



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 11:57 PM UTC

PDB ID : 3OEV / pdb_00003oev
Title : Structure of yeast 20S open-gate proteasome with Compound 25
Authors : Sintchak, M.D.
Deposited on : 2010-08-13
Resolution : 2.85 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

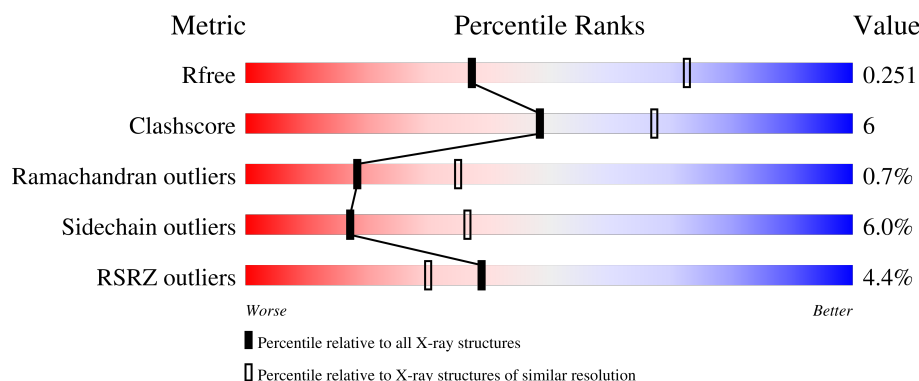
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.85 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	1407 (2.88-2.84)
Clashscore	190562	1446 (2.88-2.84)
Ramachandran outliers	187476	1406 (2.88-2.84)
Sidechain outliers	187428	1407 (2.88-2.84)
RSRZ outliers	180081	1408 (2.88-2.84)

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% 87% 12%
1	O	250	6% 83% 15%
2	B	235	7% 81% 18%
2	P	235	6% 80% 18%
3	C	241	13% 87% 12%

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Mol	Chain	Length	Quality of chain
3	Q	241	 16% 80% 17% .
4	D	260	 10% 78% 13% . 7%
4	R	260	 8% 73% 19% . 7%
5	E	233	 6% 81% 15% . .
5	S	233	 12% 79% 18% .
6	F	242	 2% 83% 11% . .
6	T	242	 2% 81% 14% . .
7	G	243	 % 79% 19% .
7	U	243	 3% 81% 19%
8	H	222	 84% 15%
8	V	222	 % 85% 14% .
9	I	204	 2% 87% 12% .
9	W	204	 % 86% 12% .
10	J	198	 4% 82% 15% .
10	X	198	 3% 81% 16% . .
11	K	212	 2% 85% 13% .
11	Y	212	 2% 85% 14% .
12	L	222	 2% 88% 10% .
12	Z	222	 3% 84% 15% .
13	1	233	 82% 16% .
13	M	233	 % 84% 14% .
14	2	196	 86% 13% .
14	N	196	 85% 15% .

2 Entry composition

There are 17 unique types of molecules in this entry. The entry contains 49398 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	242	Total	C	N	O	S	0	0	0
			1861	1162	314	378	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	197	Total	C	N	O	S	0	0	0
			1577	1000	268	304	5			

- Molecule 11 is a protein called Proteasome component PRE2.

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

- Molecule 12 is a protein called Proteasome component C5.

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

- Molecule 13 is a protein called Proteasome component PRE4.

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

- Molecule 14 is a protein called Proteasome component PRE3.

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

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

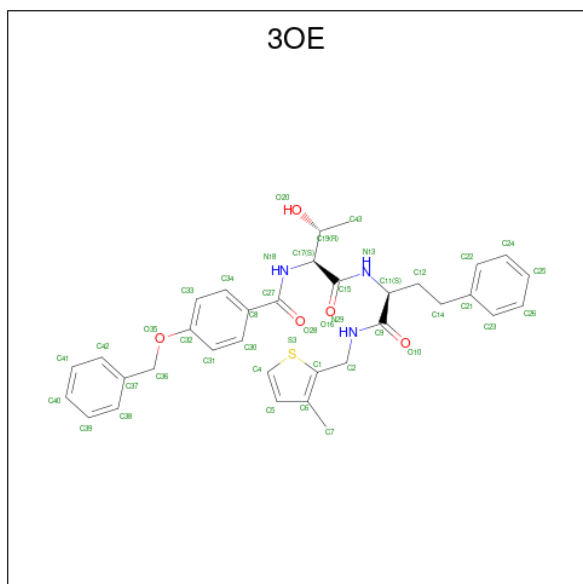
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
15	F	2	Total	Mg	0	0
			2	2		
15	G	1	Total	Mg	0	0
			1	1		

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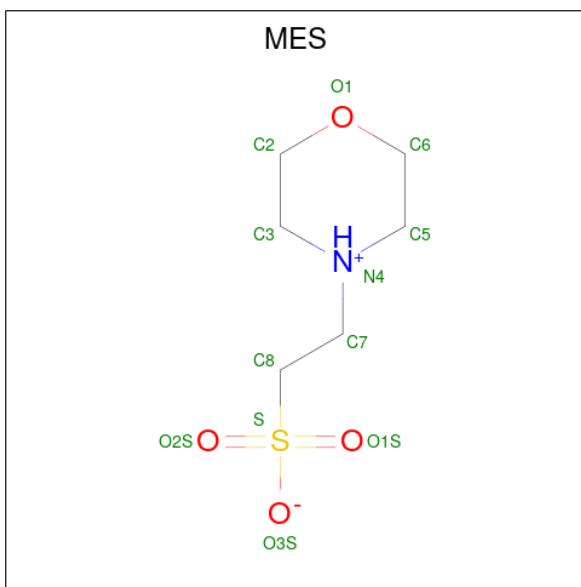
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
15	H	1	Total	Mg	0	0
			1	1		
15	I	2	Total	Mg	0	0
			2	2		
15	K	1	Total	Mg	0	0
			1	1		
15	L	2	Total	Mg	0	0
			2	2		
15	N	1	Total	Mg	0	0
			1	1		

- Molecule 16 is 4-(benzyloxy)-N-[(2S,3R)-3-hydroxy-1-{[(2S)-1-[(3-methylthiophen-2-yl)methyl]amino}-1-oxo-4-phenylbutan-2-yl]amino}-1-oxobutan-2-yl]benzamide (CCD ID: 3OE) (formula: C₃₄H₃₇N₃O₅S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
16	K	1	Total	C	N	O	S	0	0
			43	34	3	5	1		
16	Y	1	Total	C	N	O	S	0	0
			43	34	3	5	1		

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

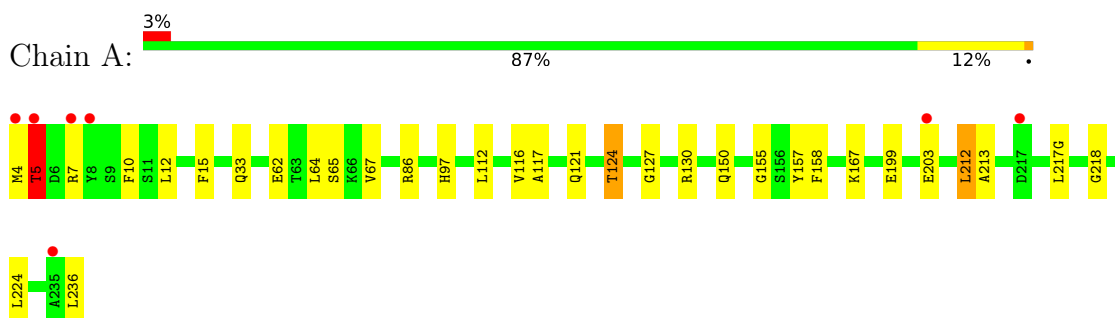


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
17	K	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
17	Y	1	Total	C	N	O	S	0	0
			12	6	1	4	1		

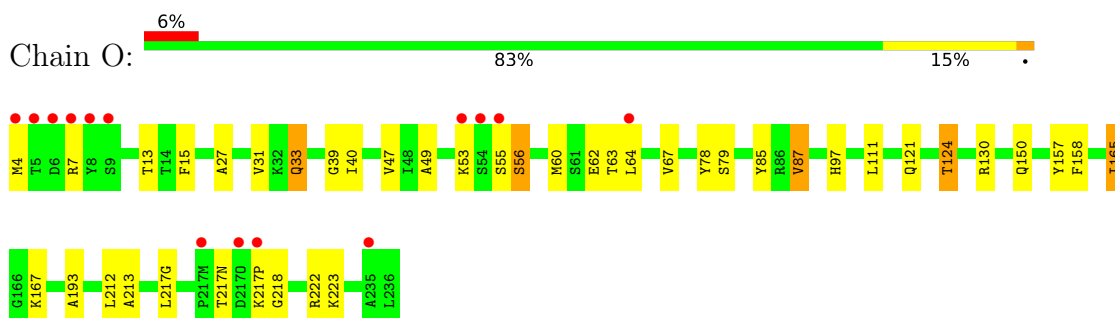
3 Residue-property plots [i](#)

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

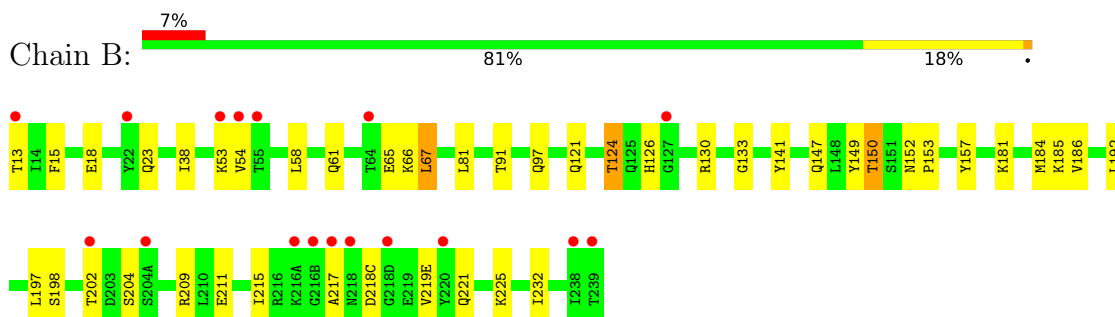
- Molecule 1: Proteasome component Y7



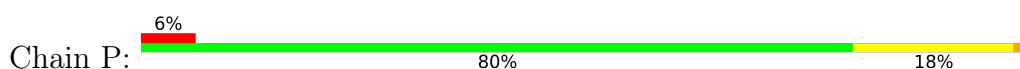
- Molecule 1: Proteasome component Y7

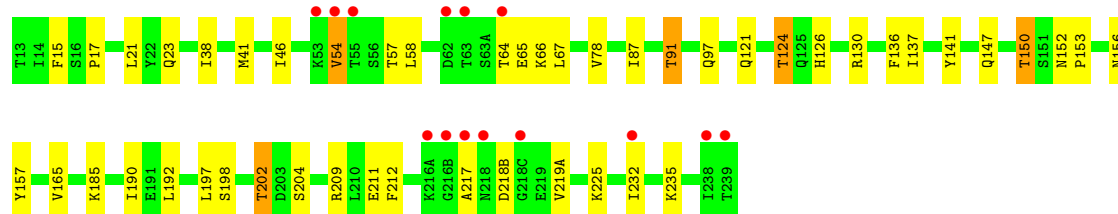


- Molecule 2: Proteasome component Y13

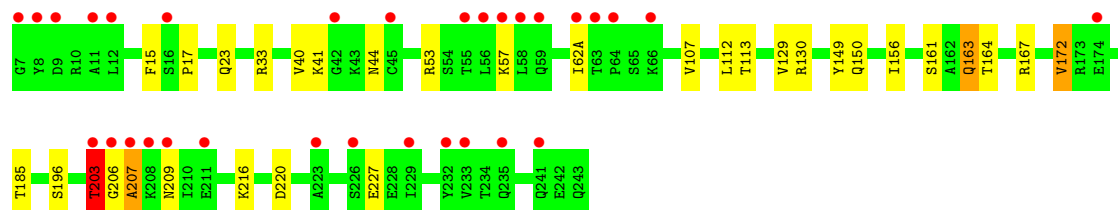
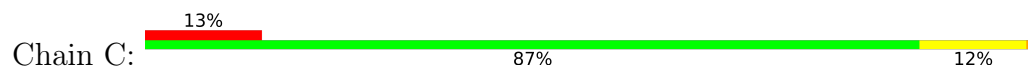


- Molecule 2: Proteasome component Y13

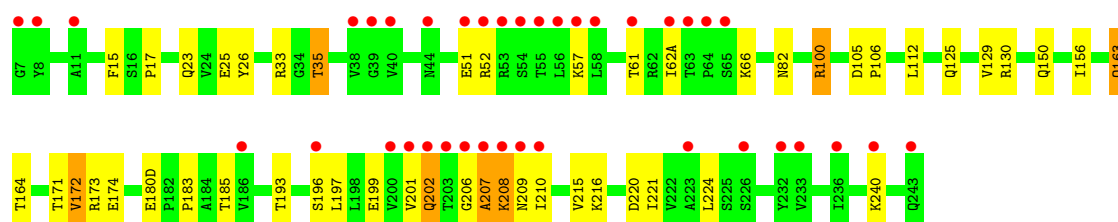
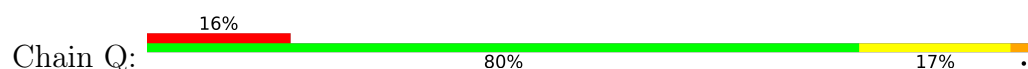




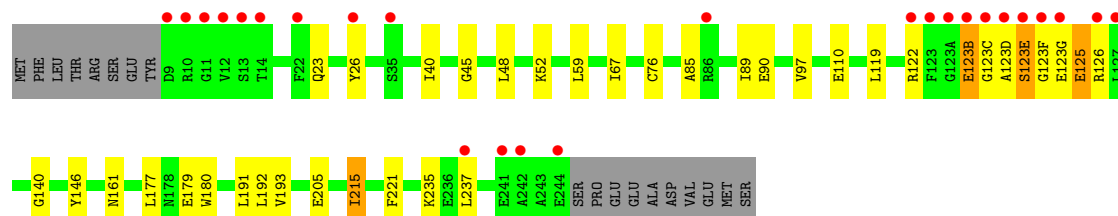
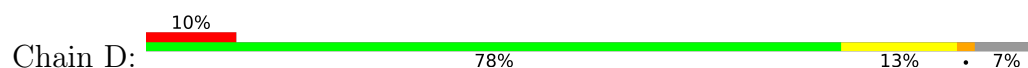
• Molecule 3: Proteasome component PRE6



• Molecule 3: Proteasome component PRE6

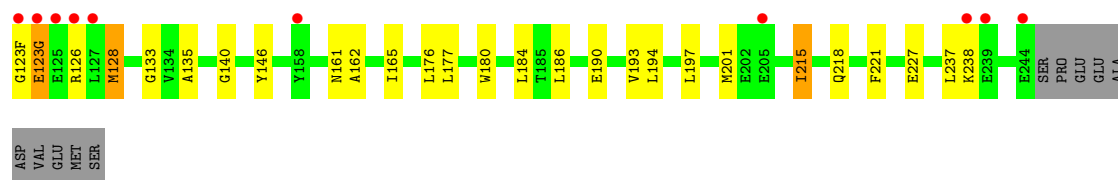


• Molecule 4: Proteasome component PUP2

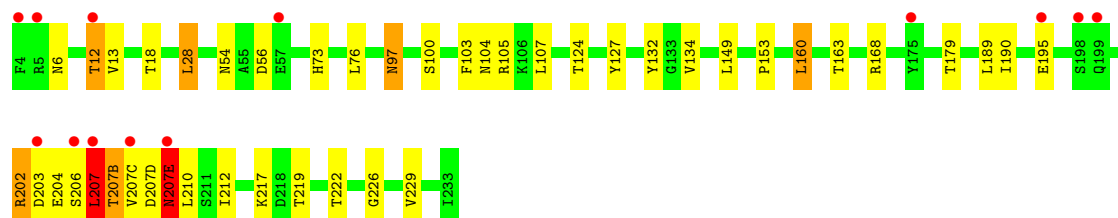
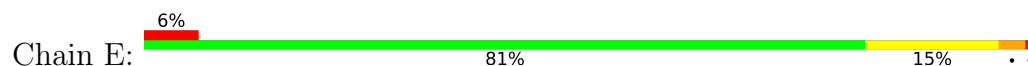


• Molecule 4: Proteasome component PUP2

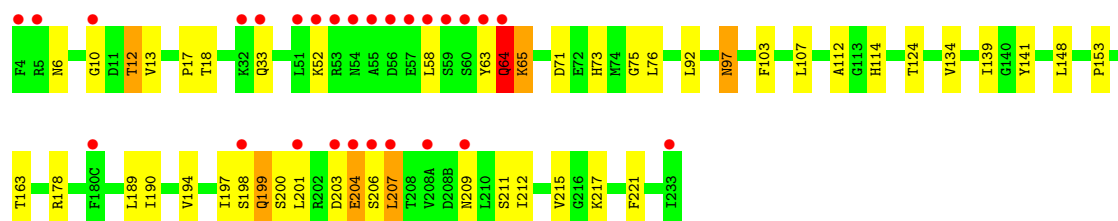
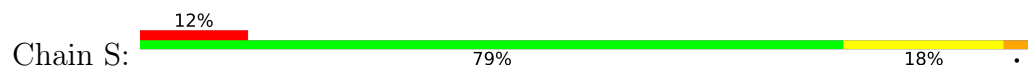




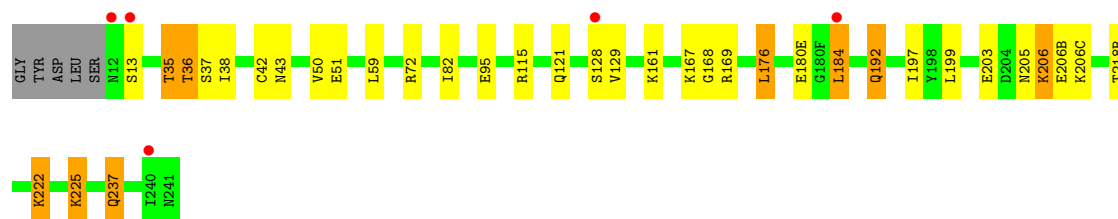
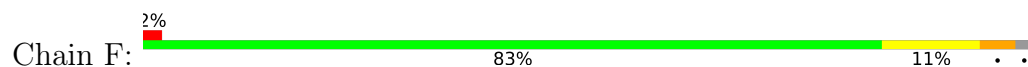
• Molecule 5: Proteasome component PRE5



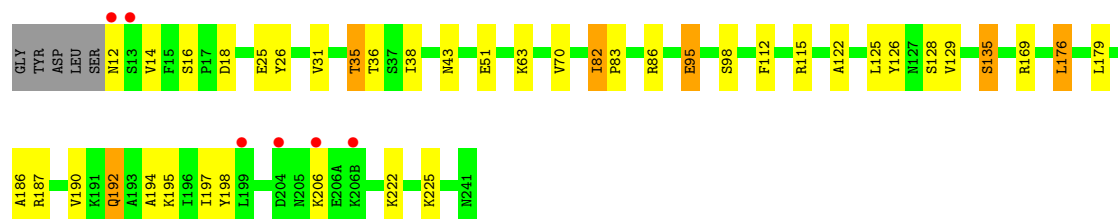
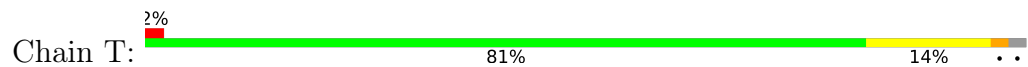
• Molecule 5: Proteasome component PRE5



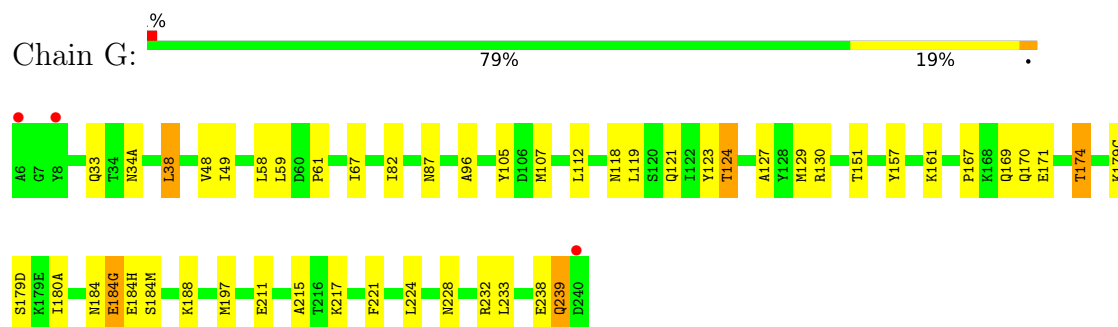
• Molecule 6: Proteasome component C1



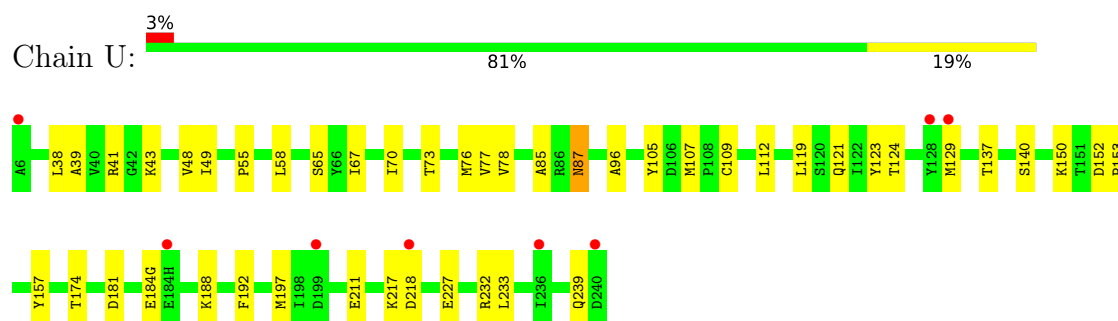
• Molecule 6: Proteasome component C1



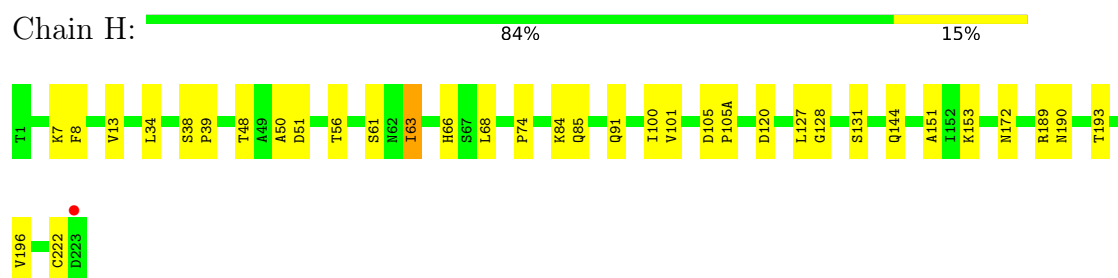
- Molecule 7: Proteasome component C7-alpha



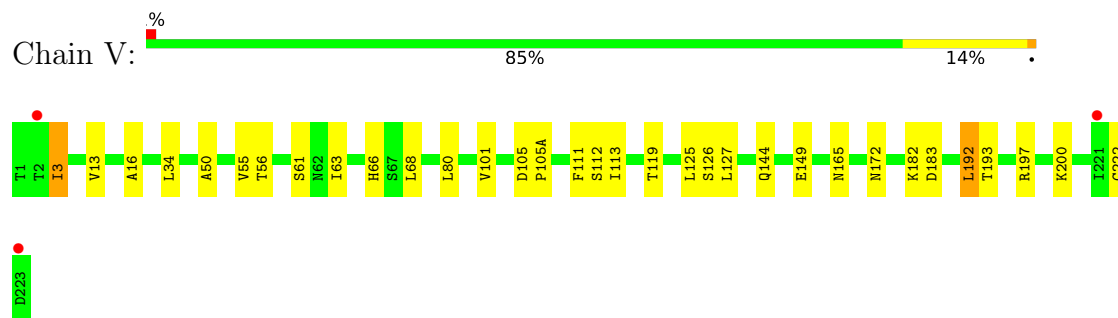
- Molecule 7: Proteasome component C7-alpha



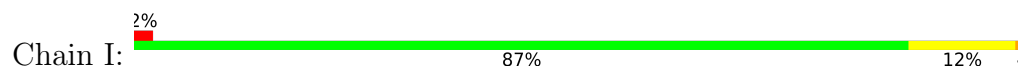
- Molecule 8: Proteasome component PUP1

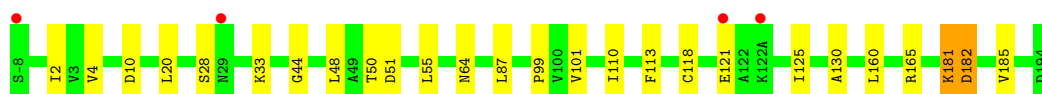


- Molecule 8: Proteasome component PUP1

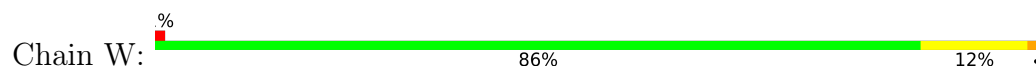


- Molecule 9: Proteasome component PUP3

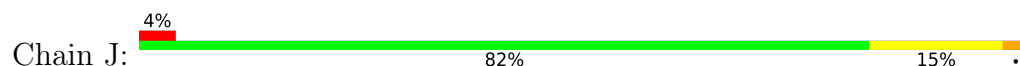




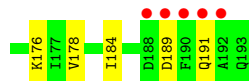
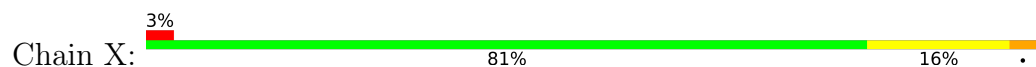
• Molecule 9: Proteasome component PUP3



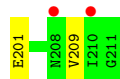
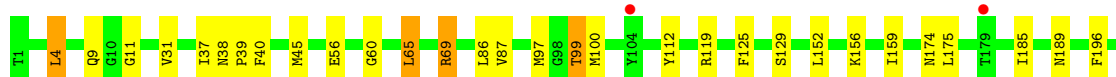
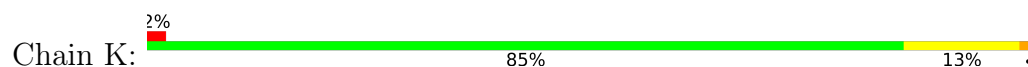
• Molecule 10: Proteasome component C11



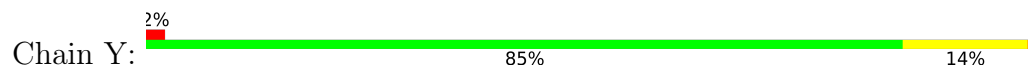
• Molecule 10: Proteasome component C11

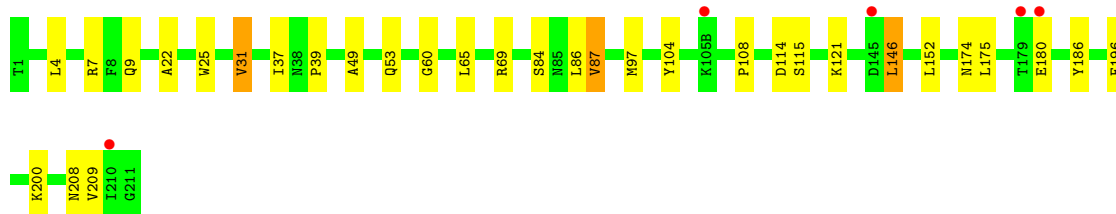


• Molecule 11: Proteasome component PRE2

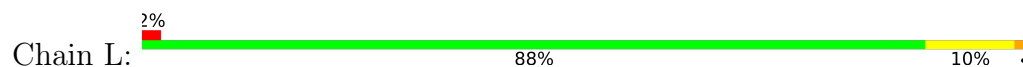


• Molecule 11: Proteasome component PRE2

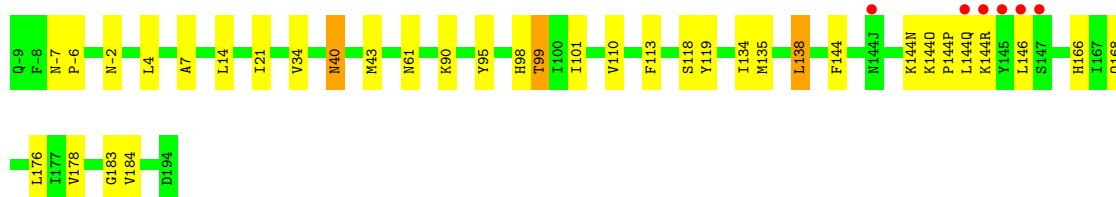
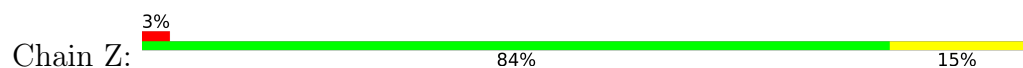




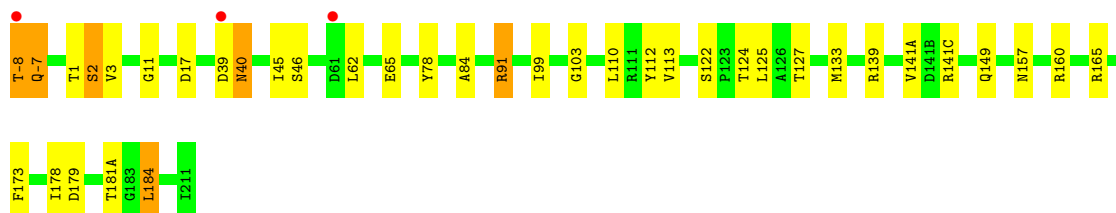
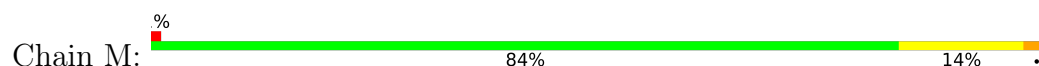
• Molecule 12: Proteasome component C5



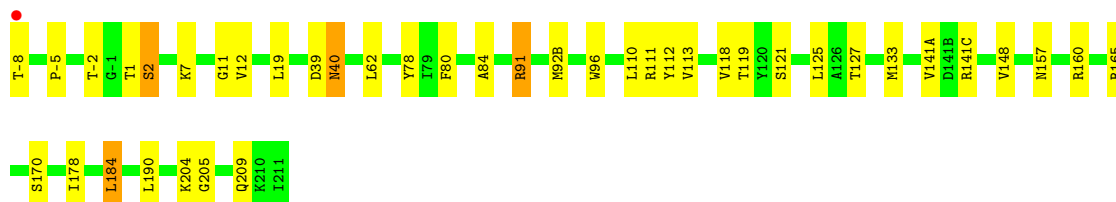
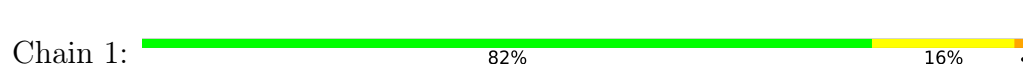
• Molecule 12: Proteasome component C5



• Molecule 13: Proteasome component PRE4



• Molecule 13: Proteasome component PRE4



• Molecule 14: Proteasome component PRE3

T1	F8	L14	T20	T31	L34	H38	D39	I55	T67	G72	K84	K91	L96	A102	K107	L115	G116	V119	T132	F133	G136	M146	E149	Q161	A162	I163	D166	G170	M175	V176	L187	I187
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- Chain 2:  86% 13%



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	136.07Å 299.95Å 145.62Å 90.00° 113.17° 90.00°	Depositor
Resolution (Å)	50.00 – 2.85 50.00 – 2.85	Depositor EDS
% Data completeness (in resolution range)	98.3 (50.00-2.85) 98.8 (50.00-2.85)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.67 (at 2.86Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.220 , 0.257 0.215 , 0.251	Depositor DCC
R_{free} test set	4967 reflections (2.01%)	wwPDB-VP
Wilson B-factor (Å ²)	55.9	Xtriage
Anisotropy	0.088	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 23.1	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	0.93	EDS
Total number of atoms	49398	wwPDB-VP
Average B, all atoms (Å ²)	53.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.26% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: 3OE, 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	0.49	0/1952	0.79	0/2642
1	O	0.51	0/1952	0.83	0/2642
2	B	0.49	0/1858	0.83	0/2516
2	P	0.49	0/1858	0.81	0/2516
3	C	0.50	0/1920	0.83	0/2598
3	Q	0.60	1/1920 (0.1%)	0.87	1/2598 (0.0%)
4	D	0.49	0/1886	0.78	0/2541
4	R	0.55	1/1886 (0.1%)	1.05	2/2541 (0.1%)
5	E	0.75	1/1823 (0.1%)	1.00	6/2463 (0.2%)
5	S	0.55	0/1815	0.80	0/2452
6	F	0.51	1/1887 (0.1%)	0.81	1/2546 (0.0%)
6	T	0.52	1/1887 (0.1%)	0.80	0/2546
7	G	0.51	1/1959 (0.1%)	0.81	1/2652 (0.0%)
7	U	0.53	0/1959	0.83	0/2652
8	H	0.54	0/1716	0.80	0/2326
8	V	0.54	0/1716	0.80	0/2326
9	I	0.58	0/1611	0.81	0/2174
9	W	0.56	0/1611	0.80	1/2174 (0.0%)
10	J	0.54	0/1610	0.82	0/2170
10	X	0.49	0/1605	0.79	1/2163 (0.0%)
11	K	0.49	0/1681	0.82	1/2274 (0.0%)
11	Y	0.48	0/1681	0.80	0/2274
12	L	0.53	0/1795	0.77	0/2420
12	Z	0.55	0/1795	0.82	1/2420 (0.0%)
13	1	0.57	0/1855	0.80	1/2514 (0.0%)
13	M	0.55	0/1855	0.80	0/2514
14	2	0.60	0/1541	0.80	0/2087
14	N	0.58	0/1541	0.78	0/2087
All	All	0.54	6/50175 (0.0%)	0.83	16/67828 (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
1	O	0	1
4	R	0	1
5	E	0	2
5	S	0	1
All	All	0	5

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	E	207	LEU	CA-C	-23.11	1.25	1.52
3	Q	180(D)	GLU	C-O	10.35	1.35	1.24
4	R	123	PHE	CA-C	8.07	1.62	1.52
6	T	82	ILE	CA-CB	5.89	1.57	1.54
6	F	82	ILE	CA-CB	5.47	1.56	1.54
7	G	82	ILE	CA-CB	5.01	1.57	1.53

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	R	123(G)	GLU	CA-C-O	26.06	157.78	120.51
5	E	207(E)	ASN	CA-C-O	23.23	148.34	120.00
4	R	123(G)	GLU	O-C-N	-22.07	93.24	122.59
5	E	207(E)	ASN	O-C-N	-16.78	97.62	122.28
12	Z	146	LEU	N-CA-C	7.07	121.19	109.95
5	E	207	LEU	CA-C-O	6.32	127.06	120.30
13	1	-2	THR	N-CA-C	6.12	119.52	109.85
11	K	11	GLY	N-CA-C	5.71	117.15	111.21
5	E	202	ARG	N-CA-C	-5.46	106.57	113.18
5	E	210	LEU	N-CA-C	5.36	118.36	109.46
7	G	161	LYS	N-CA-C	-5.27	105.62	111.36
3	Q	125	GLN	N-CA-C	5.20	117.11	110.61
10	X	49	ALA	N-CA-C	5.11	119.75	111.37
5	E	207(E)	ASN	N-CA-C	5.08	119.51	112.45
6	F	161	LYS	N-CA-C	-5.02	106.33	112.90
9	W	23	GLN	CB-CA-C	-5.01	110.41	117.23

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
5	E	204	GLU	Peptide
5	E	207(E)	ASN	Mainchain
1	O	217(N)	THR	Peptide
4	R	123(G)	GLU	Mainchain
5	S	204	GLU	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1915	0	1926	23	0
1	O	1915	0	1926	26	0
2	B	1829	0	1829	23	0
2	P	1829	0	1829	28	0
3	C	1891	0	1900	29	0
3	Q	1891	0	1900	30	0
4	D	1861	0	1836	16	0
4	R	1861	0	1835	24	0
5	E	1795	0	1797	24	0
5	S	1788	0	1790	27	0
6	F	1848	0	1844	20	0
6	T	1848	0	1844	27	0
7	G	1921	0	1910	29	0
7	U	1921	0	1910	31	0
8	H	1685	0	1688	13	0
8	V	1685	0	1688	17	0
9	I	1581	0	1574	18	0
9	W	1581	0	1574	15	0
10	J	1582	0	1583	20	0
10	X	1577	0	1581	21	0
11	K	1644	0	1595	17	0
11	Y	1644	0	1595	16	0
12	L	1757	0	1711	18	0
12	Z	1757	0	1711	30	0
13	1	1824	0	1832	25	0
13	M	1824	0	1832	26	0
14	2	1512	0	1481	15	0
14	N	1512	0	1481	18	0
15	F	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	43	0	37	2	0
16	Y	43	0	37	1	0
17	K	12	0	13	1	0
17	Y	12	0	13	0	0
All	All	49398	0	49102	546	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 (546) 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)
5:S:52:LYS:HB3	5:S:63:TYR:O	1.35	1.24
3:C:203:THR:HG22	3:C:206:GLY:N	1.65	1.05
12:Z:144(P):PRO:O	12:Z:144(R):LYS:HG2	1.53	1.05
1:O:7:ARG:HG3	6:T:128:SER:HB3	1.38	1.03
1:O:130:ARG:HH21	7:U:124:THR:HG22	1.24	1.00
7:U:96:ALA:HA	7:U:107:MET:HE2	1.43	0.98
5:E:207:LEU:HD23	5:E:207:LEU:H	1.30	0.96
3:C:203:THR:HG22	3:C:206:GLY:H	1.24	0.94
7:G:96:ALA:HA	7:G:107:MET:HE2	1.47	0.94
3:C:163:GLN:HE21	3:C:164:THR:H	1.11	0.94
4:D:123(C):GLY:HA2	4:D:125:GLU:HA	1.49	0.93
13:1:1:THR:HG23	13:1:2:SER:N	1.83	0.90
5:S:52:LYS:CB	5:S:63:TYR:O	2.22	0.88
13:1:1:THR:HG23	13:1:2:SER:H	1.40	0.87
1:A:130:ARG:HH21	7:G:124:THR:CG2	1.87	0.86
3:C:163:GLN:NE2	3:C:164:THR:H	1.72	0.86
1:A:130:ARG:HH21	7:G:124:THR:HG22	1.40	0.86
3:C:203:THR:HG22	3:C:207:ALA:H	1.39	0.85
6:F:167:LYS:HD3	6:F:205:ASN:HD21	1.41	0.85
12:Z:144(O):LYS:HG3	12:Z:144(R):LYS:NZ	1.91	0.85
12:Z:144(O):LYS:HG3	12:Z:144(R):LYS:HZ3	1.43	0.84
6:F:35:THR:HG21	6:F:51:GLU:O	1.79	0.83
7:G:38:LEU:HD23	7:G:197:MET:HE3	1.61	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:207:LEU:HA	5:E:207(E):ASN:HD22	1.44	0.83
12:L:4:LEU:HD11	12:L:138:LEU:HD21	1.61	0.82
6:F:95:GLU:HG2	6:F:115:ARG:HB3	1.60	0.81
13:M:40:ASN:H	13:M:40:ASN:HD22	1.24	0.81
13:M:157:ASN:HD22	13:M:160:ARG:HH11	1.26	0.80
1:O:130:ARG:HH21	7:U:124:THR:CG2	1.95	0.80
9:I:181:LYS:H	9:I:181:LYS:HD2	1.47	0.79
3:C:15:PHE:H	4:D:23:GLN:HE22	1.29	0.79
5:E:207(B):THR:H	5:E:207(E):ASN:HD22	1.30	0.77
12:Z:166:HIS:HD2	12:Z:168:GLN:H	1.32	0.77
14:N:34:LEU:HD13	14:N:176:VAL:HG23	1.67	0.77
3:C:163:GLN:HE21	3:C:164:THR:N	1.83	0.76
3:Q:15:PHE:H	4:R:23:GLN:HE22	1.32	0.76
14:N:161:GLN:HE21	14:2:136:GLY:HA2	1.51	0.76
7:G:107:MET:HE3	7:G:112:LEU:HD13	1.68	0.76
2:B:15:PHE:H	3:C:23:GLN:HE22	1.32	0.76
6:T:95:GLU:HG2	6:T:115:ARG:HB3	1.67	0.75
13:M:141(C):ARG:HG3	13:M:141(C):ARG:HH11	1.51	0.75
14:N:14:LEU:HD11	14:N:102:ALA:HB3	1.68	0.74
7:U:67:ILE:HD12	7:U:211:GLU:HG2	1.69	0.74
3:C:206:GLY:O	3:C:207:ALA:O	2.05	0.74
14:N:136:GLY:HA2	14:2:161:GLN:HE21	1.54	0.72
5:E:73:HIS:HE1	5:E:107:LEU:O	1.72	0.71
5:E:207:LEU:HD23	5:E:207:LEU:N	2.05	0.71
12:L:166:HIS:HD2	12:L:168:GLN:H	1.37	0.70
2:B:124:THR:HG22	3:C:130:ARG:HH21	1.55	0.70
7:G:238:GLU:O	7:G:239:GLN:HB3	1.91	0.69
11:K:31:VAL:HG11	16:K:213:3OE:S3	2.32	0.69
3:C:203:THR:CG2	3:C:206:GLY:N	2.40	0.69
12:Z:40:ASN:HD21	12:Z:183:GLY:HA2	1.57	0.69
6:F:95:GLU:HG3	6:F:115:ARG:HH11	1.57	0.68
9:I:10:ASP:HB3	9:I:181:LYS:HE2	1.74	0.68
1:O:124:THR:CG2	2:P:130:ARG:HH21	2.06	0.68
5:E:132:TYR:O	5:E:153:PRO:HB3	1.94	0.67
5:S:73:HIS:HE1	5:S:107:LEU:O	1.77	0.67
14:N:67:THR:HA	14:N:72:GLY:O	1.93	0.67
5:E:207:LEU:HA	5:E:207(E):ASN:ND2	2.10	0.67
12:Z:144(O):LYS:HE3	12:Z:144(R):LYS:HD2	1.76	0.67
4:D:97:VAL:HG21	11:K:65:LEU:HD13	1.77	0.67
1:O:217(G):LEU:HD13	1:O:218:GLY:HA2	1.77	0.67
2:P:124:THR:HG22	3:Q:130:ARG:HH21	1.60	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:2:ILE:HB	10:J:17:SER:HB3	1.77	0.66
14:2:55:ILE:HD11	14:2:95:LEU:HD13	1.77	0.66
5:E:97:ASN:HD21	12:L:61:ASN:HD21	1.44	0.66
1:A:15:PHE:H	2:B:23:GLN:HE22	1.44	0.65
11:Y:196:PHE:HZ	11:Y:209:VAL:HG21	1.61	0.65
3:C:203:THR:CG2	3:C:206:GLY:H	1.94	0.65
1:O:124:THR:HG22	2:P:130:ARG:HH21	1.61	0.65
10:J:146:MET:HE2	10:J:150:GLU:HB3	1.79	0.65
9:W:110:ILE:HD12	9:W:125:ILE:HG12	1.79	0.64
13:1:157:ASN:HD22	13:1:160:ARG:HH11	1.45	0.64
2:B:181:LYS:O	2:B:184:MET:HG3	1.98	0.64
13:M:40:ASN:HD22	13:M:40:ASN:N	1.93	0.64
13:1:111:ARG:HH11	13:1:121:SER:HB2	1.62	0.64
6:T:95:GLU:HG3	6:T:115:ARG:HH11	1.62	0.64
3:Q:163:GLN:HE21	3:Q:163:GLN:HA	1.63	0.64
3:Q:52:ARG:HB2	3:Q:209:ASN:HD22	1.62	0.64
3:Q:171:THR:O	3:Q:174:GLU:HB3	1.98	0.63
2:P:156:ASN:OD1	3:Q:82:ASN:HB2	1.99	0.63
9:I:2:ILE:HG21	9:I:130:ALA:HB3	1.81	0.63
5:S:134:VAL:O	5:S:153:PRO:HG3	1.99	0.63
14:2:88:TYR:O	14:2:91:LYS:HG2	1.99	0.62
2:P:121:GLN:O	2:P:124:THR:HB	1.99	0.62
12:Z:144(P):PRO:CD	12:Z:144(R):LYS:HZ1	2.12	0.62
7:G:96:ALA:CA	7:G:107:MET:HE2	2.27	0.62
10:J:12:VAL:HG23	10:J:108:PRO:HB2	1.81	0.62
13:M:1:THR:HG23	13:M:2:SER:N	2.13	0.62
6:T:12:ASN:C	6:T:14:VAL:H	2.07	0.62
12:L:99:THR:HG23	12:L:113:PHE:HB2	1.80	0.62
6:T:179:LEU:HD11	6:T:192:GLN:HG2	1.81	0.62
3:Q:100:ARG:NH1	3:Q:106:PRO:HG3	2.14	0.61
7:U:123:TYR:CE1	7:U:129:MET:HE2	2.35	0.61
1:O:121:GLN:O	1:O:124:THR:HB	2.00	0.61
14:2:112:THR:HG22	14:2:120:HIS:HB2	1.83	0.61
12:L:4:LEU:CD1	12:L:138:LEU:HD21	2.31	0.61
12:L:40:ASN:HD21	12:L:183:GLY:HA2	1.66	0.61
1:O:15:PHE:H	2:P:23:GLN:HE22	1.48	0.60
8:H:128:GLY:O	8:H:131:SER:HB2	2.01	0.60
1:A:130:ARG:NH2	7:G:124:THR:HG22	2.14	0.60
4:R:123(D):ALA:HB3	4:R:126:ARG:HG3	1.83	0.60
1:A:7:ARG:HD2	5:E:127:TYR:HD2	1.67	0.60
1:O:7:ARG:HG3	6:T:128:SER:CB	2.23	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:-7:ASN:HD22	12:L:-6:PRO:HD2	1.65	0.60
7:U:107:MET:HE3	7:U:112:LEU:HD13	1.83	0.60
7:U:121:GLN:O	7:U:124:THR:HB	2.02	0.60
2:P:152:ASN:HB2	2:P:153:PRO:HD2	1.84	0.59
7:U:184(G):GLU:HG2	7:U:188:LYS:CB	2.32	0.59
14:N:175:MET:HB2	14:N:187:LEU:HB2	1.84	0.59
2:B:124:THR:CG2	3:C:130:ARG:HH21	2.15	0.59
6:T:192:GLN:HE21	6:T:192:GLN:HA	1.68	0.59
7:U:184(G):GLU:HG2	7:U:188:LYS:HB2	1.85	0.59
4:R:10:ARG:HD2	5:S:10:GLY:HA2	1.84	0.59
1:A:124:THR:HG22	2:B:130:ARG:HH21	1.67	0.59
7:G:105:TYR:OH	8:H:66:HIS:HE1	1.86	0.58
7:G:121:GLN:O	7:G:124:THR:HB	2.03	0.58
11:K:174:ASN:HD21	11:K:189:ASN:HD22	1.50	0.58
2:B:65:GLU:HG3	2:B:66:LYS:HG3	1.85	0.58
6:F:37:SER:HB3	6:F:50:VAL:HG23	1.85	0.58
12:L:43:MET:HG3	12:L:101:ILE:HG22	1.85	0.58
1:O:130:ARG:NH2	7:U:124:THR:HG22	2.08	0.58
7:G:224:LEU:HB3	7:G:228:ASN:HB2	1.85	0.58
2:B:13:THR:O	3:C:130:ARG:HD3	2.03	0.58
4:R:215:ILE:HG22	4:R:221:PHE:HD2	1.69	0.57
2:B:152:ASN:HB2	2:B:153:PRO:CD	2.35	0.57
6:F:35:THR:CG2	6:F:51:GLU:O	2.52	0.57
3:Q:201:VAL:O	3:Q:202:GLN:HB2	2.03	0.57
6:T:176:LEU:HB3	7:U:58:LEU:HD21	1.87	0.57
3:C:53:ARG:HG3	3:C:167:ARG:HH12	1.70	0.56
1:O:55:SER:O	1:O:56:SER:HB3	2.04	0.56
4:R:38:ILE:HD12	4:R:197:LEU:HG	1.86	0.56
8:H:50:ALA:HB2	9:I:118:CYS:HB2	1.86	0.56
13:M:39:ASP:HA	13:M:184:LEU:HD12	1.87	0.56
12:Z:34:VAL:HG12	12:Z:176:LEU:HD22	1.87	0.56
6:F:218(B):THR:HB	6:F:222:LYS:HE3	1.88	0.56
3:Q:100:ARG:HH11	3:Q:106:PRO:HG3	1.70	0.56
8:V:3:ILE:HG22	8:V:16:ALA:HB2	1.87	0.56
7:U:96:ALA:CA	7:U:107:MET:HE2	2.27	0.55
10:X:28:LYS:HE3	11:Y:121:LYS:O	2.06	0.55
5:E:207:LEU:N	5:E:207:LEU:CD2	2.69	0.55
6:T:186:ALA:O	6:T:190:VAL:HG23	2.06	0.55
1:A:97:HIS:HD2	8:H:61:SER:OG	1.90	0.55
2:B:38:ILE:HD12	2:B:197:LEU:HG	1.89	0.55
5:S:12:THR:HG21	5:S:124:THR:HA	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:12:THR:HG21	5:E:124:THR:HA	1.89	0.55
8:H:105:ASP:HB2	8:H:105(A):PRO:HD2	1.90	0.54
3:C:203:THR:CG2	3:C:207:ALA:H	2.16	0.54
9:W:2:ILE:HG21	9:W:130:ALA:HB3	1.90	0.54
14:N:149:GLU:CD	14:N:149:GLU:H	2.15	0.54
2:P:141:TYR:CD1	2:P:219(A):VAL:HG21	2.43	0.54
4:R:123(D):ALA:C	4:R:123(F):GLY:H	2.16	0.54
2:P:38:ILE:HD12	2:P:197:LEU:HG	1.89	0.54
13:1:40:ASN:H	13:1:40:ASN:HD22	1.55	0.54
14:N:55:ILE:HD11	14:N:95:LEU:HD13	1.90	0.53
4:D:123(B):GLU:N	4:D:126:ARG:HB2	2.23	0.53
7:U:87:ASN:C	7:U:87:ASN:HD22	2.16	0.53
2:P:54:VAL:HA	2:P:209:ARG:HH12	1.73	0.53
13:1:110:LEU:HG	13:1:125:LEU:HD12	1.90	0.53
12:Z:144(P):PRO:HD2	12:Z:144(R):LYS:HZ1	1.72	0.53
13:1:19:LEU:HB2	13:1:170:SER:HB2	1.90	0.53
14:2:175:MET:HB2	14:2:187:LEU:HB2	1.90	0.53
14:N:136:GLY:HA2	14:2:161:GLN:NE2	2.23	0.53
1:O:49:ALA:HB2	1:O:212:LEU:HG	1.91	0.53
13:1:7:LYS:HB3	13:1:12:VAL:HG12	1.91	0.53
6:F:203:GLU:O	6:F:206:LYS:HG3	2.08	0.53
10:X:2:ILE:HG12	10:X:130:SER:HB3	1.91	0.53
14:2:34:LEU:HD13	14:2:176:VAL:HG23	1.90	0.53
6:T:16:SER:OG	6:T:18:ASP:OD1	2.23	0.53
8:V:197:ARG:NH1	8:V:200:LYS:HD3	2.23	0.53
13:M:139:ARG:HH11	8:V:165:ASN:HD22	1.57	0.52
1:O:60:MET:HE3	1:O:63:THR:HG21	1.92	0.52
12:L:-2:ASN:HA	12:L:21:ILE:O	2.09	0.52
5:S:92:LEU:HD11	5:S:112:ALA:HB1	1.90	0.52
10:X:168:MET:HE2	10:X:170:PHE:HB3	1.91	0.52
3:C:216:LYS:HB2	3:C:220:ASP:HB3	1.92	0.52
10:J:2:ILE:HD12	10:J:162:LEU:HD13	1.91	0.52
9:W:12:VAL:HG13	9:W:108:PRO:HB3	1.91	0.52
10:X:6:ILE:HD12	10:X:124:TYR:HB3	1.92	0.52
4:D:90:GLU:OE2	11:K:69:ARG:NH1	2.42	0.52
13:1:133:MET:HE1	13:1:165:ARG:HG3	1.92	0.52
11:K:37:ILE:HG23	11:K:60:GLY:HA2	1.92	0.52
5:S:198:SER:C	5:S:200:SER:H	2.17	0.52
7:U:152:ASP:HB2	7:U:153:PRO:CD	2.40	0.52
12:Z:4:LEU:HD11	12:Z:138:LEU:HD21	1.92	0.52
12:L:7:ALA:HB2	12:L:110:VAL:HG23	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:R:123:PHE:HB3	4:R:128:MET:HE3	1.91	0.52
10:X:113:ILE:HA	10:X:118:THR:O	2.10	0.52
4:R:45:GLY:HA2	4:R:146:TYR:CE1	2.45	0.51
4:R:67:ILE:HG22	4:R:221:PHE:HZ	1.75	0.51
12:Z:-7:ASN:HD22	12:Z:-6:PRO:HD2	1.75	0.51
2:B:121:GLN:O	2:B:124:THR:HB	2.11	0.51
13:M:40:ASN:H	13:M:40:ASN:ND2	2.02	0.51
5:S:190:ILE:HG23	5:S:212:ILE:HG21	1.93	0.51
6:T:192:GLN:NE2	6:T:195:LYS:HE3	2.26	0.51
4:R:140:GLY:HA2	4:R:215:ILE:HG12	1.93	0.51
7:U:107:MET:CE	7:U:112:LEU:HD13	2.40	0.51
12:Z:178:VAL:HG22	12:Z:184:VAL:HG22	1.92	0.51
13:1:141(C):ARG:HG3	13:1:141(C):ARG:HH11	1.76	0.51
7:G:215:ALA:HB2	7:G:221:PHE:HD2	1.76	0.51
3:C:203:THR:HG22	3:C:207:ALA:N	2.18	0.51
5:E:168:ARG:HD3	5:E:202:ARG:HE	1.76	0.51
6:T:122:ALA:HA	6:T:125:LEU:HD12	1.92	0.51
14:2:13:ILE:HG12	14:2:177:VAL:HG13	1.92	0.51
2:B:152:ASN:HB2	2:B:153:PRO:HD2	1.93	0.50
9:I:99:PRO:HB2	9:I:113:PHE:CD2	2.46	0.50
10:J:34:THR:HG21	10:J:176:LYS:NZ	2.26	0.50
2:P:124:THR:CG2	3:Q:130:ARG:HH21	2.24	0.50
12:Z:-6:PRO:O	13:1:91:ARG:NH1	2.38	0.50
12:Z:-2:ASN:HA	12:Z:21:ILE:O	2.10	0.50
6:F:237:GLN:HE21	6:F:237:GLN:HA	1.76	0.50
7:G:238:GLU:O	7:G:239:GLN:CB	2.59	0.50
12:L:144(K):LYS:HD3	12:L:144(K):LYS:C	2.36	0.50
3:C:15:PHE:N	4:D:23:GLN:HE22	2.04	0.50
3:Q:215:VAL:HG12	3:Q:221:ILE:HG12	1.93	0.50
8:V:3:ILE:HG22	8:V:16:ALA:CB	2.40	0.50
8:V:126:SER:O	8:V:127:LEU:HD23	2.11	0.50
11:Y:104:TYR:CD1	11:Y:180:GLU:HA	2.46	0.50
8:V:172:ASN:HB3	8:V:192:LEU:O	2.10	0.50
1:A:7:ARG:HG2	6:F:128:SER:HB3	1.94	0.50
14:N:38:HIS:O	14:N:39:ASP:C	2.55	0.50
2:P:126:HIS:HB3	3:Q:129:VAL:HG12	1.93	0.50
11:Y:174:ASN:ND2	11:Y:186:TYR:OH	2.44	0.50
14:N:133:PHE:HE2	14:N:166:ASP:HB2	1.76	0.50
11:K:196:PHE:HZ	11:K:209:VAL:HG21	1.76	0.49
11:Y:31:VAL:HG11	16:Y:212:3OE:S3	2.52	0.49
2:P:78:VAL:HG22	2:P:136:PHE:CE2	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:45:ILE:HG12	13:M:99:ILE:HG12	1.93	0.49
6:T:38:ILE:HG12	6:T:197:ILE:HD11	1.94	0.49
6:T:126:TYR:HB2	6:T:129:VAL:HG22	1.93	0.49
5:S:63:TYR:O	5:S:64:GLN:O	2.30	0.49
5:E:226:GLY:O	5:E:229:VAL:HG22	2.13	0.49
12:L:14:LEU:HD13	12:L:34:VAL:HG13	1.95	0.49
13:M:40:ASN:N	13:M:40:ASN:ND2	2.61	0.49
5:S:97:ASN:HD21	12:Z:61:ASN:HD21	1.60	0.49
4:D:85:ALA:O	4:D:89:ILE:HG12	2.13	0.49
9:W:51:ASP:OD2	10:X:90(B):ARG:NH2	2.46	0.49
11:Y:7:ARG:HD2	11:Y:108:PRO:O	2.13	0.49
10:J:36:GLN:HG3	10:J:184:ILE:CD1	2.43	0.49
11:K:38:ASN:O	11:K:40:PHE:N	2.46	0.49
4:R:81:LEU:HD12	4:R:133:GLY:HA3	1.94	0.49
5:S:198:SER:HA	5:S:201:LEU:HD12	1.95	0.49
1:O:13:THR:O	2:P:130:ARG:HD3	2.13	0.48
13:1:11:GLY:HA3	13:1:178:ILE:O	2.13	0.48
5:S:97:ASN:HD21	12:Z:61:ASN:ND2	2.11	0.48
12:Z:40:ASN:ND2	12:Z:183:GLY:HA2	2.27	0.48
6:T:35:THR:HG21	6:T:51:GLU:O	2.13	0.48
7:U:87:ASN:C	7:U:87:ASN:ND2	2.70	0.48
8:V:105:ASP:HB2	8:V:105(A):PRO:CD	2.44	0.48
11:K:4:LEU:HD13	11:K:159:ILE:HD11	1.96	0.48
1:A:12:LEU:HD11	7:G:127:ALA:HB2	1.94	0.48
14:2:156:LYS:HG2	14:2:187(J):LEU:HD11	1.94	0.48
7:U:39:ALA:HB2	7:U:48:VAL:HG12	1.96	0.48
14:2:176:VAL:HG12	14:2:178:LEU:HD13	1.96	0.48
5:E:100:SER:O	5:E:104:ASN:HA	2.14	0.48
3:Q:172:VAL:HG23	3:Q:196:SER:HB2	1.96	0.48
12:L:-6:PRO:O	13:M:91:ARG:NH1	2.42	0.47
12:L:135:MET:HE3	9:W:165:ARG:NH2	2.29	0.47
2:B:204:SER:OG	2:B:209:ARG:NH2	2.48	0.47
5:S:139:ILE:HD12	5:S:215:VAL:HG12	1.94	0.47
12:Z:113:PHE:CD2	12:Z:119:TYR:HB3	2.49	0.47
2:P:97:GLN:HB3	9:W:61:TYR:CD2	2.49	0.47
4:R:121:LEU:O	4:R:123:PHE:N	2.43	0.47
5:S:194:VAL:O	5:S:197:ILE:HG22	2.14	0.47
1:A:217(G):LEU:HD13	1:A:218:GLY:HA2	1.95	0.47
6:T:179:LEU:HD21	6:T:192:GLN:HG2	1.96	0.47
8:H:100:ILE:HG13	8:H:127:LEU:HD12	1.97	0.47
6:F:42:CYS:HB2	6:F:184:LEU:O	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:S:148:LEU:HD21	5:S:163:THR:HG22	1.96	0.47
6:F:36:THR:HB	6:F:168:GLY:H	1.80	0.47
10:J:167:PRO:HB3	10:X:21:THR:HG21	1.96	0.47
11:K:129:SER:HB3	17:K:214:MES:H72	1.95	0.47
2:P:78:VAL:HG22	2:P:136:PHE:HE2	1.79	0.47
3:Q:105:ASP:OD2	3:Q:106:PRO:HD2	2.15	0.47
10:X:34:THR:HG21	10:X:176:LYS:NZ	2.30	0.47
7:G:179(D):SER:C	7:G:180(A):ILE:H	2.23	0.47
3:Q:33:ARG:NH1	3:Q:33:ARG:HB2	2.30	0.47
4:R:40:ILE:HD12	4:R:193:VAL:HG23	1.96	0.47
6:T:12:ASN:C	6:T:14:VAL:N	2.73	0.47
7:U:73:THR:HG22	7:U:218:ASP:HA	1.96	0.47
14:2:38:HIS:O	14:2:39:ASP:C	2.58	0.47
14:N:91:LYS:HE2	14:N:116:GLY:O	2.15	0.47
1:A:7:ARG:CG	6:F:128:SER:HB3	2.46	0.46
1:A:86:ARG:HE	7:G:118:ASN:ND2	2.13	0.46
3:C:172:VAL:HG23	3:C:196:SER:HB2	1.96	0.46
13:1:112:TYR:HE1	13:1:127:THR:HG22	1.80	0.46
1:O:67:VAL:HG11	1:O:213:ALA:CB	2.44	0.46
1:O:150:GLN:O	1:O:157:TYR:HA	2.15	0.46
2:P:147:GLN:HG2	3:Q:62(A):ILE:HG21	1.97	0.46
8:V:50:ALA:HB2	9:W:118:CYS:HB2	1.98	0.46
1:A:86:ARG:HE	7:G:118:ASN:HD21	1.63	0.46
7:U:184(G):GLU:HG2	7:U:188:LYS:HB3	1.97	0.46
6:F:180(E):GLU:H	6:F:180(E):GLU:CD	2.23	0.46
1:A:121:GLN:O	1:A:124:THR:HB	2.15	0.46
12:L:34:VAL:HG12	12:L:176:LEU:HD22	1.96	0.46
1:O:87:VAL:HG11	7:U:121:GLN:NE2	2.31	0.46
4:D:179:GLU:HB3	4:D:192:LEU:HD21	1.98	0.46
5:E:160:LEU:HD13	5:E:163:THR:HB	1.98	0.46
11:Y:37:ILE:HG23	11:Y:60:GLY:HA2	1.97	0.46
4:D:140:GLY:HA2	4:D:215:ILE:HG12	1.97	0.46
6:F:13:SER:HB2	7:G:130:ARG:HB3	1.97	0.46
7:G:59:LEU:O	7:G:61:PRO:HD3	2.15	0.46
13:M:133:MET:HE1	13:M:165:ARG:HG3	1.98	0.46
9:W:62:LYS:HD3	9:W:82:LEU:HD11	1.97	0.46
9:I:110:ILE:HD12	9:I:125:ILE:HG12	1.98	0.46
12:L:3:ILE:HG21	12:L:44:SER:OG	2.15	0.46
13:M:157:ASN:HD22	13:M:160:ARG:NH1	2.04	0.46
5:E:134:VAL:O	5:E:153:PRO:HG3	2.16	0.46
7:G:34(A):ASN:HD22	7:G:167:PRO:HG2	1.81	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:R:215:ILE:HG13	4:R:215:ILE:O	2.15	0.46
14:2:91:LYS:HE2	14:2:116:GLY:O	2.15	0.46
11:K:45:MET:C	16:K:213:3OE:H7A	2.41	0.46
3:Q:216:LYS:HB2	3:Q:220:ASP:HB3	1.97	0.46
13:1:80:PHE:CZ	13:1:111:ARG:HG2	2.51	0.46
1:A:7:ARG:HD2	5:E:127:TYR:CD2	2.47	0.45
9:W:121:GLU:HA	9:W:121:GLU:OE2	2.16	0.45
6:F:38:ILE:HG12	6:F:197:ILE:HD11	1.98	0.45
10:J:38:SER:HB2	10:J:39:PRO:HD2	1.98	0.45
11:Y:97:MET:HG2	11:Y:115:SER:HB3	1.97	0.45
10:J:113:ILE:HA	10:J:118:THR:O	2.15	0.45
3:Q:208:LYS:HD2	3:Q:208:LYS:O	2.15	0.45
9:I:33:LYS:O	9:I:44:GLY:HA2	2.17	0.45
9:W:33:LYS:O	9:W:44:GLY:HA2	2.17	0.45
10:X:141:HIS:CB	10:X:154:LEU:HD11	2.46	0.45
13:M:179:ASP:HB3	13:M:181(A):THR:HB	1.99	0.45
14:N:8:PHE:HB2	14:N:146:MET:O	2.16	0.45
1:O:97:HIS:HD2	8:V:61:SER:OG	1.99	0.45
2:P:67:LEU:HD22	2:P:211:GLU:HB3	1.98	0.45
11:Y:49:ALA:O	11:Y:53:GLN:HB2	2.17	0.45
12:Z:113:PHE:HA	12:Z:118:SER:O	2.17	0.45
1:A:112:LEU:O	1:A:116:VAL:HG23	2.16	0.45
1:A:150:GLN:O	1:A:157:TYR:HA	2.16	0.45
6:F:192:GLN:HE21	6:F:192:GLN:HA	1.82	0.45
7:G:179(C):LYS:HE3	7:G:179(C):LYS:HA	1.98	0.45
7:G:170:GLN:HE21	7:G:174:THR:HG23	1.82	0.45
13:M:-8:THR:O	13:M:-7:GLN:HB3	2.15	0.45
14:N:163:ILE:HG23	14:N:170:GLY:HA2	1.99	0.45
5:S:103:PHE:O	13:1:78:TYR:HA	2.16	0.45
4:R:162:ALA:HB1	4:R:176:LEU:HD22	1.99	0.45
8:V:112:SER:HB3	8:V:125:LEU:HD13	1.99	0.45
10:X:2:ILE:HD13	10:X:162:LEU:HD13	1.98	0.45
13:1:113:VAL:HA	13:1:118:VAL:O	2.17	0.45
5:E:207(B):THR:H	5:E:207(E):ASN:ND2	2.06	0.45
7:G:123:TYR:CE1	7:G:129:MET:HE2	2.52	0.45
13:M:84:ALA:HA	13:M:113:VAL:HG21	1.99	0.45
2:P:41:MET:HG2	2:P:46:ILE:HG12	1.98	0.45
12:Z:7:ALA:HB2	12:Z:110:VAL:HG23	1.99	0.45
12:Z:144(P):PRO:O	12:Z:144(R):LYS:N	2.50	0.45
8:H:38:SER:HB2	8:H:39:PRO:HD2	1.98	0.45
11:K:152:LEU:HD22	11:K:175:LEU:HD13	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:U:77:VAL:CG1	7:U:137:THR:HB	2.47	0.45
7:U:192:PHE:CD1	7:U:192:PHE:C	2.94	0.44
10:X:166:MET:HE3	10:X:168:MET:HE1	1.99	0.44
13:1:39:ASP:HA	13:1:184:LEU:HD12	1.99	0.44
1:A:5:THR:HB	1:A:7:ARG:HH21	1.82	0.44
9:I:182:ASP:OD1	9:I:182:ASP:N	2.50	0.44
10:J:168:MET:HE3	10:X:167:PRO:HB2	1.98	0.44
1:O:33:GLN:H	1:O:33:GLN:HG2	1.59	0.44
4:R:31:ILE:HD13	4:R:135:ALA:HB2	2.00	0.44
9:I:20:LEU:HB3	9:I:28:SER:HB3	1.99	0.44
10:J:24:ILE:HG12	10:J:24:ILE:O	2.17	0.44
6:T:82:ILE:HB	6:T:83:PRO:HD3	1.99	0.44
8:V:80:LEU:HD12	8:V:113:ILE:HD11	1.99	0.44
3:C:113:THR:HG21	3:C:149:TYR:HB3	1.99	0.44
7:G:184(G):GLU:HG2	7:G:188:LYS:CB	2.48	0.44
13:M:110:LEU:HG	13:M:125:LEU:HD12	1.98	0.44
5:S:207:LEU:HA	5:S:209:ASN:HD22	1.83	0.44
3:Q:35:THR:HB	3:Q:51:GLU:HG3	1.99	0.44
3:Q:206:GLY:HA2	3:Q:210:ILE:HD12	2.00	0.44
2:P:202:THR:HG22	2:P:204:SER:H	1.81	0.44
5:S:65:LYS:H	5:S:65:LYS:HG2	1.43	0.44
1:A:117:ALA:HB1	1:A:155:GLY:O	2.18	0.44
10:J:141:HIS:HB2	10:J:154:LEU:HD11	1.99	0.44
2:P:15:PHE:H	3:Q:23:GLN:HE22	1.64	0.44
5:S:141:TYR:CE2	5:S:217:LYS:HA	2.53	0.44
13:1:141(A):VAL:HG23	13:1:141(A):VAL:O	2.17	0.44
2:P:65:GLU:HG3	2:P:66:LYS:HG3	2.00	0.44
2:P:87:ILE:O	2:P:91:THR:HG23	2.18	0.43
3:Q:51:GLU:HA	3:Q:209:ASN:O	2.18	0.43
5:S:75:GLY:HA3	5:S:221:PHE:CZ	2.53	0.43
7:U:41:ARG:NH2	7:U:181:ASP:O	2.46	0.43
10:X:44:SER:OG	10:X:100:LEU:HB2	2.18	0.43
2:B:126:HIS:HB3	3:C:129:VAL:HG12	2.00	0.43
13:1:84:ALA:HA	13:1:113:VAL:HG21	1.99	0.43
3:Q:197:LEU:O	3:Q:201:VAL:HG23	2.19	0.43
4:R:186:LEU:O	4:R:190:GLU:HG3	2.18	0.43
3:C:17:PRO:HA	4:D:26:TYR:CD1	2.54	0.43
4:D:40:ILE:HD12	4:D:193:VAL:HG23	2.01	0.43
5:E:28:LEU:HD12	5:E:153:PRO:HD2	2.00	0.43
8:H:84:LYS:HG3	8:H:85:GLN:N	2.33	0.43
2:P:21:LEU:HD13	2:P:124:THR:HG23	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:1:112:TYR:O	13:1:119:THR:HA	2.19	0.43
5:S:17:PRO:HA	6:T:26:TYR:CD1	2.53	0.43
5:E:190:ILE:HG23	5:E:212:ILE:HG21	2.00	0.43
11:K:112:TYR:O	11:K:119:ARG:HA	2.19	0.43
13:M:122:SER:HB3	13:M:124:THR:O	2.18	0.43
1:O:39:GLY:HA2	1:O:47:VAL:O	2.19	0.43
3:Q:163:GLN:HE22	3:Q:173:ARG:HE	1.66	0.43
7:U:150:LYS:O	7:U:157:TYR:HA	2.18	0.43
11:Y:87:VAL:CG1	11:Y:115:SER:HA	2.49	0.43
10:J:36:GLN:HG3	10:J:184:ILE:HD13	2.00	0.43
13:M:3:VAL:HG23	13:M:46:SER:HB3	2.01	0.43
1:O:40:ILE:HD12	1:O:193:ALA:HB2	2.01	0.43
3:Q:17:PRO:HA	4:R:26:TYR:CD1	2.54	0.43
8:V:182:LYS:HB3	8:V:183:ASP:H	1.70	0.43
12:Z:144(O):LYS:HG3	12:Z:144(R):LYS:HZ2	1.76	0.43
13:1:157:ASN:HD22	13:1:160:ARG:NH1	2.15	0.43
11:K:86:LEU:C	11:K:86:LEU:HD13	2.44	0.43
5:S:71:ASP:HB3	5:S:73:HIS:CD2	2.54	0.43
7:U:70:ILE:HD11	7:U:76:MET:HE2	1.99	0.43
9:I:87:LEU:HD11	9:I:99:PRO:HG2	2.01	0.43
3:Q:57:LYS:HD2	3:Q:57:LYS:HA	1.73	0.43
4:R:161:ASN:HB3	4:R:180:TRP:CE2	2.53	0.43
11:Y:152:LEU:HD23	11:Y:175:LEU:HD22	1.99	0.43
2:B:147:GLN:HG2	3:C:62(A):ILE:HG21	2.01	0.43
11:K:196:PHE:CZ	11:K:209:VAL:HG21	2.53	0.43
3:Q:163:GLN:NE2	3:Q:164:THR:H	2.16	0.43
6:T:192:GLN:HA	6:T:192:GLN:NE2	2.34	0.43
7:U:109:CYS:HB2	7:U:140:SER:OG	2.19	0.43
4:D:161:ASN:HB3	4:D:180:TRP:CE2	2.54	0.42
1:O:217(P):LYS:N	1:O:217(P):LYS:HE3	2.33	0.42
6:T:194:ALA:O	6:T:198:TYR:HD1	2.02	0.42
8:V:172:ASN:HD22	8:V:193:THR:HA	1.84	0.42
10:J:17:SER:HB2	10:J:170:PHE:HB2	2.00	0.42
2:P:17:PRO:HA	3:Q:26:TYR:CD1	2.53	0.42
8:V:113:ILE:HG12	8:V:119:THR:HG22	2.01	0.42
4:D:67:ILE:HG22	4:D:221:PHE:HZ	1.83	0.42
9:I:181:LYS:HD2	9:I:181:LYS:N	2.25	0.42
14:N:14:LEU:O	14:N:175:MET:HA	2.19	0.42
9:W:113:PHE:HA	9:W:118:CYS:O	2.19	0.42
13:1:205:GLY:HA3	13:1:209:GLN:HB3	2.01	0.42
9:I:51:ASP:OD2	10:J:90(B):ARG:NH2	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:27:ALA:O	1:O:31:VAL:HG23	2.18	0.42
3:Q:163:GLN:HE21	3:Q:163:GLN:CA	2.30	0.42
3:Q:207:ALA:C	3:Q:209:ASN:H	2.27	0.42
7:U:78:VAL:HG11	7:U:85:ALA:HB2	2.02	0.42
10:X:90(A):ILE:HD12	10:X:90(A):ILE:HA	1.89	0.42
8:H:8:PHE:HB3	8:H:151:ALA:HB2	2.00	0.42
13:1:-5:PRO:HD3	13:1:96:TRP:CE2	2.54	0.42
8:H:172:ASN:HD22	8:H:193:THR:HA	1.83	0.42
13:M:11:GLY:HA3	13:M:178:ILE:O	2.19	0.42
4:R:227:GLU:H	4:R:227:GLU:CD	2.27	0.42
9:W:87:LEU:HD11	9:W:99:PRO:HG2	2.00	0.42
11:Y:196:PHE:CZ	11:Y:209:VAL:HG21	2.49	0.42
12:Z:99:THR:HG23	12:Z:113:PHE:HB2	2.02	0.42
13:1:-8:THR:N	13:1:92(B):MET:O	2.53	0.42
1:A:10:PHE:O	1:A:127:GLY:HA2	2.19	0.42
7:G:151:THR:HG22	7:G:157:TYR:HB3	2.01	0.42
10:J:6:ILE:HD11	10:J:8:VAL:HG13	2.02	0.42
10:J:178:VAL:HG22	10:J:184:ILE:HG12	2.02	0.42
2:B:141:TYR:CD1	2:B:219(E):VAL:HG21	2.55	0.42
9:I:165:ARG:NH2	12:Z:135:MET:HE3	2.35	0.42
10:X:166:MET:HA	10:X:167:PRO:HD3	1.90	0.42
7:G:184(G):GLU:HG2	7:G:188:LYS:HB2	2.02	0.42
10:J:2:ILE:HD13	10:J:130:SER:HB3	2.02	0.42
10:J:9:GLN:HE21	10:J:9:GLN:HB3	1.67	0.42
6:T:35:THR:CG2	6:T:51:GLU:O	2.67	0.42
11:Y:22:ALA:O	11:Y:25:TRP:HB3	2.20	0.42
2:B:67:LEU:HD22	2:B:211:GLU:HB3	2.02	0.41
4:D:45:GLY:HA2	4:D:146:TYR:CE1	2.55	0.41
9:I:48:LEU:HG	9:I:50:THR:HG22	2.01	0.41
11:K:174:ASN:ND2	11:K:189:ASN:HD22	2.15	0.41
1:O:67:VAL:HG11	1:O:213:ALA:HB3	2.01	0.41
5:S:52:LYS:HD2	5:S:63:TYR:O	2.20	0.41
4:D:122:ARG:HA	4:D:126:ARG:HD3	2.01	0.41
9:I:101:VAL:O	9:I:110:ILE:HA	2.20	0.41
12:L:144(A):LYS:C	12:L:144(C):GLN:H	2.28	0.41
1:O:79:SER:HB2	1:O:165:ILE:HD12	2.01	0.41
8:V:101:VAL:HG13	8:V:111:PHE:HB2	2.02	0.41
10:X:178:VAL:HG22	10:X:184:ILE:HG12	2.02	0.41
3:C:163:GLN:HE21	3:C:163:GLN:HA	1.85	0.41
6:F:225:LYS:HD3	6:F:225:LYS:H	1.84	0.41
2:P:137:ILE:HD11	2:P:165:VAL:HG22	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:Y:86:LEU:C	11:Y:86:LEU:HD13	2.46	0.41
14:2:146:MET:HE2	14:2:150:GLU:HB3	2.03	0.41
1:A:67:VAL:HG11	1:A:213:ALA:CB	2.50	0.41
11:K:100:MET:SD	11:K:125:PHE:HB2	2.60	0.41
13:M:103:GLY:HA2	13:M:178:ILE:HD13	2.02	0.41
2:B:149:TYR:OH	3:C:62(A):ILE:HB	2.20	0.41
14:N:84:LYS:HG3	14:N:119:VAL:HG22	2.01	0.41
8:V:172:ASN:ND2	8:V:193:THR:HA	2.35	0.41
9:W:181:LYS:H	9:W:181:LYS:HD2	1.86	0.41
1:A:212:LEU:HD22	1:A:224:LEU:HD12	2.02	0.41
2:B:81:LEU:HD23	2:B:133:GLY:HA3	2.02	0.41
5:E:103:PHE:O	13:M:78:TYR:HA	2.21	0.41
8:H:63:ILE:HG23	8:H:74:PRO:HB3	2.02	0.41
7:U:65:SER:HA	7:U:211:GLU:OE2	2.21	0.41
10:X:24:ILE:O	10:X:24:ILE:HG12	2.21	0.41
10:X:141:HIS:HB2	10:X:154:LEU:HD11	2.02	0.41
2:B:215:ILE:HG12	2:B:221:GLN:HG2	2.01	0.41
4:D:123(D):ALA:O	4:D:123(E):SER:C	2.63	0.41
5:E:54:ASN:ND2	5:E:56:ASP:O	2.53	0.41
1:O:78:TYR:HB3	1:O:85:TYR:CD1	2.55	0.41
5:S:75:GLY:HA3	5:S:221:PHE:CE2	2.56	0.41
12:Z:144:PHE:CE2	12:Z:144(R):LYS:HG3	2.55	0.41
13:1:1:THR:CG2	13:1:2:SER:H	2.16	0.41
7:G:169:GLN:HE21	7:G:169:GLN:HB3	1.73	0.41
13:M:17:ASP:HA	13:M:173:PHE:CB	2.50	0.41
14:N:133:PHE:CE2	14:N:166:ASP:HB2	2.55	0.41
14:N:161:GLN:NE2	14:2:136:GLY:HA2	2.28	0.41
4:R:85:ALA:O	4:R:89:ILE:HG12	2.21	0.41
5:S:65:LYS:HB3	5:S:65:LYS:HE2	1.53	0.41
7:U:105:TYR:OH	8:V:66:HIS:HE1	2.02	0.41
9:W:20:LEU:HB3	9:W:28:SER:HB3	2.03	0.41
12:Z:4:LEU:CD1	12:Z:138:LEU:HD21	2.51	0.41
12:Z:90:LYS:HD3	12:Z:95:TYR:CE1	2.56	0.41
2:B:97:GLN:HE22	9:I:64:ASN:HD22	1.68	0.41
6:F:192:GLN:HA	6:F:192:GLN:NE2	2.36	0.41
10:J:168:MET:HA	10:X:168:MET:HA	2.03	0.41
13:M:141(A):VAL:HG23	13:M:141(A):VAL:O	2.20	0.41
4:R:37:ALA:HB3	4:R:165:ILE:HG13	2.03	0.41
4:R:51:GLU:HG3	4:R:201:MET:HE3	2.03	0.41
5:S:114:HIS:HB3	6:T:86:ARG:NH2	2.36	0.41
6:T:31:VAL:HG11	6:T:135:SER:HB2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:Z:144(N):LYS:O	12:Z:144(O):LYS:C	2.64	0.41
2:P:150:THR:O	2:P:157:TYR:HA	2.20	0.41
6:T:95:GLU:HG2	6:T:115:ARG:CB	2.44	0.41
9:W:48:LEU:HG	9:W:50:THR:HG22	2.03	0.41
2:B:150:THR:O	2:B:157:TYR:HA	2.21	0.40
12:Z:134:ILE:HG22	12:Z:138:LEU:HD22	2.02	0.40
3:C:41:LYS:HG2	3:C:161:SER:O	2.22	0.40
3:C:207:ALA:C	3:C:209:ASN:H	2.29	0.40
5:E:97:ASN:ND2	12:L:61:ASN:HD21	2.16	0.40
8:H:189:ARG:O	8:H:190:ASN:C	2.64	0.40
5:E:105:ARG:HG3	13:M:78:TYR:CZ	2.56	0.40
4:R:123:PHE:O	4:R:123:PHE:CD2	2.75	0.40
6:T:70:VAL:HG11	6:T:112:PHE:CE1	2.56	0.40
7:U:152:ASP:HB2	7:U:153:PRO:HD2	2.02	0.40
11:Y:104:TYR:CE1	11:Y:180:GLU:HA	2.57	0.40
1:A:124:THR:CG2	2:B:130:ARG:HH21	2.31	0.40
3:C:53:ARG:HG3	3:C:167:ARG:NH1	2.36	0.40
6:F:176:LEU:HB3	7:G:58:LEU:HD21	2.02	0.40
9:I:99:PRO:HB2	9:I:113:PHE:HD2	1.87	0.40
11:K:56:GLU:OE2	11:K:99:THR:OG1	2.36	0.40
2:P:190:ILE:HG23	2:P:212:PHE:CE2	2.57	0.40
6:T:206:LYS:HB2	6:T:206:LYS:HE3	1.83	0.40
7:U:78:VAL:HG11	7:U:85:ALA:CB	2.52	0.40
10:X:137:LEU:HD21	10:X:157:LEU:HB3	2.04	0.40
11:Y:114:ASP:OD1	11:Y:114:ASP:C	2.64	0.40
7:G:67:ILE:HD12	7:G:211:GLU:HG2	2.03	0.40
8:H:48:THR:HB	8:H:51:ASP:HB2	2.02	0.40
9:I:55:LEU:HA	9:I:55:LEU:HD23	1.85	0.40
13:M:112:TYR:HE1	13:M:127:THR:HG22	1.87	0.40
10:X:120:VAL:HG13	10:X:122:LEU:HG	2.03	0.40
12:Z:43:MET:HG3	12:Z:101:ILE:HG22	2.02	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%)	238 (96%)	8 (3%)	2 (1%)	16	31
1	O	248/250 (99%)	236 (95%)	10 (4%)	2 (1%)	16	31
2	B	233/235 (99%)	223 (96%)	7 (3%)	3 (1%)	9	21
2	P	233/235 (99%)	219 (94%)	11 (5%)	3 (1%)	9	21
3	C	239/241 (99%)	231 (97%)	6 (2%)	2 (1%)	16	31
3	Q	239/241 (99%)	226 (95%)	9 (4%)	4 (2%)	7	16
4	D	240/260 (92%)	222 (92%)	14 (6%)	4 (2%)	7	16
4	R	240/260 (92%)	227 (95%)	11 (5%)	2 (1%)	16	31
5	E	231/233 (99%)	217 (94%)	10 (4%)	4 (2%)	7	16
5	S	231/233 (99%)	212 (92%)	14 (6%)	5 (2%)	5	12
6	F	235/242 (97%)	224 (95%)	10 (4%)	1 (0%)	30	48
6	T	235/242 (97%)	225 (96%)	10 (4%)	0	100	100
7	G	241/243 (99%)	233 (97%)	7 (3%)	1 (0%)	30	48
7	U	241/243 (99%)	234 (97%)	5 (2%)	2 (1%)	16	31
8	H	220/222 (99%)	210 (96%)	9 (4%)	1 (0%)	24	42
8	V	220/222 (99%)	212 (96%)	8 (4%)	0	100	100
9	I	202/204 (99%)	194 (96%)	8 (4%)	0	100	100
9	W	202/204 (99%)	198 (98%)	4 (2%)	0	100	100
10	J	196/198 (99%)	187 (95%)	8 (4%)	1 (0%)	24	42
10	X	195/198 (98%)	184 (94%)	9 (5%)	2 (1%)	12	25
11	K	210/212 (99%)	204 (97%)	4 (2%)	2 (1%)	12	25
11	Y	210/212 (99%)	201 (96%)	7 (3%)	2 (1%)	12	25
12	L	220/222 (99%)	208 (94%)	12 (6%)	0	100	100
12	Z	220/222 (99%)	209 (95%)	10 (4%)	1 (0%)	24	42
13	1	231/233 (99%)	220 (95%)	11 (5%)	0	100	100
13	M	231/233 (99%)	220 (95%)	10 (4%)	1 (0%)	30	48
14	2	194/196 (99%)	188 (97%)	6 (3%)	0	100	100
14	N	194/196 (99%)	186 (96%)	8 (4%)	0	100	100
All	All	6279/6382 (98%)	5988 (95%)	246 (4%)	45 (1%)	18	35

All (45) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	217	ALA
3	C	203	THR
3	C	207	ALA
4	D	123(E)	SER
5	E	203	ASP
6	F	184	LEU
7	G	239	GLN
11	K	39	PRO
1	O	53	LYS
2	P	54	VAL
2	P	217	ALA
3	Q	202	GLN
5	S	64	GLN
5	S	203	ASP
5	S	206	SER
2	B	54	VAL
5	E	6	ASN
8	H	91	GLN
3	Q	207	ALA
5	S	199	GLN
1	A	5	THR
2	B	218(C)	ASP
4	D	123(B)	GLU
5	E	217	LYS
2	P	218(B)	ASP
4	R	123(E)	SER
4	R	128	MET
5	S	6	ASN
7	U	239	GLN
10	X	189	ASP
11	Y	39	PRO
12	Z	144(Q)	LEU
5	E	206	SER
1	O	56	SER
3	Q	183	PRO
1	A	167	LYS
4	D	123(G)	GLU
11	K	9	GLN
3	Q	208	LYS
7	U	55	PRO
13	M	-7	GLN
11	Y	146	LEU
10	X	8	VAL

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Mol	Chain	Res	Type
10	J	8	VAL
4	D	123(F)	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%)	197 (94%)	12 (6%)	18	39
1	O	209/209 (100%)	197 (94%)	12 (6%)	18	39
2	B	195/195 (100%)	180 (92%)	15 (8%)	12	25
2	P	195/195 (100%)	182 (93%)	13 (7%)	15	31
3	C	213/213 (100%)	200 (94%)	13 (6%)	17	35
3	Q	213/213 (100%)	198 (93%)	15 (7%)	14	29
4	D	198/215 (92%)	185 (93%)	13 (7%)	15	32
4	R	198/215 (92%)	182 (92%)	16 (8%)	11	23
5	E	192/192 (100%)	174 (91%)	18 (9%)	8	18
5	S	191/192 (100%)	176 (92%)	15 (8%)	11	24
6	F	196/200 (98%)	179 (91%)	17 (9%)	9	21
6	T	196/200 (98%)	182 (93%)	14 (7%)	13	28
7	G	207/207 (100%)	191 (92%)	16 (8%)	12	25
7	U	207/207 (100%)	196 (95%)	11 (5%)	20	42
8	H	181/181 (100%)	169 (93%)	12 (7%)	15	32
8	V	181/181 (100%)	170 (94%)	11 (6%)	17	35
9	I	172/172 (100%)	166 (96%)	6 (4%)	32	57
9	W	172/172 (100%)	164 (95%)	8 (5%)	23	47
10	J	174/175 (99%)	160 (92%)	14 (8%)	11	24
10	X	174/175 (99%)	164 (94%)	10 (6%)	18	39
11	K	169/169 (100%)	160 (95%)	9 (5%)	20	42
11	Y	169/169 (100%)	159 (94%)	10 (6%)	18	37

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
12	L	185/185 (100%)	180 (97%)	5 (3%)	39	63
12	Z	185/185 (100%)	180 (97%)	5 (3%)	39	63
13	1	199/199 (100%)	191 (96%)	8 (4%)	28	53
13	M	199/199 (100%)	191 (96%)	8 (4%)	28	53
14	2	162/162 (100%)	154 (95%)	8 (5%)	22	45
14	N	162/162 (100%)	156 (96%)	6 (4%)	30	55
All	All	5303/5348 (99%)	4983 (94%)	320 (6%)	17	36

All (320) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	MET
1	A	5	THR
1	A	33	GLN
1	A	62	GLU
1	A	64	LEU
1	A	65	SER
1	A	124	THR
1	A	158	PHE
1	A	199	GLU
1	A	203	GLU
1	A	212	LEU
1	A	236	LEU
2	B	18	GLU
2	B	53	LYS
2	B	58	LEU
2	B	61	GLN
2	B	67	LEU
2	B	91	THR
2	B	124	THR
2	B	150	THR
2	B	185	LYS
2	B	186	VAL
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

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Mol	Chain	Res	Type
3	C	44	ASN
3	C	57	LYS
3	C	107	VAL
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	203	THR
3	C	227	GLU
4	D	48	LEU
4	D	52	LYS
4	D	59	LEU
4	D	76	CYS
4	D	110	GLU
4	D	119	LEU
4	D	125	GLU
4	D	177	LEU
4	D	191	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	76	LEU
5	E	97	ASN
5	E	149	LEU
5	E	160	LEU
5	E	179	THR
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

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Mol	Chain	Res	Type
6	F	35	THR
6	F	36	THR
6	F	43	ASN
6	F	59	LEU
6	F	72	ARG
6	F	121	GLN
6	F	129	VAL
6	F	169	ARG
6	F	176	LEU
6	F	192	GLN
6	F	199	LEU
6	F	206	LYS
6	F	206(B)	GLU
6	F	206(C)	LYS
6	F	222	LYS
6	F	225	LYS
6	F	237	GLN
7	G	33	GLN
7	G	38	LEU
7	G	48	VAL
7	G	49	ILE
7	G	87	ASN
7	G	119	LEU
7	G	124	THR
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	217	LYS
7	G	232	ARG
7	G	233	LEU
8	H	7	LYS
8	H	13	VAL
8	H	34	LEU
8	H	56	THR
8	H	63	ILE
8	H	68	LEU
8	H	101	VAL
8	H	120	ASP
8	H	144	GLN

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Mol	Chain	Res	Type
8	H	153	LYS
8	H	196	VAL
8	H	222	CYS
9	I	4	VAL
9	I	121	GLU
9	I	160	LEU
9	I	181	LYS
9	I	182	ASP
9	I	185	VAL
10	J	6	ILE
10	J	9	GLN
10	J	24	ILE
10	J	34	THR
10	J	35	ARG
10	J	51	ASP
10	J	52	THR
10	J	68	ILE
10	J	70	GLU
10	J	137	LEU
10	J	155	LEU
10	J	160	GLN
10	J	168	MET
10	J	191	GLN
11	K	4	LEU
11	K	65	LEU
11	K	69	ARG
11	K	87	VAL
11	K	97	MET
11	K	99	THR
11	K	156	LYS
11	K	185	ILE
11	K	201	GLU
12	L	-9	GLN
12	L	14	LEU
12	L	40	ASN
12	L	99	THR
12	L	138	LEU
13	M	-8	THR
13	M	2	SER
13	M	40	ASN
13	M	62	LEU
13	M	65	GLU

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Mol	Chain	Res	Type
13	M	91	ARG
13	M	149	GLN
13	M	184	LEU
14	N	20	THR
14	N	31	THR
14	N	107	LYS
14	N	115	LEU
14	N	119	VAL
14	N	132	THR
1	O	4	MET
1	O	33	GLN
1	O	62	GLU
1	O	64	LEU
1	O	87	VAL
1	O	111	LEU
1	O	124	THR
1	O	158	PHE
1	O	165	ILE
1	O	167	LYS
1	O	222	ARG
1	O	223	LYS
2	P	57	THR
2	P	58	LEU
2	P	64	THR
2	P	91	THR
2	P	124	THR
2	P	150	THR
2	P	185	LYS
2	P	192	LEU
2	P	198	SER
2	P	202	THR
2	P	225	LYS
2	P	232	ILE
2	P	235	LYS
3	Q	25	GLU
3	Q	35	THR
3	Q	61	THR
3	Q	66	LYS
3	Q	100	ARG
3	Q	112	LEU
3	Q	150	GLN
3	Q	156	ILE

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Mol	Chain	Res	Type
3	Q	163	GLN
3	Q	172	VAL
3	Q	185	THR
3	Q	193	THR
3	Q	199	GLU
3	Q	224	LEU
3	Q	240	LYS
4	R	13	SER
4	R	28	LEU
4	R	33	LEU
4	R	48	LEU
4	R	52	LYS
4	R	59	LEU
4	R	62	ASP
4	R	119	LEU
4	R	122	ARG
4	R	177	LEU
4	R	184	LEU
4	R	194	LEU
4	R	215	ILE
4	R	218	GLN
4	R	237	LEU
4	R	238	LYS
5	S	12	THR
5	S	13	VAL
5	S	18	THR
5	S	33	GLN
5	S	58	LEU
5	S	64	GLN
5	S	65	LYS
5	S	76	LEU
5	S	97	ASN
5	S	178	ARG
5	S	189	LEU
5	S	199	GLN
5	S	204	GLU
5	S	207	LEU
5	S	211	SER
6	T	25	GLU
6	T	35	THR
6	T	36	THR
6	T	43	ASN

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Mol	Chain	Res	Type
6	T	63	LYS
6	T	95	GLU
6	T	98	SER
6	T	135	SER
6	T	169	ARG
6	T	176	LEU
6	T	187	ARG
6	T	192	GLN
6	T	222	LYS
6	T	225	LYS
7	U	38	LEU
7	U	43	LYS
7	U	49	ILE
7	U	87	ASN
7	U	119	LEU
7	U	174	THR
7	U	197	MET
7	U	217	LYS
7	U	227	GLU
7	U	232	ARG
7	U	233	LEU
8	V	3	ILE
8	V	13	VAL
8	V	34	LEU
8	V	55	VAL
8	V	56	THR
8	V	63	ILE
8	V	68	LEU
8	V	144	GLN
8	V	149	GLU
8	V	192	LEU
8	V	222	CYS
9	W	-8	SER
9	W	12	VAL
9	W	20	LEU
9	W	32	GLU
9	W	107	LYS
9	W	121	GLU
9	W	160	LEU
9	W	181	LYS
10	X	6	ILE
10	X	22	ARG

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Mol	Chain	Res	Type
10	X	34	THR
10	X	35	ARG
10	X	52	THR
10	X	68	ILE
10	X	120	VAL
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	84	SER
11	Y	87	VAL
11	Y	146	LEU
11	Y	200	LYS
11	Y	208	ASN
12	Z	14	LEU
12	Z	40	ASN
12	Z	98	HIS
12	Z	99	THR
12	Z	138	LEU
13	1	2	SER
13	1	40	ASN
13	1	62	LEU
13	1	91	ARG
13	1	148	VAL
13	1	184	LEU
13	1	190	LEU
13	1	204	LYS
14	2	9	LYS
14	2	20	THR
14	2	36	ARG
14	2	112	THR
14	2	119	VAL
14	2	132	THR
14	2	149	GLU
14	2	178	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (195) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	97	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	177	GLN
2	B	218	ASN
3	C	23	GLN
3	C	82	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	99	HIS
4	D	108	ASN
4	D	114	GLN
4	D	161	ASN
4	D	226	ASN
5	E	7	ASN
5	E	64	GLN
5	E	73	HIS
5	E	104	ASN
5	E	114	HIS
5	E	121	GLN
5	E	125	GLN
5	E	170	GLN
5	E	185	ASN
5	E	207(E)	ASN
6	F	43	ASN
6	F	90	ASN
6	F	121	GLN
6	F	205	ASN
6	F	237	GLN
7	G	34(A)	ASN
7	G	87	ASN
7	G	118	ASN
7	G	121	GLN
7	G	125	GLN

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Mol	Chain	Res	Type
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	141	HIS
8	H	144	GLN
8	H	165	ASN
8	H	172	ASN
8	H	190	ASN
9	I	23	GLN
9	I	29	ASN
9	I	56	ASN
9	I	161	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	186	GLN
11	K	85	ASN
11	K	141	ASN
11	K	174	ASN
11	K	207	ASN
12	L	-7	ASN
12	L	40	ASN
12	L	46	ASN
12	L	61	ASN
12	L	67	HIS
12	L	70(A)	ASN
12	L	123	GLN
12	L	144(B)	ASN
12	L	166	HIS
12	L	168	GLN
13	M	-7	GLN
13	M	18	ASN
13	M	40	ASN
13	M	89	GLN

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Mol	Chain	Res	Type
13	M	93	ASN
13	M	105	GLN
13	M	149	GLN
13	M	157	ASN
13	M	191	GLN
14	N	28	ASN
14	N	38	HIS
14	N	62	HIS
14	N	69	GLN
14	N	141	ASN
14	N	157	HIS
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	126	HIS
2	P	177	GLN
3	Q	23	GLN
3	Q	44	ASN
3	Q	82	ASN
3	Q	121	GLN
3	Q	125	GLN
3	Q	150	GLN
3	Q	163	GLN
3	Q	209	ASN
4	R	23	GLN
4	R	99	HIS
4	R	108	ASN
4	R	114	GLN
4	R	141	HIS
4	R	147	GLN
4	R	199	GLN
4	R	211	GLN
4	R	226	ASN
5	S	7	ASN
5	S	73	HIS
5	S	95	GLN
5	S	104	ASN

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Mol	Chain	Res	Type
5	S	121	GLN
5	S	125	GLN
5	S	170	GLN
5	S	185	ASN
5	S	209	ASN
6	T	43	ASN
6	T	90	ASN
6	T	121	GLN
6	T	147	HIS
6	T	205	ASN
6	T	241	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	178	ASN
7	U	184	ASN
8	V	30	ASN
8	V	35	HIS
8	V	66	HIS
8	V	86	HIS
8	V	165	ASN
8	V	172	ASN
8	V	190	ASN
9	W	23	GLN
9	W	29	ASN
9	W	56	ASN
9	W	81	GLN
10	X	36	GLN
10	X	54	GLN
10	X	62	ASN
10	X	77	GLN
10	X	96	GLN
10	X	106	ASN
10	X	140	HIS
10	X	141	HIS
10	X	186	GLN
11	Y	9	GLN
11	Y	85	ASN
11	Y	131	GLN

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Mol	Chain	Res	Type
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	61	ASN
12	Z	70(A)	ASN
12	Z	77	ASN
12	Z	144(J)	ASN
12	Z	166	HIS
13	1	-7	GLN
13	1	10	ASN
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	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
16	3OE	K	213	-	46,46,46	1.12	2 (4%)	58,61,61	1.05	4 (6%)
17	MES	Y	213	-	12,12,12	2.19	1 (8%)	15,16,16	1.20	1 (6%)
16	3OE	Y	212	-	46,46,46	1.11	2 (4%)	58,61,61	1.10	5 (8%)
17	MES	K	214	-	12,12,12	2.20	1 (8%)	15,16,16	1.20	1 (6%)

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	3OE	K	213	-	-	2/39/39/39	0/4/4/4
17	MES	Y	213	-	-	3/6/14/14	0/1/1/1
16	3OE	Y	212	-	-	6/39/39/39	0/4/4/4
17	MES	K	214	-	-	5/6/14/14	0/1/1/1

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	K	214	MES	C8-S	-7.30	1.67	1.77
17	Y	213	MES	C8-S	-7.26	1.67	1.77
16	K	213	3OE	C36-C37	-4.81	1.39	1.50
16	Y	212	3OE	C36-C37	-4.47	1.40	1.50
16	K	213	3OE	C5-C6	-2.72	1.35	1.42
16	Y	212	3OE	C5-C6	-2.72	1.35	1.42

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	Y	212	3OE	O35-C36-C37	4.12	121.27	109.16
16	K	213	3OE	C4-S3-C1	3.98	96.38	92.08
16	Y	212	3OE	C4-S3-C1	3.78	96.16	92.08
17	Y	213	MES	O3S-S-C8	3.05	111.97	106.00
16	K	213	3OE	C5-C6-C1	2.92	115.92	111.82
16	K	213	3OE	C5-C4-S3	-2.90	107.67	112.86
16	Y	212	3OE	C5-C4-S3	-2.87	107.71	112.86
17	K	214	MES	O3S-S-C8	2.83	111.54	106.00
16	Y	212	3OE	C5-C6-C1	2.79	115.74	111.82
16	K	213	3OE	O35-C36-C37	2.56	116.68	109.16
16	Y	212	3OE	C36-O35-C32	-2.02	112.81	117.62

There are no chirality outliers.

All (16) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
17	K	214	MES	C7-C8-S-O1S
17	K	214	MES	C7-C8-S-O3S
17	Y	213	MES	C7-C8-S-O1S
17	Y	213	MES	C7-C8-S-O2S
16	Y	212	3OE	O28-C27-C8-C34
16	Y	212	3OE	O28-C27-C8-C30
16	Y	212	3OE	N18-C27-C8-C30
16	Y	212	3OE	N18-C27-C8-C34
17	Y	213	MES	C7-C8-S-O3S
16	Y	212	3OE	C33-C32-O35-C36
16	Y	212	3OE	C31-C32-O35-C36
17	K	214	MES	C8-C7-N4-C3
16	K	213	3OE	C33-C32-O35-C36
17	K	214	MES	C7-C8-S-O2S
16	K	213	3OE	C31-C32-O35-C36
17	K	214	MES	C8-C7-N4-C5

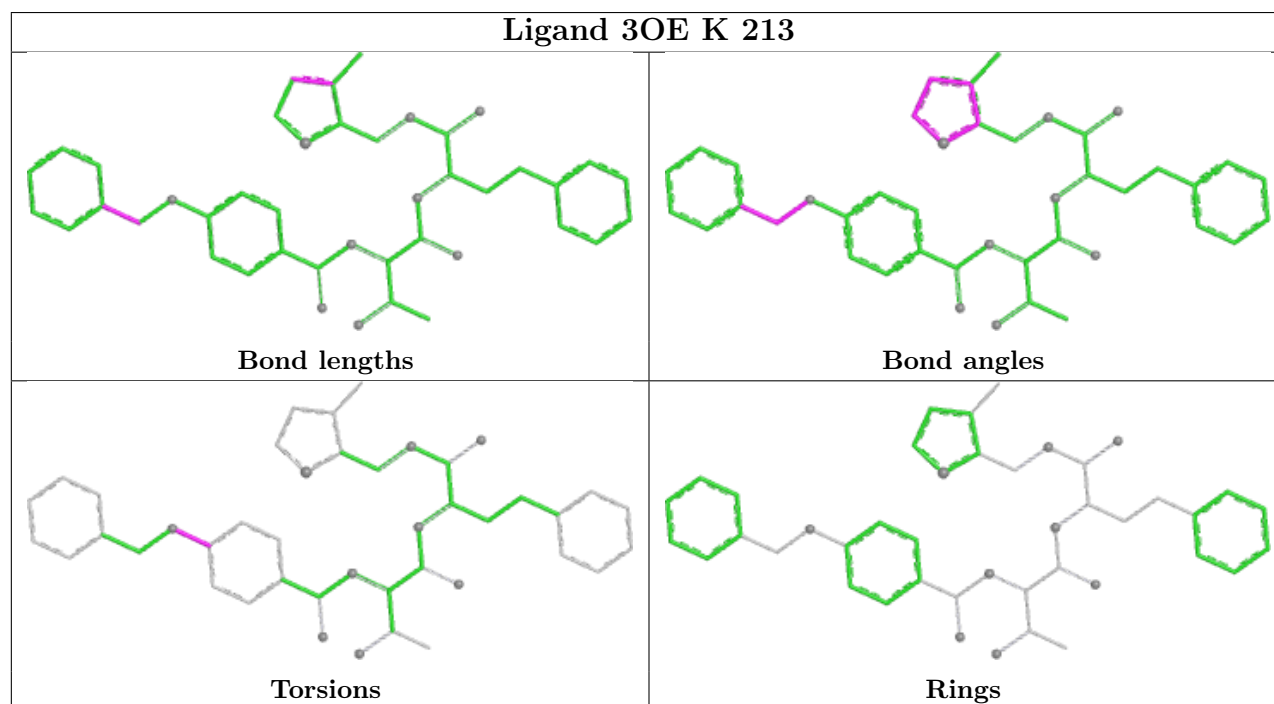
There are no ring outliers.

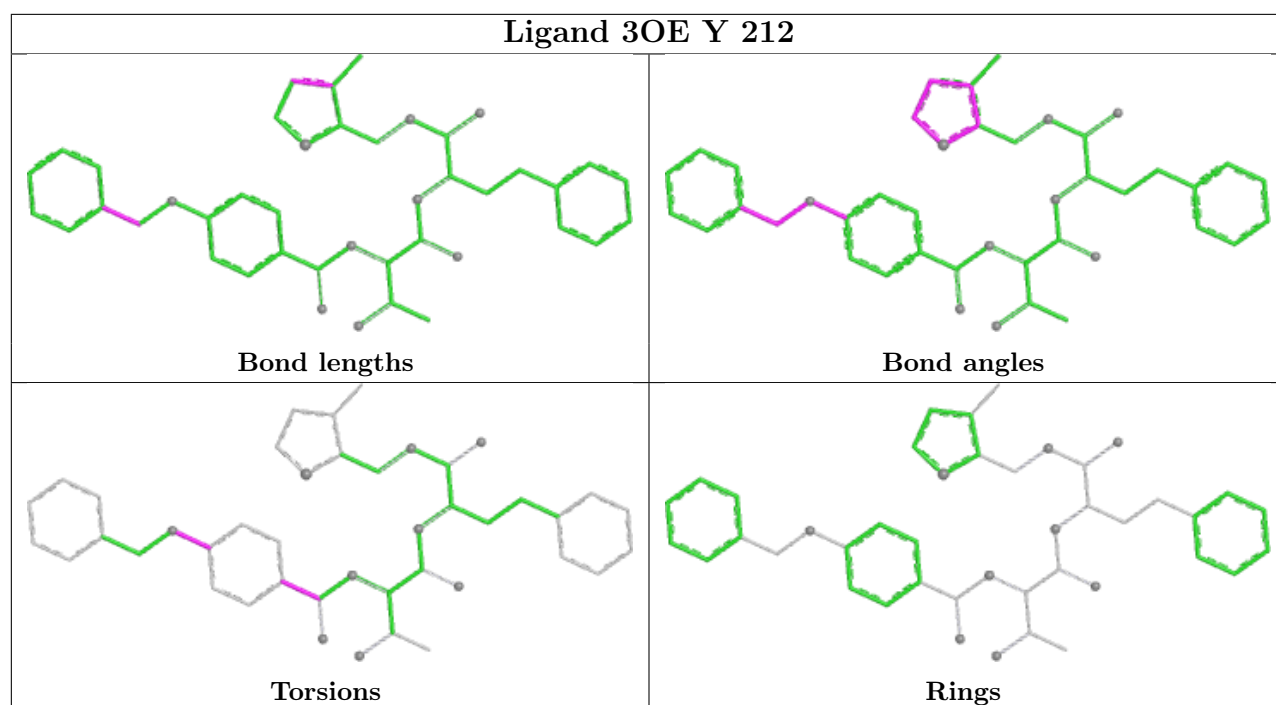
3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
16	K	213	3OE	2	0
16	Y	212	3OE	1	0
17	K	214	MES	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths,

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





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	250/250 (100%)	0.20	7 (2%) 55 46	35, 51, 76, 102	0
1	O	250/250 (100%)	0.18	14 (5%) 30 22	35, 52, 78, 104	0
2	B	235/235 (100%)	0.52	17 (7%) 21 15	33, 56, 86, 101	0
2	P	235/235 (100%)	0.39	14 (5%) 27 20	32, 56, 89, 101	0
3	C	241/241 (100%)	0.72	31 (12%) 7 5	39, 67, 108, 124	0
3	Q	241/241 (100%)	0.90	38 (15%) 5 4	39, 68, 109, 129	0
4	D	242/260 (93%)	0.57	25 (10%) 12 10	36, 59, 95, 111	0
4	R	242/260 (93%)	0.55	21 (8%) 16 12	37, 59, 98, 116	0
5	E	233/233 (100%)	0.46	13 (5%) 30 22	39, 59, 88, 110	0
5	S	233/233 (100%)	0.65	27 (11%) 9 7	39, 59, 92, 115	0
6	F	237/242 (97%)	0.16	5 (2%) 63 55	34, 51, 83, 95	0
6	T	237/242 (97%)	0.22	6 (2%) 58 49	34, 52, 81, 98	0
7	G	243/243 (100%)	-0.06	3 (1%) 76 71	31, 45, 72, 102	0
7	U	243/243 (100%)	0.00	8 (3%) 49 40	31, 46, 70, 99	0
8	H	222/222 (100%)	-0.07	1 (0%) 87 85	33, 43, 63, 92	0
8	V	222/222 (100%)	0.03	3 (1%) 73 67	33, 44, 64, 94	0
9	I	204/204 (100%)	-0.15	4 (1%) 65 57	31, 43, 60, 74	0
9	W	204/204 (100%)	-0.14	2 (0%) 79 74	31, 43, 60, 75	0
10	J	198/198 (100%)	0.05	8 (4%) 42 33	32, 46, 61, 113	0
10	X	197/198 (99%)	0.04	6 (3%) 52 44	33, 46, 61, 111	0
11	K	212/212 (100%)	0.05	4 (1%) 66 59	31, 46, 72, 81	0
11	Y	212/212 (100%)	0.07	5 (2%) 59 51	31, 46, 73, 80	0
12	L	222/222 (100%)	-0.08	5 (2%) 61 52	31, 44, 72, 80	0
12	Z	222/222 (100%)	-0.06	6 (2%) 56 47	31, 44, 70, 81	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	1	233/233 (100%)	-0.16	1 (0%) 88 87	29, 43, 56, 63	0
13	M	233/233 (100%)	-0.16	3 (1%) 75 68	29, 42, 56, 63	0
14	2	196/196 (100%)	-0.26	0 100 100	30, 40, 57, 66	0
14	N	196/196 (100%)	-0.28	0 100 100	31, 40, 57, 66	0
All	All	6335/6382 (99%)	0.17	277 (4%) 39 30	29, 49, 85, 129	0

All (277) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
10	J	-1	MET	10.3
3	Q	56	LEU	9.9
2	B	217	ALA	8.2
5	S	4	PHE	7.4
6	F	12	ASN	7.0
10	J	192	ALA	6.1
1	O	4	MET	5.9
3	C	11	ALA	5.8
10	X	192	ALA	5.8
6	T	12	ASN	5.7
4	D	123(E)	SER	5.6
3	Q	55	THR	5.5
2	P	217	ALA	5.4
13	1	-8	THR	5.3
1	A	4	MET	5.3
4	R	123(E)	SER	5.2
4	D	123(B)	GLU	5.2
1	A	5	THR	5.2
3	C	8	TYR	5.1
4	D	127	LEU	5.1
4	R	123(D)	ALA	5.1
1	A	203	GLU	5.1
4	R	127	LEU	5.0
3	C	56	LEU	4.9
2	B	54	VAL	4.8
3	C	208	LYS	4.7
4	D	123(D)	ALA	4.6
13	M	-8	THR	4.6
4	D	12	VAL	4.6
1	O	217(P)	LYS	4.6
3	C	9	ASP	4.5
4	D	123(G)	GLU	4.4

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Mol	Chain	Res	Type	RSRZ
10	X	191	GLN	4.3
3	Q	58	LEU	4.3
10	J	191	GLN	4.2
11	K	208	ASN	4.2
5	S	63	TYR	4.2
4	D	123(A)	GLY	4.2
4	R	123(F)	GLY	4.2
3	Q	54	SER	4.2
4	R	123(C)	GLY	4.2
11	K	210	ILE	4.2
3	C	55	THR	4.1
4	D	123(C)	GLY	4.1
3	Q	208	LYS	4.1
7	U	240	ASP	4.1
1	O	5	THR	4.0
3	Q	207	ALA	4.0
2	B	239	THR	4.0
2	P	54	VAL	4.0
5	E	4	PHE	4.0
5	S	206	SER	3.9
12	L	144(K)	LYS	3.9
3	Q	206	GLY	3.8
3	Q	57	LYS	3.8
3	Q	64	PRO	3.8
3	C	7	GLY	3.8
11	Y	179	THR	3.8
4	R	123(G)	GLU	3.7
5	S	55	ALA	3.6
11	Y	210	ILE	3.6
3	Q	240	LYS	3.6
12	Z	145	TYR	3.6
1	A	217	ASP	3.5
2	B	218	ASN	3.5
5	S	57	GLU	3.5
2	B	13	THR	3.4
3	C	57	LYS	3.4
4	D	242	ALA	3.4
5	S	60	SER	3.4
7	U	199	ASP	3.4
2	B	218(D)	GLY	3.4
4	D	11	GLY	3.3
5	S	5	ARG	3.3

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Mol	Chain	Res	Type	RSRZ
2	P	239	THR	3.3
4	R	123(B)	GLU	3.2
12	Z	144(Q)	LEU	3.2
1	O	6	ASP	3.2
5	S	198	SER	3.2
2	P	218	ASN	3.2
3	C	12	LEU	3.2
7	U	6	ALA	3.2
3	C	207	ALA	3.1
2	B	238	ILE	3.1
12	Z	144(R)	LYS	3.1
4	D	10	ARG	3.1
3	Q	8	TYR	3.1
4	R	123	PHE	3.0
2	B	127	GLY	3.0
4	D	123(F)	GLY	3.0
7	U	218	ASP	3.0
3	C	62(A)	ILE	2.9
9	I	121	GLU	2.9
2	B	64	THR	2.9
10	J	190	PHE	2.9
4	R	158	TYR	2.9
3	Q	62(A)	ILE	2.9
10	J	193	GLN	2.9
4	R	10	ARG	2.9
3	Q	223	ALA	2.8
2	B	22	TYR	2.8
1	A	235	ALA	2.8
3	C	233	VAL	2.8
5	S	207	LEU	2.8
3	Q	201	VAL	2.8
8	V	221	ILE	2.8
10	X	188	ASP	2.8
3	C	45	CYS	2.7
3	Q	232	TYR	2.7
3	Q	209	ASN	2.7
2	P	62	ASP	2.7
4	R	13	SER	2.7
6	F	13	SER	2.7
5	S	53	ARG	2.7
3	Q	210	ILE	2.7
5	S	56	ASP	2.7

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Mol	Chain	Res	Type	RSRZ
6	T	13	SER	2.7
4	R	125	GLU	2.7
3	Q	233	VAL	2.7
3	C	64	PRO	2.7
3	C	206	GLY	2.7
5	S	54	ASN	2.7
3	Q	236	ILE	2.6
4	D	26	TYR	2.6
3	Q	63	THR	2.6
3	C	209	ASN	2.6
2	B	53	LYS	2.6
9	W	181	LYS	2.6
12	L	144(A)	LYS	2.6
2	B	216(B)	GLY	2.6
5	S	58	LEU	2.6
5	S	209	ASN	2.6
12	L	144(B)	ASN	2.6
6	F	240	ILE	2.6
13	M	61	ASP	2.6
5	E	5	ARG	2.6
2	B	55	THR	2.6
5	E	206	SER	2.6
3	Q	53	ARG	2.6
12	Z	146	LEU	2.6
3	Q	61	THR	2.6
4	D	244	GLU	2.6
5	S	33	GLN	2.6
3	Q	44	ASN	2.6
3	C	66	LYS	2.5
2	P	238	ILE	2.5
7	U	129	MET	2.5
9	I	29	ASN	2.5
4	D	9	ASP	2.5
4	D	126	ARG	2.5
9	W	182	ASP	2.5
6	F	184	LEU	2.5
5	E	12	THR	2.5
3	C	226	SER	2.5
4	R	11	GLY	2.5
3	Q	203	THR	2.5
5	S	59	SER	2.5
9	I	-8	SER	2.5

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Mol	Chain	Res	Type	RSRZ
11	K	104	TYR	2.5
3	C	58	LEU	2.4
2	P	216(B)	GLY	2.4
3	C	42	GLY	2.4
4	D	13	SER	2.4
5	E	207	LEU	2.4
2	B	216(A)	LYS	2.4
7	U	184(H)	GLU	2.4
9	I	122(A)	LYS	2.4
5	S	51	LEU	2.4
4	R	126	ARG	2.4
3	Q	65	SER	2.4
7	G	6	ALA	2.4
3	C	229	ILE	2.4
4	R	12	VAL	2.4
5	E	207(C)	VAL	2.4
1	O	7	ARG	2.4
10	X	10	ASP	2.4
1	O	55	SER	2.4
3	C	235	GLN	2.4
2	P	53	LYS	2.3
8	V	223	ASP	2.3
1	O	64	LEU	2.3
7	U	236	ILE	2.3
4	D	14	THR	2.3
4	D	22	PHE	2.3
11	Y	180	GLU	2.3
3	C	241	GLN	2.3
5	S	201	LEU	2.3
12	Z	144(J)	ASN	2.3
3	C	174	GLU	2.3
1	O	217(O)	ASP	2.3
3	Q	202	GLN	2.3
2	P	64	THR	2.3
3	C	232	TYR	2.3
5	S	10	GLY	2.3
5	E	207(E)	ASN	2.2
7	G	240	ASP	2.2
2	P	232	ILE	2.2
1	O	8	TYR	2.2
3	Q	226	SER	2.2
10	J	168	MET	2.2

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Mol	Chain	Res	Type	RSRZ
5	S	204	GLU	2.2
6	T	199	LEU	2.2
3	Q	52	ARG	2.2
4	D	86	ARG	2.2
2	P	55	THR	2.2
1	O	53	LYS	2.2
6	T	206(B)	LYS	2.2
5	E	195	GLU	2.2
5	E	199	GLN	2.2
10	X	189	ASP	2.2
1	A	8	TYR	2.2
6	F	128	SER	2.2
5	S	32	LYS	2.2
5	S	52	LYS	2.2
4	D	241	GLU	2.2
4	R	244	GLU	2.2
5	S	233	ILE	2.2
5	S	208(A)	VAL	2.2
2	B	204(A)	SER	2.2
3	Q	196	SER	2.2
4	D	123	PHE	2.2
3	C	59	GLN	2.1
3	Q	243	GLN	2.1
5	S	64	GLN	2.1
3	Q	40	VAL	2.1
3	Q	200	VAL	2.1
4	R	9	ASP	2.1
5	S	203	ASP	2.1
4	D	237	LEU	2.1
7	U	128	TYR	2.1
1	O	9	SER	2.1
3	C	16	SER	2.1
2	P	216(A)	LYS	2.1
6	T	206	LYS	2.1
3	Q	7	GLY	2.1
10	X	190	PHE	2.1
2	B	220	TYR	2.1
4	D	122	ARG	2.1
3	C	211	GLU	2.1
4	R	238	LYS	2.1
11	Y	145	ASP	2.1
10	J	49	ALA	2.1

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Mol	Chain	Res	Type	RSRZ
3	Q	51	GLU	2.1
5	E	57	GLU	2.1
5	E	198	SER	2.1
12	Z	147	SER	2.1
4	R	57	PRO	2.1
2	P	218(C)	GLY	2.1
3	Q	39	GLY	2.1
3	C	63	THR	2.1
3	C	203	THR	2.1
5	E	203	ASP	2.1
6	T	204	ASP	2.1
8	H	223	ASP	2.1
13	M	39	ASP	2.1
3	C	223	ALA	2.1
3	Q	11	ALA	2.1
7	G	8	TYR	2.1
1	O	54	SER	2.0
4	D	35	SER	2.0
11	Y	105(B)	LYS	2.0
1	A	7	ARG	2.0
5	S	180(C)	PHE	2.0
2	P	63	THR	2.0
8	V	2	THR	2.0
1	O	235	ALA	2.0
10	J	10	ASP	2.0
4	R	239	GLU	2.0
5	E	175	TYR	2.0
3	Q	38	VAL	2.0
1	O	217(M)	PRO	2.0
2	B	202	THR	2.0
11	K	179	THR	2.0
4	R	205	GLU	2.0
12	L	144(M)	LYS	2.0
12	L	144(Q)	LYS	2.0
3	Q	186	VAL	2.0

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

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

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

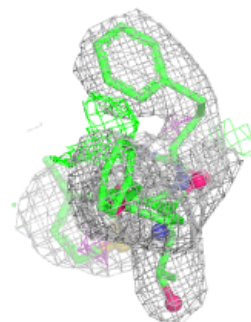
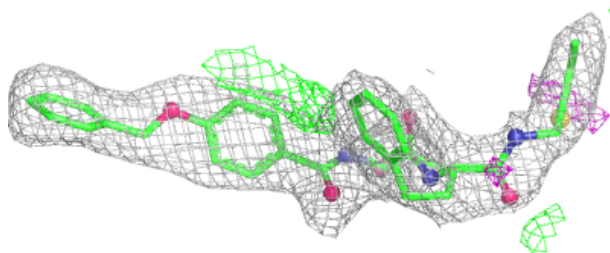
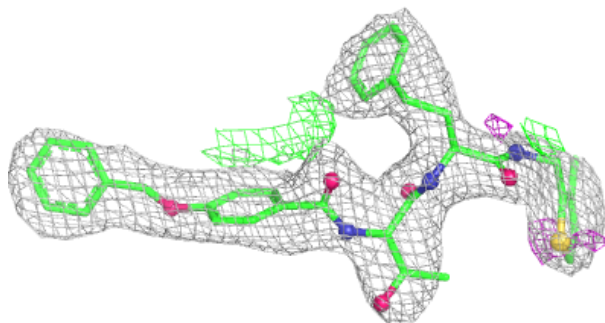
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
15	MG	I	195	1/1	0.68	0.24	57,57,57,57	0
15	MG	L	195	1/1	0.79	0.18	56,56,56,56	0
15	MG	H	224	1/1	0.84	0.15	68,68,68,68	0
16	3OE	Y	212	43/43	0.88	0.18	71,72,74,75	0
17	MES	K	214	12/12	0.90	0.19	92,93,93,93	0
17	MES	Y	213	12/12	0.90	0.21	101,102,102,102	0
15	MG	K	212	1/1	0.92	0.10	47,47,47,47	0
15	MG	F	243	1/1	0.92	0.24	105,105,105,105	0
16	3OE	K	213	43/43	0.92	0.14	55,60,68,68	0
15	MG	F	242	1/1	0.94	0.09	67,67,67,67	0
15	MG	I	196	1/1	0.96	0.09	46,46,46,46	0
15	MG	L	196	1/1	0.96	0.12	50,50,50,50	0
15	MG	N	188	1/1	0.97	0.06	36,36,36,36	0
15	MG	G	1	1/1	0.98	0.04	41,41,41,41	0

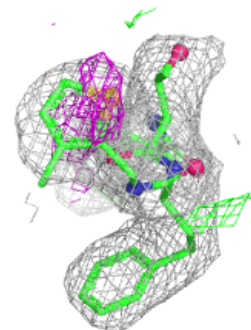
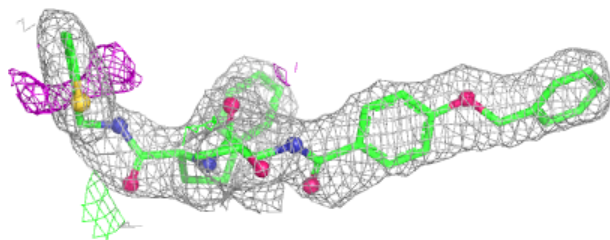
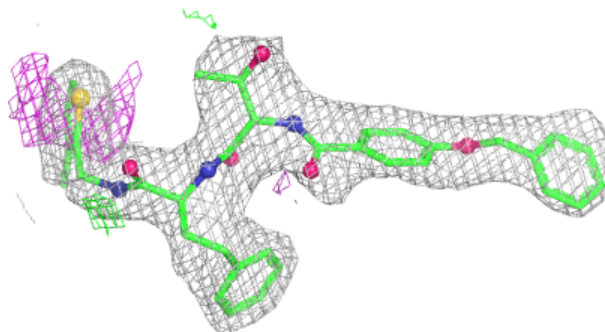
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around 3OE 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 3OE 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.