:51:GLU:O	2.51	0.57
7:G:87:ASN:C	7:G:87:ASN:HD22	2.13	0.57
10:J:34:THR:HG21	10:J:176:LYS:NZ	2.19	0.56
8:V:105:ASP:HB2	8:V:105(A):PRO:CD	2.34	0.56
12:Z:98:HIS:HB3	18:Z:218:HOH:O	2.03	0.56
12:L:166:HIS:HE1	18:L:943:HOH:O	1.87	0.56
4:R:40:ILE:HD12	4:R:193:VAL:HG23	1.86	0.56
8:H:202:LYS:HE3	12:Z:150:GLU:OE2	2.05	0.56
12:L:4:LEU:CD1	12:L:138:LEU:HD21	2.36	0.56
1:O:60:MET:HE3	1:O:63:THR:HG21	1.87	0.56
7:U:152:ASP:HB2	7:U:153:PRO:CD	2.36	0.56
4:R:233:ILE:C	4:R:236:GLU:H	2.14	0.56
7:U:191:GLU:HG3	7:U:232:ARG:HG3	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:-7:ASN:HD22	12:L:-6:PRO:HD2	1.71	0.56
11:K:73:ARG:HD3	18:K:731:HOH:O	2.06	0.56
8:H:114:HIS:HB3	18:H:582:HOH:O	2.06	0.55
6:F:166:GLY:O	6:F:169:ARG:HB3	2.06	0.55
1:O:130:ARG:NH2	7:U:124:THR:HG22	2.16	0.55
2:P:181:LYS:O	2:P:184:MET:HG3	2.07	0.55
2:B:152:ASN:HB2	2:B:153:PRO:HD2	1.88	0.55
5:S:92:LEU:HD11	5:S:112:ALA:HB1	1.87	0.55
10:J:146:MET:HE2	10:J:150:GLU:HB3	1.89	0.55
13:1:157:ASN:HD22	13:1:160:ARG:NH1	2.02	0.55
6:T:176:LEU:HB3	7:U:58:LEU:HD21	1.88	0.55
6:T:186:ALA:O	6:T:190:VAL:HG23	2.07	0.55
2:P:65:GLU:HG3	2:P:66:LYS:HG3	1.89	0.55
3:Q:122:ARG:HD2	18:Q:264:HOH:O	2.07	0.55
14:N:14:LEU:HD11	14:N:102:ALA:HB3	1.89	0.54
7:G:191:GLU:HG3	7:G:232:ARG:HG3	1.89	0.54
9:I:-8:SER:CA	18:I:834:HOH:O	2.51	0.54
11:Y:7:ARG:HD2	11:Y:108:PRO:O	2.07	0.54
2:B:152:ASN:HB2	2:B:153:PRO:CD	2.38	0.54
2:B:166:GLY:O	2:B:169:THR:HG23	2.08	0.54
7:U:87:ASN:C	7:U:87:ASN:ND2	2.63	0.54
2:P:124:THR:HG22	3:Q:130:ARG:HH21	1.73	0.54
5:S:142:ASP:HB2	18:1:616:HOH:O	2.08	0.54
2:B:225:LYS:HE2	18:B:1006:HOH:O	2.07	0.53
3:C:216:LYS:HB2	3:C:220:ASP:HB3	1.90	0.53
12:Z:-6:PRO:O	13:1:91:ARG:NH1	2.33	0.53
11:K:174:ASN:ND2	11:K:189:ASN:HD22	2.05	0.53
1:O:5:THR:HG22	1:O:6:ASP:H	1.73	0.53
2:P:64:THR:HB	18:P:356:HOH:O	2.09	0.53
5:E:54:ASN:ND2	5:E:56:ASP:O	2.42	0.53
3:Q:43:LYS:HB2	3:Q:184:ALA:HA	1.90	0.53
5:S:97:ASN:HD21	12:Z:61:ASN:ND2	2.03	0.53
6:T:114:ASP:O	6:T:118:GLN:HG2	2.09	0.53
8:V:53:GLU:HB2	18:V:878:HOH:O	2.08	0.53
1:O:32:LYS:HE2	1:O:32:LYS:HA	1.91	0.53
13:1:112:TYR:O	13:1:119:THR:HA	2.09	0.53
5:E:168:ARG:HD3	5:E:202:ARG:HE	1.72	0.53
8:H:3:ILE:HG13	8:H:100:ILE:HD12	1.91	0.53
3:C:53:ARG:HG3	3:C:167:ARG:HH12	1.73	0.53
5:E:56:ASP:HB2	18:E:1129:HOH:O	2.08	0.52
9:I:28:SER:HB2	10:J:120:VAL:HG21	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Q:84:ASP:CG	3:Q:130:ARG:HH22	2.17	0.52
1:A:150:GLN:O	1:A:157:TYR:HA	2.10	0.52
13:M:140:LYS:HD2	18:M:1084:HOH:O	2.10	0.52
6:T:187:ARG:HB2	18:T:980:HOH:O	2.08	0.52
13:1:80:PHE:CZ	13:1:111:ARG:HG2	2.44	0.52
5:E:207(B):THR:H	5:E:207(E):ASN:HD22	1.57	0.52
2:B:112:LEU:HD23	2:B:112:LEU:C	2.35	0.52
2:B:121:GLN:O	2:B:124:THR:HB	2.10	0.52
11:K:99:THR:HB	11:K:113:VAL:O	2.09	0.52
6:T:126:TYR:HB2	6:T:129:VAL:HG22	1.90	0.52
13:1:110:LEU:HG	13:1:125:LEU:HD12	1.92	0.52
2:B:15:PHE:H	3:C:23:GLN:HE22	1.56	0.52
5:S:132:TYR:O	5:S:153:PRO:HB3	2.09	0.52
10:J:24:ILE:HG22	18:J:681:HOH:O	2.10	0.52
1:O:7:ARG:CG	6:T:128:SER:HB3	2.40	0.52
12:Z:-9:GLN:HE21	12:Z:-8:PHE:N	2.07	0.52
1:O:217(P):LYS:N	1:O:217(P):LYS:HE3	2.25	0.51
6:T:207:ASP:HB3	18:T:794:HOH:O	2.09	0.51
11:Y:208:ASN:H	11:Y:208:ASN:ND2	2.08	0.51
8:V:172:ASN:HB3	8:V:192:LEU:O	2.11	0.51
7:G:121:GLN:O	7:G:124:THR:HB	2.11	0.51
8:V:172:ASN:HD22	8:V:193:THR:HA	1.75	0.51
8:H:197:ARG:HD2	18:H:788:HOH:O	2.10	0.51
11:K:12:ILE:HB	11:K:178:VAL:HB	1.93	0.51
4:R:45:GLY:HA2	4:R:146:TYR:CE1	2.45	0.51
9:W:2:ILE:HG21	9:W:130:ALA:HB3	1.93	0.51
7:G:227:GLU:HG2	18:G:387:HOH:O	2.11	0.51
8:H:172:ASN:HD22	8:H:193:THR:HA	1.75	0.51
6:T:147:HIS:HD2	18:T:686:HOH:O	1.92	0.51
13:1:8:TYR:CZ	13:1:148:VAL:HG13	2.45	0.51
4:R:67:ILE:HD12	4:R:211:GLN:HE21	1.76	0.51
11:Y:4:LEU:HD13	11:Y:159:ILE:HD11	1.93	0.51
13:M:-7:GLN:CG	18:M:784:HOH:O	2.53	0.51
5:S:139:ILE:HD12	5:S:215:VAL:HG12	1.93	0.51
1:A:121:GLN:O	1:A:124:THR:HB	2.11	0.50
10:J:24:ILE:HG12	10:J:24:ILE:O	2.10	0.50
10:J:146:MET:HE1	10:J:154:LEU:HD13	1.94	0.50
14:N:132:THR:CB	18:N:879:HOH:O	2.49	0.50
3:Q:52:ARG:HB2	3:Q:209:ASN:HD22	1.76	0.50
5:S:86:ARG:O	5:S:90:ASN:HB2	2.10	0.50
5:S:207:LEU:HA	5:S:209:ASN:ND2	2.20	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:W:12:VAL:HG23	9:W:178:ILE:HB	1.92	0.50
1:O:217(G):LEU:HD13	1:O:218:GLY:HA2	1.92	0.50
1:A:97:HIS:HD2	8:H:61:SER:OG	1.94	0.50
2:B:202:THR:HG22	2:B:204:SER:H	1.77	0.50
3:C:163:GLN:HE21	3:C:163:GLN:CA	2.20	0.50
4:D:160:TYR:CE2	5:E:59:SER:HB3	2.47	0.50
8:V:84:LYS:HE2	8:V:119:THR:HG23	1.93	0.50
13:1:-7:GLN:HB2	18:2:270:HOH:O	2.12	0.50
10:J:89:LYS:HD3	18:J:997:HOH:O	2.11	0.50
14:N:55:ILE:HD11	14:N:95:LEU:HD13	1.94	0.50
5:E:104:ASN:HB2	13:M:81:GLU:HG2	1.93	0.50
5:S:63:TYR:O	5:S:64:GLN:O	2.30	0.50
3:C:186:VAL:HG21	3:C:216:LYS:HE2	1.93	0.50
13:1:1:THR:HG23	13:1:2:SER:N	2.26	0.50
2:B:97:GLN:NE2	9:I:64:ASN:HD22	2.10	0.50
5:S:97:ASN:ND2	12:Z:61:ASN:HD21	2.03	0.50
10:J:167:PRO:HB3	10:X:21:THR:HG21	1.93	0.50
13:1:141(A):VAL:HG23	13:1:141(A):VAL:O	2.12	0.50
9:I:99:PRO:HD2	9:I:113:PHE:HB2	1.94	0.49
5:E:31:ILE:HD11	5:E:153:PRO:CD	2.42	0.49
4:R:186:LEU:O	4:R:190:GLU:HG3	2.11	0.49
5:S:207:LEU:HD23	5:S:207:LEU:H	1.77	0.49
4:R:122:ARG:HD2	18:R:394:HOH:O	2.13	0.49
10:X:34:THR:HG21	10:X:176:LYS:NZ	2.28	0.49
3:C:163:GLN:NE2	3:C:164:THR:H	2.11	0.49
14:N:67:THR:HA	14:N:72:GLY:O	2.12	0.49
6:T:192:GLN:HE22	6:T:195:LYS:CE	2.07	0.49
5:E:92:LEU:HD11	5:E:112:ALA:HB1	1.95	0.49
10:X:146:MET:CE	10:X:150:GLU:HB3	2.43	0.49
3:Q:172:VAL:HG23	3:Q:196:SER:HB2	1.95	0.49
4:R:159:ARG:HB3	5:S:60:SER:HB3	1.94	0.49
18:T:1170:HOH:O	7:U:29:LYS:HE2	2.13	0.49
7:G:105:TYR:OH	8:H:66:HIS:HE1	1.95	0.49
8:H:223:ASP:N	8:H:223:ASP:OD2	2.46	0.49
4:R:56:SER:HB2	18:R:619:HOH:O	2.12	0.49
4:R:67:ILE:HG22	4:R:221:PHE:HZ	1.77	0.49
9:I:2:ILE:HG21	9:I:130:ALA:HB3	1.95	0.49
2:B:216(B):GLY:HA2	2:B:220:TYR:HB2	1.95	0.48
5:E:160:LEU:HD23	6:F:59:LEU:HA	1.95	0.48
11:K:179:THR:O	11:K:183:GLY:HA3	2.13	0.48
2:P:78:VAL:HG22	2:P:136:PHE:HE2	1.78	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:T:126:TYR:HE1	7:U:129:MET:SD	2.36	0.48
8:V:105:ASP:HB2	8:V:105(A):PRO:HD2	1.94	0.48
5:E:15:PHE:H	6:F:23:GLN:NE2	1.99	0.48
13:1:205:GLY:HA3	13:1:209:GLN:HB3	1.95	0.48
5:S:56:ASP:HB3	5:S:58:LEU:H	1.78	0.48
16:K:213:OEU:H35	12:L:94:PRO:HG2	1.95	0.48
13:M:157:ASN:HD22	13:M:160:ARG:NH1	2.05	0.48
10:X:24:ILE:HA	18:X:893:HOH:O	2.14	0.48
7:G:170:GLN:NE2	7:G:174:THR:HG23	2.26	0.48
7:G:220:LYS:HE3	18:G:810:HOH:O	2.12	0.48
3:C:188:GLU:HG2	18:C:909:HOH:O	2.13	0.48
13:M:84:ALA:HA	13:M:113:VAL:HG21	1.96	0.48
3:Q:195:ARG:HG3	3:Q:236:ILE:HD13	1.96	0.48
13:1:40:ASN:H	13:1:40:ASN:HD22	1.62	0.48
8:H:177:VAL:HB	8:H:185:GLU:HG3	1.96	0.48
10:J:34:THR:HG21	10:J:176:LYS:HZ3	1.77	0.48
14:2:38:HIS:HD2	18:2:293:HOH:O	1.95	0.48
7:G:151:THR:HG22	7:G:157:TYR:HB3	1.94	0.48
6:T:43:ASN:HD22	6:T:44:ASP:N	2.12	0.48
4:R:162:ALA:HB1	4:R:176:LEU:HD22	1.96	0.47
2:P:152:ASN:HB2	2:P:153:PRO:CD	2.45	0.47
4:R:31:ILE:HD13	4:R:135:ALA:HB2	1.95	0.47
5:S:148:LEU:HD21	5:S:163:THR:HG22	1.96	0.47
8:V:50:ALA:HB2	9:W:118:CYS:HB2	1.96	0.47
3:Q:171:THR:O	3:Q:174:GLU:HB3	2.13	0.47
6:T:169:ARG:HD2	18:T:1108:HOH:O	2.14	0.47
6:F:104:LYS:HE3	18:F:720:HOH:O	2.14	0.47
14:N:14:LEU:HD23	14:N:44:CYS:SG	2.54	0.47
14:N:161:GLN:HE22	14:N:165:TRP:HE1	1.61	0.47
2:P:95:HIS:CE1	18:P:314:HOH:O	2.66	0.47
2:P:239:THR:HG21	18:P:680:HOH:O	2.14	0.47
3:Q:201:VAL:O	3:Q:202:GLN:CB	2.62	0.47
5:E:45:HIS:HB2	5:E:189:LEU:HD12	1.97	0.47
13:M:19:LEU:HD21	13:M:26:LEU:HD22	1.96	0.47
9:W:110:ILE:HD12	9:W:125:ILE:HG12	1.97	0.47
11:Y:19:ARG:HH21	11:Y:29:GLN:HE22	1.62	0.47
12:L:8:GLY:HA3	12:L:11:PHE:CE2	2.50	0.47
14:N:176:VAL:HG12	14:N:178:LEU:HD13	1.97	0.47
4:R:215:ILE:HG22	4:R:221:PHE:HD2	1.79	0.47
7:U:184(G):GLU:HG2	7:U:188:LYS:HB2	1.97	0.47
8:V:202:LYS:HD3	18:V:826:HOH:O	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:135:MET:HE2	9:W:165:ARG:NH2	2.29	0.47
3:Q:163:GLN:HE22	3:Q:173:ARG:HE	1.62	0.47
11:Y:67:GLU:HG3	18:Y:472:HOH:O	2.14	0.47
5:E:143:LYS:HE3	13:M:78:TYR:OH	2.15	0.47
5:E:226:GLY:O	5:E:229:VAL:HG22	2.15	0.47
9:I:28:SER:CB	10:J:120:VAL:HG21	2.45	0.47
2:P:97:GLN:NE2	9:W:64:ASN:HD22	2.12	0.47
5:S:63:TYR:O	5:S:64:GLN:C	2.57	0.47
12:Z:-7:ASN:HD22	12:Z:-6:PRO:CD	2.26	0.47
2:B:17:PRO:HA	3:C:26:TYR:CD1	2.50	0.47
5:E:29:GLU:HG3	18:E:868:HOH:O	2.15	0.47
9:I:12:VAL:HG13	9:I:108:PRO:HB3	1.96	0.47
9:W:55:LEU:HD11	9:W:97:VAL:HG21	1.97	0.47
4:D:85:ALA:O	4:D:89:ILE:HG12	2.15	0.46
12:Z:-9:GLN:HE21	12:Z:-8:PHE:H	1.60	0.46
2:B:44:ASP:OD2	2:B:44:ASP:N	2.48	0.46
3:C:35:THR:HB	3:C:51:GLU:HG3	1.97	0.46
12:L:139:ASP:O	12:L:144(A):LYS:HG3	2.15	0.46
12:L:141:GLN:HB3	12:L:154:LEU:HD21	1.97	0.46
12:Z:113:PHE:CD2	12:Z:119:TYR:HB3	2.50	0.46
13:1:113:VAL:HA	13:1:118:VAL:O	2.16	0.46
11:K:6:PHE:HA	11:K:123:ASP:O	2.14	0.46
13:M:94:PRO:HD2	18:M:784:HOH:O	2.14	0.46
6:T:95:GLU:HG2	6:T:115:ARG:CB	2.42	0.46
1:A:112:LEU:O	1:A:116:VAL:HG23	2.15	0.46
9:I:20:LEU:HB3	9:I:28:SER:HB3	1.97	0.46
2:P:78:VAL:HG22	2:P:136:PHE:CE2	2.50	0.46
9:W:192:ARG:HD2	18:W:379:HOH:O	2.16	0.46
12:L:99:THR:HG23	18:L:213:HOH:O	2.15	0.46
4:R:97:VAL:HG21	11:Y:65:LEU:HD13	1.97	0.46
4:R:122:ARG:O	4:R:128:MET:HB3	2.15	0.46
2:B:216:ARG:HB3	2:B:216(A):LYS:H	1.50	0.46
6:F:176:LEU:HD13	6:F:196:ILE:HD13	1.98	0.46
18:N:879:HOH:O	14:2:132:THR:HB	2.15	0.46
6:T:12:ASN:ND2	6:T:126:TYR:O	2.48	0.46
11:Y:49:ALA:O	11:Y:53:GLN:HB2	2.16	0.46
8:V:101:VAL:HG13	8:V:111:PHE:HB2	1.97	0.46
4:D:45:GLY:HA2	4:D:146:TYR:CE1	2.52	0.45
9:W:181:LYS:H	9:W:181:LYS:HD2	1.81	0.45
1:A:7:ARG:CG	6:F:128:SER:HB3	2.46	0.45
3:Q:216:LYS:HB2	3:Q:220:ASP:HB3	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:V:114:HIS:HB3	18:V:224:HOH:O	2.15	0.45
1:O:32:LYS:NZ	1:O:169:SER:OG	2.50	0.45
4:D:28:LEU:HA	4:D:31:ILE:HD12	1.97	0.45
2:P:45:GLY:HA2	2:P:146:TYR:CE1	2.50	0.45
11:Y:196:PHE:CZ	11:Y:209:VAL:HG21	2.50	0.45
4:D:123:PHE:HA	4:D:128:MET:HB3	1.99	0.45
7:G:152:ASP:HB2	7:G:153:PRO:CD	2.47	0.45
8:H:105:ASP:HB2	8:H:105(A):PRO:CD	2.46	0.45
6:T:38:ILE:HG12	6:T:197:ILE:HD11	1.98	0.45
12:Z:-2:ASN:HA	12:Z:21:ILE:O	2.17	0.45
9:I:-8:SER:N	18:I:368:HOH:O	2.49	0.45
5:S:198:SER:HA	5:S:201:LEU:HD12	1.98	0.45
1:A:67:VAL:HG11	1:A:213:ALA:CB	2.46	0.45
7:G:6:ALA:HB1	7:G:10:ARG:HG3	1.98	0.45
1:O:86:ARG:HH21	7:U:118:ASN:ND2	2.13	0.45
1:O:217(E):ASP:HB3	18:O:1009:HOH:O	2.16	0.45
7:U:96:ALA:CA	7:U:107:MET:CE	2.89	0.45
11:Y:105(B):LYS:HG3	18:Y:302:HOH:O	2.17	0.45
5:S:198:SER:C	5:S:200:SER:H	2.25	0.45
13:1:111:ARG:HH11	13:1:121:SER:HB2	1.82	0.45
2:B:53:LYS:HE2	18:B:546:HOH:O	2.17	0.44
14:N:149:GLU:HG3	18:N:652:HOH:O	2.17	0.44
14:N:8:PHE:HB2	14:N:146:MET:O	2.17	0.44
3:Q:71:ASP:HB3	3:Q:73:HIS:CE1	2.52	0.44
9:W:28:SER:CB	10:X:120:VAL:HG21	2.47	0.44
12:Z:1:GLY:HA3	12:Z:46:ASN:HD21	1.81	0.44
12:Z:14:LEU:HD13	12:Z:34:VAL:HG13	1.99	0.44
8:H:197:ARG:HG3	12:Z:164:GLU:CD	2.42	0.44
1:O:97:HIS:HD2	8:V:61:SER:OG	2.01	0.44
3:Q:203:THR:C	3:Q:207:ALA:H	2.26	0.44
11:K:37:ILE:HG23	11:K:60:GLY:HA2	2.00	0.44
11:Y:87:VAL:CG1	11:Y:115:SER:HA	2.48	0.44
2:B:150:THR:O	2:B:157:TYR:HA	2.18	0.44
4:D:161:ASN:HB3	4:D:180:TRP:CE2	2.52	0.44
10:J:141:HIS:HB3	10:J:154:LEU:HD11	1.99	0.44
13:M:133:MET:HE1	13:M:165:ARG:HG3	2.00	0.44
5:S:114:HIS:HB3	6:T:86:ARG:NH2	2.32	0.44
7:U:107:MET:CE	7:U:112:LEU:HD13	2.48	0.44
10:X:113:ILE:HG12	10:X:119:LYS:HG3	1.99	0.44
3:Q:163:GLN:HE21	3:Q:163:GLN:CA	2.30	0.44
6:T:206:LYS:HE3	6:T:206:LYS:HB2	1.70	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:X:2:ILE:HD13	10:X:170:PHE:CG	2.53	0.44
14:2:55:ILE:HD11	14:2:95:LEU:HD13	2.00	0.44
6:F:127:ASN:HB3	18:F:816:HOH:O	2.17	0.44
3:Q:17:PRO:HA	4:R:26:TYR:CD1	2.52	0.44
9:W:87:LEU:HD11	9:W:99:PRO:HG2	2.00	0.44
2:B:116:LEU:HD23	2:B:116:LEU:HA	1.79	0.44
7:G:192:PHE:CD1	7:G:192:PHE:C	2.95	0.44
10:J:21:THR:HG21	10:X:167:PRO:HB3	2.00	0.44
4:R:10:ARG:HD2	5:S:10:GLY:HA2	2.00	0.44
7:U:107:MET:HE3	7:U:112:LEU:HB2	2.00	0.44
8:V:197:ARG:NH1	8:V:200:LYS:HD3	2.33	0.44
8:V:211:THR:HG21	9:W:156:SER:HB3	1.99	0.44
4:D:150:HIS:O	4:D:157:PHE:HA	2.17	0.44
8:H:104:VAL:HG13	8:H:178:MET:HB3	1.99	0.44
8:H:112:SER:HB3	8:H:125:LEU:HD13	1.99	0.44
10:J:21:THR:O	10:J:22:ARG:HD3	2.18	0.44
6:T:206:LYS:C	6:T:206(B):LYS:H	2.25	0.44
9:I:174:VAL:HG21	9:I:186:LYS:HE2	2.00	0.43
12:Z:113:PHE:HA	12:Z:118:SER:O	2.17	0.43
9:I:48:LEU:HG	9:I:50:THR:HG22	2.00	0.43
3:Q:195:ARG:HA	3:Q:198:LEU:HD12	2.00	0.43
4:R:235:LYS:O	4:R:235:LYS:HG2	2.17	0.43
6:T:192:GLN:NE2	6:T:195:LYS:CE	2.71	0.43
3:Q:169:SER:HA	3:Q:172:VAL:HG13	2.00	0.43
5:S:91:TYR:O	5:S:95:GLN:HG2	2.18	0.43
11:K:211:GLY:HA3	8:V:214:LEU:HD13	2.00	0.43
8:V:197:ARG:HH21	9:W:139:GLU:HG3	1.84	0.43
13:M:1:THR:HG23	13:M:2:SER:N	2.33	0.43
2:P:150:THR:O	2:P:157:TYR:HA	2.19	0.43
3:Q:57:LYS:HD2	3:Q:57:LYS:HA	1.89	0.43
6:T:126:TYR:CE1	7:U:129:MET:SD	3.12	0.43
7:U:170:GLN:HE21	7:U:174:THR:HG23	1.84	0.43
6:F:12:ASN:C	6:F:14:VAL:H	2.26	0.43
11:K:4:LEU:CD1	11:K:159:ILE:HD11	2.48	0.43
1:O:58:LEU:HD12	7:U:173:THR:HG23	2.01	0.43
14:N:32:ASP:OD1	14:N:186:ARG:NH2	2.51	0.43
5:E:198:SER:C	5:E:200:SER:H	2.27	0.43
11:K:86:LEU:C	11:K:86:LEU:HD13	2.44	0.43
13:M:122:SER:HB3	13:M:124:THR:O	2.18	0.43
3:Q:88:LEU:HD22	3:Q:116:VAL:HG13	2.01	0.43
2:B:55:THR:HG21	18:B:263:HOH:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:97:VAL:HG11	11:K:65:LEU:HD22	2.01	0.43
6:F:95:GLU:HG2	6:F:115:ARG:CB	2.43	0.43
13:M:40:ASN:N	13:M:40:ASN:ND2	2.66	0.42
2:P:141:TYR:CD1	2:P:219(A):VAL:HG21	2.54	0.42
6:T:179:LEU:HD11	6:T:192:GLN:CG	2.46	0.42
12:Z:120:GLU:HG3	18:Z:688:HOH:O	2.18	0.42
14:2:149:GLU:HG3	18:2:280:HOH:O	2.18	0.42
2:B:169:THR:O	2:B:173:GLN:HB2	2.19	0.42
5:E:68:ILE:HB	5:E:76:LEU:CD2	2.49	0.42
5:E:75:GLY:HA3	5:E:221:PHE:CE2	2.54	0.42
7:G:215:ALA:HB2	7:G:221:PHE:HD2	1.84	0.42
12:L:137:PHE:CE1	12:L:141:GLN:HG3	2.55	0.42
2:P:53:LYS:O	2:P:54:VAL:C	2.61	0.42
3:Q:163:GLN:HG3	3:Q:164:THR:N	2.35	0.42
13:1:-7:GLN:CB	18:2:270:HOH:O	2.66	0.42
2:B:163:ILE:HG13	2:B:164:SER:N	2.35	0.42
3:C:172:VAL:HG23	3:C:196:SER:HB2	2.00	0.42
13:M:112:TYR:HE1	13:M:127:THR:HG22	1.84	0.42
9:W:28:SER:HB2	10:X:120:VAL:HG21	1.99	0.42
10:X:2:ILE:HD11	10:X:168:MET:CE	2.49	0.42
10:X:7:ARG:HG2	10:X:7:ARG:HH11	1.85	0.42
11:Y:31:VAL:HG11	16:Y:212:OEU:C3	2.49	0.42
2:B:53:LYS:O	2:B:55:THR:HG23	2.19	0.42
3:C:17:PRO:HA	4:D:26:TYR:CD1	2.54	0.42
3:Q:100:ARG:NH1	3:Q:106:PRO:HG3	2.32	0.42
7:U:152:ASP:HB2	7:U:153:PRO:HD2	2.00	0.42
8:H:34:LEU:HB2	18:H:803:HOH:O	2.19	0.42
1:O:152:ASP:HB3	1:O:153:PRO:HD2	2.02	0.42
3:Q:179:ASN:HB3	3:Q:192:LEU:HD11	2.01	0.42
8:V:84:LYS:HE2	8:V:119:THR:CG2	2.49	0.42
7:G:184(G):GLU:HG2	7:G:188:LYS:HB3	2.02	0.42
10:J:10:ASP:HB2	18:J:698:HOH:O	2.19	0.42
10:J:113:ILE:HA	10:J:118:THR:O	2.20	0.42
10:X:6:ILE:HD11	10:X:142:TYR:CD1	2.54	0.42
5:E:150:GLU:O	5:E:157:VAL:HA	2.20	0.42
4:D:123(D):ALA:O	4:D:123(F):GLY:N	2.53	0.42
7:G:123:TYR:CE1	7:G:129:MET:HE3	2.55	0.42
11:K:196:PHE:HZ	11:K:209:VAL:HG21	1.85	0.42
13:1:-5:PRO:HD3	13:1:96:TRP:CE2	2.54	0.42
3:C:12:LEU:HB2	18:C:615:HOH:O	2.20	0.41
6:F:37:SER:HB3	6:F:50:VAL:HG23	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:6:ILE:HD11	10:J:8:VAL:HG13	2.00	0.41
1:O:33:GLN:H	1:O:33:GLN:HG2	1.67	0.41
9:W:19:ARG:HD3	9:W:168:LEU:O	2.20	0.41
2:B:66:LYS:O	2:B:77:ALA:HA	2.19	0.41
7:G:49:ILE:HD13	7:G:193:ALA:HB3	2.00	0.41
1:O:39:GLY:HA2	1:O:47:VAL:O	2.20	0.41
18:B:769:HOH:O	3:C:57:LYS:HB3	2.21	0.41
7:G:87:ASN:C	7:G:87:ASN:ND2	2.73	0.41
9:I:51:ASP:OD2	10:J:90(B):ARG:NH2	2.53	0.41
11:K:37:ILE:HB	11:K:41:LEU:HB3	2.02	0.41
3:Q:152:GLU:HB2	3:Q:153:PRO:HD2	2.01	0.41
8:V:172:ASN:ND2	8:V:193:THR:HA	2.35	0.41
14:2:45:ARG:HB2	18:2:889:HOH:O	2.19	0.41
14:2:112:THR:HG22	14:2:120:HIS:HB2	2.02	0.41
13:M:197:TRP:CH2	14:2:171:GLY:HA2	2.55	0.41
14:N:161:GLN:NE2	14:N:165:TRP:HE1	2.17	0.41
3:Q:208:LYS:HD2	3:Q:208:LYS:O	2.20	0.41
5:S:52:LYS:HD2	5:S:63:TYR:O	2.21	0.41
5:S:136:LEU:HB2	5:S:151:PHE:HB3	2.02	0.41
6:T:12:ASN:C	6:T:14:VAL:N	2.75	0.41
12:Z:84:GLN:HG3	12:Z:117:GLY:O	2.20	0.41
14:2:175:MET:HB2	14:2:187:LEU:HB2	2.03	0.41
1:A:217(G):LEU:HD13	1:A:218:GLY:HA2	2.02	0.41
6:F:187:ARG:HD2	6:F:228:LEU:HD11	2.02	0.41
2:P:66:LYS:HB2	2:P:211:GLU:OE1	2.21	0.41
9:W:11:CYS:HA	9:W:104:ILE:HD11	2.03	0.41
10:X:90:SER:HG	10:X:95:TYR:H	1.69	0.41
13:1:157:ASN:ND2	13:1:160:ARG:HH11	2.06	0.41
1:A:29:THR:O	1:A:33:GLN:HG2	2.20	0.41
6:F:126:TYR:HB2	6:F:129:VAL:CG2	2.50	0.41
11:K:143:LYS:HD3	18:K:969:HOH:O	2.20	0.41
2:P:152:ASN:HB2	2:P:153:PRO:HD2	2.02	0.41
9:W:45:ILE:HG22	9:W:52:VAL:HG22	2.02	0.41
6:F:121:GLN:HE21	6:F:121:GLN:HB3	1.72	0.41
14:N:146:MET:CE	14:N:150:GLU:HB3	2.46	0.41
1:O:117:ALA:HB1	1:O:155:GLY:O	2.20	0.41
12:Z:185:ARG:HG2	18:Z:417:HOH:O	2.20	0.41
14:2:4:MET:HB3	14:2:126:ILE:HG22	2.02	0.41
10:J:138:LEU:O	10:J:142:TYR:HB3	2.20	0.41
14:N:14:LEU:O	14:N:175:MET:HA	2.21	0.41
9:W:12:VAL:HG13	9:W:108:PRO:HB3	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:13:THR:HG22	1:A:21:LEU:HD22	2.03	0.41
1:A:78:TYR:HB3	1:A:85:TYR:CD1	2.55	0.41
5:E:79:ALA:HB3	5:E:165:ILE:HD12	2.03	0.41
6:F:157:TYR:CD1	6:F:157:TYR:C	2.98	0.41
9:I:87:LEU:HD11	9:I:99:PRO:HG2	2.03	0.41
12:L:9:GLU:O	12:L:107:LYS:HA	2.20	0.41
1:O:52:LYS:HD2	1:O:61:SER:HB2	2.02	0.41
3:Q:150:GLN:HE21	3:Q:150:GLN:HB3	1.69	0.41
4:R:85:ALA:O	4:R:89:ILE:HG12	2.21	0.41
5:S:179:THR:O	5:S:179:THR:HG22	2.21	0.41
9:W:55:LEU:CD1	9:W:97:VAL:HG21	2.51	0.41
12:Z:122:GLU:OE1	12:Z:125:ARG:NH2	2.53	0.41
5:E:160:LEU:HD13	5:E:163:THR:HB	2.02	0.41
5:S:70:CYS:SG	5:S:92:LEU:HD23	2.61	0.41
5:S:103:PHE:O	13:I:78:TYR:HA	2.21	0.41
10:X:2:ILE:HD11	10:X:168:MET:HE1	2.03	0.41
4:D:32:LYS:O	4:D:167:SER:HA	2.20	0.40
7:G:10:ARG:HB2	7:G:11:HIS:HD2	1.86	0.40
10:J:2:ILE:HD12	10:J:170:PHE:CD2	2.56	0.40
10:J:24:ILE:CD1	10:X:129:TYR:HB3	2.50	0.40
2:P:222:LYS:HE2	18:P:1150:HOH:O	2.20	0.40
5:S:67:ILE:HG21	5:S:213:ALA:HB2	2.02	0.40
11:Y:37:ILE:HB	11:Y:41:LEU:HB3	2.03	0.40
5:E:207(B):THR:H	5:E:207(E):ASN:HB2	1.85	0.40
4:R:90:GLU:OE1	11:Y:69:ARG:HD2	2.21	0.40
12:Z:49:ALA:HA	18:Z:776:HOH:O	2.21	0.40
2:B:117:SER:HB3	2:B:155:GLY:O	2.22	0.40
7:G:34(A):ASN:HD22	7:G:167:PRO:HG2	1.85	0.40
13:M:205:GLY:HA3	13:M:209:GLN:HB3	2.02	0.40
7:U:65:SER:OG	7:U:211:GLU:OE2	2.38	0.40
7:U:184(G):GLU:CG	7:U:188:LYS:HB2	2.51	0.40
8:H:197:ARG:HH21	9:I:139:GLU:HG3	1.87	0.40
3:Q:35:THR:HB	3:Q:51:GLU:HG3	2.03	0.40
2:B:54:VAL:HG23	18:B:546:HOH:O	2.21	0.40
7:G:150:LYS:O	7:G:157:TYR:HA	2.21	0.40
4:R:20:ARG:HD3	4:R:25:GLU:CD	2.46	0.40
8:V:3:ILE:HG22	8:V:16:ALA:HB2	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	248/250 (99%)	240 (97%)	6 (2%)	2 (1%)	16	34
1	O	248/250 (99%)	234 (94%)	9 (4%)	5 (2%)	6	12
2	B	233/235 (99%)	221 (95%)	11 (5%)	1 (0%)	30	51
2	P	233/235 (99%)	222 (95%)	8 (3%)	3 (1%)	9	21
3	C	239/241 (99%)	231 (97%)	7 (3%)	1 (0%)	30	51
3	Q	239/241 (99%)	228 (95%)	7 (3%)	4 (2%)	7	15
4	D	240/260 (92%)	226 (94%)	11 (5%)	3 (1%)	9	21
4	R	232/260 (89%)	220 (95%)	11 (5%)	1 (0%)	30	51
5	E	231/233 (99%)	217 (94%)	11 (5%)	3 (1%)	9	21
5	S	231/233 (99%)	211 (91%)	16 (7%)	4 (2%)	7	15
6	F	235/242 (97%)	224 (95%)	10 (4%)	1 (0%)	30	51
6	T	235/242 (97%)	226 (96%)	9 (4%)	0	100	100
7	G	241/243 (99%)	234 (97%)	5 (2%)	2 (1%)	16	34
7	U	241/243 (99%)	236 (98%)	3 (1%)	2 (1%)	16	34
8	H	220/222 (99%)	212 (96%)	8 (4%)	0	100	100
8	V	220/222 (99%)	211 (96%)	8 (4%)	1 (0%)	24	46
9	I	202/204 (99%)	196 (97%)	6 (3%)	0	100	100
9	W	202/204 (99%)	196 (97%)	6 (3%)	0	100	100
10	J	196/198 (99%)	192 (98%)	3 (2%)	1 (0%)	24	46
10	X	196/198 (99%)	189 (96%)	3 (2%)	4 (2%)	6	12
11	K	210/212 (99%)	204 (97%)	5 (2%)	1 (0%)	24	46
11	Y	210/212 (99%)	205 (98%)	5 (2%)	0	100	100
12	L	220/222 (99%)	215 (98%)	5 (2%)	0	100	100
12	Z	220/222 (99%)	216 (98%)	4 (2%)	0	100	100
13	1	231/233 (99%)	225 (97%)	6 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
13	M	231/233 (99%)	222 (96%)	8 (4%)	1 (0%)	30	51
14	2	194/196 (99%)	188 (97%)	6 (3%)	0	100	100
14	N	194/196 (99%)	189 (97%)	5 (3%)	0	100	100
All	All	6272/6382 (98%)	6030 (96%)	202 (3%)	40 (1%)	21	42

All (40) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	D	123(E)	SER
5	E	206	SER
6	F	184	LEU
7	G	239	GLN
13	M	-7	GLN
2	P	54	VAL
3	Q	202	GLN
5	S	64	GLN
10	X	189	ASP
1	A	167	LYS
3	C	207	ALA
5	E	6	ASN
5	E	203	ASP
1	O	8	TYR
2	P	217	ALA
2	P	218(B)	ASP
3	Q	208	LYS
5	S	6	ASN
5	S	203	ASP
1	A	5	THR
4	D	123(D)	ALA
4	R	235	LYS
5	S	206	SER
10	X	188	ASP
7	G	217	LYS
1	O	53	LYS
3	Q	183	PRO
3	Q	207	ALA
8	V	171	SER
11	K	9	GLN
1	O	56	SER
7	U	239	GLN
10	X	8	VAL

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Mol	Chain	Res	Type
2	B	54	VAL
1	O	167	LYS
7	U	55	PRO
10	X	187	VAL
4	D	123(C)	GLY
10	J	8	VAL
1	O	204	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	209/209 (100%)	195 (93%)	14 (7%)	15	33
1	O	209/209 (100%)	193 (92%)	16 (8%)	12	27
2	B	195/195 (100%)	180 (92%)	15 (8%)	12	27
2	P	195/195 (100%)	180 (92%)	15 (8%)	12	27
3	C	213/213 (100%)	197 (92%)	16 (8%)	12	28
3	Q	213/213 (100%)	198 (93%)	15 (7%)	14	31
4	D	198/215 (92%)	185 (93%)	13 (7%)	15	34
4	R	192/215 (89%)	178 (93%)	14 (7%)	13	29
5	E	192/192 (100%)	172 (90%)	20 (10%)	7	14
5	S	191/192 (100%)	175 (92%)	16 (8%)	10	23
6	F	196/200 (98%)	183 (93%)	13 (7%)	15	34
6	T	196/200 (98%)	180 (92%)	16 (8%)	10	24
7	G	207/207 (100%)	193 (93%)	14 (7%)	14	32
7	U	207/207 (100%)	196 (95%)	11 (5%)	20	43
8	H	181/181 (100%)	174 (96%)	7 (4%)	28	55
8	V	181/181 (100%)	170 (94%)	11 (6%)	17	37
9	I	172/172 (100%)	164 (95%)	8 (5%)	23	48
9	W	172/172 (100%)	166 (96%)	6 (4%)	32	59

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
10	J	174/175 (99%)	164 (94%)	10 (6%)	18	40
10	X	174/175 (99%)	167 (96%)	7 (4%)	28	55
11	K	169/169 (100%)	160 (95%)	9 (5%)	20	43
11	Y	169/169 (100%)	159 (94%)	10 (6%)	18	38
12	L	185/185 (100%)	176 (95%)	9 (5%)	22	47
12	Z	185/185 (100%)	177 (96%)	8 (4%)	26	51
13	1	199/199 (100%)	188 (94%)	11 (6%)	19	41
13	M	199/199 (100%)	190 (96%)	9 (4%)	24	50
14	2	161/162 (99%)	157 (98%)	4 (2%)	42	69
14	N	162/162 (100%)	156 (96%)	6 (4%)	30	57
All	All	5296/5348 (99%)	4973 (94%)	323 (6%)	17	37

All (323) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	MET
1	A	5	THR
1	A	32	LYS
1	A	33	GLN
1	A	62	GLU
1	A	64	LEU
1	A	65	SER
1	A	95	VAL
1	A	124	THR
1	A	203	GLU
1	A	212	LEU
1	A	222	ARG
1	A	234	GLU
1	A	236	LEU
2	B	30	SER
2	B	55	THR
2	B	57	THR
2	B	58	LEU
2	B	61	GLN
2	B	67	LEU
2	B	82	THR
2	B	124	THR
2	B	150	THR

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Mol	Chain	Res	Type
2	B	185	LYS
2	B	192	LEU
2	B	198	SER
2	B	202	THR
2	B	225	LYS
2	B	232	ILE
3	C	33	ARG
3	C	40	VAL
3	C	44	ASN
3	C	55	THR
3	C	63	THR
3	C	87	ILE
3	C	150	GLN
3	C	156	ILE
3	C	163	GLN
3	C	172	VAL
3	C	185	THR
3	C	208	LYS
3	C	215	VAL
3	C	226	SER
3	C	235	GLN
3	C	240	LYS
4	D	28	LEU
4	D	48	LEU
4	D	59	LEU
4	D	110	GLU
4	D	119	LEU
4	D	127	LEU
4	D	177	LEU
4	D	191	LEU
4	D	194	LEU
4	D	205	GLU
4	D	215	ILE
4	D	235	LYS
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	76	LEU
5	E	78	LEU

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Mol	Chain	Res	Type
5	E	97	ASN
5	E	149	LEU
5	E	179	THR
5	E	189	LEU
5	E	195	GLU
5	E	206	SER
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	72	ARG
6	F	129	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
6	F	225	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	163	THR
7	G	169	GLN
7	G	174	THR
7	G	217	LYS
7	G	232	ARG
7	G	233	LEU
7	G	236	ILE
8	H	34	LEU
8	H	63	ILE

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Mol	Chain	Res	Type
8	H	68	LEU
8	H	144	GLN
8	H	153	LYS
8	H	197	ARG
8	H	223	ASP
9	I	4	VAL
9	I	9	LYS
9	I	121	GLU
9	I	160	LEU
9	I	171	TRP
9	I	174	VAL
9	I	181	LYS
9	I	182	ASP
10	J	6	ILE
10	J	9	GLN
10	J	24	ILE
10	J	34	THR
10	J	35	ARG
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	181	ASP
12	L	-9	GLN
12	L	14	LEU
12	L	25	SER
12	L	40	ASN
12	L	58	ARG
12	L	62	SER
12	L	99	THR
12	L	135	MET
12	L	138	LEU
13	M	-8	THR

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Mol	Chain	Res	Type
13	M	40	ASN
13	M	62	LEU
13	M	91	ARG
13	M	148	VAL
13	M	184	LEU
13	M	190	LEU
13	M	204	LYS
13	M	211	ILE
14	N	89	GLU
14	N	94	ASN
14	N	107	LYS
14	N	115	LEU
14	N	119	VAL
14	N	178	LEU
1	O	4	MET
1	O	5	THR
1	O	33	GLN
1	O	47	VAL
1	O	62	GLU
1	O	64	LEU
1	O	87	VAL
1	O	95	VAL
1	O	124	THR
1	O	158	PHE
1	O	167	LYS
1	O	170	VAL
1	O	177	GLU
1	O	203	GLU
1	O	222	ARG
1	O	224	LEU
2	P	51	GLU
2	P	58	LEU
2	P	59	LEU
2	P	61	GLN
2	P	91	THR
2	P	124	THR
2	P	150	THR
2	P	156	ASN
2	P	185	LYS
2	P	192	LEU
2	P	202	THR
2	P	219	GLU

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Mol	Chain	Res	Type
2	P	219(A)	VAL
2	P	225	LYS
2	P	235	LYS
3	Q	18	ASP
3	Q	38	VAL
3	Q	55	THR
3	Q	75	VAL
3	Q	100	ARG
3	Q	110	GLU
3	Q	112	LEU
3	Q	129	VAL
3	Q	150	GLN
3	Q	156	ILE
3	Q	163	GLN
3	Q	172	VAL
3	Q	185	THR
3	Q	199	GLU
3	Q	203	THR
4	R	35	SER
4	R	48	LEU
4	R	52	LYS
4	R	59	LEU
4	R	62	ASP
4	R	76	CYS
4	R	119	LEU
4	R	177	LEU
4	R	191	LEU
4	R	192	LEU
4	R	194	LEU
4	R	215	ILE
4	R	237	LEU
4	R	238	LYS
5	S	12	THR
5	S	13	VAL
5	S	18	THR
5	S	28	LEU
5	S	33	GLN
5	S	58	LEU
5	S	59	SER
5	S	64	GLN
5	S	65	LYS
5	S	76	LEU

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Mol	Chain	Res	Type
5	S	178	ARG
5	S	189	LEU
5	S	195	GLU
5	S	206	SER
5	S	207	LEU
5	S	222	THR
6	T	35	THR
6	T	36	THR
6	T	43	ASN
6	T	59	LEU
6	T	63	LYS
6	T	72	ARG
6	T	95	GLU
6	T	98	SER
6	T	121	GLN
6	T	127	ASN
6	T	169	ARG
6	T	176	LEU
6	T	187	ARG
6	T	205	ASN
6	T	222	LYS
6	T	225	LYS
7	U	18	GLU
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	227	GLU
7	U	232	ARG
7	U	233	LEU
8	V	13	VAL
8	V	34	LEU
8	V	55	VAL
8	V	63	ILE
8	V	68	LEU
8	V	101	VAL
8	V	121	VAL
8	V	144	GLN
8	V	149	GLU

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Mol	Chain	Res	Type
8	V	153	LYS
8	V	222	CYS
9	W	-8	SER
9	W	12	VAL
9	W	121	GLU
9	W	160	LEU
9	W	171	TRP
9	W	181	LYS
10	X	34	THR
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	65	LEU
11	Y	69	ARG
11	Y	73	ARG
11	Y	87	VAL
11	Y	145	ASP
11	Y	208	ASN
11	Y	210	ILE
12	Z	-9	GLN
12	Z	2	THR
12	Z	14	LEU
12	Z	40	ASN
12	Z	99	THR
12	Z	106	GLU
12	Z	106(A)	ASP
12	Z	138	LEU
13	1	40	ASN
13	1	62	LEU
13	1	91	ARG
13	1	121	SER
13	1	148	VAL
13	1	149	GLN
13	1	184	LEU
13	1	190	LEU
13	1	203	ILE

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Mol	Chain	Res	Type
13	1	204	LYS
13	1	211	ILE
14	2	22	THR
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 (196) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	97	HIS
1	A	150	GLN
1	A	191	HIS
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	173	GLN
2	B	218	ASN
2	B	227	GLN
3	C	23	GLN
3	C	44	ASN
3	C	120	GLN
3	C	125	GLN
3	C	150	GLN
3	C	163	GLN
3	C	168	ASN
3	C	209	ASN
4	D	23	GLN
4	D	108	ASN
4	D	147	GLN
4	D	150	HIS
4	D	161	ASN
4	D	180(C)	HIS
4	D	226	ASN
5	E	7	ASN
5	E	64	GLN
5	E	73	HIS
5	E	97	ASN
5	E	104	ASN

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Mol	Chain	Res	Type
5	E	121	GLN
5	E	125	GLN
5	E	152	GLN
5	E	156	ASN
5	E	170	GLN
5	E	185	ASN
5	E	207(E)	ASN
6	F	23	GLN
6	F	43	ASN
6	F	90	ASN
6	F	121	GLN
6	F	147	HIS
6	F	205	ASN
6	F	237	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
7	G	178	ASN
8	H	22	GLN
8	H	30	ASN
8	H	66	HIS
8	H	86	HIS
8	H	144	GLN
8	H	165	ASN
8	H	172	ASN
8	H	190	ASN
8	H	201	GLN
9	I	23	GLN
9	I	29	ASN
9	I	157	GLN
10	J	9	GLN
10	J	54	GLN
10	J	62	ASN
10	J	85	GLN
10	J	112	GLN
10	J	186	GLN
11	K	9	GLN

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Mol	Chain	Res	Type
11	K	85	ASN
11	K	141	ASN
11	K	174	ASN
11	K	207	ASN
12	L	-7	ASN
12	L	27	ASN
12	L	40	ASN
12	L	67	HIS
12	L	70(A)	ASN
12	L	143	ASN
12	L	144(B)	ASN
12	L	166	HIS
12	L	168	GLN
13	M	40	ASN
13	M	54	HIS
13	M	89	GLN
13	M	93	ASN
13	M	149	GLN
13	M	157	ASN
13	M	172	ASN
13	M	181	ASN
14	N	161	GLN
1	O	33	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	173	GLN
2	P	177	GLN
2	P	221	GLN
2	P	227	GLN
3	Q	23	GLN
3	Q	44	ASN
3	Q	59	GLN
3	Q	82	ASN
3	Q	150	GLN
3	Q	163	GLN
3	Q	209	ASN
4	R	23	GLN
4	R	108	ASN

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Mol	Chain	Res	Type
4	R	147	GLN
4	R	150	HIS
4	R	161	ASN
4	R	199	GLN
4	R	211	GLN
4	R	226	ASN
5	S	73	HIS
5	S	97	ASN
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	147	HIS
6	T	180(B)	HIS
6	T	192	GLN
6	T	205	ASN
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	170	GLN
7	U	178	ASN
7	U	182	HIS
7	U	184	ASN
8	V	30	ASN
8	V	66	HIS
8	V	144	GLN
8	V	165	ASN
8	V	172	ASN
8	V	190	ASN
9	W	23	GLN
9	W	56	ASN
9	W	81	GLN

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Mol	Chain	Res	Type
10	X	36	GLN
10	X	54	GLN
10	X	62	ASN
10	X	85	GLN
10	X	96	GLN
10	X	112	GLN
10	X	141	HIS
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	20	ASN
12	Z	27	ASN
12	Z	40	ASN
12	Z	46	ASN
12	Z	67	HIS
12	Z	70(A)	ASN
12	Z	140	ASN
12	Z	141	GLN
12	Z	144(J)	ASN
12	Z	166	HIS
12	Z	168	GLN
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	161	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 13 ligands modelled in this entry, 9 are monoatomic - leaving 4 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
16	OEU	K	213	-	41,41,41	0.63	1 (2%)	54,54,54	0.85	3 (5%)
17	MES	K	214	-	12,12,12	2.18	1 (8%)	15,16,16	1.13	1 (6%)
17	MES	Y	213	-	12,12,12	2.26	1 (8%)	15,16,16	1.21	1 (6%)
16	OEU	Y	212	-	41,41,41	0.63	1 (2%)	54,54,54	0.80	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
16	OEU	K	213	-	-	1/35/35/35	0/3/3/3
17	MES	K	214	-	-	5/6/14/14	0/1/1/1
17	MES	Y	213	-	-	0/6/14/14	0/1/1/1
16	OEU	Y	212	-	-	0/35/35/35	0/3/3/3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	Y	213	MES	C8-S	-7.50	1.67	1.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	K	214	MES	C8-S	-7.18	1.67	1.77
16	Y	212	OEU	C38-C33	2.19	1.55	1.51
16	K	213	OEU	C38-C33	2.01	1.54	1.51

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	Y	213	MES	O3S-S-C8	2.74	111.37	106.00
17	K	214	MES	O3S-S-C8	2.62	111.13	106.00
16	K	213	OEU	C8-C1-C6	2.58	124.48	121.08
16	K	213	OEU	C20-C18-N19	-2.15	105.99	111.70
16	K	213	OEU	C8-C1-C2	-2.02	116.51	120.98

There are no chirality outliers.

All (6) 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-O3S
16	K	213	OEU	C9-C31-C32-C33
17	K	214	MES	C7-C8-S-O1S
17	K	214	MES	C7-C8-S-O2S

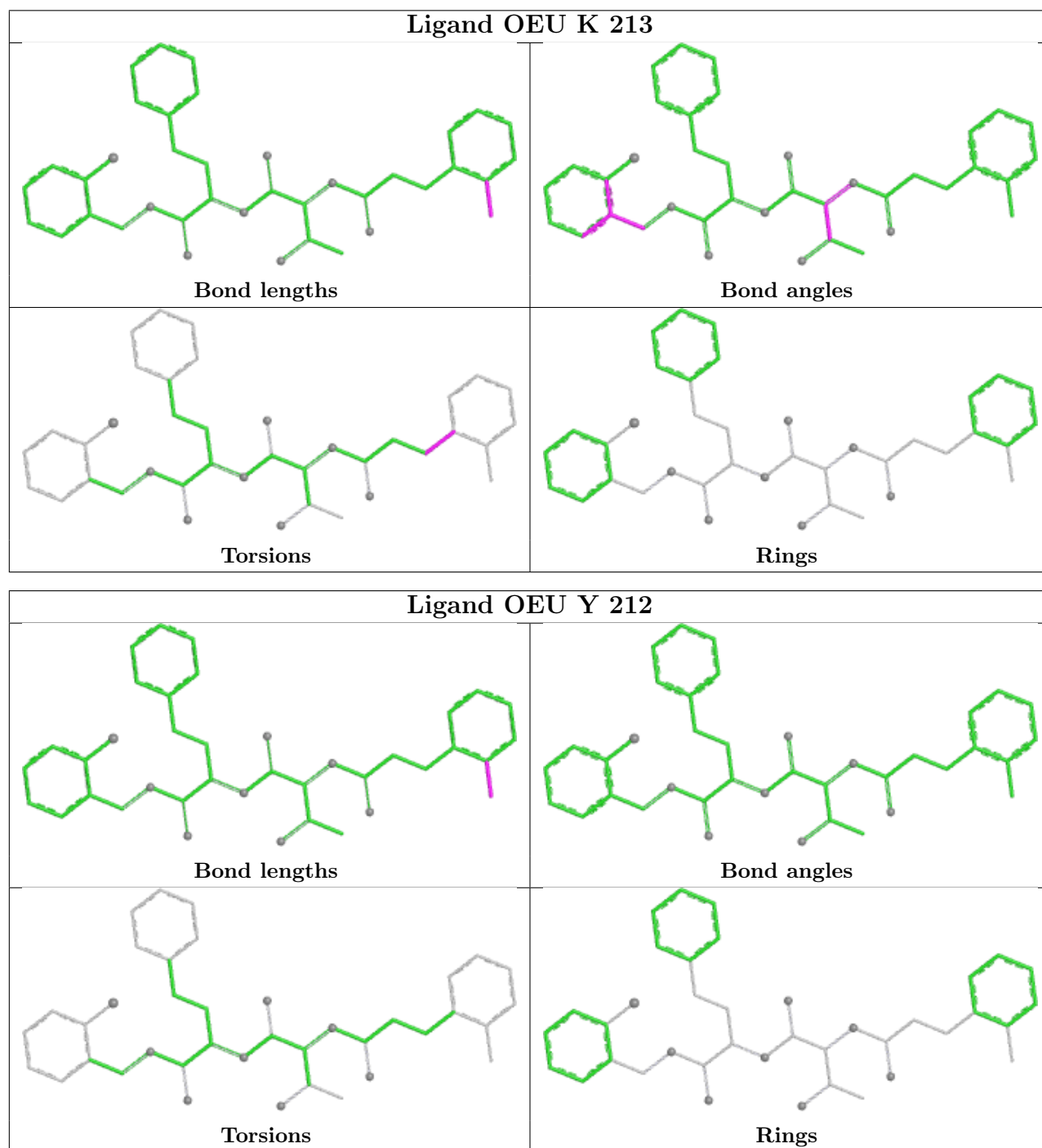
There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
16	K	213	OEU	3	0
16	Y	212	OEU	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 ⓘ

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%)	0.01	8 (3%)	50	44	36, 50, 76, 106	0
1	O	250/250 (100%)	0.19	10 (4%)	42	37	41, 56, 87, 111	0
2	B	235/235 (100%)	0.28	13 (5%)	30	25	37, 56, 87, 103	0
2	P	235/235 (100%)	0.39	13 (5%)	30	25	38, 59, 93, 110	0
3	C	241/241 (100%)	0.54	22 (9%)	15	11	40, 65, 114, 137	0
3	Q	241/241 (100%)	1.02	47 (19%)	3	2	43, 71, 123, 148	0
4	D	242/260 (93%)	0.44	21 (8%)	16	12	37, 60, 96, 116	0
4	R	236/260 (90%)	0.39	14 (5%)	28	23	37, 60, 94, 118	0
5	E	233/233 (100%)	0.27	5 (2%)	63	58	42, 56, 84, 112	0
5	S	233/233 (100%)	0.54	21 (9%)	15	11	40, 60, 96, 123	0
6	F	237/242 (97%)	0.10	9 (3%)	44	38	34, 52, 87, 104	0
6	T	237/242 (97%)	0.09	4 (1%)	69	64	36, 53, 79, 110	0
7	G	243/243 (100%)	-0.12	7 (2%)	53	48	32, 48, 75, 109	0
7	U	243/243 (100%)	-0.14	5 (2%)	63	58	33, 48, 71, 104	0
8	H	222/222 (100%)	-0.16	1 (0%)	87	85	32, 44, 62, 95	0
8	V	222/222 (100%)	-0.07	3 (1%)	73	69	36, 48, 65, 104	0
9	I	204/204 (100%)	-0.33	2 (0%)	79	76	32, 43, 60, 76	0
9	W	204/204 (100%)	-0.18	0	100	100	33, 46, 66, 79	0
10	J	198/198 (100%)	-0.05	8 (4%)	42	37	32, 47, 64, 119	0
10	X	198/198 (100%)	-0.01	7 (3%)	47	41	35, 50, 66, 118	0
11	K	212/212 (100%)	-0.25	2 (0%)	81	78	34, 45, 65, 80	0
11	Y	212/212 (100%)	-0.19	1 (0%)	87	85	36, 45, 64, 73	0
12	L	222/222 (100%)	-0.18	1 (0%)	87	85	34, 46, 68, 79	0
12	Z	222/222 (100%)	-0.20	2 (0%)	81	78	32, 45, 66, 81	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	1	233/233 (100%)	-0.37	1 (0%) 88 86	31, 42, 57, 65	0
13	M	233/233 (100%)	-0.27	3 (1%) 75 71	33, 45, 59, 64	0
14	2	196/196 (100%)	-0.36	0 100 100	34, 42, 62, 79	0
14	N	196/196 (100%)	-0.39	0 100 100	32, 42, 58, 73	0
All	All	6330/6382 (99%)	0.05	230 (3%) 46 40	31, 50, 87, 148	0

All (230) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
10	X	-1	MET	12.9
10	J	-1	MET	11.6
3	Q	56	LEU	8.9
6	F	12	ASN	7.8
2	B	217	ALA	6.5
6	T	12	ASN	6.3
5	S	4	PHE	6.0
2	P	217	ALA	5.7
5	E	4	PHE	5.6
4	D	12	VAL	5.6
4	D	123(E)	SER	5.5
4	D	123(D)	ALA	5.5
3	C	56	LEU	5.3
4	D	123(B)	GLU	5.2
1	O	4	MET	5.2
4	D	127	LEU	5.1
10	J	192	ALA	5.1
13	M	-8	THR	5.0
4	R	123(A)	GLY	5.0
3	Q	55	THR	4.9
4	D	123(G)	GLU	4.9
2	P	216(B)	GLY	4.9
1	A	4	MET	4.6
3	C	7	GLY	4.6
11	K	208	ASN	4.5
3	Q	208	LYS	4.5
3	Q	210	ILE	4.5
3	Q	207	ALA	4.4
1	A	5	THR	4.4
1	O	217(O)	ASP	4.4
3	Q	64	PRO	4.4
4	R	10	ARG	4.4

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Mol	Chain	Res	Type	RSRZ
3	Q	58	LEU	4.4
3	C	11	ALA	4.3
10	X	192	ALA	4.2
2	P	54	VAL	4.2
7	U	240	ASP	4.2
10	X	191	GLN	4.2
4	D	123(C)	GLY	4.1
2	B	127	GLY	4.1
6	T	13	SER	4.1
3	C	208	LYS	4.1
3	C	12	LEU	4.0
3	Q	57	LYS	4.0
3	Q	233	VAL	4.0
3	C	207	ALA	3.9
4	D	242	ALA	3.9
3	C	8	TYR	3.9
1	O	5	THR	3.9
4	R	12	VAL	3.8
4	D	9	ASP	3.8
7	G	240	ASP	3.8
2	P	239	THR	3.7
5	E	207	LEU	3.7
6	F	13	SER	3.7
2	B	22	TYR	3.7
3	Q	62(A)	ILE	3.7
3	Q	206	GLY	3.7
4	R	125	GLU	3.7
10	J	191	GLN	3.7
7	U	6	ALA	3.6
2	B	13	THR	3.6
5	S	63	TYR	3.6
3	Q	198	LEU	3.5
3	Q	8	TYR	3.4
11	K	210	ILE	3.4
5	S	206	SER	3.4
3	Q	236	ILE	3.4
4	D	123(A)	GLY	3.4
1	A	235	ALA	3.4
3	Q	63	THR	3.3
5	S	5	ARG	3.2
8	V	221	ILE	3.2
10	J	190	PHE	3.2

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Mol	Chain	Res	Type	RSRZ
1	O	64	LEU	3.2
2	P	63	THR	3.2
4	D	10	ARG	3.2
5	S	32	LYS	3.2
4	D	244	GLU	3.2
2	B	64	THR	3.2
4	D	11	GLY	3.2
10	J	49	ALA	3.2
2	B	54	VAL	3.2
4	D	126	ARG	3.2
2	B	239	THR	3.1
3	C	55	THR	3.1
5	S	55	ALA	3.1
1	O	217(P)	LYS	3.1
3	Q	224	LEU	3.1
5	S	51	LEU	3.1
5	S	207	LEU	3.0
3	Q	209	ASN	3.0
3	Q	196	SER	3.0
2	P	218	ASN	3.0
13	M	61	ASP	3.0
6	T	240	ILE	3.0
3	Q	240	LYS	3.0
13	1	-8	THR	3.0
3	Q	201	VAL	3.0
3	C	58	LEU	2.9
3	Q	200	VAL	2.9
7	G	6	ALA	2.9
3	Q	232	TYR	2.9
3	Q	180	TYR	2.8
3	Q	11	ALA	2.8
2	B	218	ASN	2.8
7	U	239	GLN	2.8
1	A	217	ASP	2.8
3	Q	184	ALA	2.7
4	D	22	PHE	2.7
3	Q	65	SER	2.7
4	D	241	GLU	2.7
10	X	188	ASP	2.7
6	F	128	SER	2.7
3	C	9	ASP	2.7
10	X	10	ASP	2.7

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Mol	Chain	Res	Type	RSRZ
2	B	216(B)	GLY	2.7
2	B	218(D)	GLY	2.6
5	S	33	GLN	2.6
6	F	240	ILE	2.6
11	Y	210	ILE	2.6
4	R	11	GLY	2.6
6	F	184	LEU	2.6
3	C	240	LYS	2.6
5	S	208(A)	VAL	2.6
3	Q	13	SER	2.6
4	D	122	ARG	2.6
3	Q	59	GLN	2.6
8	V	197	ARG	2.5
1	A	8	TYR	2.5
4	R	242	ALA	2.5
10	X	190	PHE	2.5
3	Q	234	THR	2.5
3	Q	54	SER	2.5
4	R	126	ARG	2.5
5	E	203	ASP	2.5
4	D	238	LYS	2.4
5	S	65	LYS	2.4
12	Z	144(R)	LYS	2.4
3	C	203	THR	2.4
3	Q	61	THR	2.4
8	V	223	ASP	2.4
3	C	206	GLY	2.4
3	Q	222	VAL	2.4
3	Q	53	ARG	2.4
5	S	53	ARG	2.4
3	Q	51	GLU	2.4
2	P	59	LEU	2.4
1	A	55	SER	2.4
1	A	56	SER	2.4
10	J	193	GLN	2.4
3	C	233	VAL	2.4
4	R	9	ASP	2.3
3	Q	185	THR	2.3
3	Q	44	ASN	2.3
5	S	209	ASN	2.3
6	F	180(F)	GLY	2.3
6	T	170	GLN	2.3

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Mol	Chain	Res	Type	RSRZ
1	O	8	TYR	2.3
6	F	206	LYS	2.3
12	L	144(Q)	LYS	2.3
2	P	218(C)	GLY	2.3
4	R	123	PHE	2.3
1	A	203	GLU	2.3
4	R	205	GLU	2.3
3	C	52	ARG	2.3
4	D	86	ARG	2.3
3	Q	12	LEU	2.3
2	B	55	THR	2.2
5	E	12	THR	2.2
5	S	54	ASN	2.2
5	S	203	ASP	2.2
8	H	170	GLY	2.2
12	Z	144(Q)	LEU	2.2
3	C	14	ILE	2.2
5	S	8	TYR	2.2
3	Q	243	GLN	2.2
2	B	59	LEU	2.2
4	R	127	LEU	2.2
3	C	57	LYS	2.2
3	Q	52	ARG	2.2
1	O	53	LYS	2.2
3	Q	7	GLY	2.2
5	S	10	GLY	2.2
9	I	182	ASP	2.2
3	Q	211	GLU	2.2
5	S	57	GLU	2.2
2	P	55	THR	2.2
3	Q	203	THR	2.2
5	S	52	LYS	2.2
2	P	127	GLY	2.2
7	G	218	ASP	2.2
10	J	187	VAL	2.2
4	R	122	ARG	2.1
2	P	61	GLN	2.1
2	P	220	TYR	2.1
4	R	238	LYS	2.1
7	U	199	ASP	2.1
5	S	198	SER	2.1
4	D	230	ALA	2.1

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Mol	Chain	Res	Type	RSRZ
5	E	5	ARG	2.1
9	I	181	LYS	2.1
4	R	158	TYR	2.1
3	Q	186	VAL	2.1
7	G	49	ILE	2.1
10	X	189	ASP	2.1
3	C	17	PRO	2.1
7	G	8	TYR	2.1
1	O	210	ILE	2.1
2	B	238	ILE	2.1
10	J	24	ILE	2.1
6	F	204	ASP	2.1
1	O	217(N)	THR	2.1
3	C	209	ASN	2.1
4	D	123(F)	GLY	2.1
2	P	238	ILE	2.1
7	G	128	TYR	2.1
7	U	236	ILE	2.1
3	Q	40	VAL	2.1
6	F	129	VAL	2.1
3	C	18	ASP	2.0
3	Q	144(A)	ASP	2.0
7	G	129	MET	2.0
13	M	29	ASN	2.0
3	C	186	VAL	2.0
3	C	232	TYR	2.0
3	Q	10	ARG	2.0
5	S	168	ARG	2.0
3	Q	217	PRO	2.0
1	O	7	ARG	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 ⓘ

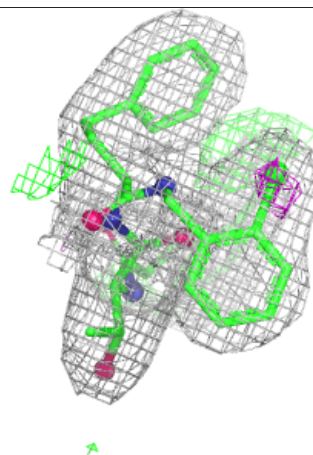
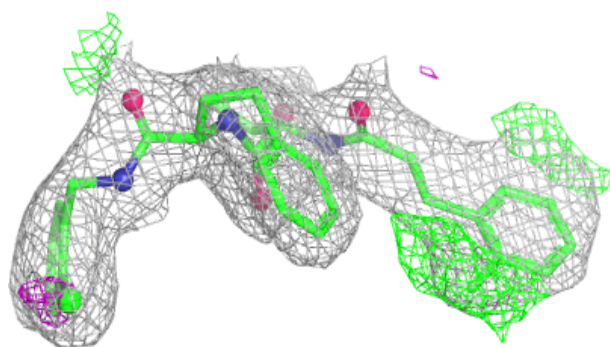
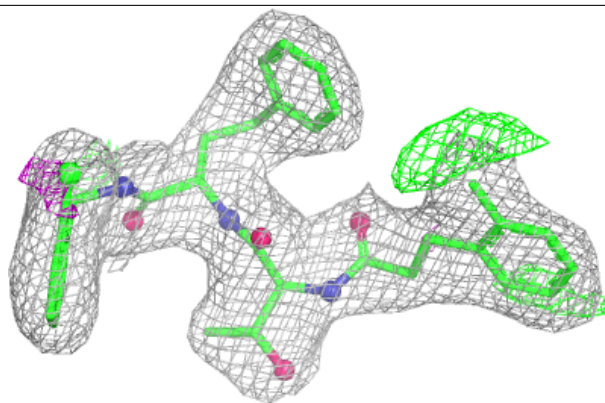
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	F	242	1/1	0.57	0.47	136,136,136,136	0
15	MG	L	196	1/1	0.90	0.10	72,72,72,72	0
17	MES	Y	213	12/12	0.90	0.18	87,89,89,89	0
17	MES	K	214	12/12	0.91	0.17	87,88,89,89	0
15	MG	I	196	1/1	0.91	0.13	64,64,64,64	0
15	MG	I	195	1/1	0.92	0.13	65,65,65,65	0
16	OEUE	Y	212	39/39	0.93	0.10	40,45,49,49	0
16	OEUE	K	213	39/39	0.94	0.09	38,45,50,50	0
15	MG	H	224	1/1	0.95	0.13	51,51,51,51	0
15	MG	K	212	1/1	0.96	0.10	79,79,79,79	0
15	MG	G	1	1/1	0.97	0.10	61,61,61,61	0
15	MG	N	188	1/1	0.97	0.12	68,68,68,68	0
15	MG	L	195	1/1	0.97	0.07	75,75,75,75	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.

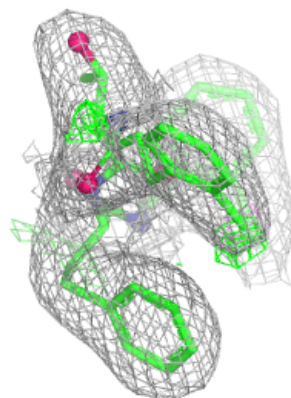
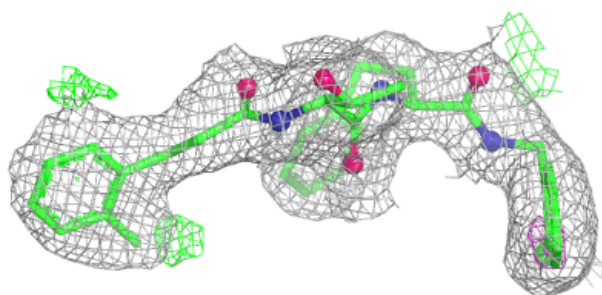
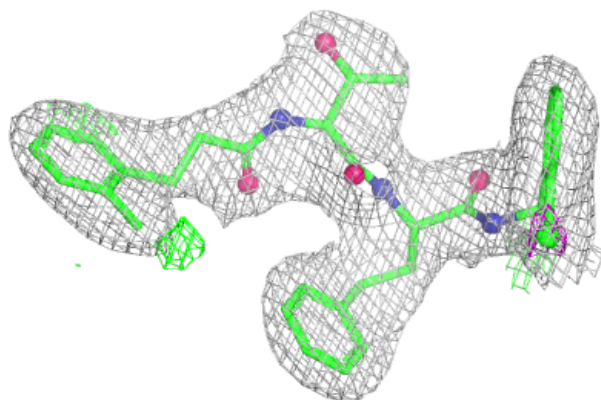
Electron density around OEU Y 212:

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



Electron density around OEU 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)



6.5 Other polymers [i](#)

There are no such residues in this entry.