



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 09:35 AM UTC

PDB ID : 3SDK / pdb_00003sdk
Title : Structure of yeast 20S open-gate proteasome with Compound 34
Authors : Sintchak, M.D.
Deposited on : 2011-06-09
Resolution : 2.70 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

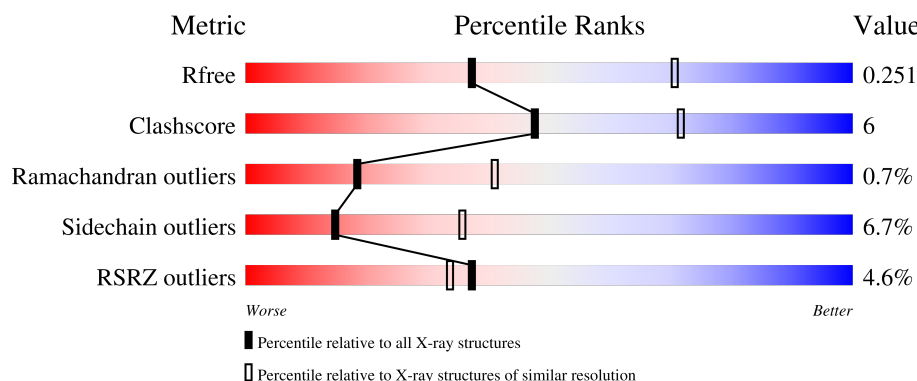
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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	3538 (2.70-2.70)
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (2.70-2.70)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	250	4% 81% 17% .
1	O	250	5% 83% 15% .
2	B	235	9% 82% 16% .
2	P	235	8% 80% 18% .
3	C	241	10% 83% 14% .

Continued on next page...

Continued from previous page...

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

2 Entry composition

There are 17 unique types of molecules in this entry. The entry contains 49255 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	233	Total	C	N	O	S	0	0	0
			1794	1123	302	362	7			
4	R	232	Total	C	N	O	S	0	0	0
			1786	1120	298	361	7			

- Molecule 5 is a protein called Proteasome component PRE5.

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

- Molecule 6 is a protein called Proteasome component C1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	236	Total	C	N	O	S	0	0	0
			1840	1171	321	344	4			
6	T	236	Total	C	N	O	S	0	0	0
			1840	1171	321	344	4			

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

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

- Molecule 8 is a protein called Proteasome component PUP1.

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

- Molecule 9 is a protein called Proteasome component PUP3.

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

- Molecule 10 is a protein called Proteasome component C11.

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

Continued on next page...

Continued from previous page...

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
			1512	955	250	300	7			

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

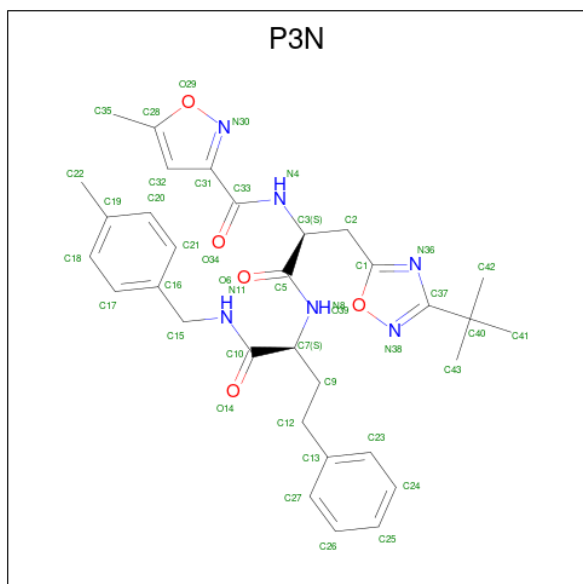
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
15	F	2	Total	Mg	0	0
			2	2		
15	G	1	Total	Mg	0	0
			1	1		

Continued on next page...

Continued from previous page...

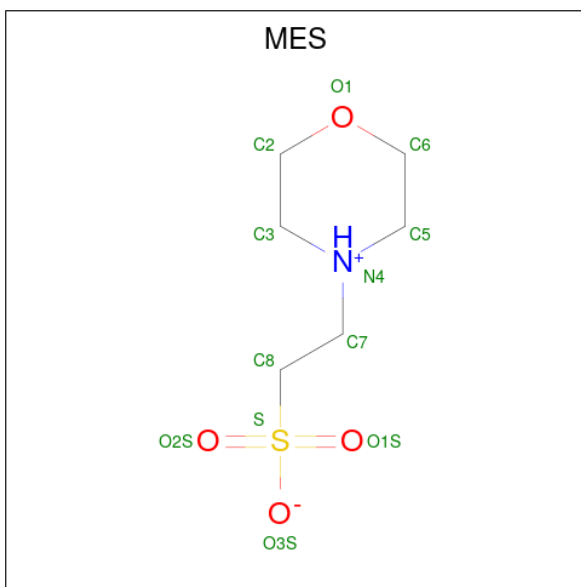
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
15	H	1	Total	Mg	0	0
			1	1		
15	I	2	Total	Mg	0	0
			2	2		
15	K	1	Total	Mg	0	0
			1	1		
15	L	2	Total	Mg	0	0
			2	2		
15	N	1	Total	Mg	0	0
			1	1		

- Molecule 16 is N-[(2S)-3-(3-tert-butyl-1,2,4-oxadiazol-5-yl)-1-({(2S)-1-[(4-methylbenzyl)amino]-1-oxo-4-phenylbutan-2-yl}amino)-1-oxopropan-2-yl]-5-methyl-1,2-oxazole-3-carboxamide (CCD ID: P3N) (formula: C₃₂H₃₈N₆O₅).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
16	K	1	Total	C	N	O	0	0
			43	32	6	5		
16	Y	1	Total	C	N	O	0	0
			43	32	6	5		

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

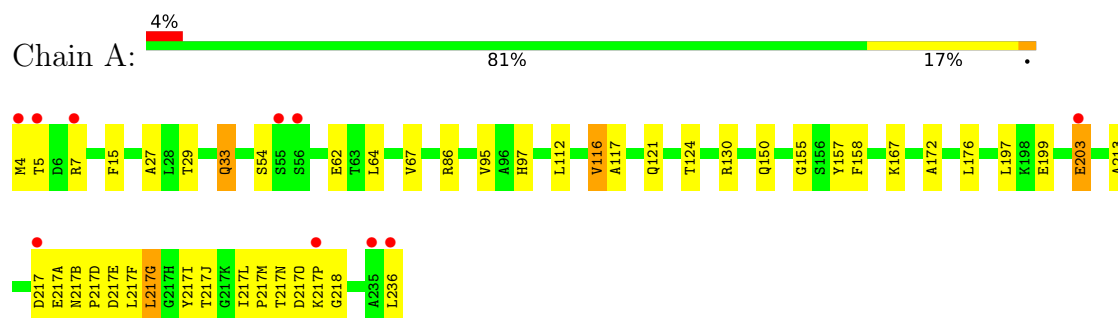


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
17	K	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
17	Y	1	Total	C	N	O	S	0	0
			12	6	1	4	1		

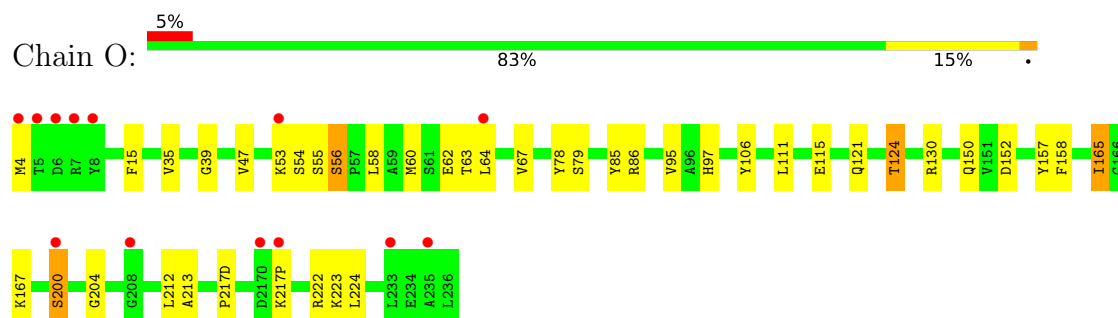
3 Residue-property plots

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.

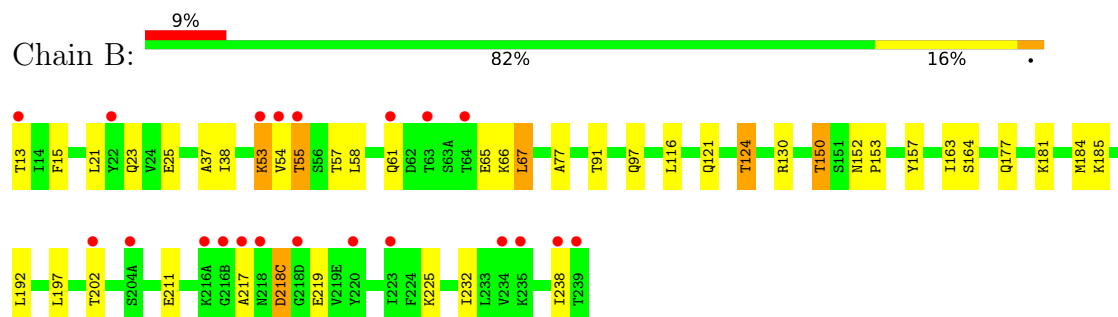
• Molecule 1: Proteasome component Y7



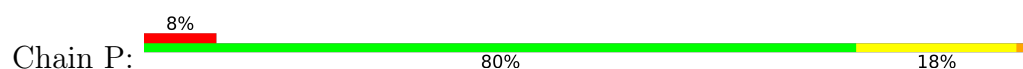
• Molecule 1: Proteasome component Y7

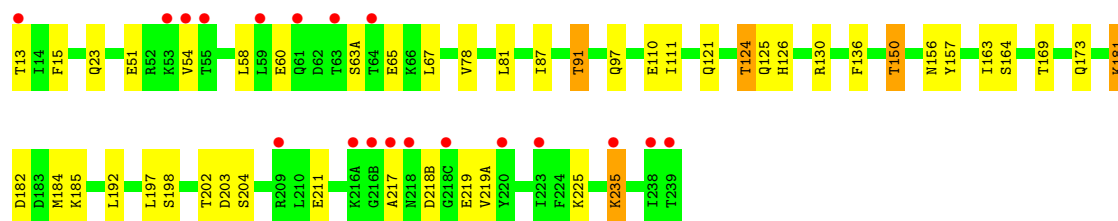


• Molecule 2: Proteasome component Y13

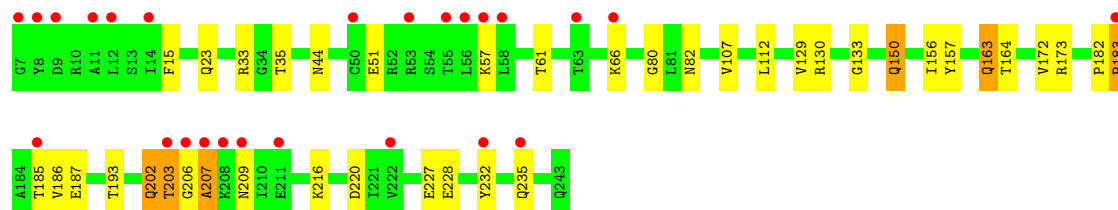
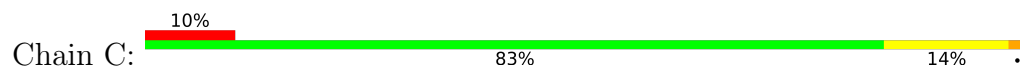


• Molecule 2: Proteasome component Y13

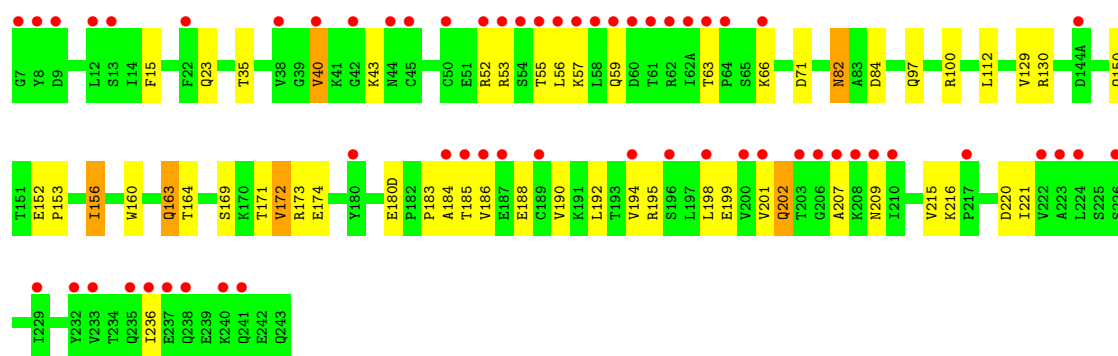
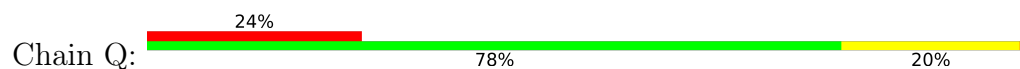




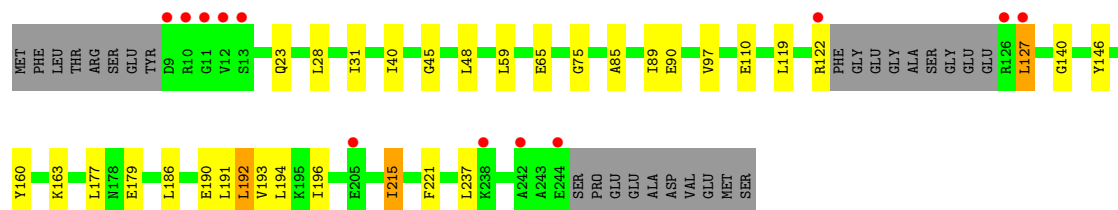
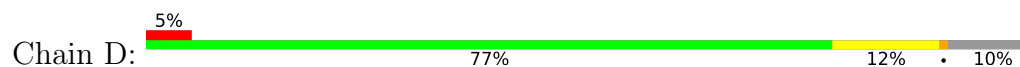
• Molecule 3: Proteasome component PRE6



• Molecule 3: Proteasome component PRE6

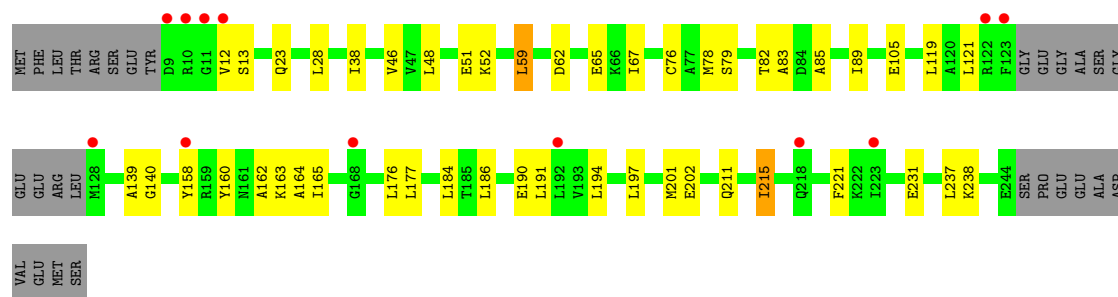


• Molecule 4: Proteasome component PUP2

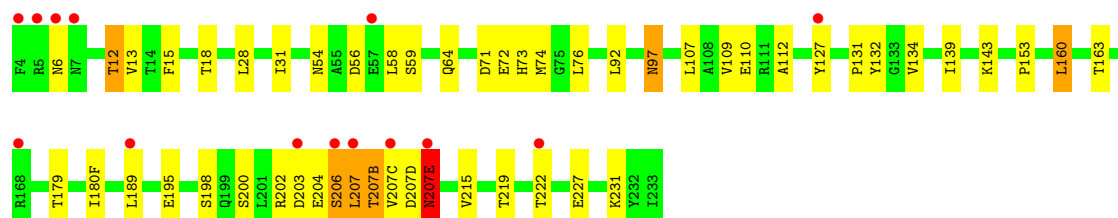
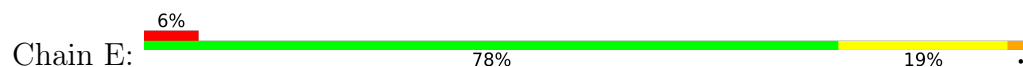


• Molecule 4: Proteasome component PUP2

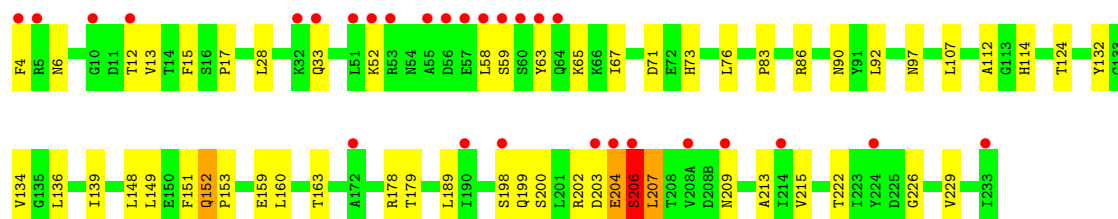
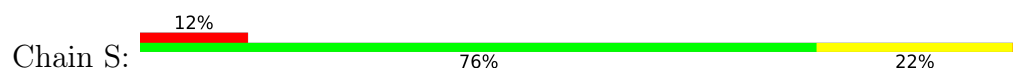




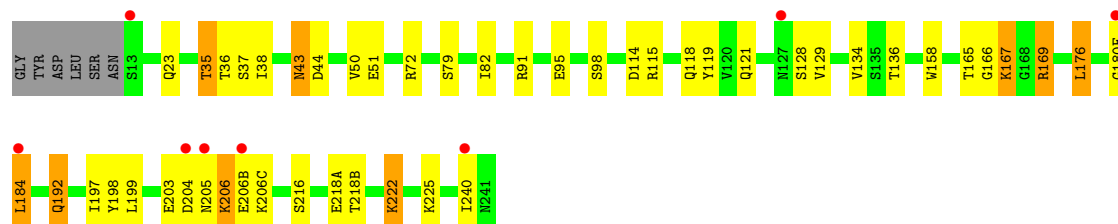
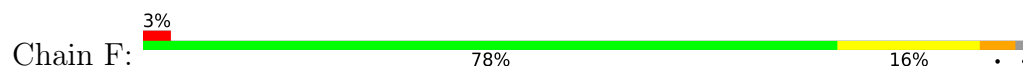
- Molecule 5: Proteasome component PRE5



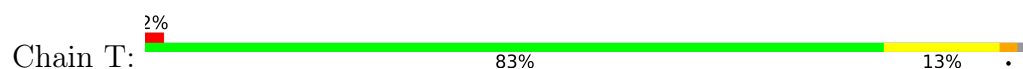
- Molecule 5: Proteasome component PRE5



- Molecule 6: Proteasome component C1

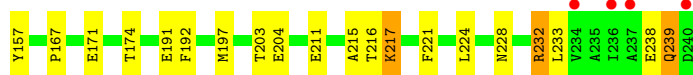
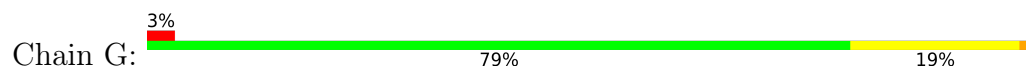


- Molecule 6: Proteasome component C1

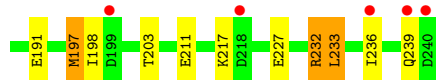
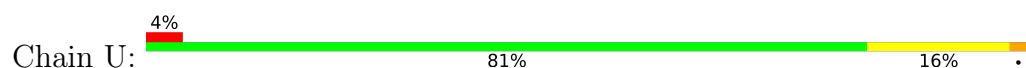




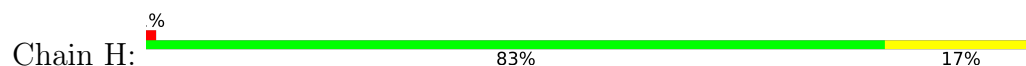
- Molecule 7: Proteasome component C7-alpha



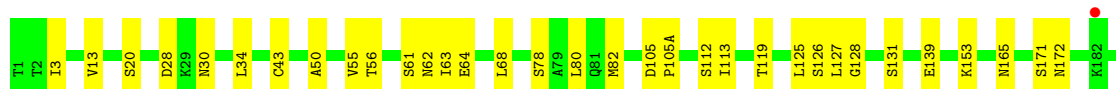
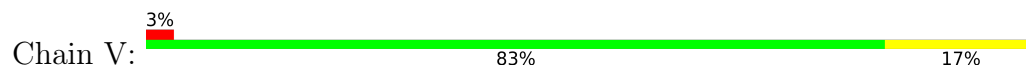
- Molecule 7: Proteasome component C7-alpha



- Molecule 8: Proteasome component PUP1

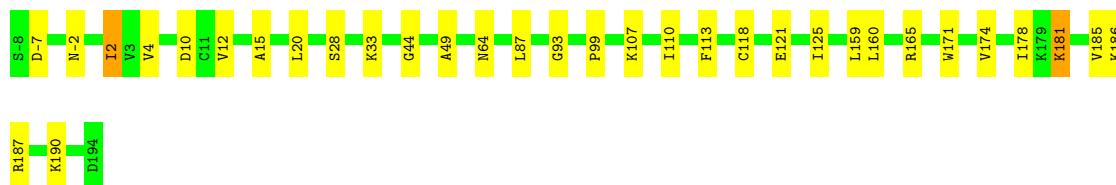


- Molecule 8: Proteasome component PUP1



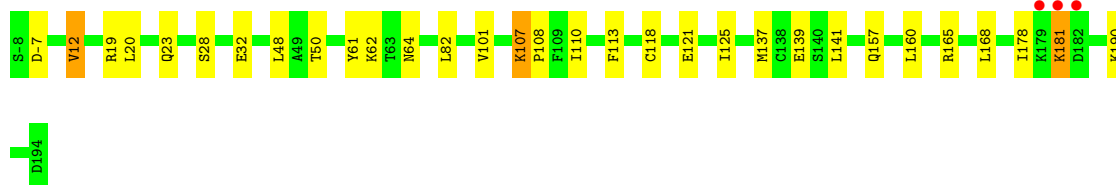
- Molecule 9: Proteasome component PUP3

Chain I:  84% 15% .



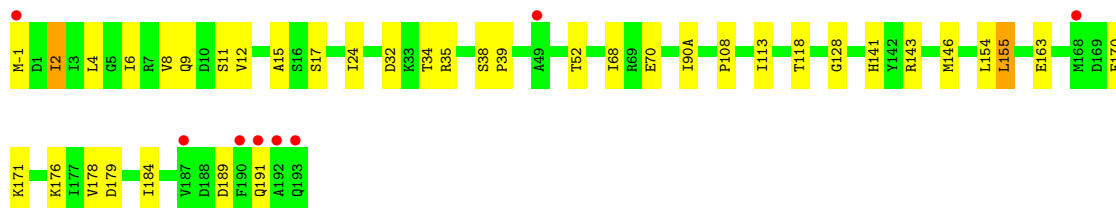
• Molecule 9: Proteasome component PUP3

Chain W:  85% 14% .



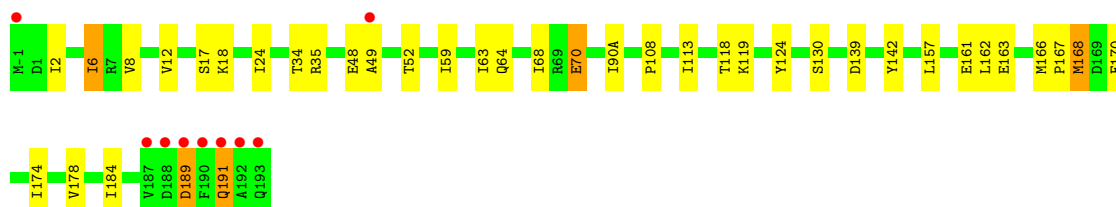
• Molecule 10: Proteasome component C11

Chain J:  81% 18% .



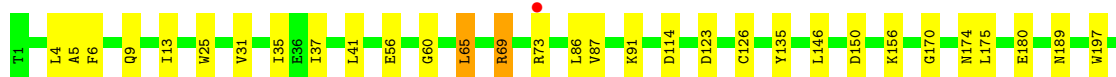
• Molecule 10: Proteasome component C11

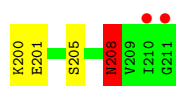
Chain X:  80% 17% .



• Molecule 11: Proteasome component PRE2

Chain K:  83% 15% .

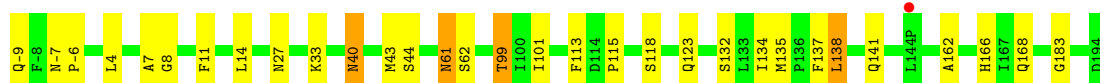




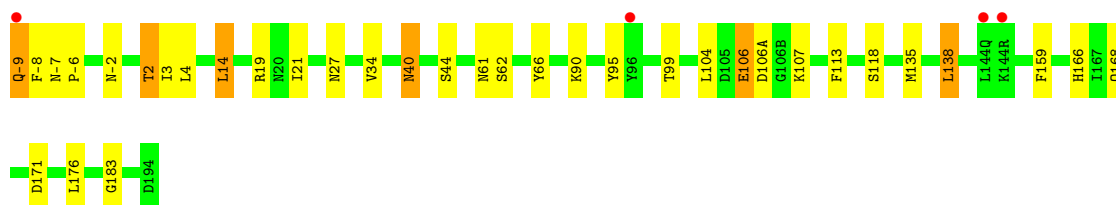
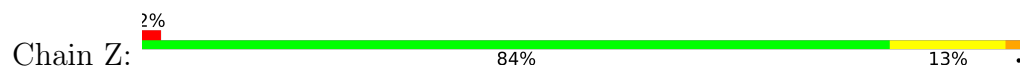
- Molecule 11: Proteasome component PRE2



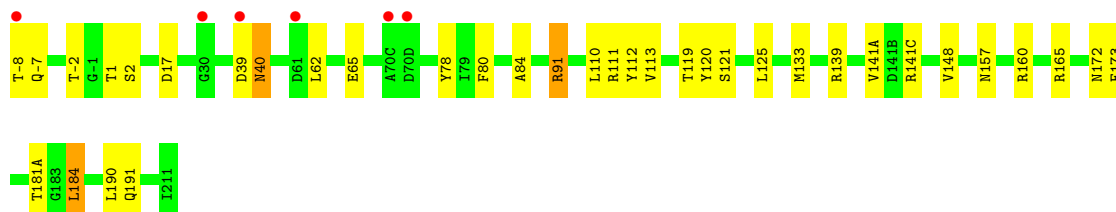
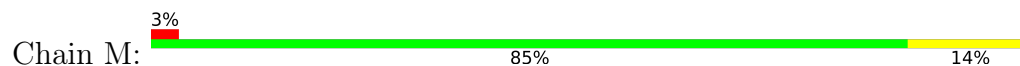
- Molecule 12: Proteasome component C5



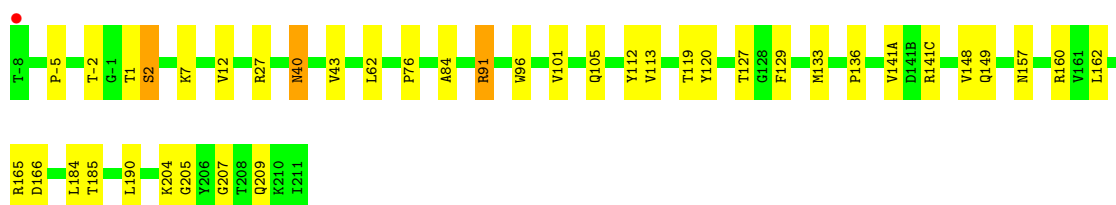
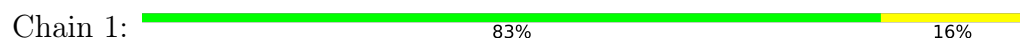
- Molecule 12: Proteasome component C5



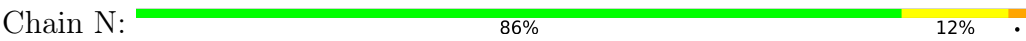
- Molecule 13: Proteasome component PRE4



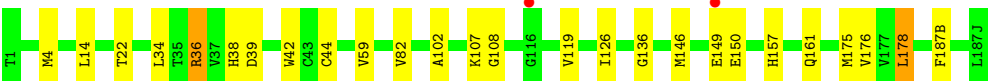
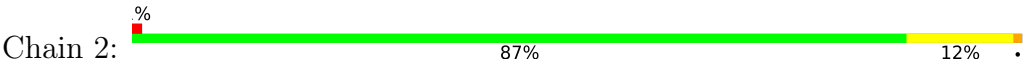
- Molecule 13: Proteasome component PRE4



● 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	136.12Å 299.40Å 146.24Å 90.00° 112.92° 90.00°	Depositor
Resolution (Å)	50.00 – 2.70 50.00 – 2.70	Depositor EDS
% Data completeness (in resolution range)	95.0 (50.00-2.70) 95.1 (50.00-2.70)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.43 (at 2.69Å)	Xtriage
Refinement program	REFMAC 5.5.0110	Depositor
R, R_{free}	0.223 , 0.259 0.219 , 0.251	Depositor DCC
R_{free} test set	5652 reflections (2.02%)	wwPDB-VP
Wilson B-factor (Å ²)	54.4	Xtriage
Anisotropy	0.156	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 25.7	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	49255	wwPDB-VP
Average B, all atoms (Å ²)	52.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.28% 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: P3N, 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	0.55	0/1952	0.82	0/2642
1	O	0.63	2/1952 (0.1%)	0.84	3/2642 (0.1%)
2	B	0.56	0/1858	0.85	1/2516 (0.0%)
2	P	0.56	0/1858	0.83	0/2516
3	C	0.57	0/1920	0.85	0/2598
3	Q	0.60	2/1920 (0.1%)	0.88	0/2598
4	D	0.55	0/1817	0.81	0/2449
4	R	0.52	0/1810	0.82	0/2440
5	E	0.64	3/1823 (0.2%)	0.85	2/2463 (0.1%)
5	S	0.57	2/1823 (0.1%)	0.83	4/2463 (0.2%)
6	F	0.56	1/1879 (0.1%)	0.83	0/2535
6	T	0.57	1/1879 (0.1%)	0.84	0/2535
7	G	0.61	1/1959 (0.1%)	0.85	1/2652 (0.0%)
7	U	0.58	1/1959 (0.1%)	0.85	0/2652
8	H	0.55	0/1716	0.83	0/2326
8	V	0.59	0/1716	0.81	0/2326
9	I	0.65	1/1611 (0.1%)	0.83	3/2174 (0.1%)
9	W	0.67	0/1611	0.86	1/2174 (0.0%)
10	J	0.63	0/1613	0.82	0/2173
10	X	0.58	0/1610	0.83	1/2170 (0.0%)
11	K	0.58	0/1681	0.86	2/2274 (0.1%)
11	Y	0.53	0/1681	0.81	0/2274
12	L	0.57	0/1795	0.80	0/2420
12	Z	0.59	0/1795	0.82	0/2420
13	1	0.62	0/1855	0.83	2/2514 (0.1%)
13	M	0.61	1/1855 (0.1%)	0.82	0/2514
14	2	0.68	0/1541	0.84	0/2087
14	N	0.71	1/1541 (0.1%)	0.82	0/2087
All	All	0.59	16/50030 (0.0%)	0.83	20/67634 (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
5	E	0	2
5	S	0	1
14	N	0	1
All	All	0	5

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	E	207(E)	ASN	C-O	12.41	1.39	1.24
1	O	200	SER	C-O	11.93	1.39	1.24
3	Q	180(D)	GLU	C-O	9.51	1.36	1.24
14	N	181	ALA	C-O	8.14	1.34	1.24
1	O	200	SER	CA-C	7.29	1.62	1.52
5	E	206	SER	N-CA	6.74	1.54	1.46
6	F	82	ILE	CA-CB	6.67	1.57	1.54
7	U	82	ILE	CA-CB	6.33	1.58	1.53
13	M	181(A)	THR	C-O	5.82	1.31	1.24
5	S	206	SER	N-CA	5.77	1.53	1.46
6	T	82	ILE	CA-CB	5.73	1.57	1.53
5	E	207(E)	ASN	CA-C	5.64	1.60	1.52
5	S	204	GLU	C-O	5.24	1.30	1.23
7	G	82	ILE	CA-CB	5.20	1.57	1.53
9	I	2	ILE	C-O	-5.08	1.18	1.23
3	Q	180(D)	GLU	CA-C	5.06	1.57	1.52

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	S	152	GLN	CA-C-N	7.36	127.03	119.82
5	S	152	GLN	C-N-CA	7.36	127.03	119.82
5	E	202	ARG	N-CA-C	-6.10	105.87	113.38
1	O	152	ASP	CA-C-N	5.89	127.20	119.84
1	O	152	ASP	C-N-CA	5.89	127.20	119.84
9	W	23	GLN	CB-CA-C	-5.76	109.39	117.23
13	1	-2	THR	N-CA-C	5.61	118.21	109.52
9	I	-2	ASN	N-CA-C	5.54	120.32	113.50
2	B	238	ILE	N-CA-C	-5.51	107.91	113.20
5	S	202	ARG	N-CA-C	-5.47	105.34	112.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	K	208	ASN	N-CA-C	-5.44	106.64	113.28
7	G	155	GLY	N-CA-C	-5.41	107.81	115.43
10	X	191	GLN	N-CA-C	5.34	116.79	110.97
1	O	200	SER	CA-C-O	-5.31	112.91	120.51
11	K	170	GLY	N-CA-C	5.28	117.14	110.38
13	1	27	ARG	N-CA-C	5.07	117.78	111.24
5	E	207(E)	ASN	CA-C-O	-5.05	114.16	119.97
5	S	204	GLU	O-C-N	-5.03	118.88	123.41
9	I	-7	ASP	CA-C-N	5.00	124.78	119.28
9	I	-7	ASP	C-N-CA	5.00	124.78	119.28

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
14	N	181	ALA	Mainchain
1	O	200	SER	Mainchain
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	28	0
1	O	1915	0	1926	24	0
2	B	1829	0	1829	25	0
2	P	1829	0	1829	27	0
3	C	1891	0	1900	27	0
3	Q	1891	0	1900	38	0
4	D	1794	0	1778	21	0
4	R	1786	0	1763	19	0
5	E	1795	0	1797	22	0
5	S	1795	0	1797	27	0
6	F	1840	0	1838	30	0
6	T	1840	0	1838	21	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	G	1921	0	1910	34	0
7	U	1921	0	1910	34	0
8	H	1685	0	1688	17	0
8	V	1685	0	1688	21	0
9	I	1581	0	1574	17	0
9	W	1581	0	1574	23	0
10	J	1585	0	1590	14	0
10	X	1582	0	1583	20	0
11	K	1644	0	1595	16	0
11	Y	1644	0	1595	13	0
12	L	1757	0	1711	21	0
12	Z	1757	0	1711	25	0
13	1	1824	0	1832	24	0
13	M	1824	0	1832	27	0
14	2	1512	0	1481	16	0
14	N	1512	0	1481	14	0
15	F	2	0	0	0	0
15	G	1	0	0	0	0
15	H	1	0	0	0	0
15	I	2	0	0	0	0
15	K	1	0	0	0	0
15	L	2	0	0	0	0
15	N	1	0	0	0	0
16	K	43	0	38	2	0
16	Y	43	0	38	1	0
17	K	12	0	13	1	0
17	Y	12	0	13	1	0
All	All	49255	0	48978	549	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 (549) 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)
4:D:127:LEU:HD12	4:D:127:LEU:N	1.53	1.02
4:D:127:LEU:H	4:D:127:LEU:CD1	1.70	1.01
1:A:130:ARG:HH21	7:G:124:THR:CG2	1.78	0.97
4:D:127:LEU:C	4:D:127:LEU:HD13	1.89	0.96
4:D:127:LEU:HD12	4:D:127:LEU:H	0.81	0.95
7:U:96:ALA:HA	7:U:107:MET:HE2	1.49	0.94

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:130:ARG:HH21	7:U:124:THR:HG22	1.29	0.94
13:M:157:ASN:HD22	13:M:160:ARG:HH11	1.09	0.92
11:K:208:ASN:ND2	10:X:124:TYR:OH	2.03	0.91
7:G:96:ALA:HA	7:G:107:MET:HE2	1.51	0.90
4:D:127:LEU:N	4:D:127:LEU:CD1	2.30	0.88
3:C:202:GLN:O	3:C:203:THR:HG22	1.73	0.88
14:N:161:GLN:HE21	14:2:136:GLY:HA2	1.37	0.88
1:A:124:THR:HG22	2:B:130:ARG:HH21	1.39	0.87
3:C:15:PHE:H	4:D:23:GLN:HE22	1.22	0.86
1:O:130:ARG:HH21	7:U:124:THR:CG2	1.90	0.84
4:D:127:LEU:HD13	4:D:127:LEU:O	1.80	0.82
5:E:97:ASN:HD21	12:L:61:ASN:HD21	1.28	0.81
5:E:15:PHE:H	6:F:23:GLN:HE22	1.29	0.81
3:Q:15:PHE:H	4:R:23:GLN:HE22	1.28	0.81
13:1:157:ASN:HD22	13:1:160:ARG:HH11	1.29	0.80
1:A:130:ARG:HH21	7:G:124:THR:HG22	1.45	0.80
14:N:136:GLY:HA2	14:2:161:GLN:HE21	1.46	0.80
3:C:202:GLN:O	3:C:203:THR:CG2	2.30	0.79
5:E:207(B):THR:H	5:E:207(E):ASN:HD22	1.30	0.79
2:B:124:THR:HG22	3:C:130:ARG:HH21	1.49	0.77
1:O:15:PHE:H	2:P:23:GLN:HE22	1.32	0.77
3:C:202:GLN:C	3:C:203:THR:HG22	2.10	0.77
5:S:134:VAL:O	5:S:153:PRO:HG3	1.85	0.77
3:C:202:GLN:O	3:C:203:THR:CB	2.33	0.76
6:F:95:GLU:HG2	6:F:115:ARG:HB3	1.66	0.76
3:C:163:GLN:NE2	3:C:164:THR:H	1.84	0.76
4:D:127:LEU:CD1	4:D:127:LEU:C	2.57	0.76
11:Y:174:ASN:HD21	11:Y:189:ASN:HD22	1.33	0.76
1:O:86:ARG:HE	7:U:118:ASN:HD21	1.35	0.75
13:M:141(C):ARG:HG3	13:M:141(C):ARG:HH11	1.51	0.75
12:Z:166:HIS:HD2	12:Z:168:GLN:H	1.34	0.74
6:T:192:GLN:HE21	6:T:195:LYS:HE3	1.52	0.74
1:O:124:THR:CG2	2:P:130:ARG:HH21	2.00	0.74
1:O:124:THR:HG22	2:P:130:ARG:HH21	1.50	0.73
13:M:40:ASN:H	13:M:40:ASN:HD22	1.32	0.73
12:Z:4:LEU:HD13	12:Z:138:LEU:HD21	1.71	0.73
7:U:121:GLN:O	7:U:124:THR:HB	1.89	0.72
7:U:87:ASN:C	7:U:87:ASN:HD22	1.97	0.72
2:B:124:THR:CG2	3:C:130:ARG:HH21	2.03	0.72
2:P:202:THR:HG22	2:P:204:SER:H	1.55	0.72
13:1:2:SER:HB3	13:1:127:THR:O	1.90	0.72

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:13:THR:O	3:C:130:ARG:HD3	1.88	0.72
7:G:96:ALA:HA	7:G:107:MET:CE	2.19	0.71
12:L:4:LEU:HD13	12:L:138:LEU:HD21	1.71	0.71
6:F:95:GLU:HG3	6:F:115:ARG:HH11	1.54	0.70
12:L:166:HIS:HD2	12:L:168:GLN:H	1.37	0.70
12:L:4:LEU:CD1	12:L:138:LEU:HD21	2.21	0.70
3:Q:201:VAL:O	3:Q:202:GLN:HB2	1.92	0.70
11:Y:174:ASN:ND2	11:Y:189:ASN:HD22	1.88	0.70
7:U:184(G):GLU:HG2	7:U:188:LYS:CB	2.21	0.70
12:L:-7:ASN:HD22	12:L:-6:PRO:HD2	1.55	0.69
13:M:157:ASN:HD22	13:M:160:ARG:NH1	1.88	0.69
3:C:163:GLN:HE21	3:C:164:THR:H	1.38	0.69
7:U:184(G):GLU:HG2	7:U:188:LYS:HB2	1.74	0.69
3:C:202:GLN:O	3:C:203:THR:HB	1.93	0.68
3:Q:195:ARG:HG3	3:Q:236:ILE:HD13	1.74	0.68
1:A:124:THR:CG2	2:B:130:ARG:HH21	2.07	0.68
2:B:15:PHE:H	3:C:23:GLN:HE22	1.42	0.68
7:G:123:TYR:CE1	7:G:129:MET:HE3	2.29	0.67
1:A:112:LEU:O	1:A:116:VAL:HG23	1.95	0.67
10:J:2:ILE:HB	10:J:17:SER:HB3	1.75	0.67
5:S:139:ILE:HD12	5:S:215:VAL:HG12	1.76	0.67
5:S:132:TYR:O	5:S:153:PRO:HB3	1.95	0.67
7:U:107:MET:HE3	7:U:112:LEU:HD13	1.77	0.67
1:O:130:ARG:NH2	7:U:124:THR:HG22	2.09	0.66
5:S:73:HIS:HE1	5:S:107:LEU:O	1.78	0.66
3:Q:171:THR:O	3:Q:174:GLU:HB3	1.95	0.66
9:I:181:LYS:H	9:I:181:LYS:HD2	1.60	0.66
5:E:73:HIS:HE1	5:E:107:LEU:O	1.79	0.66
2:B:152:ASN:HB2	2:B:153:PRO:CD	2.26	0.65
12:L:40:ASN:HD21	12:L:183:GLY:HA2	1.61	0.65
5:E:132:TYR:O	5:E:153:PRO:HB3	1.97	0.65
6:F:35:THR:HG21	6:F:51:GLU:O	1.97	0.65
6:F:37:SER:HB3	6:F:50:VAL:HG23	1.78	0.65
2:P:121:GLN:O	2:P:124:THR:HB	1.95	0.65
2:P:126:HIS:HB3	3:Q:129:VAL:HG12	1.77	0.65
9:W:137:MET:HE3	9:W:141:LEU:HD11	1.79	0.65
3:C:163:GLN:HE21	3:C:163:GLN:HA	1.62	0.64
1:O:121:GLN:O	1:O:124:THR:HB	1.97	0.64
6:T:35:THR:HG21	6:T:51:GLU:O	1.97	0.64
12:Z:-7:ASN:HD22	12:Z:-6:PRO:HD2	1.62	0.64
3:Q:82:ASN:H	3:Q:82:ASN:HD22	1.43	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:7:ARG:HD2	5:E:127:TYR:CD2	2.33	0.64
4:D:140:GLY:HA2	4:D:215:ILE:HG12	1.80	0.64
2:B:121:GLN:O	2:B:124:THR:HB	1.97	0.63
4:R:140:GLY:HA2	4:R:215:ILE:HG12	1.80	0.63
4:D:179:GLU:HB3	4:D:192:LEU:HD21	1.79	0.63
5:S:97:ASN:HD21	12:Z:61:ASN:HD21	1.46	0.63
1:A:130:ARG:HH21	7:G:124:THR:HG23	1.64	0.63
14:N:176:VAL:HG12	14:N:178:LEU:HD13	1.79	0.63
8:V:80:LEU:HD12	8:V:113:ILE:HD11	1.80	0.62
2:B:38:ILE:HD12	2:B:197:LEU:HG	1.80	0.62
11:K:208:ASN:ND2	10:X:139:ASP:OD1	2.32	0.62
10:X:18:LYS:HD3	10:X:174:ILE:HG13	1.82	0.62
6:F:216:SER:HB3	6:F:218(A):GLU:HB2	1.81	0.61
1:A:15:PHE:H	2:B:23:GLN:HE22	1.48	0.61
7:U:123:TYR:CE1	7:U:129:MET:HE2	2.35	0.61
2:B:67:LEU:HD22	2:B:211:GLU:HB3	1.83	0.61
5:S:52:LYS:HB2	5:S:63:TYR:HB3	1.82	0.61
5:S:12:THR:HG21	5:S:124:THR:HA	1.82	0.61
6:T:192:GLN:HE21	6:T:195:LYS:CE	2.13	0.61
12:Z:-9:GLN:HE21	12:Z:-8:PHE:N	1.99	0.61
11:K:174:ASN:HD21	11:K:189:ASN:HD22	1.47	0.61
16:K:302:P3N:H23	17:K:303:MES:H82	1.82	0.61
6:F:192:GLN:HE21	6:F:192:GLN:HA	1.66	0.60
13:1:1:THR:HG23	13:1:2:SER:N	2.17	0.60
3:Q:160:TRP:CZ2	4:R:59:LEU:HD23	2.37	0.60
8:V:3:ILE:HD11	8:V:127:LEU:HB2	1.82	0.60
14:2:176:VAL:HG12	14:2:178:LEU:HD13	1.84	0.60
11:Y:208:ASN:H	11:Y:208:ASN:HD22	1.50	0.59
2:B:65:GLU:HG3	2:B:66:LYS:HG3	1.83	0.59
6:T:95:GLU:HG2	6:T:115:ARG:HB3	1.82	0.59
9:I:174:VAL:HG21	9:I:186:LYS:HE2	1.83	0.59
7:U:87:ASN:C	7:U:87:ASN:ND2	2.59	0.59
3:Q:163:GLN:HE22	3:Q:173:ARG:HE	1.48	0.59
1:A:7:ARG:HG2	6:F:128:SER:HB3	1.85	0.59
1:A:130:ARG:NH2	7:G:124:THR:CG2	2.59	0.59
1:A:86:ARG:HE	7:G:118:ASN:HD21	1.50	0.59
1:A:7:ARG:HD2	5:E:127:TYR:HD2	1.66	0.59
1:A:130:ARG:NH2	7:G:124:THR:HG22	2.18	0.59
12:L:43:MET:HG3	12:L:101:ILE:HG22	1.84	0.59
13:M:40:ASN:HD22	13:M:40:ASN:N	1.98	0.59
8:H:50:ALA:HB2	9:I:118:CYS:HB2	1.84	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:R:186:LEU:O	4:R:190:GLU:HG3	2.03	0.58
3:Q:52:ARG:HB2	3:Q:209:ASN:HD22	1.68	0.58
3:Q:152:GLU:HB2	3:Q:153:PRO:CD	2.33	0.58
1:O:86:ARG:HE	7:U:118:ASN:ND2	2.01	0.58
8:V:50:ALA:HB2	9:W:118:CYS:HB2	1.86	0.58
8:V:113:ILE:HG12	8:V:119:THR:HG22	1.86	0.58
8:H:214:LEU:HD13	11:Y:211:GLY:HA3	1.85	0.58
2:P:15:PHE:H	3:Q:23:GLN:HE22	1.52	0.57
5:E:31:ILE:HD11	5:E:153:PRO:HD3	1.86	0.57
9:I:190:LYS:HZ2	11:Y:197:TRP:CD1	2.22	0.57
13:1:133:MET:HE1	13:1:165:ARG:HG3	1.87	0.57
1:A:121:GLN:O	1:A:124:THR:HB	2.04	0.57
2:P:67:LEU:HD22	2:P:211:GLU:HB3	1.85	0.57
6:T:95:GLU:HG3	6:T:115:ARG:HH11	1.69	0.57
8:V:128:GLY:O	8:V:131:SER:HB2	2.03	0.57
1:A:86:ARG:HH21	7:G:118:ASN:HD22	1.52	0.57
5:S:52:LYS:HD2	5:S:63:TYR:O	2.04	0.57
7:U:152:ASP:HB2	7:U:153:PRO:CD	2.35	0.57
13:1:157:ASN:HD22	13:1:160:ARG:NH1	2.01	0.57
12:Z:14:LEU:HD13	12:Z:34:VAL:HG13	1.86	0.56
3:C:163:GLN:HE21	3:C:164:THR:N	2.02	0.56
11:K:197:TRP:CD1	9:W:190:LYS:HZ1	2.23	0.56
3:Q:163:GLN:HE21	3:Q:163:GLN:HA	1.69	0.56
1:A:97:HIS:HD2	8:H:61:SER:OG	1.89	0.56
1:A:67:VAL:HG11	1:A:213:ALA:CB	2.36	0.56
3:C:186:VAL:HG21	3:C:216:LYS:HE2	1.88	0.56
14:2:14:LEU:HD23	14:2:44:CYS:SG	2.46	0.56
13:M:165:ARG:HD3	8:V:139:GLU:OE1	2.07	0.55
7:G:123:TYR:HE1	7:G:129:MET:HE3	1.68	0.55
13:M:157:ASN:ND2	13:M:160:ARG:HH11	1.91	0.55
14:N:161:GLN:NE2	14:2:136:GLY:HA2	2.17	0.55
10:X:2:ILE:HG12	10:X:130:SER:HB3	1.88	0.55
10:J:12:VAL:HG23	10:J:108:PRO:HB2	1.87	0.55
14:N:14:LEU:HD11	14:N:102:ALA:HB3	1.89	0.55
5:S:114:HIS:HB3	6:T:86:ARG:NH2	2.22	0.55
12:Z:-6:PRO:O	13:1:91:ARG:NH1	2.34	0.55
13:1:40:ASN:H	13:1:40:ASN:HD22	1.54	0.55
4:D:97:VAL:HG21	11:K:65:LEU:HD13	1.88	0.54
10:X:166:MET:HE3	10:X:168:MET:HE1	1.87	0.54
13:1:7:LYS:HB3	13:1:12:VAL:HG12	1.89	0.54
5:S:198:SER:C	5:S:200:SER:H	2.15	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:181:LYS:O	2:P:184:MET:HG3	2.06	0.54
3:Q:43:LYS:HB2	3:Q:184:ALA:HA	1.90	0.54
4:R:121:LEU:HD21	5:S:83:PRO:HB3	1.89	0.54
3:C:163:GLN:HE22	3:C:173:ARG:HE	1.54	0.54
7:G:67:ILE:HD12	7:G:211:GLU:HG2	1.90	0.54
10:J:143:ARG:O	10:J:146:MET:HG3	2.07	0.54
5:S:207:LEU:HA	5:S:209:ASN:HD22	1.73	0.54
12:Z:40:ASN:HD21	12:Z:183:GLY:HA2	1.72	0.54
6:F:192:GLN:HA	6:F:192:GLN:NE2	2.23	0.54
9:I:33:LYS:O	9:I:44:GLY:HA2	2.08	0.54
14:N:136:GLY:HA2	14:2:161:GLN:NE2	2.19	0.54
2:P:97:GLN:HE21	9:W:61:TYR:HA	1.73	0.54
8:H:3:ILE:HG13	8:H:100:ILE:HD12	1.90	0.53
12:L:99:THR:HG23	12:L:113:PHE:HB2	1.89	0.53
13:M:39:ASP:HA	13:M:184:LEU:HD12	1.90	0.53
2:P:97:GLN:HE22	9:W:64:ASN:HD22	1.56	0.53
1:A:150:GLN:O	1:A:157:TYR:HA	2.09	0.53
5:E:31:ILE:HD11	5:E:153:PRO:CD	2.39	0.53
13:M:84:ALA:HA	13:M:113:VAL:HG21	1.91	0.53
3:C:163:GLN:HE21	3:C:163:GLN:CA	2.21	0.53
5:E:207:LEU:HD23	5:E:207:LEU:H	1.74	0.53
6:T:43:ASN:N	6:T:43:ASN:HD22	2.07	0.53
5:E:134:VAL:O	5:E:153:PRO:HG3	2.09	0.53
14:N:67:THR:HA	14:N:72:GLY:O	2.09	0.53
6:T:176:LEU:HB3	7:U:58:LEU:HD21	1.90	0.53
5:S:97:ASN:HD21	12:Z:61:ASN:ND2	2.05	0.53
6:F:180(F):GLY:O	6:F:184:LEU:CB	2.57	0.52
7:G:238:GLU:O	7:G:239:GLN:HB2	2.08	0.52
12:L:134:ILE:HD11	12:L:162:ALA:HB2	1.91	0.52
13:1:1:THR:HG23	13:1:2:SER:H	1.73	0.52
10:J:171:LYS:NZ	10:X:163:GLU:O	2.42	0.52
14:2:146:MET:HE2	14:2:150:GLU:HB3	1.91	0.52
3:C:35:THR:HB	3:C:51:GLU:HG3	1.91	0.52
3:Q:156:ILE:HD12	4:R:83:ALA:HB2	1.90	0.52
3:Q:163:GLN:HE21	3:Q:164:THR:H	1.57	0.52
3:Q:169:SER:HA	3:Q:172:VAL:HG13	1.91	0.52
14:2:34:LEU:HD13	14:2:176:VAL:HG23	1.91	0.52
2:B:152:ASN:HB2	2:B:153:PRO:HD2	1.91	0.52
11:K:86:LEU:C	11:K:86:LEU:HD13	2.35	0.52
2:P:124:THR:HG22	3:Q:130:ARG:HH21	1.74	0.52
6:T:114:ASP:O	6:T:118:GLN:HG2	2.10	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:U:191:GLU:HG3	7:U:232:ARG:HG3	1.92	0.52
2:B:218(C):ASP:OD2	2:B:219:GLU:HB2	2.09	0.52
4:D:160:TYR:CE2	5:E:59:SER:HB3	2.45	0.52
9:W:101:VAL:O	9:W:110:ILE:HA	2.09	0.52
12:Z:4:LEU:CD1	12:Z:138:LEU:HD21	2.38	0.52
7:G:105:TYR:OH	8:H:66:HIS:HE1	1.92	0.51
9:I:20:LEU:HB3	9:I:28:SER:HB3	1.93	0.51
10:J:-1:MET:SD	10:J:128:GLY:HA3	2.50	0.51
5:S:15:PHE:H	6:T:23:GLN:HE22	1.57	0.51
10:X:178:VAL:HG22	10:X:184:ILE:HG12	1.91	0.51
14:2:175:MET:HE3	14:2:187(B):PHE:CE2	2.45	0.51
1:A:7:ARG:CG	6:F:128:SER:HB3	2.41	0.51
8:V:62:ASN:HB3	8:V:82:MET:HE1	1.91	0.51
6:F:35:THR:CG2	6:F:51:GLU:O	2.59	0.51
16:K:302:P3N:H41	12:L:115:PRO:HD3	1.92	0.51
12:L:-7:ASN:HD22	12:L:-6:PRO:CD	2.24	0.51
3:Q:84:ASP:CG	3:Q:130:ARG:HH22	2.18	0.51
6:F:79:SER:OG	6:F:165:THR:HG23	2.11	0.51
9:I:110:ILE:HD12	9:I:125:ILE:HG12	1.92	0.51
11:K:6:PHE:HA	11:K:123:ASP:O	2.11	0.51
14:N:140:LYS:NZ	14:2:157:HIS:HD2	2.09	0.51
13:M:139:ARG:HH11	8:V:165:ASN:HD22	1.57	0.51
6:T:35:THR:CG2	6:T:51:GLU:O	2.58	0.50
9:W:110:ILE:HD12	9:W:125:ILE:HG12	1.92	0.50
14:2:14:LEU:HD11	14:2:102:ALA:HB3	1.93	0.50
4:D:28:LEU:HA	4:D:31:ILE:HD12	1.93	0.50
8:H:216:GLU:HG3	9:I:187:ARG:HG2	1.93	0.50
9:I:165:ARG:NH2	12:Z:135:MET:HE3	2.26	0.50
11:K:37:ILE:HG23	11:K:60:GLY:HA2	1.94	0.50
2:P:87:ILE:O	2:P:91:THR:HG23	2.12	0.50
9:W:12:VAL:HG13	9:W:108:PRO:HB3	1.92	0.50
4:D:40:ILE:HD12	4:D:193:VAL:HG23	1.92	0.50
10:J:113:ILE:HA	10:J:118:THR:O	2.11	0.50
4:R:46:VAL:HG11	4:R:139:ALA:HB1	1.94	0.50
4:R:38:ILE:HD12	4:R:197:LEU:HG	1.94	0.50
7:U:151:THR:HG22	7:U:157:TYR:CB	2.41	0.50
14:2:4:MET:HB3	14:2:126:ILE:HG22	1.94	0.50
5:S:97:ASN:ND2	12:Z:61:ASN:HD21	2.09	0.50
13:1:112:TYR:O	13:1:119:THR:HA	2.12	0.50
6:F:114:ASP:O	6:F:118:GLN:HG2	2.12	0.50
10:J:17:SER:HB2	10:J:170:PHE:HB2	1.93	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:78:TYR:HB3	1:O:85:TYR:CD1	2.47	0.50
5:E:160:LEU:HD13	5:E:163:THR:HB	1.94	0.50
7:G:65:SER:HA	7:G:211:GLU:OE2	2.12	0.50
11:Y:33:LYS:HA	11:Y:45:MET:HE3	1.94	0.50
2:P:124:THR:CG2	3:Q:130:ARG:HH21	2.25	0.49
8:V:197:ARG:NH1	8:V:200:LYS:HD3	2.27	0.49
8:V:112:SER:HB3	8:V:125:LEU:HD13	1.95	0.49
10:X:6:ILE:HD11	10:X:142:TYR:CD1	2.48	0.49
7:G:215:ALA:HB2	7:G:221:PHE:HD2	1.77	0.49
11:Y:129:SER:HB3	17:Y:302:MES:H72	1.94	0.49
13:1:76:PRO:HD2	13:1:105:GLN:OE1	2.13	0.49
3:C:82:ASN:N	3:C:82:ASN:HD22	2.10	0.49
6:F:198:TYR:HB3	6:F:240:ILE:HD12	1.95	0.49
9:I:113:PHE:HA	9:I:118:CYS:O	2.12	0.49
7:G:121:GLN:O	7:G:124:THR:HB	2.13	0.49
10:J:141:HIS:HB3	10:J:154:LEU:HD11	1.94	0.49
1:O:212:LEU:HD22	1:O:224:LEU:HD12	1.95	0.49
2:B:97:GLN:HE22	9:I:64:ASN:HD22	1.60	0.48
4:D:45:GLY:HA2	4:D:146:TYR:CE1	2.48	0.48
1:O:55:SER:O	1:O:56:SER:HB3	2.13	0.48
2:B:53:LYS:O	2:B:55:THR:HG23	2.13	0.48
10:J:32:ASP:OD1	10:J:176:LYS:NZ	2.46	0.48
10:X:161:GLU:OE2	10:X:161:GLU:HA	2.13	0.48
6:T:167:LYS:HD3	6:T:205:ASN:OD1	2.13	0.48
7:U:65:SER:HA	7:U:211:GLU:OE2	2.13	0.48
12:Z:104:LEU:HA	12:Z:107:LYS:O	2.13	0.48
5:S:71:ASP:HB3	5:S:73:HIS:CD2	2.48	0.48
5:S:226:GLY:O	5:S:229:VAL:HG22	2.13	0.48
6:T:43:ASN:H	6:T:43:ASN:ND2	2.11	0.48
1:A:86:ARG:HE	7:G:118:ASN:ND2	2.10	0.48
5:S:92:LEU:HD11	5:S:112:ALA:HB1	1.96	0.48
11:Y:31:VAL:HG11	16:Y:301:P3N:C18	2.44	0.48
2:P:197:LEU:O	2:P:202:THR:OG1	2.30	0.48
6:T:126:TYR:HB2	6:T:129:VAL:HG22	1.95	0.48
13:M:110:LEU:HG	13:M:125:LEU:HD12	1.96	0.48
14:N:38:HIS:O	14:N:39:ASP:C	2.56	0.48
3:Q:201:VAL:O	3:Q:202:GLN:CB	2.61	0.48
10:X:12:VAL:HG23	10:X:108:PRO:HB2	1.95	0.48
7:G:191:GLU:HG3	7:G:232:ARG:HG3	1.95	0.48
9:I:12:VAL:HG23	9:I:178:ILE:HB	1.95	0.48
13:M:112:TYR:O	13:M:119:THR:HA	2.14	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:67:VAL:HG11	1:O:213:ALA:HB3	1.96	0.47
4:R:162:ALA:HB1	4:R:176:LEU:HD22	1.96	0.47
8:H:84:LYS:HG3	8:H:85:GLN:N	2.28	0.47
3:Q:163:GLN:NE2	3:Q:164:THR:H	2.11	0.47
10:X:113:ILE:HG12	10:X:119:LYS:HG3	1.96	0.47
5:E:92:LEU:HD11	5:E:112:ALA:HB1	1.95	0.47
9:I:10:ASP:HB3	9:I:181:LYS:HE2	1.95	0.47
8:V:126:SER:O	8:V:127:LEU:HD23	2.14	0.47
8:H:112:SER:HB3	8:H:125:LEU:HD13	1.96	0.47
9:I:20:LEU:HD21	9:I:49:ALA:HB2	1.95	0.47
10:J:15:ALA:HB2	10:J:155:LEU:HD11	1.95	0.47
13:M:141(A):VAL:HG23	13:M:141(A):VAL:O	2.15	0.47
1:O:79:SER:HB2	1:O:165:ILE:HD12	1.96	0.47
1:O:60:MET:HE3	1:O:63:THR:HG21	1.97	0.47
3:Q:216:LYS:HB2	3:Q:220:ASP:HB3	1.97	0.47
6:T:199:LEU:O	6:T:203:GLU:HB2	2.15	0.47
12:Z:-2:ASN:HA	12:Z:21:ILE:O	2.15	0.47
13:1:157:ASN:ND2	13:1:160:ARG:HH11	2.07	0.47
6:F:203:GLU:O	6:F:206:LYS:HG3	2.15	0.47
8:H:134:ALA:HB1	8:H:158:ALA:HB1	1.97	0.47
8:V:128:GLY:O	8:V:131:SER:CB	2.63	0.47
9:W:113:PHE:HA	9:W:118:CYS:O	2.15	0.47
13:1:112:TYR:HE1	13:1:127:THR:HG22	1.79	0.47
7:G:34(A):ASN:HD22	7:G:167:PRO:HG2	1.80	0.47
7:G:87:ASN:C	7:G:87:ASN:HD22	2.23	0.47
13:1:84:ALA:HA	13:1:113:VAL:HG21	1.97	0.47
2:B:150:THR:O	2:B:157:TYR:HA	2.15	0.47
3:Q:55:THR:O	3:Q:56:LEU:HD13	2.14	0.47
12:Z:2:THR:HG22	12:Z:159:PHE:CE2	2.50	0.47
13:1:205:GLY:HA3	13:1:209:GLN:HB3	1.97	0.47
1:O:35:VAL:O	1:O:79:SER:OG	2.31	0.46
1:O:97:HIS:HD2	8:V:61:SER:OG	1.98	0.46
14:N:55:ILE:HD11	14:N:95:LEU:HD13	1.97	0.46
4:R:78:MET:HG3	4:R:82:THR:HG22	1.98	0.46
1:O:111:LEU:O	1:O:115:GLU:HG2	2.16	0.46
1:A:27:ALA:HB2	7:G:15:PHE:CE2	2.51	0.46
11:K:126:CYS:HB2	11:K:135:TYR:CE1	2.50	0.46
7:U:151:THR:HG22	7:U:157:TYR:HB3	1.96	0.46
6:F:218(B):THR:HB	6:F:222:LYS:HE3	1.97	0.46
11:K:35:ILE:HG21	11:K:56:GLU:HB3	1.98	0.46
12:L:27:ASN:HB3	13:M:120:TYR:CE1	2.51	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:150:GLN:O	1:O:157:TYR:HA	2.16	0.46
6:F:38:ILE:HG12	6:F:197:ILE:HD11	1.97	0.46
3:Q:82:ASN:H	3:Q:82:ASN:ND2	2.13	0.46
4:R:215:ILE:O	4:R:215:ILE:HG13	2.13	0.46
5:S:86:ARG:O	5:S:90:ASN:HB2	2.16	0.46
8:V:197:ARG:HH21	9:W:139:GLU:HG3	1.80	0.46
9:W:107:LYS:HA	9:W:108:PRO:HD3	1.84	0.46
12:L:135:MET:HE3	9:W:165:ARG:NH2	2.31	0.46
6:F:180(F):GLY:O	6:F:184:LEU:HB2	2.16	0.46
7:U:172:ILE:HD13	7:U:197:MET:HE1	1.98	0.46
13:1:141(C):ARG:HG3	13:1:141(C):ARG:HH11	1.80	0.46
14:2:59:VAL:HG22	14:2:82:VAL:HG12	1.97	0.46
4:D:186:LEU:O	4:D:190:GLU:HG3	2.16	0.45
13:1:141(A):VAL:HG23	13:1:141(A):VAL:O	2.16	0.45
3:C:207:ALA:C	3:C:209:ASN:H	2.25	0.45
5:E:143:LYS:HE3	13:M:78:TYR:OH	2.17	0.45
7:U:233:LEU:O	7:U:236:ILE:HG13	2.16	0.45
12:L:137:PHE:CE1	12:L:141:GLN:HG3	2.52	0.45
1:O:217(D):PRO:HA	1:O:217(P):LYS:O	2.16	0.45
11:Y:196:PHE:HZ	11:Y:209:VAL:HG21	1.81	0.45
14:N:175:MET:HB2	14:N:187:LEU:HB2	1.98	0.45
13:1:40:ASN:HD22	13:1:40:ASN:N	2.14	0.45
3:C:228:GLU:O	3:C:232:TYR:HD1	2.00	0.45
4:R:158:TYR:HB3	4:R:160:TYR:CE1	2.52	0.45
5:S:179:THR:O	5:S:179:THR:HG22	2.17	0.45
3:Q:97:GLN:NE2	10:X:64:GLN:HB2	2.32	0.45
4:R:67:ILE:HD12	4:R:211:GLN:HE21	1.82	0.45
8:V:105:ASP:HB2	8:V:105(A):PRO:CD	2.46	0.45
6:F:176:LEU:HB3	7:G:58:LEU:HD21	1.99	0.45
2:P:51:GLU:OE2	2:P:202:THR:HG23	2.17	0.45
2:P:78:VAL:HG22	2:P:136:PHE:HE2	1.82	0.45
4:R:51:GLU:HG3	4:R:201:MET:HG2	1.99	0.45
1:A:67:VAL:HG11	1:A:213:ALA:HB3	1.98	0.45
1:A:217(G):LEU:HD13	1:A:218:GLY:HA2	1.99	0.45
13:M:40:ASN:N	13:M:40:ASN:ND2	2.65	0.45
7:U:77:VAL:HG12	7:U:137:THR:HB	1.99	0.45
2:P:169:THR:O	2:P:173:GLN:HB2	2.17	0.44
1:A:117:ALA:HB1	1:A:155:GLY:O	2.16	0.44
1:O:58:LEU:HD12	7:U:173:THR:HG23	1.99	0.44
7:U:166:GLY:O	7:U:169:GLN:HB2	2.18	0.44
12:L:33:LYS:O	12:L:44:SER:OG	2.34	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:T:122:ALA:HA	6:T:125:LEU:HD12	1.98	0.44
7:U:37:SER:HA	7:U:49:ILE:O	2.17	0.44
11:K:5:ALA:HA	11:K:13:ILE:O	2.18	0.44
12:L:8:GLY:HA3	12:L:11:PHE:CE2	2.53	0.44
2:P:163:ILE:HG13	2:P:164:SER:N	2.32	0.44
9:W:19:ARG:HD3	9:W:168:LEU:O	2.18	0.44
7:U:198:ILE:HG23	7:U:203:THR:O	2.17	0.44
9:W:181:LYS:H	9:W:181:LYS:HD2	1.83	0.44
10:X:90(A):ILE:HD12	10:X:90(A):ILE:HA	1.86	0.44
1:A:67:VAL:HG11	1:A:213:ALA:HB2	2.00	0.44
5:E:198:SER:C	5:E:200:SER:H	2.26	0.44
5:S:67:ILE:HG21	5:S:213:ALA:HB2	2.00	0.44
8:H:207:PRO:O	8:H:210:THR:OG1	2.34	0.44
7:G:39:ALA:HB2	7:G:48:VAL:HG12	2.00	0.44
9:W:137:MET:CE	9:W:141:LEU:HD11	2.46	0.44
10:X:2:ILE:HD12	10:X:170:PHE:CG	2.52	0.44
12:Z:34:VAL:HG12	12:Z:176:LEU:HD22	2.00	0.44
3:C:163:GLN:NE2	3:C:163:GLN:HA	2.30	0.44
4:D:192:LEU:O	4:D:196:ILE:HG13	2.18	0.44
6:F:169:ARG:HE	6:F:169:ARG:HB3	1.64	0.44
10:J:178:VAL:HG22	10:J:184:ILE:HG12	2.00	0.44
14:N:24:ALA:HB3	13:1:129:PHE:HE2	1.83	0.44
3:Q:186:VAL:O	3:Q:190:VAL:HG23	2.18	0.44
2:B:21:LEU:O	2:B:25:GLU:HG2	2.18	0.43
6:F:43:ASN:HD22	6:F:44:ASP:N	2.16	0.43
6:T:192:GLN:NE2	6:T:195:LYS:HE3	2.28	0.43
7:U:150:LYS:O	7:U:157:TYR:HA	2.18	0.43
8:V:172:ASN:ND2	8:V:193:THR:HA	2.33	0.43
8:V:206:PHE:CZ	9:W:157:GLN:HG3	2.53	0.43
14:2:36:ARG:HG3	14:2:42:TRP:CE2	2.52	0.43
6:F:167:LYS:HD3	6:F:205:ASN:HD21	1.83	0.43
2:P:125:GLN:HG3	3:Q:130:ARG:HG3	2.00	0.43
7:U:67:ILE:HD12	7:U:211:GLU:HG2	2.00	0.43
5:E:74:MET:HE2	5:E:109:VAL:HA	2.00	0.43
10:J:11:SER:HB3	10:J:179:ASP:HB3	2.01	0.43
11:K:25:TRP:CZ3	12:L:132:SER:HA	2.53	0.43
1:O:130:ARG:NH2	7:U:124:THR:CG2	2.71	0.43
2:P:150:THR:O	2:P:157:TYR:HA	2.18	0.43
11:Y:87:VAL:CG1	11:Y:115:SER:HA	2.49	0.43
14:2:38:HIS:O	14:2:39:ASP:C	2.61	0.43
3:C:203:THR:O	3:C:203:THR:OG1	2.34	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:160:TYR:CZ	4:D:163:LYS:HD3	2.54	0.43
3:Q:57:LYS:HD2	3:Q:57:LYS:HA	1.92	0.43
4:R:105:GLU:OE1	12:Z:66:TYR:OH	2.31	0.43
12:Z:106:GLU:H	12:Z:106:GLU:HG2	1.59	0.43
4:D:90:GLU:OE1	11:K:69:ARG:HD2	2.19	0.43
7:G:151:THR:HG22	7:G:157:TYR:HB3	2.01	0.43
13:M:80:PHE:CZ	13:M:111:ARG:HG2	2.53	0.43
2:P:97:GLN:NE2	9:W:64:ASN:HD22	2.17	0.43
12:Z:-9:GLN:HE21	12:Z:-8:PHE:H	1.65	0.43
2:B:37:ALA:O	2:B:164:SER:HA	2.18	0.43
7:G:192:PHE:CD1	7:G:192:PHE:C	2.96	0.43
13:M:172:ASN:ND2	13:M:191:GLN:HG2	2.34	0.43
2:P:111:ILE:HG12	10:X:70:GLU:OE2	2.19	0.43
2:P:156:ASN:OD1	3:Q:82:ASN:HB2	2.18	0.43
3:Q:40:VAL:HG21	3:Q:192:LEU:HD23	2.00	0.43
5:E:139:ILE:HD12	5:E:215:VAL:HG12	2.01	0.43
3:Q:71:ASP:OD1	3:Q:100:ARG:NH1	2.48	0.43
8:H:5:GLY:O	8:H:124:TYR:HA	2.19	0.43
9:W:48:LEU:HG	9:W:50:THR:HG22	2.01	0.43
5:E:12:THR:HG21	5:E:131:PRO:HG3	2.00	0.42
8:H:30:ASN:O	8:H:189:ARG:NH2	2.52	0.42
9:W:137:MET:HE3	9:W:141:LEU:CD1	2.48	0.42
12:Z:19:ARG:NE	12:Z:171:ASP:OD2	2.45	0.42
13:1:-5:PRO:HD3	13:1:96:TRP:CE2	2.54	0.42
1:A:29:THR:O	1:A:33:GLN:HG2	2.19	0.42
2:B:163:ILE:HG13	2:B:164:SER:N	2.34	0.42
8:H:52:THR:HG22	8:H:97:ALA:HA	2.02	0.42
8:H:172:ASN:ND2	8:H:193:THR:HG22	2.34	0.42
6:F:166:GLY:O	6:F:169:ARG:HB3	2.19	0.42
5:S:136:LEU:HB2	5:S:151:PHE:HB3	2.02	0.42
13:1:43:VAL:HG22	13:1:101:VAL:HG22	2.02	0.42
13:1:162:LEU:O	13:1:166:ASP:HB3	2.20	0.42
11:Y:86:LEU:C	11:Y:86:LEU:HD13	2.45	0.42
2:B:116:LEU:HD23	2:B:116:LEU:HA	1.83	0.42
2:P:60:GLU:O	2:P:63(A):SER:HB2	2.20	0.42
9:W:62:LYS:HD3	9:W:82:LEU:HD11	2.01	0.42
4:R:85:ALA:O	4:R:89:ILE:HG12	2.20	0.42
10:X:166:MET:HA	10:X:167:PRO:HD3	1.87	0.42
1:A:197:LEU:HD12	1:A:197:LEU:HA	1.94	0.42
7:G:224:LEU:HB3	7:G:228:ASN:HB2	2.00	0.42
11:K:146:LEU:HD22	11:K:150:ASP:HB3	2.01	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:111:ARG:HH11	13:M:121:SER:HB2	1.85	0.42
11:Y:5:ALA:HA	11:Y:13:ILE:O	2.19	0.42
2:B:97:GLN:NE2	9:I:64:ASN:HD22	2.17	0.42
11:K:200:LYS:HG3	11:K:205:SER:O	2.20	0.42
1:O:106:TYR:OH	8:V:64:GLU:OE2	2.38	0.42
4:R:79:SER:HB3	4:R:165:ILE:HD12	2.01	0.42
12:Z:3:ILE:HG21	12:Z:44:SER:OG	2.19	0.42
2:B:66:LYS:O	2:B:77:ALA:HA	2.19	0.42
3:C:150:GLN:O	3:C:157:TYR:HA	2.19	0.42
12:L:27:ASN:HB3	13:M:120:TYR:CD1	2.55	0.42
3:Q:59:GLN:HE22	3:Q:63:THR:HG21	1.85	0.42
5:E:15:PHE:H	6:F:23:GLN:NE2	2.06	0.42
5:E:54:ASN:ND2	5:E:56:ASP:O	2.53	0.42
6:F:35:THR:HG23	6:F:51:GLU:HB3	2.00	0.42
2:P:202:THR:HG22	2:P:203:ASP:N	2.35	0.42
2:P:235:LYS:H	2:P:235:LYS:HG2	1.57	0.42
4:R:67:ILE:HG22	4:R:221:PHE:HZ	1.85	0.42
2:B:181:LYS:O	2:B:184:MET:HG3	2.20	0.41
3:Q:82:ASN:ND2	3:Q:82:ASN:N	2.68	0.41
5:S:148:LEU:HD21	5:S:163:THR:HG22	2.02	0.41
6:T:194:ALA:O	6:T:198:TYR:HD1	2.03	0.41
13:1:133:MET:C	13:1:136:PRO:HD2	2.45	0.41
14:2:107:LYS:HB3	14:2:108:GLY:H	1.78	0.41
3:C:182:PRO:O	3:C:183:PRO:C	2.63	0.41
10:J:90(A):ILE:HD12	10:J:90(A):ILE:HA	1.96	0.41
5:S:152:GLN:HA	5:S:153:PRO:HD3	1.91	0.41
10:X:2:ILE:HB	10:X:17:SER:HB3	2.01	0.41
1:A:172:ALA:O	1:A:176:LEU:HG	2.20	0.41
4:D:75:GLY:HA3	4:D:221:PHE:CE2	2.55	0.41
4:D:85:ALA:O	4:D:89:ILE:HG12	2.20	0.41
8:H:3:ILE:HD11	8:H:127:LEU:HB2	2.02	0.41
12:L:113:PHE:HA	12:L:118:SER:O	2.21	0.41
13:M:1:THR:O	13:M:2:SER:C	2.61	0.41
7:U:184(G):GLU:HG2	7:U:188:LYS:HB3	1.99	0.41
10:X:2:ILE:HD13	10:X:162:LEU:HD13	2.02	0.41
10:X:113:ILE:HA	10:X:118:THR:O	2.20	0.41
6:T:216:SER:HB3	6:T:218(A):GLU:HB2	2.03	0.41
7:U:38:LEU:C	7:U:38:LEU:HD12	2.46	0.41
7:U:151:THR:HA	7:U:156:TYR:O	2.20	0.41
12:Z:113:PHE:HA	12:Z:118:SER:O	2.20	0.41
9:I:87:LEU:HD11	9:I:99:PRO:HG2	2.03	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:-8:THR:O	13:M:-7:GLN:HB3	2.21	0.41
13:M:133:MET:HE1	13:M:165:ARG:HG3	2.02	0.41
7:G:109:CYS:HB2	7:G:140:SER:OG	2.21	0.41
8:H:172:ASN:HD22	8:H:193:THR:HA	1.85	0.41
12:L:-6:PRO:O	13:M:91:ARG:NH1	2.45	0.41
7:U:170:GLN:HE21	7:U:174:THR:HG23	1.85	0.41
9:W:20:LEU:HB3	9:W:28:SER:HB3	2.03	0.41
12:L:7:ALA:HB3	12:L:123:GLN:HE21	1.86	0.41
3:C:80:GLY:HA3	3:C:133:GLY:O	2.21	0.41
6:F:203:GLU:O	6:F:206:LYS:CG	2.69	0.41
7:G:77:VAL:CG1	7:G:137:THR:HB	2.50	0.41
13:M:141(C):ARG:HH11	13:M:141(C):ARG:CG	2.28	0.41
1:O:39:GLY:HA2	1:O:47:VAL:O	2.20	0.41
3:Q:194:VAL:O	3:Q:198:LEU:HG	2.20	0.41
3:Q:215:VAL:HG12	3:Q:221:ILE:HG12	2.03	0.41
9:W:12:VAL:HG23	9:W:178:ILE:HB	2.03	0.41
12:Z:90:LYS:HD3	12:Z:95:TYR:CZ	2.56	0.41
6:F:91:ARG:HG2	6:F:119:TYR:CD2	2.56	0.41
7:G:216:THR:O	7:G:217:LYS:C	2.64	0.41
9:I:15:ALA:HB1	9:I:159:LEU:HD13	2.03	0.41
13:M:172:ASN:HD22	13:M:191:GLN:HG2	1.86	0.41
3:Q:52:ARG:HB2	3:Q:209:ASN:HA	2.03	0.41
3:Q:185:THR:HB	3:Q:188:GLU:HG2	2.03	0.41
6:T:43:ASN:HD22	6:T:43:ASN:H	1.67	0.41
10:X:59:ILE:O	10:X:63:ILE:HG12	2.21	0.41
12:Z:27:ASN:HB3	13:1:120:TYR:CE1	2.56	0.41
5:E:71:ASP:OD2	5:E:72:GLU:N	2.54	0.40
6:F:158:TRP:CZ3	7:G:64:VAL:HA	2.56	0.40
5:S:17:PRO:HA	6:T:26:TYR:CD1	2.56	0.40
12:Z:113:PHE:CD1	12:Z:113:PHE:N	2.88	0.40
7:G:76:MET:HE3	7:G:78:VAL:CG2	2.51	0.40
11:K:114:ASP:OD1	11:K:114:ASP:C	2.65	0.40
7:U:151:THR:HG22	7:U:157:TYR:HB2	2.03	0.40
8:V:78:SER:O	8:V:82:MET:HG3	2.20	0.40
10:J:38:SER:HB2	10:J:39:PRO:HD2	2.03	0.40
5:S:52:LYS:CB	5:S:63:TYR:HB3	2.49	0.40
5:S:149:LEU:HD12	5:S:159:GLU:HG3	2.04	0.40
7:G:87:ASN:C	7:G:87:ASN:ND2	2.80	0.40
13:M:17:ASP:HA	13:M:173:PHE:CB	2.52	0.40
14:N:14:LEU:O	14:N:175:MET:HA	2.21	0.40
3:Q:84:ASP:OD2	3:Q:130:ARG:NH2	2.53	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:R:163:LYS:HG3	4:R:164:ALA:N	2.37	0.40
8:V:20:SER:OG	8:V:28:ASP:HB3	2.20	0.40
8:V:197:ARG:NH2	9:W:139:GLU:HG3	2.37	0.40
2:B:21:LEU:HD13	2:B:124:THR:HG23	2.04	0.40
3:C:216:LYS:HB2	3:C:220:ASP:HB3	2.04	0.40
6:F:199:LEU:O	6:F:203:GLU:HB2	2.20	0.40
7:G:203:THR:HG22	7:G:204:GLU:O	2.22	0.40
8:H:223:ASP:OD2	8:H:223:ASP:N	2.53	0.40
14:N:129:SER:O	14:N:132:THR:HG23	2.19	0.40
11:Y:45:MET:HB3	11:Y:52:CYS:HB3	2.02	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	248/250 (99%)	239 (96%)	6 (2%)	3 (1%)	10	27
1	O	248/250 (99%)	234 (94%)	12 (5%)	2 (1%)	16	37
2	B	233/235 (99%)	223 (96%)	7 (3%)	3 (1%)	9	25
2	P	233/235 (99%)	218 (94%)	11 (5%)	4 (2%)	7	19
3	C	239/241 (99%)	229 (96%)	6 (2%)	4 (2%)	7	19
3	Q	239/241 (99%)	230 (96%)	6 (2%)	3 (1%)	9	25
4	D	229/260 (88%)	218 (95%)	11 (5%)	0	100	100
4	R	228/260 (88%)	219 (96%)	9 (4%)	0	100	100
5	E	231/233 (99%)	217 (94%)	9 (4%)	5 (2%)	5	14
5	S	231/233 (99%)	216 (94%)	11 (5%)	4 (2%)	7	19
6	F	234/242 (97%)	223 (95%)	10 (4%)	1 (0%)	30	54
6	T	234/242 (97%)	221 (94%)	13 (6%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
7	G	241/243 (99%)	234 (97%)	6 (2%)	1 (0%)	30	54
7	U	241/243 (99%)	232 (96%)	7 (3%)	2 (1%)	16	37
8	H	220/222 (99%)	211 (96%)	8 (4%)	1 (0%)	24	48
8	V	220/222 (99%)	213 (97%)	6 (3%)	1 (0%)	24	48
9	I	202/204 (99%)	192 (95%)	9 (4%)	1 (0%)	24	48
9	W	202/204 (99%)	198 (98%)	4 (2%)	0	100	100
10	J	196/198 (99%)	188 (96%)	7 (4%)	1 (0%)	24	48
10	X	196/198 (99%)	185 (94%)	8 (4%)	3 (2%)	8	22
11	K	210/212 (99%)	201 (96%)	8 (4%)	1 (0%)	24	48
11	Y	210/212 (99%)	204 (97%)	6 (3%)	0	100	100
12	L	220/222 (99%)	213 (97%)	7 (3%)	0	100	100
12	Z	220/222 (99%)	213 (97%)	7 (3%)	0	100	100
13	1	231/233 (99%)	221 (96%)	9 (4%)	1 (0%)	30	54
13	M	231/233 (99%)	214 (93%)	17 (7%)	0	100	100
14	2	194/196 (99%)	186 (96%)	8 (4%)	0	100	100
14	N	194/196 (99%)	189 (97%)	5 (3%)	0	100	100
All	All	6255/6382 (98%)	5981 (96%)	233 (4%)	41 (1%)	18	41

All (41) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	54	VAL
3	C	203	THR
3	C	207	ALA
5	E	6	ASN
6	F	184	LEU
7	G	239	GLN
11	K	180	GLU
2	P	54	VAL
3	Q	202	GLN
5	S	6	ASN
5	S	203	ASP
1	A	5	THR
1	A	167	LYS
2	B	217	ALA
2	B	218(C)	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	C	206	GLY
5	E	203	ASP
5	E	206	SER
8	H	91	GLN
3	Q	207	ALA
5	S	199	GLN
1	O	53	LYS
2	P	217	ALA
2	P	218(B)	ASP
5	S	206	SER
7	U	239	GLN
7	U	55	PRO
1	A	203	GLU
5	E	231	LYS
2	P	182	ASP
8	V	171	SER
10	X	189	ASP
10	J	8	VAL
3	Q	183	PRO
10	X	49	ALA
9	I	93	GLY
13	1	207	GLY
10	X	8	VAL
3	C	183	PRO
1	O	204	GLY
5	E	180(F)	ILE

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%)	184 (88%)	25 (12%)	5	12
1	O	209/209 (100%)	197 (94%)	12 (6%)	18	43
2	B	195/195 (100%)	180 (92%)	15 (8%)	12	30
2	P	195/195 (100%)	179 (92%)	16 (8%)	10	27

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	C	213/213 (100%)	195 (92%)	18 (8%)	10	25
3	Q	213/213 (100%)	202 (95%)	11 (5%)	21	47
4	D	192/215 (89%)	179 (93%)	13 (7%)	14	35
4	R	191/215 (89%)	172 (90%)	19 (10%)	7	19
5	E	192/192 (100%)	171 (89%)	21 (11%)	6	16
5	S	192/192 (100%)	178 (93%)	14 (7%)	13	32
6	F	195/200 (98%)	176 (90%)	19 (10%)	8	20
6	T	195/200 (98%)	180 (92%)	15 (8%)	12	30
7	G	207/207 (100%)	194 (94%)	13 (6%)	16	39
7	U	207/207 (100%)	198 (96%)	9 (4%)	26	54
8	H	181/181 (100%)	169 (93%)	12 (7%)	15	36
8	V	181/181 (100%)	171 (94%)	10 (6%)	19	45
9	I	172/172 (100%)	164 (95%)	8 (5%)	23	51
9	W	172/172 (100%)	165 (96%)	7 (4%)	27	56
10	J	175/175 (100%)	161 (92%)	14 (8%)	11	28
10	X	174/175 (99%)	162 (93%)	12 (7%)	14	34
11	K	169/169 (100%)	156 (92%)	13 (8%)	12	30
11	Y	169/169 (100%)	162 (96%)	7 (4%)	27	56
12	L	185/185 (100%)	178 (96%)	7 (4%)	29	58
12	Z	185/185 (100%)	176 (95%)	9 (5%)	22	49
13	1	199/199 (100%)	189 (95%)	10 (5%)	22	48
13	M	199/199 (100%)	191 (96%)	8 (4%)	28	56
14	2	162/162 (100%)	157 (97%)	5 (3%)	35	65
14	N	162/162 (100%)	152 (94%)	10 (6%)	16	39
All	All	5290/5348 (99%)	4938 (93%)	352 (7%)	15	36

All (352) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	MET
1	A	33	GLN
1	A	54	SER
1	A	62	GLU
1	A	64	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	95	VAL
1	A	116	VAL
1	A	158	PHE
1	A	199	GLU
1	A	203	GLU
1	A	217	ASP
1	A	217(A)	GLU
1	A	217(B)	ASN
1	A	217(D)	PRO
1	A	217(E)	ASP
1	A	217(F)	LEU
1	A	217(G)	LEU
1	A	217(I)	TYR
1	A	217(J)	THR
1	A	217(L)	ILE
1	A	217(M)	PRO
1	A	217(N)	THR
1	A	217(O)	ASP
1	A	217(P)	LYS
1	A	236	LEU
2	B	53	LYS
2	B	55	THR
2	B	57	THR
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	177	GLN
2	B	185	LYS
2	B	192	LEU
2	B	202	THR
2	B	225	LYS
2	B	232	ILE
3	C	33	ARG
3	C	44	ASN
3	C	57	LYS
3	C	61	THR
3	C	66	LYS
3	C	107	VAL
3	C	112	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	C	129	VAL
3	C	150	GLN
3	C	156	ILE
3	C	163	GLN
3	C	172	VAL
3	C	185	THR
3	C	187	GLU
3	C	193	THR
3	C	202	GLN
3	C	227	GLU
3	C	235	GLN
4	D	48	LEU
4	D	59	LEU
4	D	65	GLU
4	D	110	GLU
4	D	119	LEU
4	D	122	ARG
4	D	127	LEU
4	D	177	LEU
4	D	191	LEU
4	D	192	LEU
4	D	194	LEU
4	D	215	ILE
4	D	237	LEU
5	E	12	THR
5	E	13	VAL
5	E	18	THR
5	E	28	LEU
5	E	58	LEU
5	E	64	GLN
5	E	76	LEU
5	E	97	ASN
5	E	110	GLU
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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
5	E	219	THR
5	E	222	THR
5	E	227	GLU
6	F	35	THR
6	F	36	THR
6	F	43	ASN
6	F	72	ARG
6	F	98	SER
6	F	121	GLN
6	F	129	VAL
6	F	134	VAL
6	F	136	THR
6	F	167	LYS
6	F	169	ARG
6	F	176	LEU
6	F	192	GLN
6	F	204	ASP
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	54	VAL
7	G	87	ASN
7	G	119	LEU
7	G	124	THR
7	G	171	GLU
7	G	174	THR
7	G	197	MET
7	G	217	LYS
7	G	232	ARG
7	G	233	LEU
8	H	13	VAL
8	H	31	CYS
8	H	34	LEU
8	H	55	VAL
8	H	63	ILE
8	H	68	LEU
8	H	101	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
8	H	113	ILE
8	H	144	GLN
8	H	148	LYS
8	H	182	LYS
8	H	196	VAL
9	I	2	ILE
9	I	4	VAL
9	I	107	LYS
9	I	121	GLU
9	I	160	LEU
9	I	171	TRP
9	I	181	LYS
9	I	185	VAL
10	J	2	ILE
10	J	4	LEU
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	163	GLU
10	J	189	ASP
10	J	191	GLN
11	K	4	LEU
11	K	9	GLN
11	K	31	VAL
11	K	41	LEU
11	K	65	LEU
11	K	69	ARG
11	K	73	ARG
11	K	87	VAL
11	K	91	LYS
11	K	156	LYS
11	K	175	LEU
11	K	201	GLU
11	K	208	ASN
12	L	-9	GLN
12	L	14	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
12	L	40	ASN
12	L	61	ASN
12	L	62	SER
12	L	99	THR
12	L	138	LEU
13	M	-2	THR
13	M	40	ASN
13	M	62	LEU
13	M	65	GLU
13	M	91	ARG
13	M	148	VAL
13	M	184	LEU
13	M	190	LEU
14	N	1	THR
14	N	20	THR
14	N	36	ARG
14	N	73	THR
14	N	94	ASN
14	N	107	LYS
14	N	115	LEU
14	N	119	VAL
14	N	132	THR
14	N	178	LEU
1	O	4	MET
1	O	54	SER
1	O	56	SER
1	O	62	GLU
1	O	64	LEU
1	O	95	VAL
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	13	THR
2	P	58	LEU
2	P	65	GLU
2	P	81	LEU
2	P	91	THR
2	P	110	GLU
2	P	124	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	P	150	THR
2	P	181	LYS
2	P	185	LYS
2	P	192	LEU
2	P	198	SER
2	P	219	GLU
2	P	219(A)	VAL
2	P	225	LYS
2	P	235	LYS
3	Q	35	THR
3	Q	40	VAL
3	Q	53	ARG
3	Q	66	LYS
3	Q	82	ASN
3	Q	112	LEU
3	Q	150	GLN
3	Q	156	ILE
3	Q	163	GLN
3	Q	172	VAL
3	Q	199	GLU
4	R	12	VAL
4	R	13	SER
4	R	28	LEU
4	R	48	LEU
4	R	52	LYS
4	R	59	LEU
4	R	62	ASP
4	R	65	GLU
4	R	76	CYS
4	R	119	LEU
4	R	177	LEU
4	R	184	LEU
4	R	191	LEU
4	R	194	LEU
4	R	202	GLU
4	R	215	ILE
4	R	231	GLU
4	R	237	LEU
4	R	238	LYS
5	S	4	PHE
5	S	13	VAL
5	S	28	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
5	S	33	GLN
5	S	58	LEU
5	S	59	SER
5	S	65	LYS
5	S	76	LEU
5	S	160	LEU
5	S	178	ARG
5	S	189	LEU
5	S	206	SER
5	S	207	LEU
5	S	222	THR
6	T	25	GLU
6	T	35	THR
6	T	36	THR
6	T	43	ASN
6	T	72	ARG
6	T	95	GLU
6	T	98	SER
6	T	135	SER
6	T	165	THR
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	49	ILE
7	U	87	ASN
7	U	119	LEU
7	U	124	THR
7	U	197	MET
7	U	217	LYS
7	U	227	GLU
7	U	232	ARG
7	U	233	LEU
8	V	13	VAL
8	V	30	ASN
8	V	34	LEU
8	V	43	CYS
8	V	55	VAL
8	V	56	THR
8	V	63	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
8	V	68	LEU
8	V	153	LYS
8	V	218	ILE
9	W	-7	ASP
9	W	12	VAL
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	24	ILE
10	X	34	THR
10	X	35	ARG
10	X	48	GLU
10	X	52	THR
10	X	68	ILE
10	X	70	GLU
10	X	157	LEU
10	X	168	MET
10	X	189	ASP
10	X	191	GLN
11	Y	4	LEU
11	Y	31	VAL
11	Y	69	ARG
11	Y	87	VAL
11	Y	146	LEU
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	62	SER
12	Z	99	THR
12	Z	106	GLU
12	Z	106(A)	ASP
12	Z	138	LEU
13	1	2	SER
13	1	40	ASN
13	1	62	LEU
13	1	91	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
13	1	148	VAL
13	1	149	GLN
13	1	184	LEU
13	1	185	THR
13	1	190	LEU
13	1	204	LYS
14	2	22	THR
14	2	36	ARG
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 (195) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	33	GLN
1	A	97	HIS
1	A	150	GLN
1	A	191	HIS
2	B	23	GLN
2	B	97	GLN
2	B	121	GLN
2	B	125	GLN
2	B	156	ASN
2	B	177	GLN
2	B	218	ASN
2	B	221	GLN
3	C	20	HIS
3	C	23	GLN
3	C	44	ASN
3	C	82	ASN
3	C	121	GLN
3	C	125	GLN
3	C	150	GLN
3	C	163	GLN
3	C	168	ASN
3	C	235	GLN
4	D	23	GLN
4	D	108	ASN
4	D	150	HIS
4	D	161	ASN
4	D	199	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
4	D	226	ASN
5	E	6	ASN
5	E	7	ASN
5	E	64	GLN
5	E	73	HIS
5	E	97	ASN
5	E	104	ASN
5	E	121	GLN
5	E	125	GLN
5	E	152	GLN
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	180(C)	HIS
6	F	192	GLN
6	F	205	ASN
6	F	241	ASN
7	G	34(A)	ASN
7	G	87	ASN
7	G	118	ASN
7	G	121	GLN
7	G	125	GLN
7	G	169	GLN
7	G	178	ASN
8	H	22	GLN
8	H	30	ASN
8	H	66	HIS
8	H	86	HIS
8	H	109	HIS
8	H	144	GLN
8	H	172	ASN
8	H	190	ASN
9	I	29	ASN
10	J	36	GLN
10	J	54	GLN
10	J	77	GLN
10	J	85	GLN
10	J	112	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
10	J	141	HIS
10	J	186	GLN
11	K	9	GLN
11	K	85	ASN
11	K	141	ASN
11	K	174	ASN
11	K	190	HIS
11	K	207	ASN
11	K	208	ASN
12	L	-7	ASN
12	L	27	ASN
12	L	40	ASN
12	L	67	HIS
12	L	70(A)	ASN
12	L	123	GLN
12	L	143	ASN
12	L	144(B)	ASN
12	L	166	HIS
12	L	168	GLN
13	M	10	ASN
13	M	40	ASN
13	M	89	GLN
13	M	157	ASN
13	M	172	ASN
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	181	ASN
2	P	23	GLN
2	P	97	GLN
2	P	121	GLN
2	P	125	GLN
2	P	173	GLN
2	P	177	GLN
3	Q	20	HIS
3	Q	23	GLN
3	Q	44	ASN
3	Q	59	GLN
3	Q	82	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	Q	97	GLN
3	Q	121	GLN
3	Q	125	GLN
3	Q	150	GLN
3	Q	163	GLN
3	Q	179	ASN
3	Q	209	ASN
3	Q	235	GLN
4	R	23	GLN
4	R	99	HIS
4	R	108	ASN
4	R	147	GLN
4	R	150	HIS
4	R	199	GLN
4	R	211	GLN
4	R	226	ASN
5	S	73	HIS
5	S	104	ASN
5	S	121	GLN
5	S	125	GLN
5	S	156	ASN
5	S	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	192	GLN
7	U	34(A)	ASN
7	U	87	ASN
7	U	118	ASN
7	U	121	GLN
7	U	125	GLN
7	U	170	GLN
7	U	178	ASN
7	U	182	HIS
8	V	30	ASN
8	V	35	HIS
8	V	57	GLN
8	V	66	HIS
8	V	86	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
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
9	W	145	ASN
10	X	36	GLN
10	X	54	GLN
10	X	77	GLN
10	X	96	GLN
10	X	106	ASN
10	X	112	GLN
10	X	141	HIS
10	X	186	GLN
11	Y	85	ASN
11	Y	141	ASN
11	Y	174	ASN
11	Y	207	ASN
11	Y	208	ASN
12	Z	-9	GLN
12	Z	-7	ASN
12	Z	40	ASN
12	Z	61	ASN
12	Z	67	HIS
12	Z	70	HIS
12	Z	70(A)	ASN
12	Z	84	GLN
12	Z	141	GLN
12	Z	166	HIS
13	1	-7	GLN
13	1	10	ASN
13	1	18	ASN
13	1	40	ASN
13	1	89	GLN
13	1	149	GLN
13	1	157	ASN
14	2	38	HIS
14	2	69	GLN
14	2	157	HIS
14	2	161	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 14 ligands modelled in this entry, 10 are monoatomic - leaving 4 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
17	MES	Y	302	-	12,12,12	2.31	1 (8%)	15,16,16	1.30	1 (6%)
16	P3N	K	302	-	46,46,46	1.29	5 (10%)	61,64,64	1.81	9 (14%)
17	MES	K	303	-	12,12,12	2.28	1 (8%)	15,16,16	1.16	1 (6%)
16	P3N	Y	301	-	46,46,46	1.26	6 (13%)	61,64,64	1.75	7 (11%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
17	MES	Y	302	-	-	3/6/14/14	0/1/1/1
16	P3N	K	302	-	-	0/40/40/40	0/4/4/4
17	MES	K	303	-	-	1/6/14/14	0/1/1/1
16	P3N	Y	301	-	-	7/40/40/40	0/4/4/4

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	Y	302	MES	C8-S	-7.73	1.66	1.77
17	K	303	MES	C8-S	-7.61	1.66	1.77
16	K	302	P3N	C1-N36	5.62	1.35	1.29
16	Y	301	P3N	C1-N36	5.09	1.34	1.29
16	Y	301	P3N	C32-C31	-2.85	1.34	1.41
16	K	302	P3N	C32-C31	-2.68	1.34	1.41
16	Y	301	P3N	O39-C1	2.65	1.36	1.34
16	K	302	P3N	C31-C33	2.61	1.53	1.48
16	Y	301	P3N	C40-C37	2.55	1.55	1.51
16	Y	301	P3N	C31-C33	2.49	1.53	1.48
16	K	302	P3N	C40-C37	2.46	1.55	1.51
16	K	302	P3N	C2-C1	2.41	1.53	1.49
16	Y	301	P3N	C2-C1	2.01	1.52	1.49

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	K	302	P3N	O29-C28-C35	6.33	124.60	115.89
16	Y	301	P3N	O29-C28-C35	5.84	123.92	115.89
16	K	302	P3N	O39-C1-N36	-5.63	109.06	113.62
16	Y	301	P3N	O39-C1-N36	-5.58	109.11	113.62
16	K	302	P3N	C35-C28-C32	-4.97	125.46	134.05
16	K	302	P3N	O39-N38-C37	4.75	107.13	103.14
16	Y	301	P3N	O39-N38-C37	4.49	106.91	103.14
16	Y	301	P3N	C35-C28-C32	-4.32	126.58	134.05
16	Y	301	P3N	N36-C37-N38	-4.12	109.56	114.74
16	K	302	P3N	N36-C37-N38	-3.95	109.78	114.74
16	Y	301	P3N	O39-C1-C2	3.76	122.11	117.11
16	K	302	P3N	C40-C37-N36	3.25	127.13	122.92
16	K	302	P3N	C28-O29-N30	-2.87	105.55	108.47
17	Y	302	MES	O3S-S-C8	2.70	111.29	106.00
17	K	303	MES	O3S-S-C8	2.70	111.28	106.00
16	K	302	P3N	O39-C1-C2	2.47	120.39	117.11
16	K	302	P3N	C3-C2-C1	-2.41	107.82	113.72
16	Y	301	P3N	C28-O29-N30	-2.21	106.21	108.47

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
17	Y	302	MES	C7-C8-S-O1S

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
17	Y	302	MES	C7-C8-S-O3S
16	Y	301	P3N	N38-C37-C40-C41
16	Y	301	P3N	N38-C37-C40-C42
16	Y	301	P3N	N38-C37-C40-C43
17	Y	302	MES	C7-C8-S-O2S
16	Y	301	P3N	N36-C37-C40-C43
16	Y	301	P3N	C32-C31-C33-N4
16	Y	301	P3N	N36-C37-C40-C42
16	Y	301	P3N	N36-C37-C40-C41
17	K	303	MES	C7-C8-S-O3S

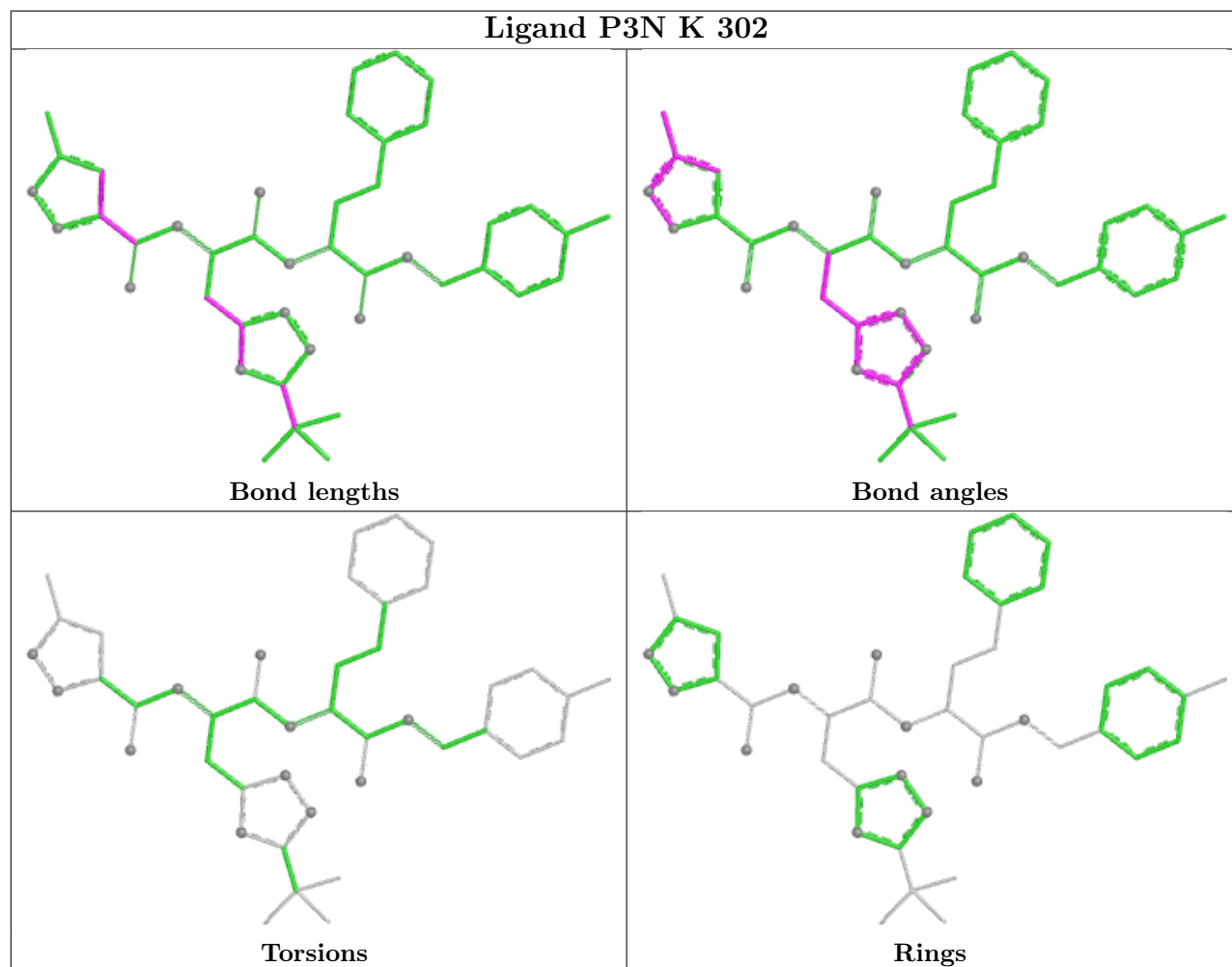
There are no ring outliers.

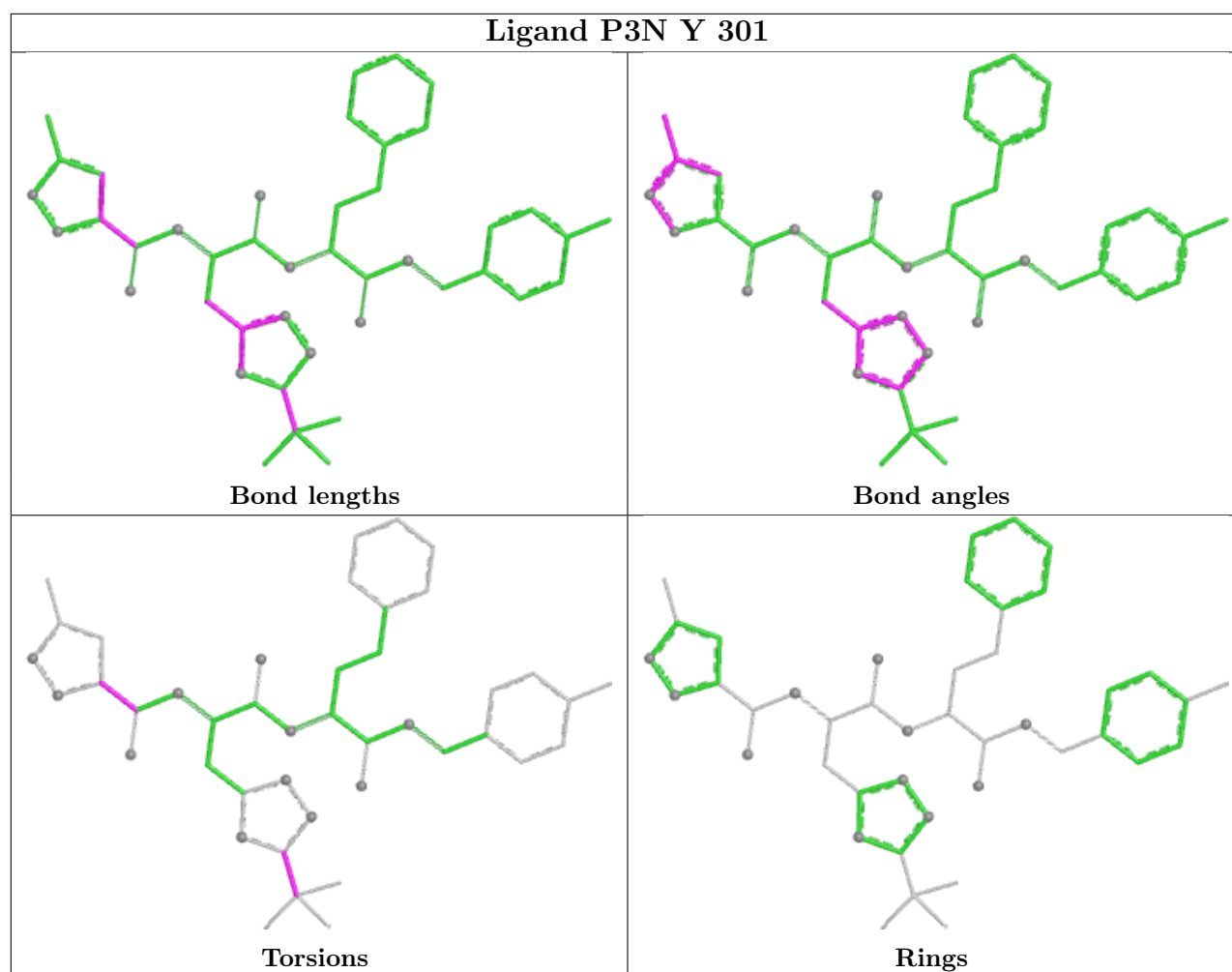
4 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
17	Y	302	MES	1	0
16	K	302	P3N	2	0
17	K	303	MES	1	0
16	Y	301	P3N	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.

Ligand P3N K 302





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%)	0.24	10 (4%) 42 38	35, 50, 71, 89	0
1	O	250/250 (100%)	0.33	13 (5%) 33 29	37, 55, 83, 94	0
2	B	235/235 (100%)	0.53	21 (8%) 15 13	34, 53, 86, 91	0
2	P	235/235 (100%)	0.53	19 (8%) 18 15	33, 55, 85, 94	0
3	C	241/241 (100%)	0.71	25 (10%) 11 10	38, 61, 100, 118	0
3	Q	241/241 (100%)	1.21	59 (24%) 2 1	42, 65, 110, 128	0
4	D	233/260 (89%)	0.44	12 (5%) 33 29	36, 56, 81, 97	0
4	R	232/260 (89%)	0.50	12 (5%) 33 29	35, 57, 80, 94	0
5	E	233/233 (100%)	0.60	14 (6%) 27 24	42, 58, 84, 94	0
5	S	233/233 (100%)	0.81	28 (12%) 9 7	40, 60, 90, 102	0
6	F	236/242 (97%)	0.28	8 (3%) 48 44	33, 51, 80, 88	0
6	T	236/242 (97%)	0.37	6 (2%) 58 55	32, 52, 77, 98	0
7	G	243/243 (100%)	0.09	8 (3%) 49 45	30, 47, 72, 96	0
7	U	243/243 (100%)	0.09	9 (3%) 45 41	31, 47, 70, 86	0
8	H	222/222 (100%)	-0.00	2 (0%) 81 80	34, 44, 61, 88	0
8	V	222/222 (100%)	0.13	6 (2%) 56 53	37, 47, 64, 87	0
9	I	204/204 (100%)	-0.14	0 100 100	31, 43, 57, 64	0
9	W	204/204 (100%)	-0.02	3 (1%) 72 70	31, 44, 61, 66	0
10	J	198/198 (100%)	0.07	8 (4%) 42 38	33, 45, 58, 110	0
10	X	198/198 (100%)	0.15	9 (4%) 38 34	36, 46, 62, 111	0
11	K	212/212 (100%)	-0.06	3 (1%) 73 72	33, 42, 59, 72	0
11	Y	212/212 (100%)	-0.03	1 (0%) 87 86	32, 44, 60, 65	0
12	L	222/222 (100%)	-0.01	1 (0%) 87 86	32, 44, 65, 72	0
12	Z	222/222 (100%)	0.01	4 (1%) 67 65	32, 44, 64, 73	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	1	233/233 (100%)	-0.02	1 (0%) 88 87	31, 43, 59, 64	0
13	M	233/233 (100%)	0.07	6 (2%) 57 54	33, 45, 59, 62	0
14	2	196/196 (100%)	-0.12	2 (1%) 79 78	33, 41, 58, 72	0
14	N	196/196 (100%)	-0.13	0 100 100	32, 41, 57, 71	0
All	All	6315/6382 (98%)	0.25	290 (4%) 37 34	30, 48, 83, 128	0

All (290) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
10	X	-1	MET	9.6
3	Q	56	LEU	9.6
2	B	217	ALA	6.9
5	E	4	PHE	6.8
3	Q	55	THR	6.7
10	J	192	ALA	6.7
5	S	4	PHE	6.6
13	M	-8	THR	6.6
10	J	-1	MET	5.8
3	C	55	THR	5.8
3	C	56	LEU	5.5
3	C	208	LYS	5.4
2	P	217	ALA	5.4
10	X	192	ALA	5.4
6	T	13	SER	5.3
2	P	54	VAL	5.1
2	B	54	VAL	5.1
2	B	239	THR	5.0
6	F	13	SER	5.0
1	O	4	MET	4.7
13	1	-8	THR	4.7
3	Q	54	SER	4.7
7	U	6	ALA	4.6
7	U	240	ASP	4.6
4	D	12	VAL	4.6
3	Q	57	LYS	4.5
3	Q	207	ALA	4.5
1	A	4	MET	4.5
3	C	7	GLY	4.3
3	Q	59	GLN	4.3
1	O	5	THR	4.3
3	Q	64	PRO	4.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
11	K	210	ILE	4.2
4	D	10	ARG	4.1
6	F	205	ASN	4.0
3	Q	58	LEU	4.0
3	Q	232	TYR	4.0
3	Q	208	LYS	3.9
2	P	218	ASN	3.8
3	C	8	TYR	3.8
1	O	217(P)	LYS	3.8
5	S	209	ASN	3.8
10	J	191	GLN	3.8
3	C	11	ALA	3.8
5	E	5	ARG	3.8
4	D	11	GLY	3.7
5	S	206	SER	3.7
6	T	240	ILE	3.7
2	P	216(B)	GLY	3.7
8	V	197	ARG	3.6
4	D	127	LEU	3.6
3	Q	44	ASN	3.6
2	P	239	THR	3.6
6	F	204	ASP	3.6
3	C	57	LYS	3.6
3	Q	9	ASP	3.5
2	B	55	THR	3.5
5	S	51	LEU	3.5
8	V	223	ASP	3.5
2	B	216(B)	GLY	3.5
3	Q	233	VAL	3.5
2	B	216(A)	LYS	3.5
7	U	199	ASP	3.5
13	M	61	ASP	3.5
3	C	207	ALA	3.5
6	F	184	LEU	3.4
4	R	10	ARG	3.4
11	Y	210	ILE	3.4
1	A	5	THR	3.4
2	B	13	THR	3.4
2	B	218	ASN	3.4
5	S	63	TYR	3.4
5	S	57	GLU	3.4
3	C	185	THR	3.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
3	C	9	ASP	3.3
3	Q	240	LYS	3.3
10	J	168	MET	3.3
1	O	235	ALA	3.3
10	J	190	PHE	3.3
3	C	14	ILE	3.2
1	O	217(O)	ASP	3.2
4	D	13	SER	3.2
3	Q	184	ALA	3.2
4	D	242	ALA	3.2
5	S	55	ALA	3.2
10	X	191	GLN	3.1
5	S	12	THR	3.1
7	G	6	ALA	3.1
4	D	126	ARG	3.1
3	Q	236	ILE	3.1
12	Z	144(R)	LYS	3.1
5	E	206	SER	3.1
7	G	240	ASP	3.1
13	M	39	ASP	3.1
5	S	5	ARG	3.1
3	Q	201	VAL	3.1
3	Q	180	TYR	3.0
3	Q	224	LEU	3.0
6	F	206(B)	GLU	3.0
5	E	203	ASP	3.0
3	C	58	LEU	3.0
3	Q	8	TYR	3.0
3	Q	144(A)	ASP	3.0
3	Q	63	THR	3.0
3	Q	200	VAL	3.0
1	A	203	GLU	3.0
7	U	218	ASP	2.9
3	Q	206	GLY	2.9
4	R	123	PHE	2.9
5	E	207(C)	VAL	2.9
6	F	180(F)	GLY	2.9
3	Q	187	GLU	2.9
5	E	7	ASN	2.9
3	C	12	LEU	2.9
3	Q	186	VAL	2.9
9	W	181	LYS	2.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
3	Q	13	SER	2.9
5	S	60	SER	2.9
1	A	217	ASP	2.9
3	Q	62(A)	ILE	2.8
5	S	32	LYS	2.8
3	Q	223	ALA	2.8
5	E	207	LEU	2.8
7	G	237	ALA	2.8
3	Q	52	ARG	2.8
2	P	61	GLN	2.8
2	P	238	ILE	2.8
3	C	209	ASN	2.8
2	P	53	LYS	2.8
3	C	66	LYS	2.8
2	P	13	THR	2.8
4	D	9	ASP	2.8
5	S	203	ASP	2.8
4	D	244	GLU	2.8
3	Q	189	CYS	2.8
5	E	168	ARG	2.8
1	O	6	ASP	2.8
3	Q	7	GLY	2.7
4	R	11	GLY	2.7
1	A	235	ALA	2.7
3	Q	185	THR	2.7
3	Q	222	VAL	2.7
9	W	182	ASP	2.7
3	Q	229	ILE	2.7
3	C	206	GLY	2.7
2	B	64	THR	2.7
2	P	63	THR	2.7
3	Q	22	PHE	2.7
1	A	7	ARG	2.6
3	Q	62	ARG	2.6
8	V	221	ILE	2.6
11	K	211	GLY	2.6
10	X	188	ASP	2.6
5	S	58	LEU	2.6
2	P	216(A)	LYS	2.6
2	P	55	THR	2.6
3	Q	61	THR	2.6
5	S	33	GLN	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
12	L	144(P)	LEU	2.6
3	Q	209	ASN	2.6
5	E	207(E)	ASN	2.6
10	X	190	PHE	2.6
3	C	203	THR	2.5
5	S	56	ASP	2.5
5	S	10	GLY	2.5
3	Q	217	PRO	2.5
3	Q	45	CYS	2.5
5	S	59	SER	2.5
1	O	64	LEU	2.5
2	P	59	LEU	2.5
6	T	203	GLU	2.5
7	U	239	GLN	2.5
4	R	158	TYR	2.5
2	B	61	GLN	2.5
5	S	208(A)	VAL	2.5
3	Q	50	CYS	2.5
3	Q	66	LYS	2.5
3	Q	12	LEU	2.5
4	D	122	ARG	2.5
7	U	236	ILE	2.5
3	C	53	ARG	2.4
4	R	9	ASP	2.4
7	U	55	PRO	2.4
3	C	222	VAL	2.4
8	V	213	VAL	2.4
5	S	198	SER	2.4
5	S	53	ARG	2.4
3	Q	203	THR	2.4
2	B	53	LYS	2.4
10	J	193	GLN	2.4
2	P	220	TYR	2.4
1	A	236	LEU	2.4
2	B	202	THR	2.4
8	H	221	ILE	2.4
13	M	70(D)	ASP	2.4
2	P	218(C)	GLY	2.4
14	2	116	GLY	2.4
2	B	238	ILE	2.3
6	F	240	ILE	2.3
3	Q	237	GLU	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	55	SER	2.3
4	R	12	VAL	2.3
10	X	49	ALA	2.3
2	P	64	THR	2.3
4	R	128	MET	2.3
14	2	149	GLU	2.3
10	X	189	ASP	2.3
4	R	192	LEU	2.3
3	C	211	GLU	2.3
6	F	127	ASN	2.3
2	P	209	ARG	2.3
1	O	208	GLY	2.3
3	Q	238	GLN	2.3
3	C	232	TYR	2.3
5	E	57	GLU	2.3
1	O	200	SER	2.3
8	H	223	ASP	2.3
11	K	73	ARG	2.3
12	Z	-9	GLN	2.3
3	Q	198	LEU	2.3
10	J	49	ALA	2.2
13	M	70(C)	ALA	2.2
3	C	63	THR	2.2
2	B	22	TYR	2.2
10	X	193	GLN	2.2
3	Q	38	VAL	2.2
3	Q	210	ILE	2.2
4	D	238	LYS	2.2
12	Z	96	TYR	2.2
2	B	204(A)	SER	2.2
3	Q	42	GLY	2.2
1	A	217(P)	LYS	2.2
1	O	53	LYS	2.2
3	Q	60	ASP	2.2
5	E	189	LEU	2.2
9	W	179	LYS	2.2
2	P	223	ILE	2.2
6	T	22	PHE	2.2
8	V	218	ILE	2.2
2	B	220	TYR	2.2
4	R	218	GLN	2.2
8	V	182	LYS	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	B	218(D)	GLY	2.2
12	Z	144(Q)	LEU	2.2
3	Q	194	VAL	2.2
1	O	7	ARG	2.1
1	O	8	TYR	2.1
3	Q	241	GLN	2.1
3	Q	226	SER	2.1
5	S	214	ILE	2.1
7	G	234	VAL	2.1
10	J	187	VAL	2.1
4	R	122	ARG	2.1
2	B	63	THR	2.1
2	B	235	LYS	2.1
3	Q	235	GLN	2.1
5	E	127	TYR	2.1
7	G	8	TYR	2.1
4	R	168	GLY	2.1
2	B	223	ILE	2.1
5	S	190	ILE	2.1
7	G	236	ILE	2.1
5	S	172	ALA	2.1
5	S	52	LYS	2.1
7	G	129	MET	2.1
1	O	233	LEU	2.1
3	C	50	CYS	2.1
2	B	234	VAL	2.1
3	Q	40	VAL	2.1
6	T	227	ASP	2.1
5	S	204	GLU	2.1
6	T	238	LYS	2.1
3	Q	53	ARG	2.0
3	Q	196	SER	2.0
2	P	235	LYS	2.0
5	E	222	THR	2.0
3	C	183	PRO	2.0
7	U	129	MET	2.0
3	C	235	GLN	2.0
5	S	64	GLN	2.0
5	E	6	ASN	2.0
4	R	223	ILE	2.0
7	U	7	GLY	2.0
13	M	30	GLY	2.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
10	X	187	VAL	2.0
4	D	205	GLU	2.0
7	G	57	LYS	2.0
1	A	56	SER	2.0
5	S	233	ILE	2.0
5	S	224	TYR	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

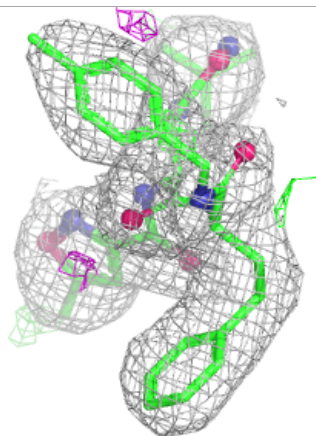
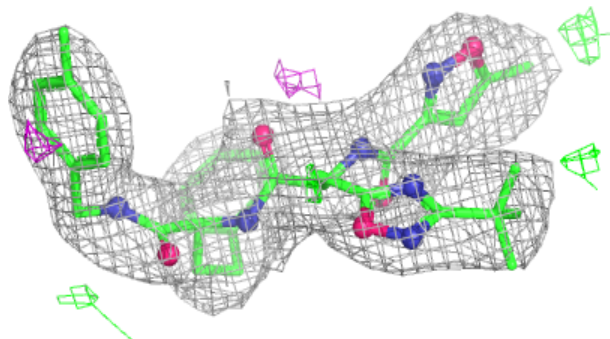
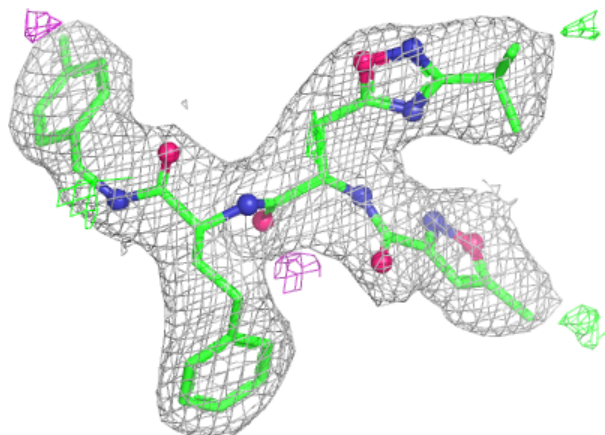
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
15	MG	I	201	1/1	0.69	0.20	58,58,58,58	0
15	MG	L	201	1/1	0.74	0.19	56,56,56,56	0
15	MG	L	202	1/1	0.86	0.15	54,54,54,54	0
15	MG	H	301	1/1	0.91	0.13	66,66,66,66	0
15	MG	F	302	1/1	0.91	0.22	107,107,107,107	0
15	MG	F	301	1/1	0.93	0.09	61,61,61,61	0
16	P3N	K	302	43/43	0.93	0.11	38,45,57,58	0
16	P3N	Y	301	43/43	0.93	0.11	40,45,58,59	0
15	MG	G	301	1/1	0.94	0.11	59,59,59,59	0
15	MG	N	201	1/1	0.94	0.08	47,47,47,47	0
17	MES	K	303	12/12	0.94	0.12	62,66,69,69	0
17	MES	Y	302	12/12	0.94	0.12	66,69,71,71	0
15	MG	I	202	1/1	0.96	0.13	57,57,57,57	0
15	MG	K	301	1/1	0.97	0.08	53,53,53,53	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers

as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

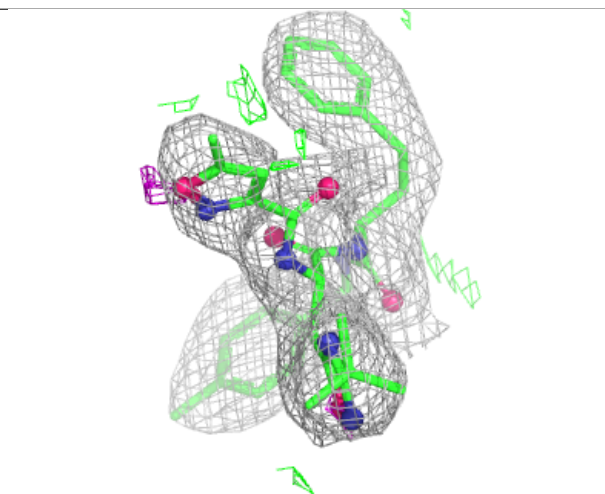
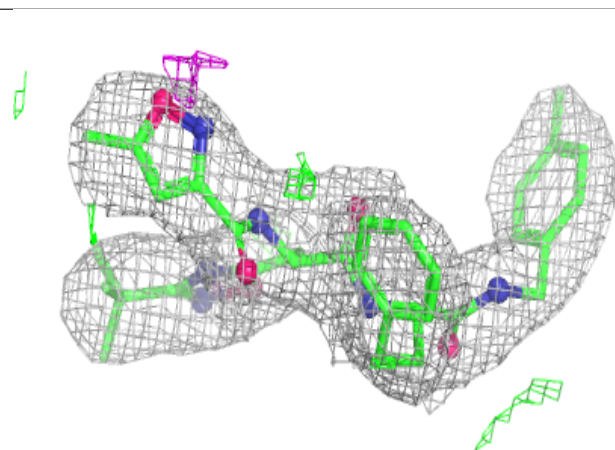
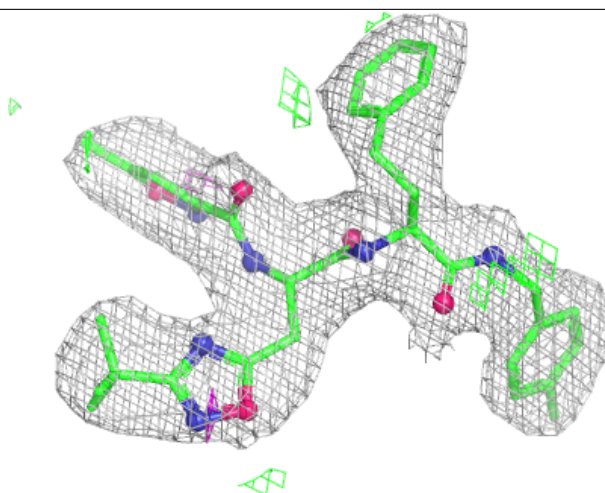
Electron density around P3N K 302:

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



Electron density around P3N Y 301:

$2mF_o-DF_c$ (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.