



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 06:45 PM UTC

PDB ID : 7B12 / pdb_00007b12
Title : HUMAN IMMUNOPROTEASOME 20S PARTICLE IN COMPLEX WITH [2-(3-ethylphenyl)-1-[(2S)-3-phenyl-2-[(pyrazin-2-yl)formamido]propanamido]ethyl]boronic acid
Authors : Musil, D.; Klein, M.; Crosignani, S.
Deposited on : 2020-11-23
Resolution : 2.43 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

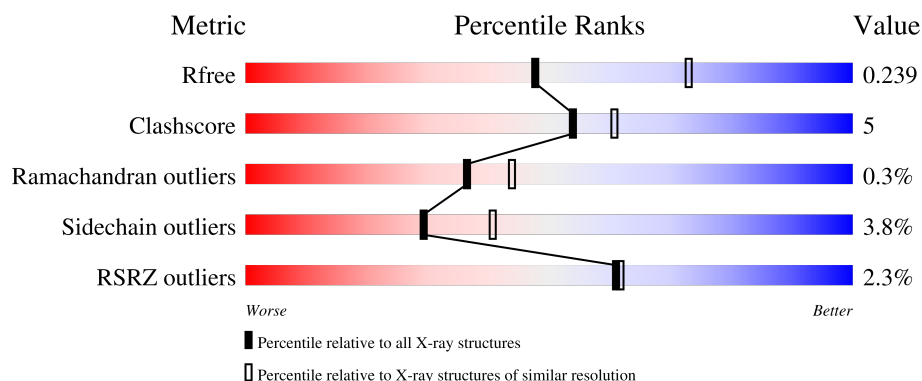
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.43 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	2340 (2.46-2.42)
Clashscore	190562	2400 (2.46-2.42)
Ramachandran outliers	187476	2379 (2.46-2.42)
Sidechain outliers	187428	2379 (2.46-2.42)
RSRZ outliers	180081	2340 (2.46-2.42)

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	1	213	% 87% 11% .
1	M	213	88% 11% .
2	2	214	% 85% 14% .
2	N	214	83% 16% .

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Mol	Chain	Length	Quality of chain
3	A	242	
3	O	242	
4	B	229	
4	P	229	
5	C	248	
5	Q	248	
6	D	235	
6	r	235	
7	E	232	
7	s	232	
8	F	236	
8	T	236	
9	G	244	
9	U	244	
10	H	199	
10	V	199	
11	J	204	
11	X	204	
12	K	197	
12	Y	197	
13	L	203	
13	Z	203	
14	i	223	
14	w	223	

2 Entry composition

There are 18 unique types of molecules in this entry. The entry contains 49338 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 subunit beta type-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	1	213	Total	C	N	O	S	54	0	0
			1654	1047	284	313	10			
1	M	213	Total	C	N	O	S	36	0	0
			1654	1047	284	313	10			

- Molecule 2 is a protein called Proteasome subunit beta type-4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	2	214	Total	C	N	O	S	20	0	0
			1673	1055	289	317	12			
2	N	214	Total	C	N	O	S	25	0	0
			1673	1055	289	317	12			

- Molecule 3 is a protein called Proteasome subunit alpha type-6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	A	240	Total	C	N	O	S	154	0	0
			1866	1185	309	359	13			
3	O	240	Total	C	N	O	S	114	0	0
			1866	1182	312	359	13			

- Molecule 4 is a protein called Proteasome subunit alpha type-2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	B	229	Total	C	N	O	S	123	0	0
			1787	1144	301	336	6			
4	P	229	Total	C	N	O	S	98	0	0
			1787	1144	301	336	6			

- Molecule 5 is a protein called Proteasome subunit alpha type-4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	C	241	Total	C	N	O	S	156	0	0
			1898	1202	325	361	10			
5	Q	245	Total	C	N	O	S	156	0	0
			1931	1220	332	369	10			

- Molecule 6 is a protein called Proteasome subunit alpha type-7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	D	227	Total	C	N	O	S	182	0	0
			1798	1132	318	343	5			
6	r	229	Total	C	N	O	S	239	0	0
			1816	1143	322	346	5			

- Molecule 7 is a protein called Proteasome subunit alpha type-5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	E	230	Total	C	N	O	S	117	0	0
			1758	1103	291	353	11			
7	s	230	Total	C	N	O	S	134	0	0
			1752	1100	290	351	11			

- Molecule 8 is a protein called Proteasome subunit alpha type-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	F	236	Total	C	N	O	S	109	0	0
			1857	1162	334	350	11			
8	T	236	Total	C	N	O	S	129	0	0
			1857	1162	334	350	11			

- Molecule 9 is a protein called Proteasome subunit alpha type-3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	G	242	Total	C	N	O	S	149	0	0
			1893	1201	323	358	11			
9	U	243	Total	C	N	O	S	134	0	0
			1899	1204	324	360	11			

- Molecule 10 is a protein called Proteasome subunit beta type-9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	H	199	Total	C	N	O	S	26	0	0
			1493	939	254	291	9			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	V	199	Total	C	N	O	S	34	0	0
			1493	939	254	291	9			

- Molecule 11 is a protein called Proteasome subunit beta type-3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	J	204	Total	C	N	O	S	33	0	0
			1591	1013	265	294	19			
11	X	204	Total	C	N	O	S	23	0	0
			1591	1013	265	294	19			

- Molecule 12 is a protein called Proteasome subunit beta type-2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	K	196	Total	C	N	O	S	56	0	0
			1571	1006	267	289	9			
12	Y	197	Total	C	N	O	S	51	0	0
			1578	1011	268	290	9			

- Molecule 13 is a protein called Proteasome subunit beta type-8.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	L	203	Total	C	N	O	S	18	0	0
			1576	984	276	301	15			
13	Z	203	Total	C	N	O	S	37	0	0
			1576	984	276	301	15			

- Molecule 14 is a protein called Proteasome subunit beta type-10.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	i	219	Total	C	N	O	S	76	0	0
			1609	1010	286	305	8			
14	w	220	Total	C	N	O	S	69	0	0
			1616	1014	287	307	8			

- Molecule 15 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



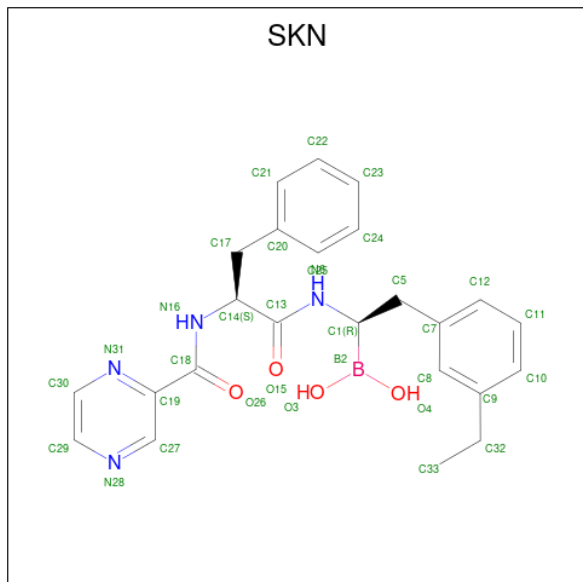
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
15	1	1	Total	O	S	0	0
			5	4	1		
15	1	1	Total	O	S	0	0
			5	4	1		
15	K	1	Total	O	S	0	0
			5	4	1		
15	L	1	Total	O	S	0	0
			5	4	1		
15	Y	1	Total	O	S	0	0
			5	4	1		

- Molecule 16 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
16	A	1	Total	Na	0	0
			1	1		
16	L	1	Total	Na	0	0
			1	1		
16	O	1	Total	Na	0	0
			1	1		
16	Z	1	Total	Na	0	0
			1	1		
16	i	1	Total	Na	0	0
			1	1		
16	w	1	Total	Na	0	0
			1	1		

- Molecule 17 is ((R)-2-(3-ethylphenyl)-1-((S)-3-phenyl-2-(pyrazine-2-carboxamido)propan

amido)ethyl)boronic acid (CCD ID: SKN) (formula: C₂₄H₂₇BN₄O₄) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
17	H	1	Total	B	C	N	O	0	0
			33	1	24	4	4		
17	L	1	Total	B	C	N	O	0	0
			33	1	24	4	4		
17	V	1	Total	B	C	N	O	0	0
			33	1	24	4	4		
17	Z	1	Total	B	C	N	O	0	0
			33	1	24	4	4		
17	i	1	Total	B	C	N	O	0	0
			33	1	24	4	4		
17	w	1	Total	B	C	N	O	0	0
			33	1	24	4	4		

- Molecule 18 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
18	1	56	Total	O	0	0
			56	56		
18	2	60	Total	O	0	0
			60	60		
18	A	32	Total	O	0	0
			32	32		
18	B	26	Total	O	0	0
			26	26		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
18	C	36	Total O 36 36	0	0
18	D	18	Total O 18 18	0	0
18	E	28	Total O 28 28	0	0
18	F	23	Total O 23 23	0	0
18	G	21	Total O 21 21	0	0
18	H	32	Total O 32 32	0	0
18	J	59	Total O 59 59	0	0
18	K	16	Total O 16 16	0	0
18	L	41	Total O 41 41	0	0
18	M	43	Total O 43 43	0	0
18	N	54	Total O 54 54	0	0
18	O	34	Total O 34 34	0	0
18	P	28	Total O 28 28	0	0
18	Q	33	Total O 33 33	0	0
18	T	38	Total O 38 38	0	0
18	U	33	Total O 33 33	0	0
18	V	42	Total O 42 42	0	0
18	X	47	Total O 47 47	0	0
18	Y	28	Total O 28 28	0	0
18	Z	38	Total O 38 38	0	0
18	i	35	Total O 35 35	0	0

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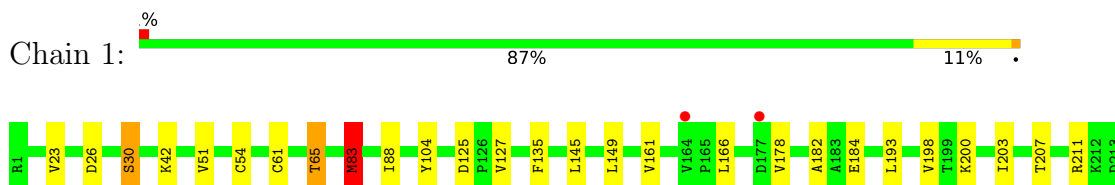
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
18	r	27	Total 27	O 27	0	0
18	s	20	Total 20	O 20	0	0
18	w	48	Total 48	O 48	0	0

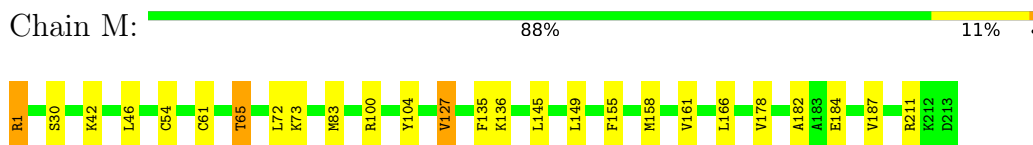
3 Residue-property plots [i](#)

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

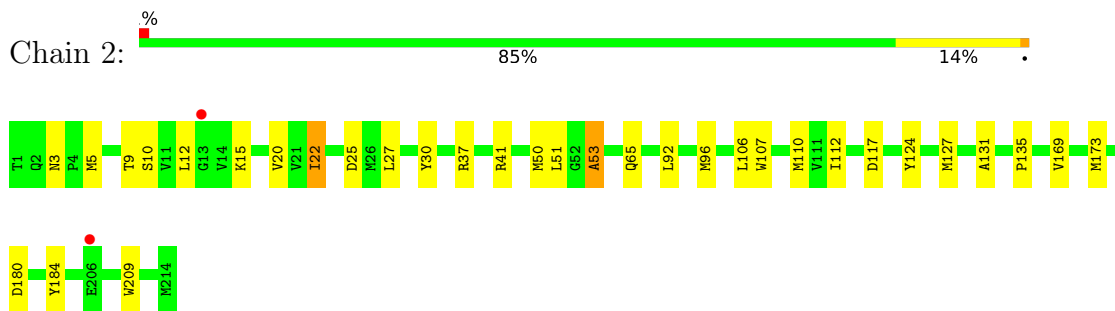
- Molecule 1: Proteasome subunit beta type-1



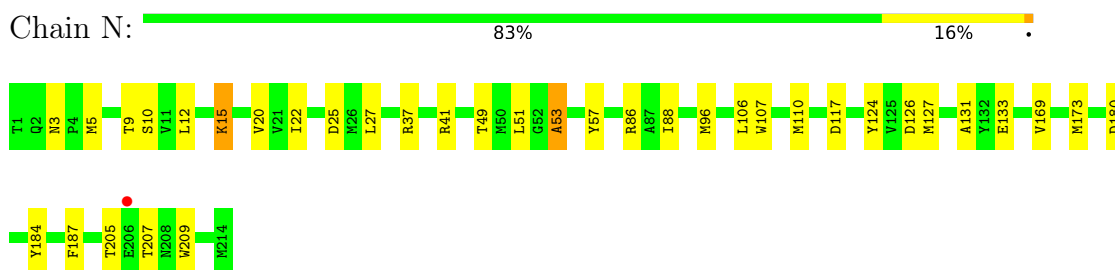
- Molecule 1: Proteasome subunit beta type-1



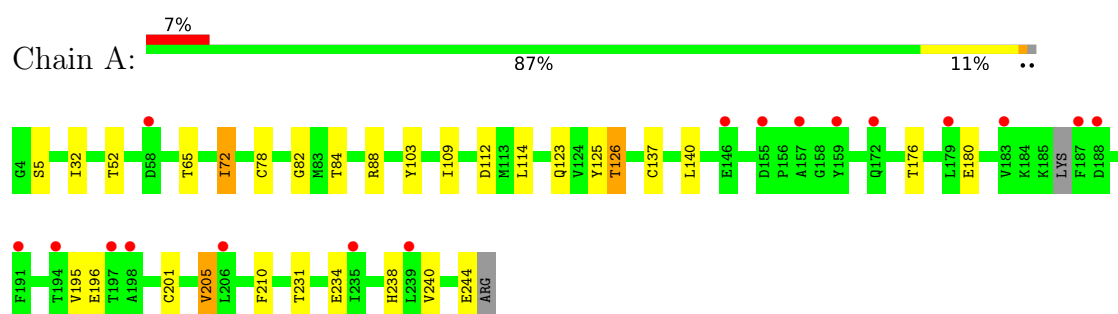
- Molecule 2: Proteasome subunit beta type-4



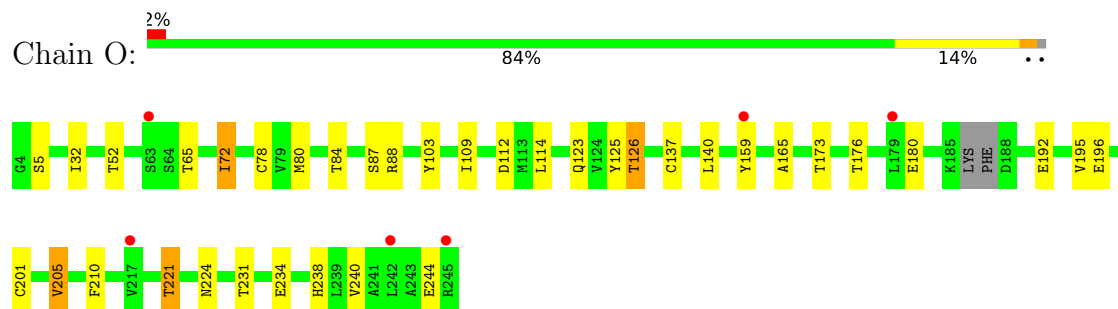
- Molecule 2: Proteasome subunit beta type-4



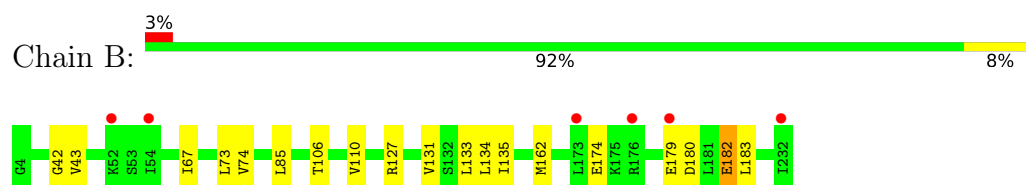
- Molecule 3: Proteasome subunit alpha type-6



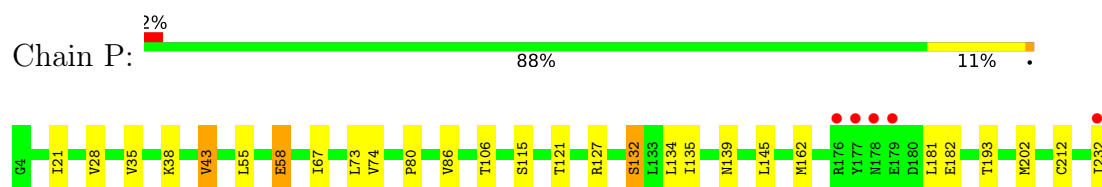
• Molecule 3: Proteasome subunit alpha type-6



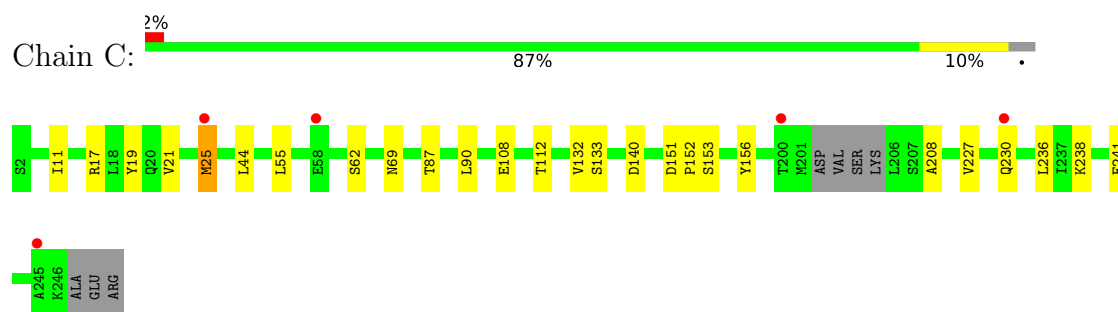
• Molecule 4: Proteasome subunit alpha type-2



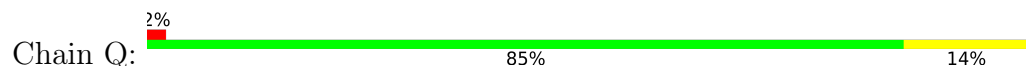
• Molecule 4: Proteasome subunit alpha type-2

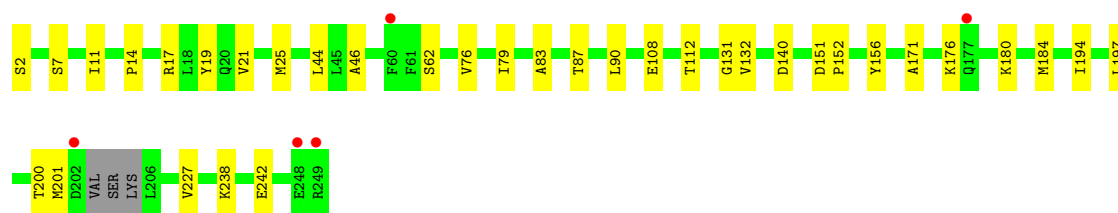


• Molecule 5: Proteasome subunit alpha type-4

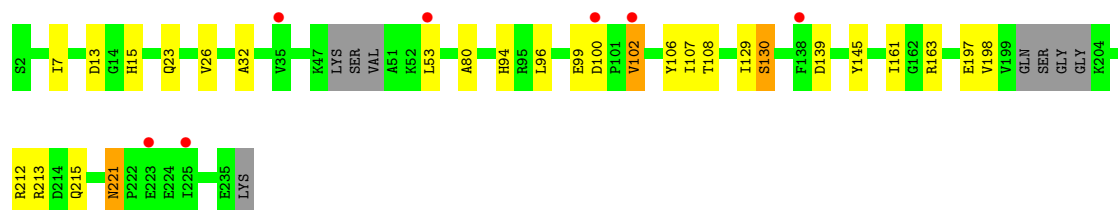
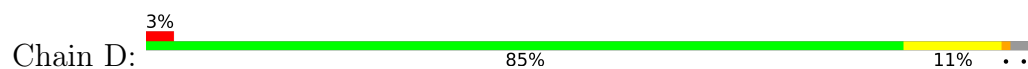


• Molecule 5: Proteasome subunit alpha type-4

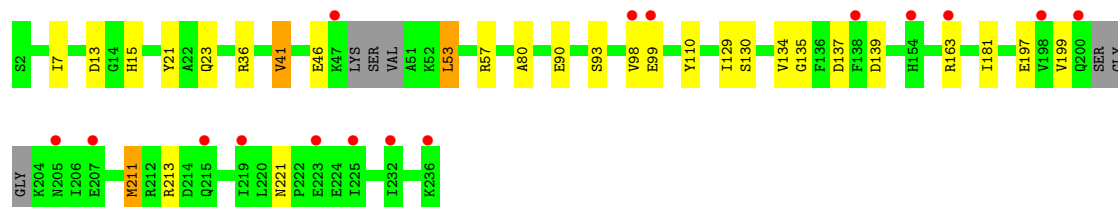
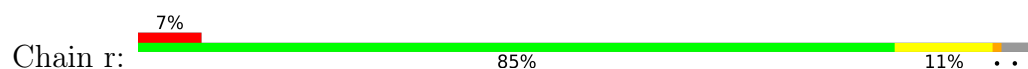




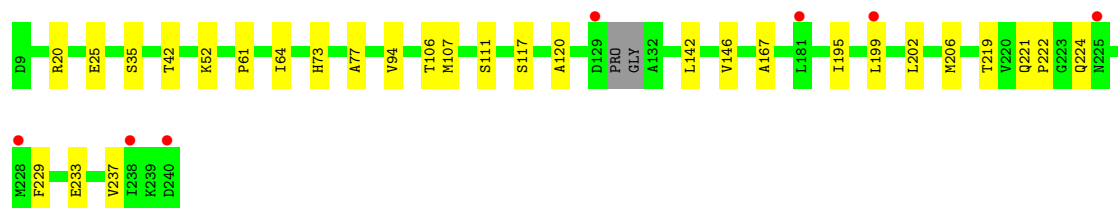
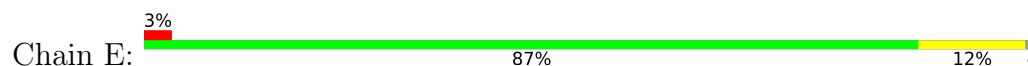
• Molecule 6: Proteasome subunit alpha type-7



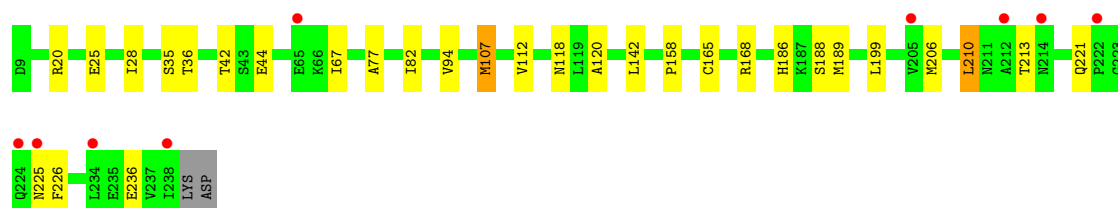
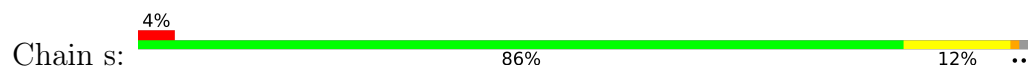
• Molecule 6: Proteasome subunit alpha type-7



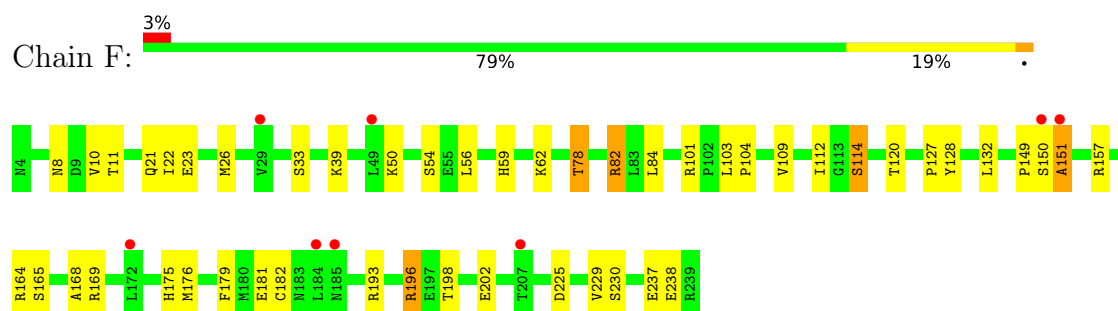
• Molecule 7: Proteasome subunit alpha type-5



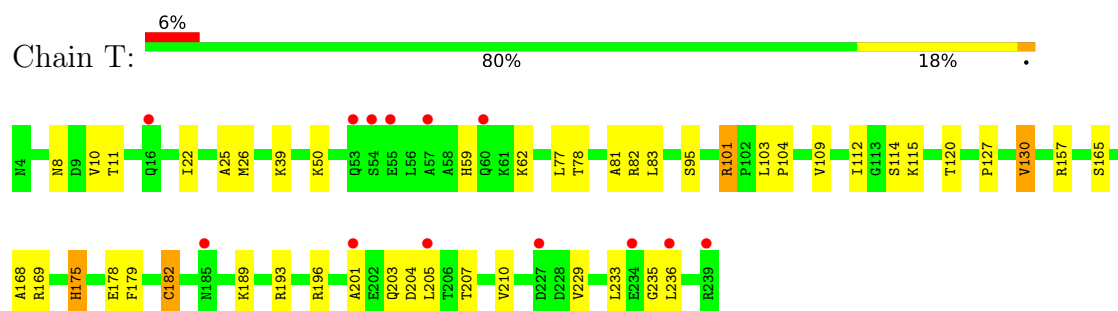
• Molecule 7: Proteasome subunit alpha type-5



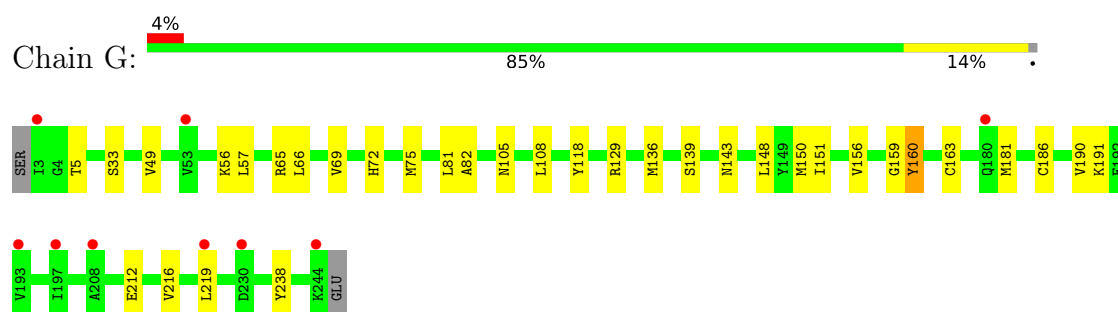
- Molecule 8: Proteasome subunit alpha type-1



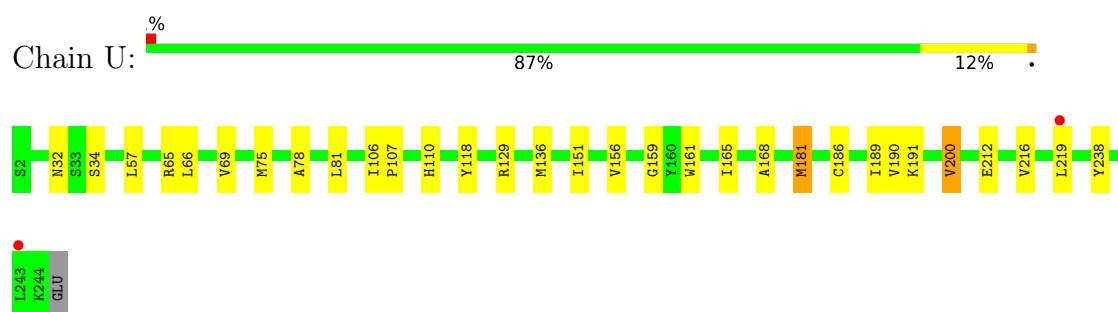
- Molecule 8: Proteasome subunit alpha type-1



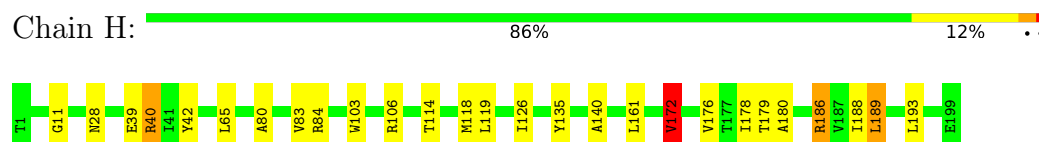
- Molecule 9: Proteasome subunit alpha type-3



- Molecule 9: Proteasome subunit alpha type-3



- Molecule 10: Proteasome subunit beta type-9



- Molecule 10: Proteasome subunit beta type-9

Chain V:  87% 11%



- Molecule 11: Proteasome subunit beta type-3

Chain J:  80% 18%



- Molecule 11: Proteasome subunit beta type-3

Chain X:  82% 16%



- Molecule 12: Proteasome subunit beta type-2

Chain K:  83% 15%



- Molecule 12: Proteasome subunit beta type-2

Chain Y:  82% 17%

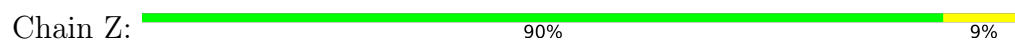


- Molecule 13: Proteasome subunit beta type-8

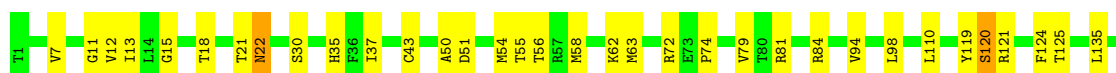
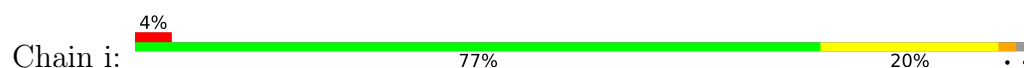
Chain L:  89% 10%



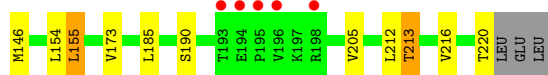
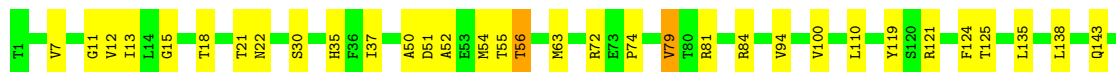
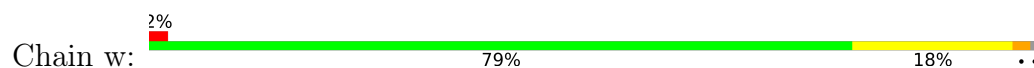
- Molecule 13: Proteasome subunit beta type-8



- Molecule 14: Proteasome subunit beta type-10



- Molecule 14: Proteasome subunit beta type-10



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	119.00Å 201.74Å 161.93Å 90.00° 106.83° 90.00°	Depositor
Resolution (Å)	107.89 – 2.43 107.89 – 2.43	Depositor EDS
% Data completeness (in resolution range)	93.4 (107.89-2.43) 64.7 (107.89-2.43)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.83 (at 2.42Å)	Xtriage
Refinement program	BUSTER 2.11.7 (18-SEP-2020)	Depositor
R, R_{free}	0.180 , 0.225 0.196 , 0.239	Depositor DCC
R_{free} test set	8735 reflections (4.93%)	wwPDB-VP
Wilson B-factor (Å ²)	50.3	Xtriage
Anisotropy	0.074	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 59.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	49338	wwPDB-VP
Average B, all atoms (Å ²)	60.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.37% 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: NA, SKN, SO4

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	1	0.88	2/1684 (0.1%)	1.10	1/2268 (0.0%)
1	M	0.85	1/1684 (0.1%)	1.12	1/2268 (0.0%)
2	2	0.79	0/1706	1.11	4/2309 (0.2%)
2	N	0.80	0/1706	1.10	5/2309 (0.2%)
3	A	0.75	0/1899	1.14	6/2567 (0.2%)
3	O	0.76	0/1898	1.15	6/2565 (0.2%)
4	B	0.78	0/1826	1.12	1/2474 (0.0%)
4	P	0.80	0/1826	1.15	0/2474
5	C	0.75	0/1927	1.14	3/2595 (0.1%)
5	Q	0.75	0/1960	1.12	3/2639 (0.1%)
6	D	0.74	0/1822	1.04	1/2458 (0.0%)
6	r	0.74	0/1840	1.06	1/2481 (0.0%)
7	E	0.76	0/1783	1.08	1/2406 (0.0%)
7	s	0.77	1/1779 (0.1%)	1.08	1/2404 (0.0%)
8	F	0.82	0/1891	1.21	9/2555 (0.4%)
8	T	0.82	0/1891	1.23	10/2555 (0.4%)
9	G	0.76	0/1928	1.12	4/2596 (0.2%)
9	U	0.80	0/1934	1.14	2/2604 (0.1%)
10	H	0.82	2/1521 (0.1%)	1.14	6/2062 (0.3%)
10	V	0.80	0/1521	1.14	5/2062 (0.2%)
11	J	0.82	1/1620 (0.1%)	1.14	3/2184 (0.1%)
11	X	0.81	2/1620 (0.1%)	1.13	3/2184 (0.1%)
12	K	0.81	0/1603	1.13	3/2168 (0.1%)
12	Y	0.78	0/1611	1.08	0/2180
13	L	0.79	1/1609 (0.1%)	1.15	4/2170 (0.2%)
13	Z	0.76	1/1609 (0.1%)	1.12	2/2170 (0.1%)
14	i	0.80	0/1635	1.11	3/2222 (0.1%)
14	w	0.79	0/1642	1.14	3/2232 (0.1%)
All	All	0.79	11/48975 (0.0%)	1.13	91/66161 (0.1%)

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1	83	MET	SD-CE	-9.04	1.56	1.79
7	s	107	MET	SD-CE	-6.86	1.62	1.79
1	M	83	MET	SD-CE	-6.69	1.62	1.79
13	L	45	MET	SD-CE	-6.31	1.63	1.79
13	Z	45	MET	SD-CE	-5.92	1.64	1.79
11	X	183	MET	SD-CE	-5.82	1.65	1.79
10	H	186	ARG	C-N	-5.51	1.26	1.33
1	1	26	ASP	CA-C	5.46	1.60	1.53
11	X	45	MET	SD-CE	-5.43	1.66	1.79
11	J	45	MET	SD-CE	-5.04	1.67	1.79
10	H	103	TRP	CA-C	5.03	1.58	1.52

All (91) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	69	ASN	CA-CB-CG	10.35	122.95	112.60
13	L	38	ASN	CA-CB-CG	7.59	120.19	112.60
12	K	119	ASP	CA-CB-CG	7.54	120.14	112.60
11	J	115	LYS	CA-C-N	7.13	135.16	121.54
11	J	115	LYS	C-N-CA	7.13	135.16	121.54
13	L	115	ASP	CA-CB-CG	7.00	119.60	112.60
6	r	98	VAL	N-CA-C	-6.74	102.70	110.05
8	T	8	ASN	N-CA-C	6.67	118.21	111.07
2	2	180	ASP	CA-CB-CG	6.67	119.27	112.60
8	F	8	ASN	N-CA-C	6.64	118.17	111.07
14	i	22	ASN	CA-CB-CG	6.32	118.92	112.60
10	H	172	VAL	N-CA-CB	-6.26	101.96	112.47
8	T	204	ASP	CA-CB-CG	6.24	118.84	112.60
14	w	37	ILE	N-CA-C	-6.20	106.72	111.62
2	N	180	ASP	CA-CB-CG	6.20	118.80	112.60
3	A	210	PHE	N-CA-C	6.17	118.74	110.35
8	F	150	SER	N-CA-C	-6.16	99.97	109.76
2	N	106	LEU	N-CA-C	-6.12	98.75	108.73
3	O	210	PHE	N-CA-C	6.08	118.62	110.35
8	T	175	HIS	CA-C-N	6.00	129.82	120.82
8	T	175	HIS	C-N-CA	6.00	129.82	120.82
8	F	175	HIS	CA-C-N	5.96	129.76	120.82
8	F	175	HIS	C-N-CA	5.96	129.76	120.82
3	O	5	SER	N-CA-C	5.94	118.37	110.53
8	F	114	SER	CA-C-N	5.90	128.18	120.28
8	F	114	SER	C-N-CA	5.90	128.18	120.28
2	2	106	LEU	N-CA-C	-5.88	99.15	108.73
9	G	118	TYR	N-CA-C	-5.87	104.96	111.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	T	201	ALA	CA-C-N	5.87	128.62	120.29
8	T	201	ALA	C-N-CA	5.87	128.62	120.29
13	L	115	ASP	N-CA-CB	-5.86	101.36	111.55
11	J	69	PHE	CA-CB-CG	5.81	119.61	113.80
11	X	69	PHE	CA-CB-CG	5.81	119.61	113.80
14	i	37	ILE	N-CA-C	-5.80	106.57	111.56
3	A	5	SER	N-CA-C	5.79	118.17	110.53
3	A	109	ILE	N-CA-C	5.78	115.26	108.96
5	Q	2	SER	CA-C-N	5.76	128.47	120.29
5	Q	2	SER	C-N-CA	5.76	128.47	120.29
8	T	168	ALA	CA-C-N	5.76	128.00	120.28
8	T	168	ALA	C-N-CA	5.76	128.00	120.28
13	Z	17	ASP	N-CA-CB	-5.75	102.45	110.38
9	U	118	TYR	N-CA-C	-5.65	105.20	111.36
5	C	140	ASP	CA-CB-CG	5.61	118.21	112.60
1	1	104	TYR	N-CA-C	-5.60	100.06	108.96
14	w	11	GLY	N-CA-C	5.56	118.08	110.58
3	O	109	ILE	N-CA-C	5.55	115.01	108.96
2	N	53	ALA	N-CA-C	5.50	118.05	108.76
10	V	103	TRP	CA-C-N	5.50	131.36	122.29
10	V	103	TRP	C-N-CA	5.50	131.36	122.29
2	2	53	ALA	N-CA-C	5.46	118.36	109.24
14	i	11	GLY	N-CA-C	5.43	117.92	110.58
13	L	17	ASP	N-CA-CB	-5.43	102.88	110.38
2	N	25	ASP	CA-CB-CG	5.41	118.01	112.60
10	H	83	VAL	CA-C-N	5.37	127.79	120.54
10	H	83	VAL	C-N-CA	5.37	127.79	120.54
5	C	69	ASN	N-CA-CB	-5.35	102.38	111.31
10	V	11	GLY	N-CA-C	5.32	117.10	110.29
4	B	182	GLU	N-CA-C	-5.31	102.63	110.48
6	D	221	ASN	CA-CB-CG	5.30	117.90	112.60
10	V	26	VAL	CA-C-N	5.30	128.32	120.74
10	V	26	VAL	C-N-CA	5.30	128.32	120.74
2	N	126	ASP	CA-CB-CG	5.30	117.90	112.60
13	Z	115	ASP	CA-CB-CG	5.29	117.89	112.60
7	s	120	ALA	N-CA-C	5.28	116.84	111.14
1	M	104	TYR	N-CA-C	-5.27	100.59	108.96
3	O	125	TYR	CA-C-N	5.18	129.37	120.72
3	O	125	TYR	C-N-CA	5.18	129.37	120.72
5	Q	140	ASP	CA-CB-CG	5.17	117.77	112.60
9	G	160	TYR	N-CA-C	5.14	117.62	109.50
10	H	11	GLY	N-CA-C	5.14	116.87	110.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	K	123	ALA	N-CA-C	-5.13	100.94	109.46
3	O	72	ILE	N-CA-C	-5.12	106.08	110.74
14	w	205	VAL	N-CA-CB	5.12	114.84	110.08
12	K	24	ASN	CA-CB-CG	5.11	117.71	112.60
8	F	225	ASP	N-CA-C	5.09	119.23	112.72
3	A	72	ILE	N-CA-C	-5.07	106.12	110.74
10	H	180	ALA	CA-C-N	5.07	127.08	120.28
10	H	180	ALA	C-N-CA	5.07	127.08	120.28
11	X	117	PHE	CA-C-N	5.07	128.29	121.20
11	X	117	PHE	C-N-CA	5.07	128.29	121.20
8	F	179	PHE	N-CA-C	5.06	116.48	111.07
8	T	130	VAL	CA-C-N	5.05	125.08	121.65
8	T	130	VAL	C-N-CA	5.05	125.08	121.65
7	E	120	ALA	N-CA-C	5.04	116.63	111.03
9	U	32	ASN	CA-CB-CG	5.04	117.64	112.60
8	F	238	GLU	N-CA-C	5.04	115.18	108.38
2	2	25	ASP	CA-CB-CG	5.01	117.61	112.60
3	A	125	TYR	CA-C-N	5.01	129.08	120.72
3	A	125	TYR	C-N-CA	5.01	129.08	120.72
9	G	33	SER	CA-C-N	5.00	128.31	120.75
9	G	33	SER	C-N-CA	5.00	128.31	120.75

There are no chirality outliers.

There are no planarity outliers.

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	1	1654	0	1656	14	0
1	M	1654	0	1656	10	0
2	2	1673	0	1650	20	0
2	N	1673	0	1650	18	0
3	A	1866	0	1865	16	0
3	O	1866	0	1870	19	0
4	B	1787	0	1782	13	0
4	P	1787	0	1782	19	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	C	1898	0	1917	13	0
5	Q	1931	0	1945	17	0
6	D	1798	0	1820	15	0
6	r	1816	0	1841	13	0
7	E	1758	0	1742	21	0
7	s	1752	0	1736	13	0
8	F	1857	0	1845	25	0
8	T	1857	0	1845	22	0
9	G	1893	0	1882	19	0
9	U	1899	0	1887	17	0
10	H	1493	0	1457	12	0
10	V	1493	0	1457	12	0
11	J	1591	0	1609	25	0
11	X	1591	0	1609	17	0
12	K	1571	0	1573	20	0
12	Y	1578	0	1580	19	0
13	L	1576	0	1522	14	0
13	Z	1576	0	1522	13	0
14	i	1609	0	1645	28	0
14	w	1616	0	1652	25	0
15	1	10	0	0	0	0
15	K	5	0	0	0	0
15	L	5	0	0	0	0
15	Y	5	0	0	0	0
16	A	1	0	0	0	0
16	L	1	0	0	0	0
16	O	1	0	0	0	0
16	Z	1	0	0	0	0
16	i	1	0	0	0	0
16	w	1	0	0	0	0
17	H	33	0	0	0	0
17	L	33	0	0	0	0
17	V	33	0	0	0	0
17	Z	33	0	0	0	0
17	i	33	0	0	2	0
17	w	33	0	0	0	0
18	1	56	0	0	1	0
18	2	60	0	0	1	0
18	A	32	0	0	0	0
18	B	26	0	0	0	0
18	C	36	0	0	0	0
18	D	18	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
18	E	28	0	0	0	0
18	F	23	0	0	1	0
18	G	21	0	0	0	0
18	H	32	0	0	0	0
18	J	59	0	0	1	0
18	K	16	0	0	0	0
18	L	41	0	0	0	0
18	M	43	0	0	0	0
18	N	54	0	0	0	0
18	O	34	0	0	0	0
18	P	28	0	0	0	0
18	Q	33	0	0	0	0
18	T	38	0	0	0	0
18	U	33	0	0	0	0
18	V	42	0	0	1	0
18	X	47	0	0	0	0
18	Y	28	0	0	1	0
18	Z	38	0	0	0	0
18	i	35	0	0	0	0
18	r	27	0	0	0	0
18	s	20	0	0	0	0
18	w	48	0	0	0	0
All	All	49338	0	47997	433	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 5.

All (433) 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)
9:U:34:SER:HB2	9:U:65:ARG:HH12	1.25	0.99
7:E:221:GLN:HG3	7:E:224:GLN:HB2	1.49	0.93
9:U:34:SER:HB2	9:U:65:ARG:NH1	1.90	0.86
1:1:145:LEU:HD21	1:1:182:ALA:HB2	1.59	0.84
14:i:18:THR:HB	14:i:30:SER:HA	1.58	0.84
14:w:18:THR:HB	14:w:30:SER:HA	1.59	0.83
1:M:145:LEU:HD21	1:M:182:ALA:HB2	1.60	0.83
3:O:231:THR:HB	3:O:234:GLU:HG3	1.63	0.79
9:G:136:MET:HE3	9:G:163:CYS:HB3	1.65	0.78
9:U:168:ALA:HB1	9:U:200:VAL:HG22	1.68	0.76
9:G:49:VAL:HG11	9:G:65:ARG:HD3	1.66	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:J:45:MET:HE3	11:J:71:LEU:HD22	1.68	0.74
7:E:167:ALA:HB3	8:F:56:LEU:HD13	1.69	0.74
11:X:45:MET:HE3	11:X:71:LEU:HD22	1.70	0.74
4:P:43:VAL:HG23	4:P:212:CYS:HB3	1.68	0.74
6:D:102:VAL:HG22	6:D:106:TYR:CD1	2.23	0.73
12:Y:21:ALA:HB3	12:Y:29:LYS:HB2	1.71	0.72
7:s:107:MET:HE3	7:s:112:VAL:HG22	1.70	0.72
12:K:21:ALA:HB3	12:K:29:LYS:HB2	1.72	0.71
12:Y:37:LYS:HB3	18:Y:306:HOH:O	1.91	0.70
4:B:73:LEU:CD1	4:B:135:ILE:HG12	2.23	0.68
11:J:199:THR:OG1	14:i:213:THR:HB	1.94	0.68
4:B:74:VAL:HG12	4:B:134:LEU:HB2	1.75	0.67
3:O:72:ILE:HG21	3:O:114:LEU:HD21	1.76	0.67
13:Z:115:ASP:HB2	13:Z:119:THR:HB	1.77	0.67
2:2:15:LYS:HB3	2:2:20:VAL:HG22	1.77	0.67
11:J:114:PRO:C	11:J:116:THR:H	2.03	0.67
9:U:65:ARG:HH21	9:U:78:ALA:HA	1.60	0.67
2:N:15:LYS:HB3	2:N:20:VAL:HG22	1.78	0.66
3:A:72:ILE:HG21	3:A:114:LEU:HD21	1.77	0.66
12:Y:35:MET:HG2	12:Y:45:LEU:HG	1.76	0.65
3:A:195:VAL:HG11	3:A:238:HIS:CD2	2.32	0.65
8:T:189:LYS:HB3	8:T:193:ARG:HH21	1.60	0.65
11:J:66:ARG:HD2	18:J:350:HOH:O	1.96	0.65
3:O:192:GLU:O	3:O:196:GLU:HG3	1.97	0.65
14:w:51:ASP:O	14:w:55:THR:HG23	1.98	0.64
12:K:35:MET:HG2	12:K:45:LEU:HG	1.78	0.64
1:1:198:VAL:HG22	1:1:203:ILE:HG12	1.80	0.64
5:Q:197:LEU:HB3	5:Q:201:MET:HE3	1.80	0.64
6:D:212:ARG:HB3	6:D:215:GLN:HG2	1.80	0.63
14:w:63:MET:CE	14:w:74:PRO:HB3	2.28	0.63
6:D:102:VAL:HG11	6:D:107:ILE:HB	1.81	0.63
6:D:99:GLU:O	6:D:99:GLU:HG2	1.97	0.63
8:F:128:TYR:O	8:F:149:PRO:HB3	1.99	0.63
14:i:51:ASP:O	14:i:55:THR:HG23	1.98	0.63
5:Q:171:ALA:HB2	5:Q:200:THR:HG21	1.81	0.62
8:T:81:ALA:HB2	8:T:130:VAL:HG21	1.81	0.62
9:G:108:LEU:HD13	9:G:139:SER:HB2	1.80	0.62
11:J:83:LYS:HG2	11:J:114:PRO:HG3	1.81	0.62
2:N:9:THR:O	2:N:41:ARG:NH2	2.32	0.62
6:r:41:VAL:HG23	6:r:211:MET:HB2	1.81	0.62
7:E:20:ARG:HE	7:E:25:GLU:CG	2.13	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:K:2:GLU:HG2	12:K:34:LYS:NZ	2.14	0.62
14:i:63:MET:CE	14:i:74:PRO:HB3	2.28	0.62
7:s:20:ARG:HE	7:s:25:GLU:CG	2.13	0.62
12:Y:118:MET:HE2	12:Y:124:LEU:HD13	1.81	0.62
10:H:188:ILE:HG22	10:H:193:LEU:HD23	1.81	0.62
4:P:28:VAL:HG11	4:P:132:SER:HB2	1.82	0.62
14:w:63:MET:HE3	14:w:74:PRO:HB3	1.82	0.62
8:F:10:VAL:HG11	8:F:127:PRO:HD3	1.82	0.61
10:V:188:ILE:HG22	10:V:193:LEU:HD23	1.82	0.61
7:E:219:THR:HG23	7:E:229:PHE:CE1	2.34	0.61
12:Y:2:GLU:HG2	12:Y:34:LYS:NZ	2.16	0.61
11:J:116:THR:HG22	11:J:192:LYS:HB2	1.81	0.61
4:P:73:LEU:CD1	4:P:135:ILE:HG12	2.31	0.61
6:r:13:ASP:CG	6:r:15:HIS:HD2	2.09	0.60
13:L:8:PHE:CE1	13:L:13:ILE:HG12	2.36	0.60
2:N:209:TRP:HB2	10:V:189:LEU:HG	1.83	0.60
6:D:13:ASP:CG	6:D:15:HIS:HD2	2.09	0.60
8:T:165:SER:OG	8:T:169:ARG:NH2	2.34	0.60
4:P:134:LEU:HD12	4:P:162:MET:HE2	1.84	0.60
14:i:63:MET:HE3	14:i:74:PRO:HB3	1.83	0.60
9:G:136:MET:HE2	9:G:148:LEU:HD11	1.84	0.60
2:2:5:MET:HG2	2:2:30:TYR:HE1	1.65	0.59
2:2:15:LYS:HE2	2:2:135:PRO:HA	1.83	0.59
6:D:99:GLU:OE1	13:L:120:ARG:NH1	2.32	0.59
7:s:77:ALA:HB3	7:s:142:LEU:HB2	1.85	0.59
2:2:9:THR:O	2:2:41:ARG:NH2	2.35	0.59
13:Z:174:VAL:HG22	13:Z:192:VAL:HG12	1.84	0.59
7:s:20:ARG:HE	7:s:25:GLU:HG2	1.68	0.59
7:E:77:ALA:HB3	7:E:142:LEU:HB2	1.85	0.59
8:F:84:LEU:HD23	8:F:132:LEU:HD11	1.85	0.59
8:F:169:ARG:HG2	9:G:57:LEU:CD1	2.32	0.59
7:E:20:ARG:HE	7:E:25:GLU:HG2	1.68	0.59
3:O:195:VAL:HG11	3:O:238:HIS:CD2	2.37	0.58
6:D:102:VAL:HG22	6:D:106:TYR:HD1	1.67	0.58
4:B:74:VAL:CG1	4:B:134:LEU:HB2	2.33	0.58
7:E:117:SER:HB3	8:F:82:ARG:NH2	2.19	0.58
11:X:199:THR:OG1	14:w:213:THR:HB	2.03	0.58
3:O:103:TYR:O	14:w:81:ARG:HD3	2.04	0.58
4:P:106:THR:H	4:P:139:ASN:HD21	1.51	0.57
14:w:143:GLN:O	14:w:146:MET:HG3	2.03	0.57
13:Z:8:PHE:CE1	13:Z:13:ILE:HG12	2.38	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:i:143:GLN:O	14:i:146:MET:HG3	2.05	0.57
7:E:202:LEU:O	7:E:206:MET:HG3	2.05	0.57
12:Y:151:ILE:HG13	12:Y:155:ARG:HD2	1.87	0.57
14:w:7:VAL:HG22	14:w:12:VAL:HG22	1.86	0.57
5:C:208:ALA:HB3	5:C:230:GLN:HG2	1.87	0.57
7:E:219:THR:HG23	7:E:229:PHE:HE1	1.69	0.57
12:Y:184:ASP:OD1	12:Y:189:HIS:NE2	2.38	0.57
2:2:5:MET:HG2	2:2:30:TYR:CE1	2.40	0.56
8:F:165:SER:OG	8:F:169:ARG:NH1	2.38	0.56
11:J:14:MET:HB3	11:J:163:LEU:HD11	1.86	0.56
1:M:61:CYS:O	1:M:65:THR:HB	2.06	0.56
14:i:7:VAL:HG22	14:i:12:VAL:HG22	1.87	0.56
4:B:179:GLU:O	4:B:180:ASP:HB2	2.05	0.56
12:Y:51:GLY:HA3	13:Z:117:HIS:O	2.05	0.56
14:i:163:ILE:HG23	14:i:170:GLY:HA2	1.88	0.56
12:K:107:TYR:CE1	12:K:185:LYS:HA	2.41	0.56
11:J:28:PHE:HB2	11:J:39:PHE:HB2	1.88	0.55
8:T:95:SER:OG	8:T:101:ARG:NH2	2.34	0.55
2:2:51:LEU:HD11	2:2:110:MET:HB3	1.88	0.55
13:L:161:ALA:HA	13:L:192:VAL:CG1	2.37	0.55
11:X:28:PHE:HB2	11:X:39:PHE:HB2	1.89	0.54
3:A:103:TYR:O	14:i:81:ARG:HD3	2.07	0.54
2:N:27:LEU:HD22	2:N:184:TYR:HB2	1.90	0.54
2:2:27:LEU:HD22	2:2:184:TYR:HB2	1.90	0.54
7:E:233:GLU:O	7:E:237:VAL:HG23	2.07	0.54
8:F:101:ARG:HG3	8:F:101:ARG:O	2.06	0.54
2:N:49:THR:HG21	2:N:88:ILE:HG13	1.90	0.54
3:A:65:THR:HG21	9:G:159:GLY:HA3	1.88	0.54
2:N:187:PHE:CE1	2:N:205:THR:HG23	2.43	0.54
5:Q:151:ASP:HB2	5:Q:152:PRO:CD	2.39	0.53
3:O:165:ALA:HB3	4:P:55:LEU:HD22	1.89	0.53
14:i:84:ARG:HD3	14:i:119:TYR:HB3	1.90	0.53
9:G:136:MET:CE	9:G:163:CYS:HB3	2.36	0.53
3:O:65:THR:HG21	9:U:159:GLY:HA3	1.89	0.53
4:B:67:ILE:HD11	4:B:73:LEU:HD22	1.91	0.53
3:O:221:THR:HG22	3:O:224:ASN:H	1.72	0.53
4:B:42:GLY:HA3	4:B:183:LEU:HD22	1.91	0.53
14:w:84:ARG:HD3	14:w:119:TYR:HB3	1.91	0.52
4:P:58:GLU:CD	4:P:58:GLU:H	2.17	0.52
6:r:135:GLY:HA2	6:r:211:MET:HE2	1.92	0.52
5:Q:176:LYS:HA	6:r:53:LEU:HD21	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:42:LYS:HB3	1:1:54:CYS:O	2.10	0.52
8:T:10:VAL:HG11	8:T:127:PRO:HD3	1.90	0.52
6:D:96:LEU:HG	12:K:62:LYS:HG2	1.91	0.52
4:P:35:VAL:HG11	4:P:193:THR:HG21	1.91	0.51
14:w:110:LEU:HD21	14:w:125:THR:HG22	1.92	0.51
2:2:65:GLN:HB2	18:2:321:HOH:O	2.10	0.51
7:E:52:LYS:HE2	7:E:61:PRO:O	2.10	0.51
8:T:22:ILE:HG22	8:T:26:MET:HE2	1.91	0.51
14:w:52:ALA:O	14:w:56:THR:HB	2.10	0.51
1:1:127:VAL:HG23	13:Z:50:ALA:HB2	1.92	0.51
8:T:189:LYS:HB3	8:T:193:ARG:NH2	2.26	0.51
1:1:200:LYS:HG3	18:1:442:HOH:O	2.09	0.51
11:X:20:VAL:HG12	11:X:190:ILE:HB	1.92	0.51
14:i:110:LEU:HD21	14:i:125:THR:HG22	1.93	0.51
5:Q:87:THR:HA	5:Q:90:LEU:HD12	1.93	0.51
14:i:58:MET:HE3	14:i:62:LYS:HE3	1.92	0.50
4:B:85:LEU:HD13	4:B:133:LEU:HD11	1.92	0.50
7:E:199:LEU:HD22	7:E:237:VAL:HG12	1.93	0.50
5:Q:108:GLU:O	5:Q:112:THR:HG23	2.12	0.50
3:A:32:ILE:HD13	3:A:137:CYS:HB2	1.93	0.50
4:P:67:ILE:HD11	4:P:73:LEU:HD22	1.93	0.50
1:1:61:CYS:O	1:1:65:THR:HB	2.12	0.49
11:J:14:MET:HB2	11:J:167:ILE:HD12	1.94	0.49
8:T:11:THR:HA	9:U:129:ARG:HB2	1.93	0.49
2:2:107:TRP:CE2	2:2:127:MET:HE1	2.46	0.49
3:A:240:VAL:O	3:A:244:GLU:HG2	2.12	0.49
11:J:37:THR:OG1	11:J:183:MET:HB3	2.12	0.49
2:N:107:TRP:CE2	2:N:127:MET:HE1	2.47	0.49
5:Q:17:ARG:HH21	5:Q:19:TYR:HE1	1.59	0.49
14:w:79:VAL:CG2	14:w:100:VAL:HG11	2.43	0.49
5:C:11:ILE:HG22	6:D:7:ILE:HG23	1.95	0.49
8:F:39:LYS:HE2	8:F:157:ARG:HA	1.95	0.49
2:N:187:PHE:HE1	2:N:205:THR:HG23	1.78	0.49
8:T:50:LYS:HB3	8:T:59:HIS:HB3	1.95	0.49
6:r:80:ALA:HB2	6:r:129:ILE:HG21	1.94	0.49
5:C:108:GLU:O	5:C:112:THR:HG23	2.13	0.49
8:F:22:ILE:O	8:F:26:MET:HG3	2.12	0.49
10:H:172:VAL:HG22	10:H:189:LEU:HA	1.93	0.49
2:2:209:TRP:HB2	10:H:189:LEU:HG	1.93	0.49
6:D:80:ALA:HB2	6:D:129:ILE:HG21	1.95	0.49
8:T:82:ARG:NH1	7:s:118:ASN:OD1	2.46	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:Z:174:VAL:CG2	13:Z:192:VAL:HG12	2.43	0.48
3:O:32:ILE:HD13	3:O:137:CYS:HB2	1.95	0.48
8:T:39:LYS:HE2	8:T:157:ARG:HA	1.95	0.48
10:V:152:ARG:O	10:V:156:THR:OG1	2.25	0.48
13:L:169:TYR:CE2	11:X:32:ALA:HB2	2.48	0.48
3:O:240:VAL:O	3:O:244:GLU:HG2	2.14	0.48
5:Q:108:GLU:OE1	6:r:57:ARG:NH2	2.44	0.48
5:Q:79:ILE:HD13	5:Q:131:GLY:HA3	1.95	0.48
11:J:201:LYS:HB2	14:i:212:LEU:HG	1.95	0.48
8:T:189:LYS:CD	8:T:236:LEU:HG	2.44	0.48
14:i:35:HIS:NE2	17:i:301:SKN:C33	2.76	0.48
12:K:85:ARG:HH12	12:K:86:ARG:NH2	2.11	0.48
5:C:17:ARG:HE	5:C:19:TYR:HE1	1.62	0.48
8:T:205:LEU:HB3	8:T:210:VAL:HG21	1.96	0.48
14:w:124:PHE:HB2	14:w:138:LEU:HD13	1.95	0.48
8:F:176:MET:HE1	9:G:56:LYS:HB3	1.96	0.48
2:2:96:MET:HE3	2:2:127:MET:HA	1.96	0.47
11:J:58:THR:OG1	12:K:121:LEU:O	2.30	0.47
2:N:207:THR:O	10:V:191:ASN:OD1	2.31	0.47
11:J:190:ILE:HG23	11:J:195:ILE:CD1	2.44	0.47
5:Q:21:VAL:O	5:Q:25:MET:HG2	2.15	0.47
5:Q:46:ALA:HB1	5:Q:197:LEU:HD11	1.95	0.47
14:w:35:HIS:CG	14:w:56:THR:HG21	2.50	0.47
1:1:184:GLU:OE2	1:1:211:ARG:HD2	2.14	0.47
4:P:106:THR:H	4:P:139:ASN:ND2	2.11	0.47
13:Z:7:LYS:HB2	13:Z:124:ASN:HB2	1.96	0.47
13:L:7:LYS:HB2	13:L:124:ASN:HB2	1.96	0.47
2:N:96:MET:HE3	2:N:127:MET:HA	1.97	0.47
4:B:73:LEU:HD11	4:B:135:ILE:HG12	1.94	0.47
5:C:112:THR:HG22	5:C:156:TYR:CE1	2.48	0.47
7:s:165:CYS:SG	7:s:168:ARG:HD3	2.55	0.47
5:C:87:THR:HA	5:C:90:LEU:HD12	1.97	0.47
1:M:145:LEU:HD22	1:M:178:VAL:HB	1.96	0.47
9:U:186:CYS:HB2	9:U:219:LEU:HD12	1.95	0.47
12:Y:44:LEU:HD11	12:Y:102:LEU:HD13	1.97	0.47
6:r:137:ASP:HB3	6:r:139:ASP:OD1	2.14	0.47
12:Y:107:TYR:CE2	12:Y:185:LYS:HA	2.50	0.47
8:F:169:ARG:HG2	9:G:57:LEU:HD11	1.96	0.47
6:D:94:HIS:CE1	6:D:100:ASP:O	2.68	0.47
6:r:36:ARG:HA	6:r:41:VAL:HG12	1.96	0.47
10:H:28:ASN:ND2	14:i:120:SER:OG	2.42	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:U:161:TRP:HB3	9:U:181:MET:HE3	1.97	0.46
8:F:164:ARG:HD2	8:F:198:THR:O	2.14	0.46
12:Y:180:VAL:HG21	12:Y:194:ILE:HG12	1.98	0.46
14:w:84:ARG:HD3	14:w:119:TYR:CD1	2.50	0.46
12:K:180:VAL:HG21	12:K:194:ILE:HG12	1.97	0.46
1:M:155:PHE:HA	1:M:158:MET:HE2	1.97	0.46
11:J:154:TRP:CH2	11:J:156:PRO:HA	2.50	0.46
1:M:46:LEU:HB3	1:M:72:LEU:HD11	1.97	0.46
5:Q:112:THR:HG22	5:Q:156:TYR:CE1	2.50	0.46
7:s:206:MET:HE1	7:s:210:LEU:HD12	1.97	0.46
5:C:21:VAL:HG12	5:C:25:MET:HE3	1.98	0.46
12:Y:4:LEU:HD22	12:Y:45:LEU:HB3	1.98	0.46
6:r:211:MET:HE3	6:r:211:MET:HB3	1.90	0.46
4:B:174:GLU:HA	5:C:55:LEU:HD21	1.98	0.46
13:L:164:THR:HB	13:L:171:GLY:HA2	1.97	0.46
14:i:124:PHE:HB2	14:i:138:LEU:HD13	1.97	0.46
6:D:108:THR:HG21	6:D:145:TYR:HB3	1.96	0.46
4:P:38:LYS:HA	4:P:43:VAL:HG13	1.98	0.46
11:X:14:MET:HB2	11:X:167:ILE:HD12	1.97	0.46
11:J:194:LYS:HA	14:i:219:LEU:HG	1.96	0.46
10:V:83:VAL:HG12	10:V:114:THR:HG21	1.97	0.46
12:Y:49:GLU:HB2	12:Y:99:HIS:HB3	1.98	0.46
2:2:169:VAL:O	2:2:173:MET:HG2	2.16	0.46
11:J:129:CYS:HB2	14:i:50:ALA:HB2	1.98	0.46
13:L:164:THR:OG1	13:L:192:VAL:HG11	2.16	0.46
2:N:169:VAL:O	2:N:173:MET:HG2	2.16	0.46
7:E:94:VAL:HG22	13:L:65:LEU:HD21	1.96	0.45
5:Q:238:LYS:O	5:Q:242:GLU:HG3	2.16	0.45
2:2:51:LEU:HD13	2:2:112:ILE:HG12	1.99	0.45
8:F:23:GLU:HA	8:F:26:MET:HE2	1.99	0.45
12:K:23:SER:O	12:K:24:ASN:HB3	2.16	0.45
14:i:84:ARG:HD3	14:i:119:TYR:CD1	2.50	0.45
1:1:145:LEU:HD22	1:1:178:VAL:HB	1.97	0.45
3:A:176:THR:O	3:A:180:GLU:HG2	2.16	0.45
12:K:51:GLY:HA3	13:L:117:HIS:O	2.16	0.45
2:2:124:TYR:O	2:2:131:ALA:HA	2.16	0.45
7:E:52:LYS:HE2	7:E:64:ILE:HB	1.99	0.45
3:O:176:THR:O	3:O:180:GLU:HG2	2.17	0.45
9:U:110:HIS:HD2	18:V:306:HOH:O	1.98	0.45
1:1:135:PHE:CD2	1:1:149:LEU:HB3	2.52	0.45
8:F:11:THR:HA	9:G:129:ARG:HB2	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:H:140:ALA:HB2	10:V:161:LEU:HD11	1.99	0.45
13:L:161:ALA:HA	13:L:192:VAL:HG13	1.97	0.45
11:X:53:LEU:HB2	11:X:60:VAL:HG13	1.98	0.45
2:2:53:ALA:HB2	2:2:110:MET:HG2	1.98	0.45
5:C:151:ASP:HB2	5:C:152:PRO:CD	2.47	0.45
11:J:184:GLY:HA2	11:J:202:ALA:HB3	1.99	0.45
12:K:64:VAL:HG22	12:K:75:LEU:HD12	1.98	0.45
14:i:35:HIS:CE1	17:i:301:SKN:C33	3.00	0.45
11:J:53:LEU:HB2	11:J:60:VAL:HG13	1.98	0.45
13:L:144:ARG:HG3	13:L:147:LEU:HG	1.99	0.45
8:F:181:GLU:HG2	18:F:311:HOH:O	2.18	0.44
1:M:42:LYS:HB3	1:M:54:CYS:O	2.17	0.44
1:M:184:GLU:OE2	1:M:211:ARG:HD2	2.17	0.44
5:Q:11:ILE:HG22	6:r:7:ILE:HG23	1.99	0.44
9:U:136:MET:HE2	9:U:165:ILE:HG12	1.98	0.44
12:Y:160:LEU:O	12:Y:164:LEU:HG	2.17	0.44
12:Y:182:ILE:HG13	12:Y:191:LEU:HD11	1.99	0.44
14:w:55:THR:HG21	14:w:94:VAL:HG11	1.99	0.44
11:J:34:MET:HE3	13:Z:166:ARG:HD3	1.99	0.44
8:T:22:ILE:HD11	8:T:120:THR:HB	1.99	0.44
8:T:109:VAL:HA	8:T:112:ILE:HD12	1.99	0.44
8:T:175:HIS:HD2	8:T:178:GLU:OE2	2.00	0.44
13:Z:157:ARG:HD3	13:Z:195:LEU:HD21	1.99	0.44
2:2:22:ILE:HD12	2:2:50:MET:HE3	1.98	0.44
12:Y:9:GLY:HA3	12:Y:12:TYR:CE1	2.52	0.44
1:1:23:VAL:HG21	1:1:51:VAL:HG23	1.99	0.44
1:1:30:SER:HB3	14:i:167:LEU:HD11	2.00	0.44
7:E:199:LEU:CD2	7:E:237:VAL:HG12	2.48	0.44
8:F:22:ILE:HD11	8:F:120:THR:HB	1.99	0.44
11:J:20:VAL:HG13	11:J:190:ILE:HD12	1.99	0.44
12:K:4:LEU:HD22	12:K:45:LEU:HB3	1.99	0.44
14:i:35:HIS:CD2	14:i:56:THR:HG21	2.53	0.44
3:A:195:VAL:CG1	3:A:238:HIS:CD2	3.00	0.44
11:X:14:MET:HE1	11:X:166:THR:HG22	1.99	0.44
13:Z:173:VAL:HG12	13:Z:191:ASP:HA	1.99	0.44
7:E:107:MET:HE2	7:E:111:SER:HB3	1.98	0.44
8:F:193:ARG:HA	8:F:196:ARG:HG2	2.00	0.44
9:G:186:CYS:HB2	9:G:219:LEU:HD12	2.00	0.44
4:P:21:ILE:HD11	4:P:121:THR:HB	2.00	0.44
8:T:196:ARG:HH22	8:T:236:LEU:HB3	1.82	0.44
11:X:34:MET:HE3	11:X:34:MET:HB3	1.95	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:Y:2:GLU:HG2	12:Y:34:LYS:HZ2	1.83	0.44
11:J:34:MET:HE3	11:J:34:MET:HB3	1.95	0.44
8:F:168:ALA:HB2	8:F:198:THR:CG2	2.46	0.44
1:M:135:PHE:CD1	1:M:149:LEU:HB3	2.53	0.44
2:2:107:TRP:NE1	2:2:127:MET:HE1	2.32	0.43
2:N:86:ARG:NH1	2:N:133:GLU:OE2	2.51	0.43
12:K:182:ILE:HG13	12:K:191:LEU:HD11	2.00	0.43
7:s:44:GLU:O	7:s:221:GLN:HB3	2.18	0.43
7:E:146:VAL:HG11	7:E:222:PRO:HG3	2.00	0.43
2:N:53:ALA:HB2	2:N:110:MET:HG2	1.99	0.43
2:N:124:TYR:O	2:N:131:ALA:HA	2.18	0.43
14:i:15:GLY:HA3	14:i:155:LEU:HD21	2.00	0.43
14:i:55:THR:HG21	14:i:94:VAL:HG11	2.00	0.43
3:A:84:THR:O	3:A:88:ARG:HG2	2.17	0.43
8:F:109:VAL:HA	8:F:112:ILE:HD12	2.00	0.43
11:J:65:GLN:OE1	12:K:86:ARG:NH2	2.51	0.43
10:V:75:LEU:HD21	10:V:106:ARG:HD2	2.01	0.43
6:D:26:VAL:HG11	6:D:130:SER:HB2	1.99	0.43
4:P:35:VAL:HG21	4:P:193:THR:HG23	2.00	0.43
3:A:231:THR:HB	3:A:234:GLU:HG3	2.01	0.43
7:E:73:HIS:CE1	7:E:106:THR:HB	2.54	0.43
10:H:39:GLU:O	10:H:40:ARG:HB2	2.18	0.43
3:O:84:THR:O	3:O:88:ARG:HG2	2.18	0.43
11:X:154:TRP:CH2	11:X:156:PRO:HA	2.53	0.43
11:X:184:GLY:HA2	11:X:202:ALA:HB3	2.00	0.43
5:Q:14:PRO:HA	6:r:21:TYR:CD1	2.53	0.43
3:A:112:ASP:OD2	14:i:72:ARG:NH2	2.52	0.43
12:K:9:GLY:HA3	12:K:12:TYR:CE1	2.52	0.43
3:O:112:ASP:OD1	14:w:72:ARG:NH2	2.51	0.43
12:Y:64:VAL:HG22	12:Y:75:LEU:HD12	2.00	0.43
5:C:208:ALA:CB	5:C:230:GLN:HG2	2.49	0.43
10:H:118:MET:HE3	2:N:57:TYR:HD2	1.84	0.43
11:J:159:ASP:OD2	11:J:162:HIS:HB2	2.19	0.43
8:T:169:ARG:HG2	9:U:57:LEU:CD1	2.48	0.43
3:O:123:GLN:O	3:O:126:THR:HB	2.19	0.43
11:X:201:LYS:HB2	14:w:212:LEU:HG	2.00	0.43
13:L:5:ALA:HA	13:L:13:ILE:O	2.19	0.42
9:U:151:ILE:HA	9:U:156:VAL:O	2.19	0.42
7:s:225:ASN:O	7:s:226:PHE:C	2.62	0.42
1:1:83:MET:HE2	1:1:88:ILE:HA	2.00	0.42
10:H:161:LEU:HD11	10:V:140:ALA:HB2	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:X:196:THR:HG23	14:w:216:VAL:HG22	2.00	0.42
9:G:150:MET:HB3	9:G:160:TYR:CE1	2.54	0.42
2:N:209:TRP:CZ3	10:V:29:ARG:HD2	2.55	0.42
7:s:28:ILE:HD13	7:s:158:PRO:HD2	2.00	0.42
2:2:22:ILE:HB	2:2:50:MET:HE3	2.01	0.42
4:B:106:THR:O	4:B:110:VAL:HG23	2.19	0.42
8:F:78:THR:O	8:F:82:ARG:HG3	2.19	0.42
8:F:151:ALA:HB3	9:G:82:ALA:HB1	2.02	0.42
14:w:50:ALA:O	14:w:54:MET:HG2	2.19	0.42
3:A:126:THR:HG22	4:B:127:ARG:HH21	1.84	0.42
8:T:25:ALA:HB2	8:T:127:PRO:HG2	2.00	0.42
10:V:126:ILE:HD11	10:V:135:TYR:CD1	2.54	0.42
13:L:97:MET:HE2	13:L:97:MET:HB3	1.92	0.42
2:N:107:TRP:NE1	2:N:127:MET:HE1	2.34	0.42
3:O:78:CYS:HB3	3:O:140:LEU:HD23	2.02	0.42
13:Z:65:LEU:HD21	7:s:94:VAL:HG22	2.00	0.42
4:P:73:LEU:HD23	4:P:86:VAL:HG22	2.01	0.42
8:T:103:LEU:HD12	8:T:104:PRO:HD2	2.00	0.42
9:U:65:ARG:NH2	9:U:78:ALA:HA	2.30	0.42
9:G:191:LYS:HB3	9:G:238:TYR:CD2	2.55	0.42
6:D:94:HIS:ND1	6:D:100:ASP:O	2.52	0.42
3:O:159:TYR:CZ	4:P:80:PRO:HD3	2.55	0.42
5:Q:180:LYS:O	5:Q:184:MET:HG2	2.19	0.42
11:X:164:PHE:CE1	11:X:198:ARG:HD2	2.55	0.42
3:A:201:CYS:O	3:A:205:VAL:HB	2.20	0.41
7:E:195:ILE:O	7:E:199:LEU:HD13	2.20	0.41
10:H:80:ALA:HB1	10:H:119:LEU:HD11	2.02	0.41
5:Q:76:VAL:HG11	5:Q:83:ALA:HB1	2.02	0.41
13:Z:5:ALA:HA	13:Z:13:ILE:O	2.21	0.41
14:w:63:MET:HG3	14:w:79:VAL:HG12	2.01	0.41
5:C:151:ASP:OD2	5:C:153:SER:OG	2.32	0.41
7:E:219:THR:CG2	7:E:229:PHE:HE1	2.33	0.41
10:H:118:MET:HE3	2:N:57:TYR:CD2	2.55	0.41
10:H:126:ILE:HD11	10:H:135:TYR:CD1	2.55	0.41
9:U:191:LYS:HB3	9:U:238:TYR:CD2	2.55	0.41
2:2:96:MET:HE2	2:2:110:MET:HE1	2.02	0.41
4:B:134:LEU:HG	4:B:162:MET:SD	2.61	0.41
3:A:123:GLN:O	3:A:126:THR:HB	2.19	0.41
4:B:134:LEU:HD23	4:B:134:LEU:HA	1.95	0.41
1:M:1:ARG:HA	1:M:1:ARG:HD3	1.81	0.41
11:X:14:MET:HB3	11:X:163:LEU:HD11	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:i:43:CYS:SG	14:i:98:LEU:HB3	2.60	0.41
7:s:67:ILE:HG22	7:s:226:PHE:HZ	1.85	0.41
14:w:15:GLY:HA3	14:w:155:LEU:HD21	2.02	0.41
5:C:238:LYS:HA	5:C:241:GLU:HB2	2.02	0.41
12:K:2:GLU:CB	12:K:47:VAL:HG22	2.50	0.41
6:r:13:ASP:OD2	6:r:15:HIS:HD2	2.02	0.41
7:s:186:HIS:O	7:s:189:MET:HG2	2.20	0.41
3:A:78:CYS:HB3	3:A:140:LEU:HD23	2.03	0.41
9:G:72:HIS:CE1	9:G:105:ASN:HB3	2.56	0.41
9:G:75:MET:HA	9:G:136:MET:O	2.21	0.41
12:K:118:MET:HE2	12:K:124:LEU:HD13	2.03	0.41
14:i:50:ALA:O	14:i:54:MET:HG2	2.20	0.41
14:w:146:MET:HE1	14:w:154:LEU:HD23	2.03	0.41
5:C:151:ASP:HB2	5:C:152:PRO:HD2	2.03	0.41
8:F:50:LYS:CB	8:F:59:HIS:HB3	2.51	0.41
9:G:108:LEU:HD13	9:G:139:SER:CB	2.49	0.41
1:M:100:ARG:HD2	1:M:127:VAL:HG11	2.03	0.41
3:O:80:MET:HE2	3:O:87:SER:HA	2.03	0.41
8:T:50:LYS:CB	8:T:59:HIS:HB3	2.50	0.41
8:T:179:PHE:O	8:T:182:CYS:HB2	2.21	0.41
14:w:173:VAL:HB	14:w:190:SER:HB3	2.02	0.41
1:1:127:VAL:HG23	13:Z:50:ALA:CB	2.49	0.41
7:E:206:MET:HE3	7:E:206:MET:HB2	1.92	0.41
9:G:66:LEU:HD12	9:G:212:GLU:HB3	2.02	0.41
9:G:151:ILE:HA	9:G:156:VAL:O	2.21	0.41
12:K:107:TYR:CD1	12:K:185:LYS:HA	2.55	0.41
11:X:129:CYS:HB2	14:w:50:ALA:HB2	2.03	0.41
11:X:153:LEU:HB3	11:X:166:THR:HG23	2.02	0.41
14:i:173:VAL:HB	14:i:190:SER:HB3	2.01	0.41
6:r:90:GLU:HG2	6:r:110:TYR:CD1	2.55	0.41
2:2:92:LEU:CD2	2:2:112:ILE:HD11	2.51	0.41
8:F:103:LEU:HD12	8:F:104:PRO:HD2	2.01	0.41
11:J:164:PHE:CE1	11:J:198:ARG:HD2	2.56	0.41
12:K:2:GLU:HG2	12:K:34:LYS:HZ2	1.83	0.41
3:O:126:THR:HG22	4:P:127:ARG:HH21	1.85	0.41
1:1:193:LEU:O	1:1:207:THR:HA	2.20	0.40
8:F:10:VAL:HG12	8:F:21:GLN:HB3	2.03	0.40
10:H:42:TYR:HB2	10:H:178:ILE:HD11	2.03	0.40
13:L:115:ASP:HB3	13:L:119:THR:HB	2.03	0.40
4:P:134:LEU:HD22	4:P:145:LEU:HD11	2.02	0.40
10:V:11:GLY:HA2	10:V:109:GLY:HA3	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:K:4:LEU:HB2	12:K:132:HIS:HB2	2.02	0.40
4:P:73:LEU:HD11	4:P:135:ILE:HG12	2.03	0.40
9:U:66:LEU:HD12	9:U:212:GLU:HB3	2.03	0.40
4:P:28:VAL:CG1	4:P:132:SER:HB2	2.50	0.40
9:U:75:MET:HA	9:U:136:MET:O	2.21	0.40
9:U:106:ILE:HA	9:U:107:PRO:HD3	1.96	0.40
6:D:32:ALA:HB3	6:D:161:ILE:HG13	2.03	0.40
3:O:201:CYS:O	3:O:205:VAL:HB	2.21	0.40
12:Y:35:MET:HE2	12:Y:45:LEU:HD21	2.03	0.40
3:A:32:ILE:HA	3:A:82:GLY:HA2	2.04	0.40
11:J:114:PRO:C	11:J:116:THR:N	2.74	0.40
10:V:99:MET:HE3	10:V:99:MET:HB2	1.97	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	1	211/213 (99%)	207 (98%)	4 (2%)	0	100	100
1	M	211/213 (99%)	206 (98%)	5 (2%)	0	100	100
2	2	212/214 (99%)	202 (95%)	10 (5%)	0	100	100
2	N	212/214 (99%)	202 (95%)	10 (5%)	0	100	100
3	A	236/242 (98%)	232 (98%)	4 (2%)	0	100	100
3	O	236/242 (98%)	234 (99%)	2 (1%)	0	100	100
4	B	227/229 (99%)	222 (98%)	5 (2%)	0	100	100
4	P	227/229 (99%)	218 (96%)	9 (4%)	0	100	100
5	C	237/248 (96%)	233 (98%)	4 (2%)	0	100	100
5	Q	241/248 (97%)	233 (97%)	8 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
6	D	221/235 (94%)	216 (98%)	3 (1%)	2 (1%)	14	16
6	r	223/235 (95%)	216 (97%)	5 (2%)	2 (1%)	14	16
7	E	226/232 (97%)	219 (97%)	7 (3%)	0	100	100
7	s	228/232 (98%)	220 (96%)	8 (4%)	0	100	100
8	F	234/236 (99%)	222 (95%)	10 (4%)	2 (1%)	14	16
8	T	234/236 (99%)	223 (95%)	10 (4%)	1 (0%)	30	36
9	G	240/244 (98%)	235 (98%)	5 (2%)	0	100	100
9	U	241/244 (99%)	232 (96%)	9 (4%)	0	100	100
10	H	197/199 (99%)	191 (97%)	6 (3%)	0	100	100
10	V	197/199 (99%)	191 (97%)	5 (2%)	1 (0%)	24	29
11	J	202/204 (99%)	191 (95%)	7 (4%)	4 (2%)	6	4
11	X	202/204 (99%)	196 (97%)	3 (2%)	3 (2%)	8	7
12	K	194/197 (98%)	186 (96%)	7 (4%)	1 (0%)	24	29
12	Y	195/197 (99%)	188 (96%)	6 (3%)	1 (0%)	24	29
13	L	201/203 (99%)	198 (98%)	3 (2%)	0	100	100
13	Z	201/203 (99%)	197 (98%)	4 (2%)	0	100	100
14	i	217/223 (97%)	209 (96%)	8 (4%)	0	100	100
14	w	218/223 (98%)	211 (97%)	7 (3%)	0	100	100
All	All	6121/6238 (98%)	5930 (97%)	174 (3%)	17 (0%)	36	44

All (17) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
6	D	213	ARG
6	r	213	ARG
11	J	156	PRO
11	X	156	PRO
6	D	163	ARG
8	F	151	ALA
11	J	116	THR
11	X	17	LYS
6	r	163	ARG
12	K	122	ALA
8	F	54	SER
11	J	115	LYS
10	V	115	LEU

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Mol	Chain	Res	Type
12	Y	50	ALA
8	T	235	GLY
11	J	101	GLY
11	X	101	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	1	178/178 (100%)	172 (97%)	6 (3%)	32	45
1	M	178/178 (100%)	169 (95%)	9 (5%)	21	29
2	2	177/177 (100%)	171 (97%)	6 (3%)	32	45
2	N	177/177 (100%)	168 (95%)	9 (5%)	21	29
3	A	204/206 (99%)	200 (98%)	4 (2%)	48	62
3	O	204/206 (99%)	199 (98%)	5 (2%)	42	54
4	B	188/188 (100%)	185 (98%)	3 (2%)	55	68
4	P	188/188 (100%)	179 (95%)	9 (5%)	23	32
5	C	202/208 (97%)	195 (96%)	7 (4%)	32	44
5	Q	205/208 (99%)	199 (97%)	6 (3%)	37	49
6	D	193/199 (97%)	185 (96%)	8 (4%)	27	38
6	r	195/199 (98%)	182 (93%)	13 (7%)	15	19
7	E	193/194 (100%)	191 (99%)	2 (1%)	68	77
7	s	192/194 (99%)	183 (95%)	9 (5%)	23	33
8	F	202/202 (100%)	191 (95%)	11 (5%)	20	27
8	T	202/202 (100%)	190 (94%)	12 (6%)	18	24
9	G	199/201 (99%)	192 (96%)	7 (4%)	32	44
9	U	200/201 (100%)	193 (96%)	7 (4%)	32	44
10	H	153/153 (100%)	143 (94%)	10 (6%)	15	20
10	V	153/153 (100%)	147 (96%)	6 (4%)	28	40

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
11	J	173/173 (100%)	168 (97%)	5 (3%)	37	49
11	X	173/173 (100%)	166 (96%)	7 (4%)	28	39
12	K	167/168 (99%)	165 (99%)	2 (1%)	63	74
12	Y	168/168 (100%)	163 (97%)	5 (3%)	36	48
13	L	165/165 (100%)	163 (99%)	2 (1%)	63	74
13	Z	165/165 (100%)	164 (99%)	1 (1%)	78	85
14	i	171/175 (98%)	160 (94%)	11 (6%)	16	21
14	w	172/175 (98%)	161 (94%)	11 (6%)	16	21
All	All	5137/5174 (99%)	4944 (96%)	193 (4%)	29	41

All (193) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	1	30	SER
1	1	65	THR
1	1	83	MET
1	1	125	ASP
1	1	161	VAL
1	1	166	LEU
2	2	3	ASN
2	2	10	SER
2	2	12	LEU
2	2	22	ILE
2	2	37	ARG
2	2	117	ASP
3	A	52	THR
3	A	126	THR
3	A	196	GLU
3	A	205	VAL
4	B	43	VAL
4	B	131	VAL
4	B	182	GLU
5	C	25	MET
5	C	44	LEU
5	C	62	SER
5	C	132	VAL
5	C	133	SER
5	C	227	VAL
5	C	236	LEU

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Mol	Chain	Res	Type
6	D	23	GLN
6	D	53	LEU
6	D	102	VAL
6	D	130	SER
6	D	139	ASP
6	D	197	GLU
6	D	198	VAL
6	D	221	ASN
7	E	35	SER
7	E	42	THR
8	F	33	SER
8	F	62	LYS
8	F	78	THR
8	F	82	ARG
8	F	114	SER
8	F	182	CYS
8	F	196	ARG
8	F	202	GLU
8	F	229	VAL
8	F	230	SER
8	F	237	GLU
9	G	5	THR
9	G	69	VAL
9	G	81	LEU
9	G	143	ASN
9	G	181	MET
9	G	190	VAL
9	G	216	VAL
10	H	40	ARG
10	H	65	LEU
10	H	84	ARG
10	H	106	ARG
10	H	114	THR
10	H	172	VAL
10	H	176	VAL
10	H	179	THR
10	H	186	ARG
10	H	189	LEU
11	J	11	VAL
11	J	14	MET
11	J	81	GLN
11	J	94	LEU

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Mol	Chain	Res	Type
11	J	108	VAL
12	K	13	VAL
12	K	47	VAL
13	L	73	ARG
13	L	144	ARG
1	M	1	ARG
1	M	30	SER
1	M	65	THR
1	M	73	LYS
1	M	127	VAL
1	M	136	LYS
1	M	161	VAL
1	M	166	LEU
1	M	187	VAL
2	N	3	ASN
2	N	5	MET
2	N	10	SER
2	N	12	LEU
2	N	15	LYS
2	N	22	ILE
2	N	37	ARG
2	N	51	LEU
2	N	117	ASP
3	O	52	THR
3	O	126	THR
3	O	173	THR
3	O	205	VAL
3	O	221	THR
4	P	43	VAL
4	P	58	GLU
4	P	74	VAL
4	P	115	SER
4	P	132	SER
4	P	181	LEU
4	P	182	GLU
4	P	202	MET
4	P	232	ILE
5	Q	7	SER
5	Q	44	LEU
5	Q	62	SER
5	Q	132	VAL
5	Q	194	ILE

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Mol	Chain	Res	Type
5	Q	227	VAL
8	T	62	LYS
8	T	77	LEU
8	T	78	THR
8	T	83	LEU
8	T	101	ARG
8	T	114	SER
8	T	115	LYS
8	T	182	CYS
8	T	203	GLN
8	T	207	THR
8	T	229	VAL
8	T	233	LEU
9	U	69	VAL
9	U	81	LEU
9	U	181	MET
9	U	189	ILE
9	U	190	VAL
9	U	200	VAL
9	U	216	VAL
10	V	40	ARG
10	V	65	LEU
10	V	114	THR
10	V	176	VAL
10	V	179	THR
10	V	189	LEU
11	X	11	VAL
11	X	20	VAL
11	X	81	GLN
11	X	108	VAL
11	X	116	THR
11	X	121	ILE
11	X	175	VAL
12	Y	13	VAL
12	Y	85	ARG
12	Y	102	LEU
12	Y	173	LEU
12	Y	185	LYS
13	Z	97	MET
14	i	13	ILE
14	i	21	THR
14	i	22	ASN

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Mol	Chain	Res	Type
14	i	79	VAL
14	i	120	SER
14	i	121	ARG
14	i	135	LEU
14	i	155	LEU
14	i	164	LEU
14	i	185	LEU
14	i	213	THR
6	r	23	GLN
6	r	41	VAL
6	r	46	GLU
6	r	53	LEU
6	r	93	SER
6	r	99	GLU
6	r	130	SER
6	r	134	VAL
6	r	181	ILE
6	r	197	GLU
6	r	199	VAL
6	r	211	MET
6	r	221	ASN
7	s	35	SER
7	s	36	THR
7	s	42	THR
7	s	82	ILE
7	s	188	SER
7	s	199	LEU
7	s	210	LEU
7	s	213	THR
7	s	236	GLU
14	w	13	ILE
14	w	21	THR
14	w	22	ASN
14	w	56	THR
14	w	79	VAL
14	w	121	ARG
14	w	135	LEU
14	w	155	LEU
14	w	185	LEU
14	w	213	THR
14	w	220	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (75)

such sidechains are listed below:

Mol	Chain	Res	Type
1	1	36	HIS
1	1	151	ASN
1	1	152	GLN
2	2	89	HIS
2	2	162	GLN
3	A	75	ASN
4	B	122	GLN
5	C	30	HIS
5	C	40	ASN
5	C	51	ASN
5	C	240	HIS
6	D	15	HIS
6	D	92	GLN
7	E	41	GLN
7	E	152	GLN
7	E	164	GLN
8	F	16	GLN
8	F	203	GLN
9	G	143	ASN
10	H	97	HIS
10	H	191	ASN
11	J	33	GLN
11	J	72	ASN
11	J	169	GLN
12	K	32	HIS
12	K	61	GLN
13	L	85	ASN
13	L	203	ASN
1	M	151	ASN
1	M	160	ASN
2	N	65	GLN
2	N	89	HIS
2	N	162	GLN
3	O	68	HIS
3	O	75	ASN
4	P	95	GLN
4	P	111	GLN
4	P	139	ASN
5	Q	30	HIS
5	Q	40	ASN
5	Q	166	ASN
5	Q	198	ASN

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Mol	Chain	Res	Type
5	Q	240	HIS
8	T	16	GLN
8	T	86	ASN
8	T	146	GLN
8	T	166	GLN
8	T	175	HIS
8	T	190	HIS
9	U	110	HIS
10	V	97	HIS
10	V	122	GLN
10	V	191	ASN
12	Y	27	GLN
12	Y	32	HIS
12	Y	55	GLN
12	Y	61	GLN
12	Y	87	ASN
13	Z	53	GLN
13	Z	203	ASN
14	i	9	GLN
14	i	93	HIS
14	i	109	GLN
14	i	131	GLN
14	i	172	ASN
6	r	15	HIS
6	r	122	ASN
6	r	175	ASN
7	s	41	GLN
7	s	152	GLN
7	s	164	GLN
14	w	109	GLN
14	w	131	GLN
14	w	145	ASN
14	w	152	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 [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 17 ligands modelled in this entry, 6 are monoatomic - leaving 11 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	SKN	H	201	10	31,35,35	0.19	0	41,46,46	0.46	0
15	SO4	1	302	-	4,4,4	0.38	0	6,6,6	0.10	0
17	SKN	V	201	10	31,35,35	0.14	0	41,46,46	0.50	0
17	SKN	Z	301	13	31,35,35	0.28	0	41,46,46	0.42	0
15	SO4	L	303	-	4,4,4	0.41	0	6,6,6	0.22	0
17	SKN	L	301	13	31,35,35	0.24	0	41,46,46	0.99	1 (2%)
15	SO4	K	201	-	4,4,4	0.30	0	6,6,6	0.16	0
15	SO4	1	301	-	4,4,4	0.41	0	6,6,6	0.36	0
17	SKN	w	301	14	31,35,35	0.31	0	41,46,46	0.67	1 (2%)
17	SKN	i	301	14	31,35,35	0.23	0	41,46,46	0.48	0
15	SO4	Y	201	-	4,4,4	0.26	0	6,6,6	0.14	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
17	SKN	H	201	10	-	5/25/30/30	0/3/3/3
17	SKN	Z	301	13	-	2/25/30/30	0/3/3/3
17	SKN	V	201	10	-	3/25/30/30	0/3/3/3
17	SKN	L	301	13	-	2/25/30/30	0/3/3/3
17	SKN	w	301	14	-	3/25/30/30	0/3/3/3
17	SKN	i	301	14	-	2/25/30/30	0/3/3/3

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	L	301	SKN	C5-C1-N6	-5.81	102.88	110.39
17	w	301	SKN	C1-N6-C13	-2.45	116.80	122.99

There are no chirality outliers.

All (17) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
17	H	201	SKN	C1-C5-C7-C12
17	L	301	SKN	C1-C5-C7-C8
17	L	301	SKN	C1-C5-C7-C12
17	Z	301	SKN	C1-C5-C7-C8
17	Z	301	SKN	C1-C5-C7-C12
17	i	301	SKN	C1-C5-C7-C8
17	i	301	SKN	C1-C5-C7-C12
17	w	301	SKN	B2-C1-C5-C7
17	w	301	SKN	C1-C5-C7-C8
17	w	301	SKN	C1-C5-C7-C12
17	H	201	SKN	N16-C18-C19-C27
17	H	201	SKN	O26-C18-C19-C27
17	V	201	SKN	C13-C14-N16-C18
17	H	201	SKN	C1-C5-C7-C8
17	V	201	SKN	C1-C5-C7-C12
17	V	201	SKN	C1-C5-C7-C8
17	H	201	SKN	C33-C32-C9-C8

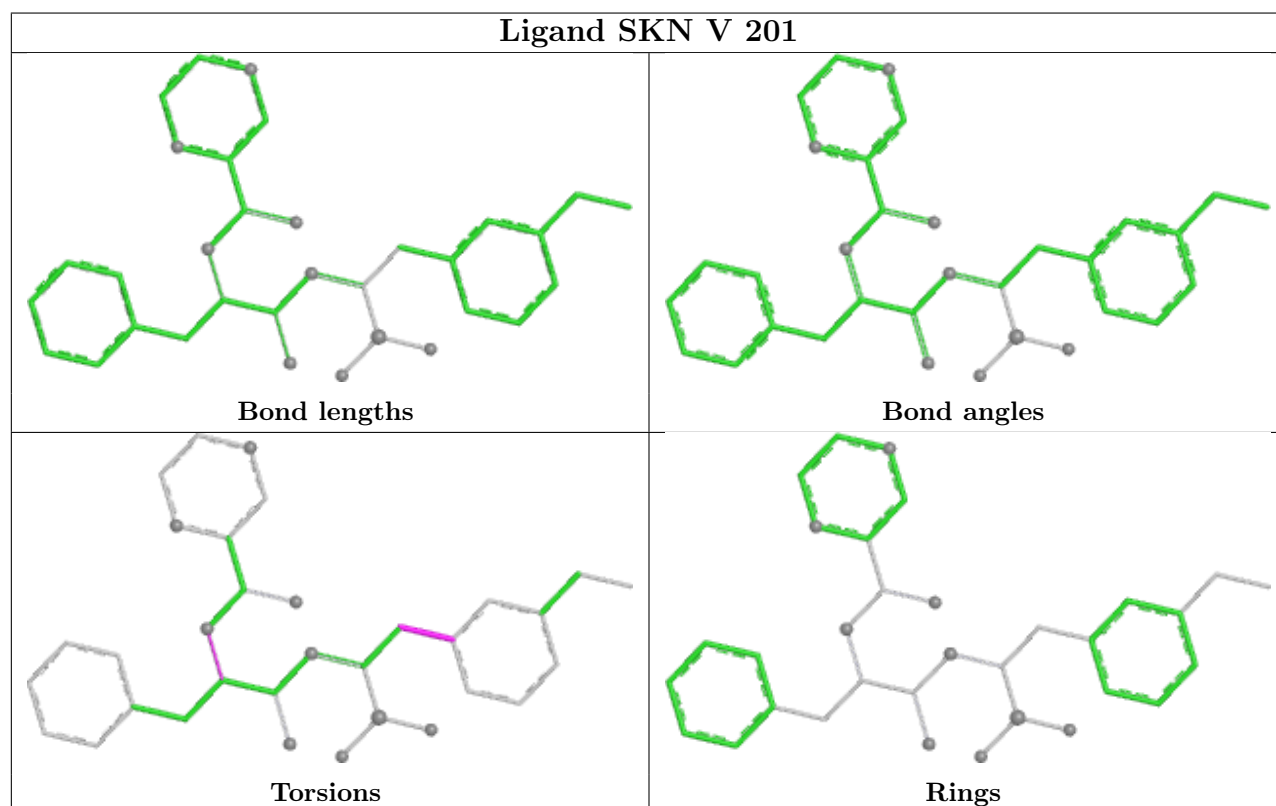
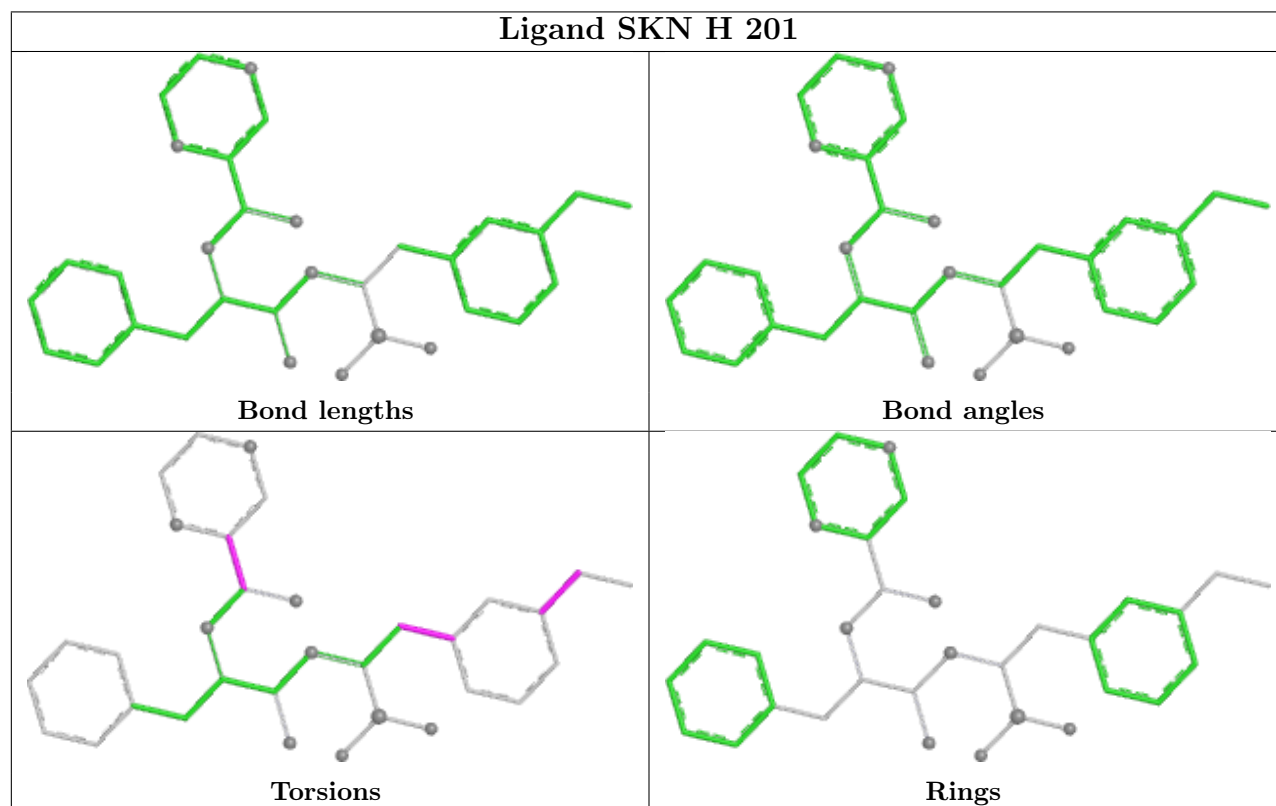
There are no ring outliers.

1 monomer is involved in 2 short contacts:

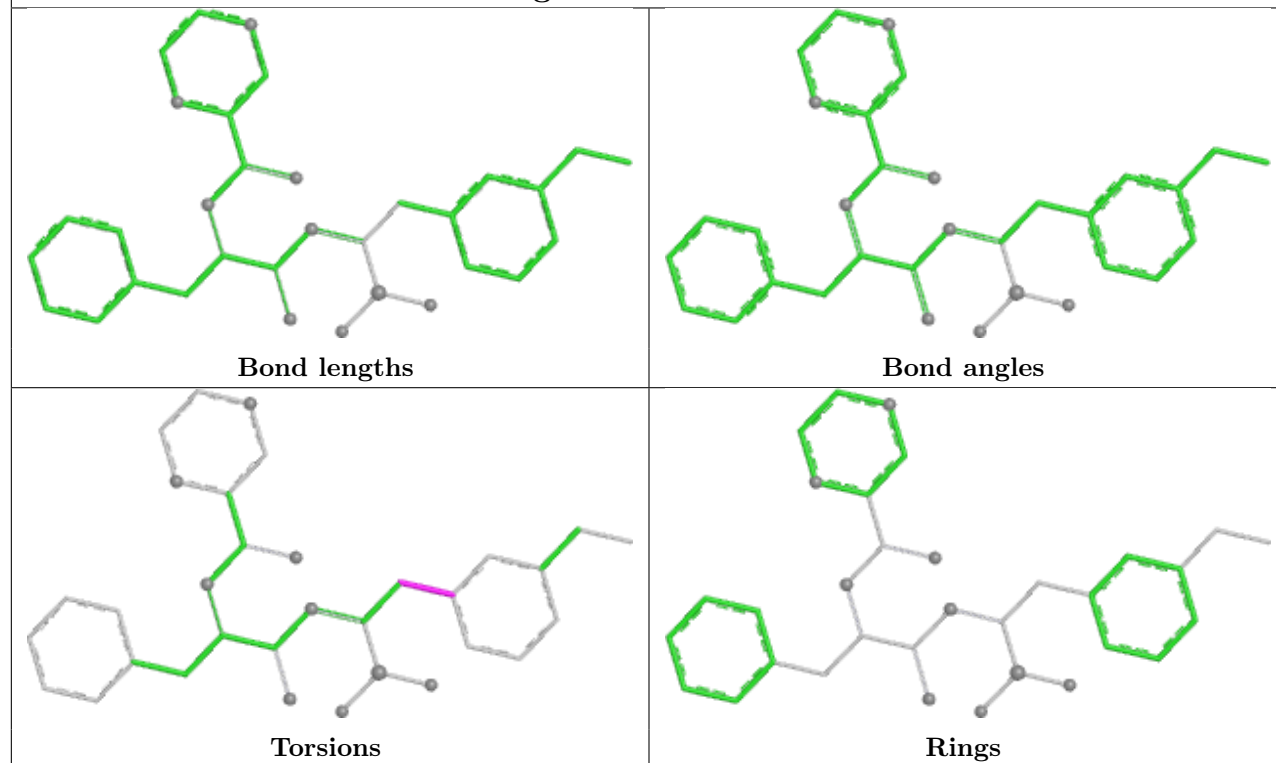
Mol	Chain	Res	Type	Clashes	Symm-Clashes
17	i	301	SKN	2	0

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

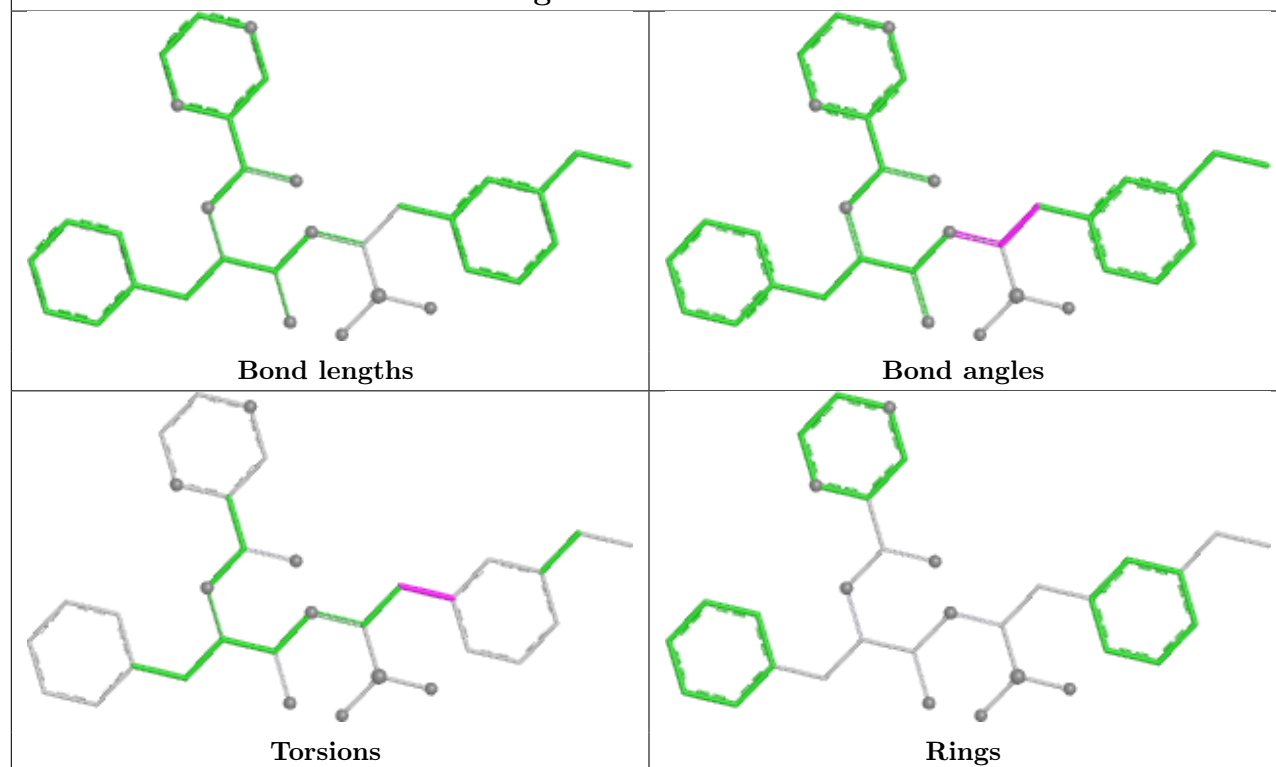
average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

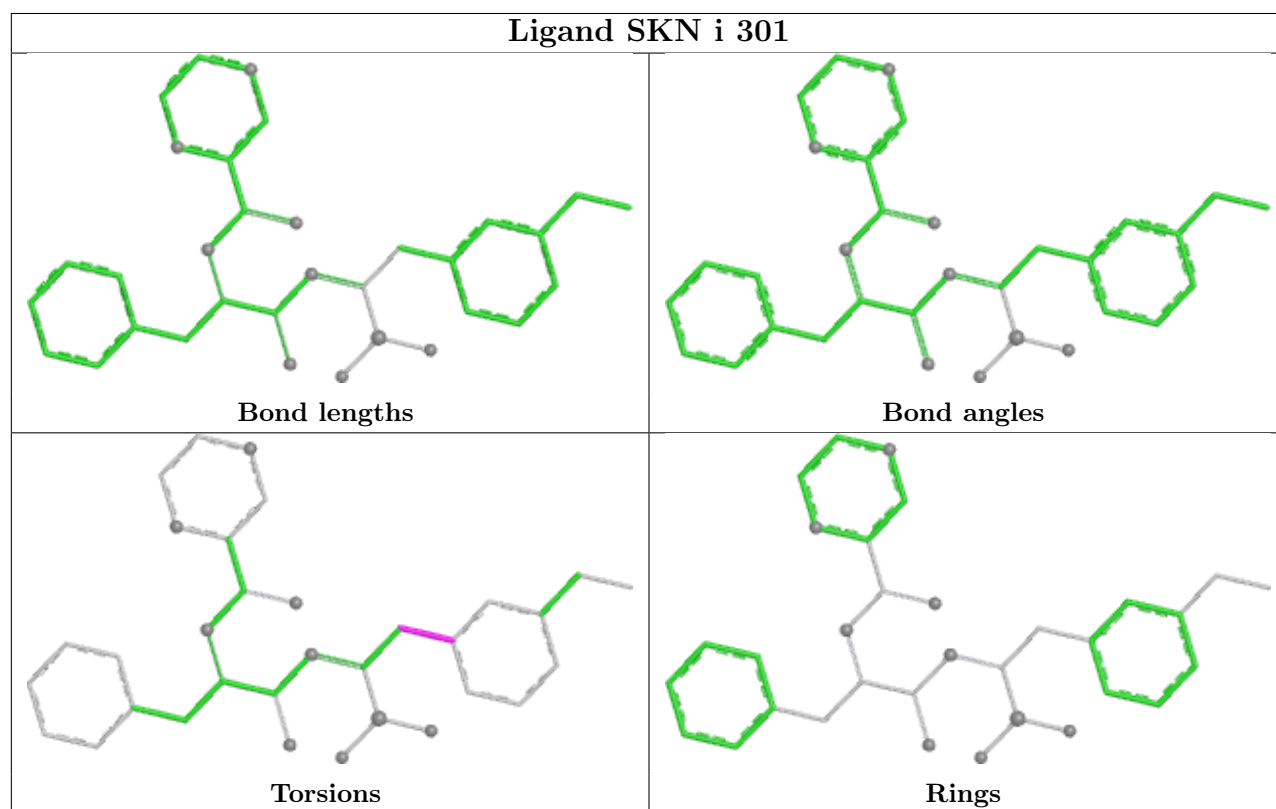
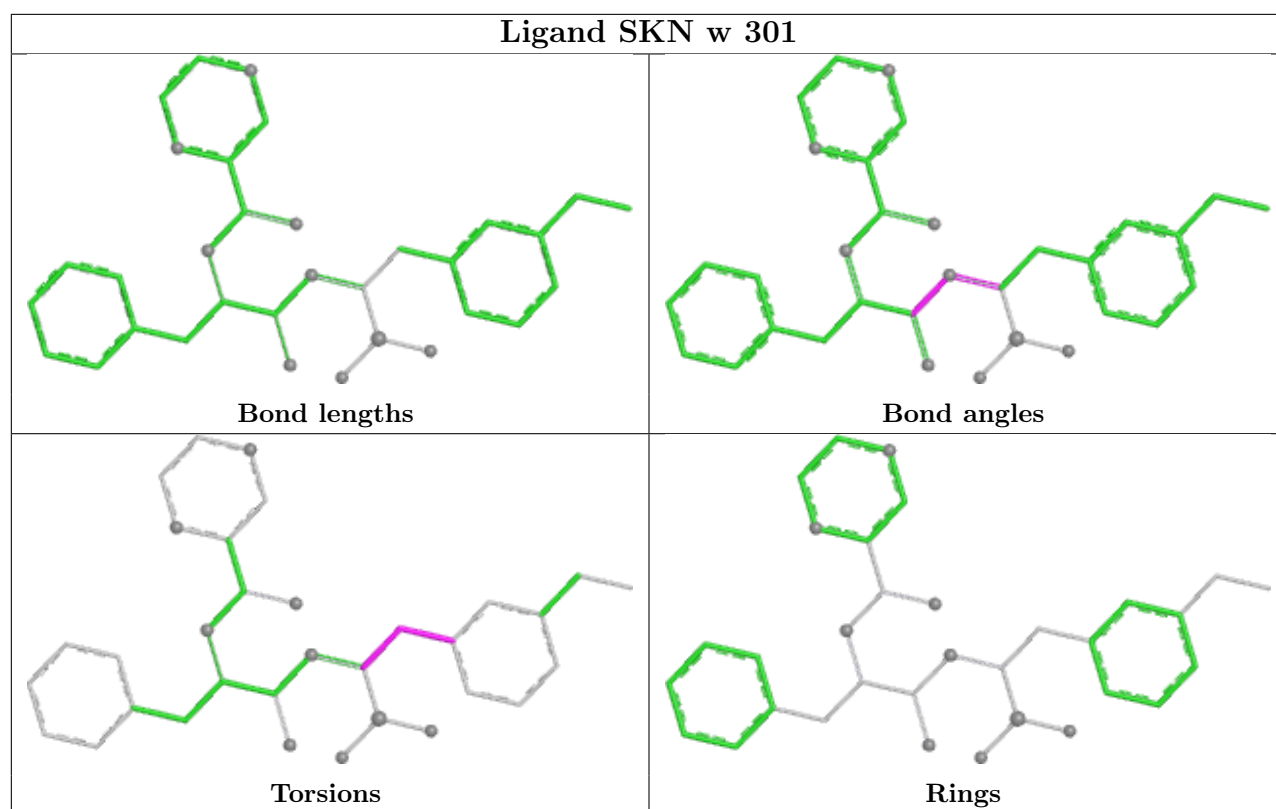


Ligand SKN Z 301



Ligand SKN L 301





5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	1	213/213 (100%)	-0.23	2 (0%) 81 82	19, 43, 62, 86	18 (8%)
1	M	213/213 (100%)	-0.23	0 100 100	25, 45, 66, 85	16 (7%)
2	2	214/214 (100%)	-0.27	2 (0%) 81 82	27, 42, 65, 85	9 (4%)
2	N	214/214 (100%)	-0.24	1 (0%) 87 89	32, 45, 62, 86	13 (6%)
3	A	240/242 (99%)	0.42	17 (7%) 22 18	25, 58, 93, 114	58 (24%)
3	O	240/242 (99%)	0.04	6 (2%) 58 59	22, 48, 72, 99	44 (18%)
4	B	229/229 (100%)	0.23	6 (2%) 57 57	25, 57, 83, 99	41 (17%)
4	P	229/229 (100%)	0.06	5 (2%) 62 63	27, 51, 72, 84	33 (14%)
5	C	241/248 (97%)	0.33	5 (2%) 63 64	29, 57, 82, 117	55 (22%)
5	Q	245/248 (98%)	0.22	5 (2%) 65 66	27, 52, 73, 104	54 (22%)
6	D	227/235 (96%)	0.58	7 (3%) 51 50	26, 63, 99, 119	60 (26%)
6	r	229/235 (97%)	0.63	16 (6%) 22 19	26, 63, 107, 164	81 (35%)
7	E	230/232 (99%)	0.38	7 (3%) 52 52	33, 61, 86, 100	45 (19%)
7	s	230/232 (99%)	0.50	9 (3%) 43 40	28, 60, 89, 101	58 (25%)
8	F	236/236 (100%)	0.37	8 (3%) 48 46	27, 59, 96, 116	42 (17%)
8	T	236/236 (100%)	0.30	13 (5%) 30 28	26, 53, 86, 106	45 (19%)
9	G	242/244 (99%)	0.45	9 (3%) 45 43	20, 58, 91, 110	53 (21%)
9	U	243/244 (99%)	0.02	2 (0%) 82 83	22, 48, 68, 82	51 (20%)
10	H	199/199 (100%)	-0.13	0 100 100	29, 46, 62, 67	11 (5%)
10	V	199/199 (100%)	-0.25	0 100 100	22, 41, 59, 66	11 (5%)
11	J	204/204 (100%)	-0.12	3 (1%) 72 73	32, 47, 68, 83	11 (5%)
11	X	204/204 (100%)	-0.22	1 (0%) 87 89	29, 45, 61, 76	8 (3%)
12	K	196/197 (99%)	-0.05	0 100 100	24, 49, 62, 74	17 (8%)
12	Y	197/197 (100%)	-0.07	1 (0%) 87 89	27, 48, 62, 83	20 (10%)

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	L	203/203 (100%)	-0.13	0 100 100	30, 47, 66, 79	6 (2%)
13	Z	203/203 (100%)	-0.15	1 (0%) 87 89	30, 47, 66, 76	12 (5%)
14	i	219/223 (98%)	0.07	9 (4%) 41 39	26, 48, 73, 104	25 (11%)
14	w	220/223 (98%)	-0.03	5 (2%) 61 62	27, 45, 69, 99	23 (10%)
All	All	6195/6238 (99%)	0.10	140 (2%) 61 62	19, 50, 82, 164	920 (14%)

All (140) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
7	E	240	ASP	4.4
7	s	238	ILE	4.0
8	T	53	GLN	3.8
4	P	179	GLU	3.8
4	B	232	ILE	3.8
9	G	193	VAL	3.7
4	B	176	ARG	3.7
9	G	230	ASP	3.5
5	C	58	GLU	3.5
5	C	25	MET	3.4
11	J	116	THR	3.4
9	G	244	LYS	3.4
3	A	188	ASP	3.3
4	P	178	ASN	3.3
5	Q	202	ASP	3.3
6	D	225	ILE	3.2
3	O	159	TYR	3.2
8	T	236	LEU	3.1
9	U	219	LEU	3.0
4	P	232	ILE	2.9
6	r	205	ASN	2.9
14	i	196	VAL	2.9
8	T	55	GLU	2.9
4	P	177	TYR	2.9
6	D	138	PHE	2.9
6	r	138	PHE	2.9
3	O	242	LEU	2.8
14	i	203	HIS	2.8
2	2	13	GLY	2.8
3	A	179	LEU	2.8
14	w	198	ARG	2.8
3	O	179	LEU	2.8

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Mol	Chain	Res	Type	RSRZ
6	D	53	LEU	2.8
11	X	116	THR	2.8
4	P	176	ARG	2.7
14	i	194	GLU	2.7
14	i	202	TYR	2.7
14	w	196	VAL	2.7
8	T	60	GLN	2.7
7	E	129	ASP	2.7
6	r	219	ILE	2.7
4	B	54	ILE	2.7
8	T	234	GLU	2.6
3	A	159	TYR	2.6
6	D	100	ASP	2.6
7	s	214	ASN	2.6
9	G	219	LEU	2.6
3	A	146	GLU	2.6
8	F	184	LEU	2.6
6	r	236	LYS	2.6
5	Q	249	ARG	2.6
8	F	172	LEU	2.6
6	r	198	VAL	2.6
3	O	63	SER	2.6
11	J	115	LYS	2.6
4	B	179	GLU	2.5
1	1	164	VAL	2.5
3	A	183	VAL	2.5
8	F	29	VAL	2.5
3	A	198	ALA	2.5
7	E	238	ILE	2.5
7	E	199	LEU	2.5
8	F	185	ASN	2.5
6	r	223	GLU	2.5
14	i	199	SER	2.4
6	r	99	GLU	2.4
5	C	245	ALA	2.4
5	C	200	THR	2.4
12	Y	197	PRO	2.4
3	O	245	ARG	2.4
3	A	187	PHE	2.4
7	s	65	GLU	2.4
14	i	193	THR	2.4
3	A	239	LEU	2.4

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Mol	Chain	Res	Type	RSRZ
8	T	239	ARG	2.4
3	A	235	ILE	2.3
5	Q	177	GLN	2.3
14	w	193	THR	2.3
3	A	206	LEU	2.3
6	r	215	GLN	2.3
7	s	224	GLN	2.3
3	A	58	ASP	2.3
7	s	234	LEU	2.3
9	G	197	ILE	2.3
3	A	191	PHE	2.3
8	T	185	ASN	2.2
3	A	172	GLN	2.2
4	B	52	LYS	2.2
3	A	155	ASP	2.2
6	D	223	GLU	2.2
6	D	102	VAL	2.2
6	r	163	ARG	2.2
14	w	195	PRO	2.2
8	T	57	ALA	2.2
14	w	194	GLU	2.2
6	r	98	VAL	2.2
7	s	222	PRO	2.2
7	E	225	ASN	2.2
8	F	207	THR	2.2
6	r	225	ILE	2.2
8	T	54	SER	2.2
14	i	198	ARG	2.2
9	G	208	ALA	2.2
3	A	197	THR	2.2
5	Q	60	PHE	2.2
6	D	35	VAL	2.1
5	C	230	GLN	2.1
7	E	181	LEU	2.1
8	T	227	ASP	2.1
6	r	47	LYS	2.1
7	E	228	MET	2.1
9	G	180	GLN	2.1
3	A	157	ALA	2.1
7	s	212	ALA	2.1
3	A	194	THR	2.1
14	i	200	GLY	2.1

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Mol	Chain	Res	Type	RSRZ
6	r	232	ILE	2.1
9	G	3	ILE	2.1
13	Z	72	GLU	2.1
8	F	150	SER	2.1
3	O	217	VAL	2.1
8	T	16	GLN	2.1
9	G	53	VAL	2.1
8	T	201	ALA	2.1
8	F	49	LEU	2.1
8	T	205	LEU	2.1
5	Q	248	GLU	2.1
7	s	205	VAL	2.1
2	2	206	GLU	2.1
14	i	195	PRO	2.1
6	r	200	GLN	2.0
9	U	243	LEU	2.0
2	N	206	GLU	2.0
6	r	207	GLU	2.0
11	J	117	PHE	2.0
4	B	173	LEU	2.0
8	F	151	ALA	2.0
7	s	225	ASN	2.0
1	1	177	ASP	2.0
6	r	154	HIS	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](#)

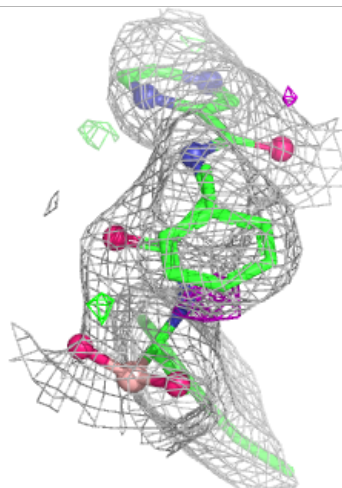
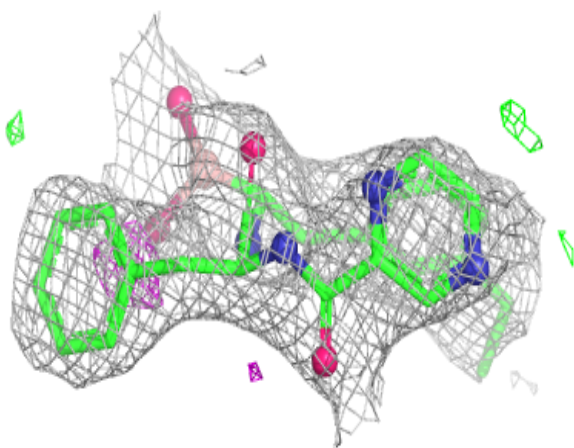
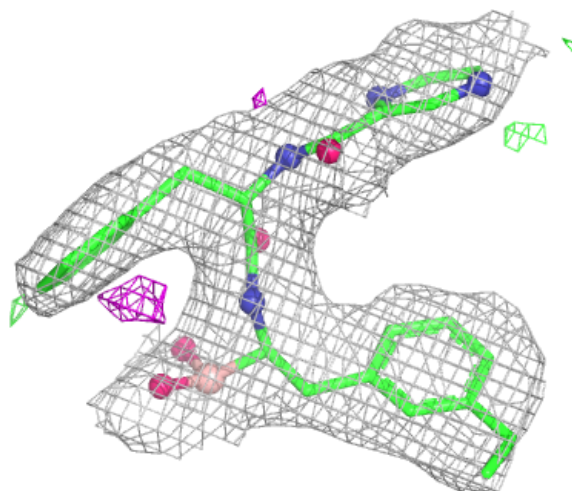
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	SO4	1	302	5/5	0.83	0.12	99,99,99,99	0
15	SO4	1	301	5/5	0.89	0.16	77,77,78,78	0
15	SO4	L	303	5/5	0.90	0.12	101,101,101,101	0
15	SO4	Y	201	5/5	0.90	0.11	104,104,104,104	0
15	SO4	K	201	5/5	0.93	0.12	109,109,109,109	0
16	NA	w	302	1/1	0.93	0.07	60,60,60,60	0
17	SKN	i	301	33/33	0.93	0.09	47,49,55,55	0
17	SKN	w	301	33/33	0.93	0.09	45,46,54,54	0
17	SKN	H	201	33/33	0.94	0.09	37,39,40,41	0
17	SKN	Z	301	33/33	0.94	0.08	34,40,44,44	0
17	SKN	V	201	33/33	0.95	0.09	39,42,46,46	0
16	NA	A	301	1/1	0.95	0.06	42,42,42,42	0
17	SKN	L	301	33/33	0.96	0.07	40,44,46,46	0
16	NA	i	302	1/1	0.97	0.06	47,47,47,47	0
16	NA	Z	302	1/1	0.97	0.04	47,47,47,47	0
16	NA	L	302	1/1	0.98	0.05	30,30,30,30	0
16	NA	O	301	1/1	0.99	0.04	33,33,33,33	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.

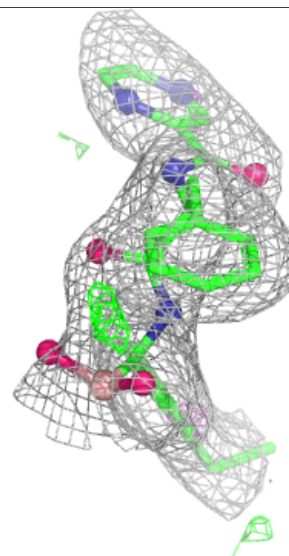
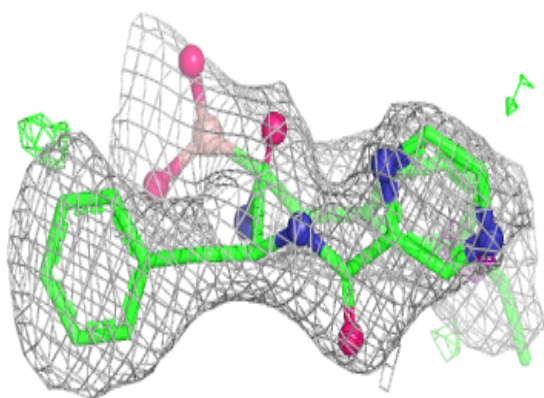
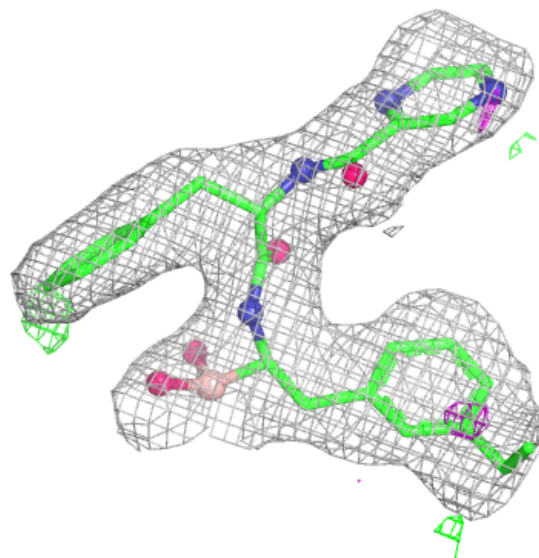
Electron density around SKN i 301:

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



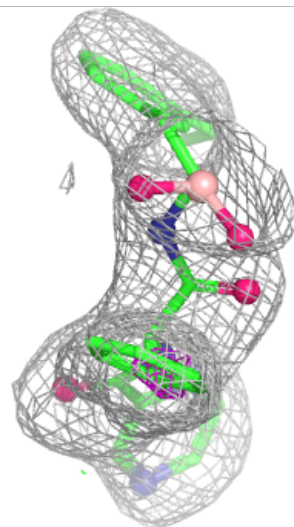
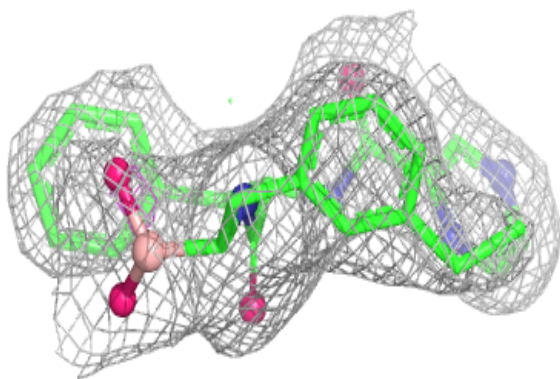
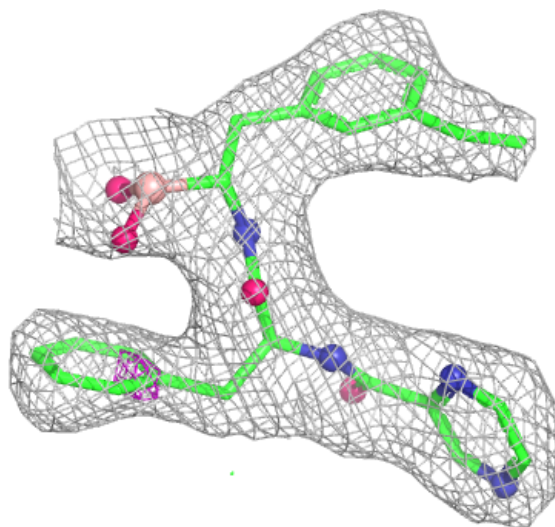
Electron density around SKN w 301:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



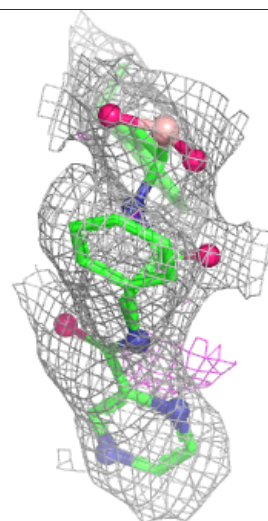
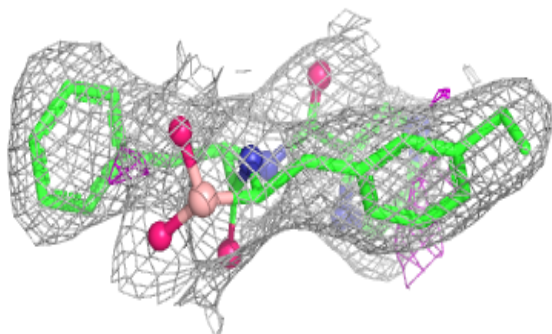
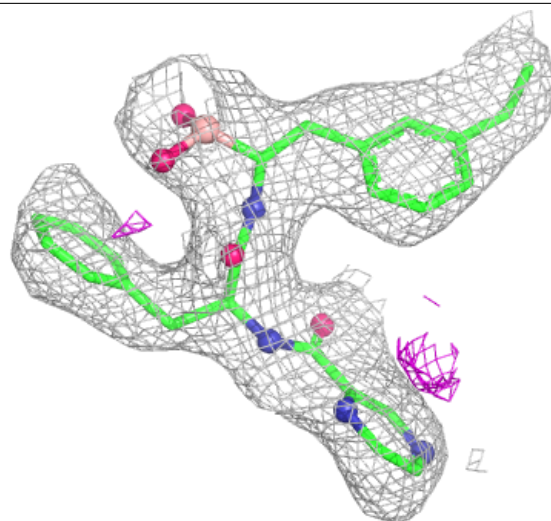
Electron density around SKN H 201:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



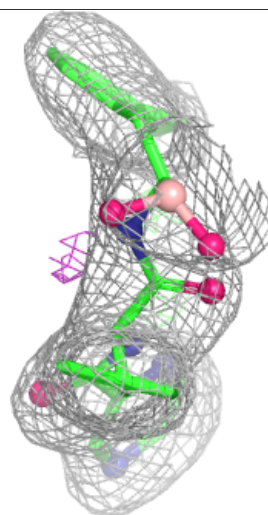
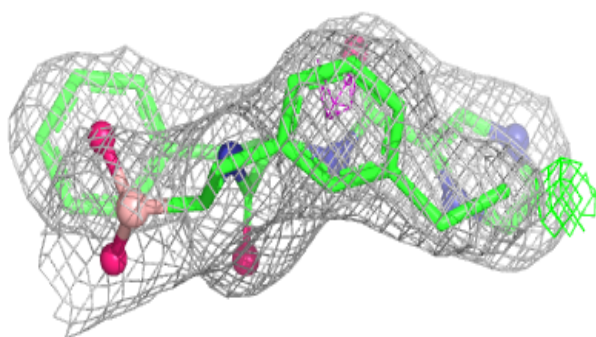
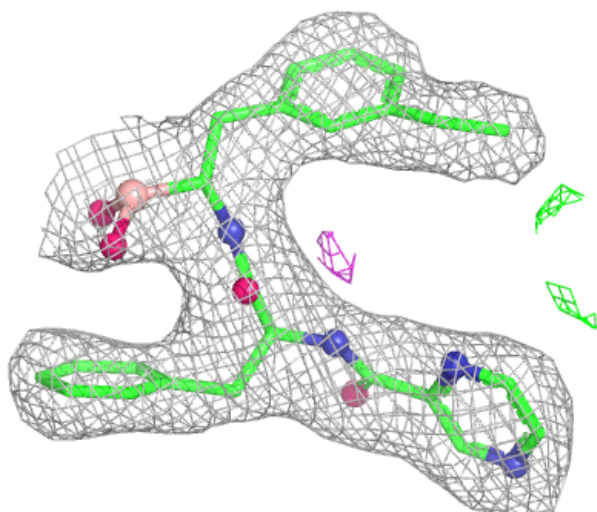
Electron density around SKN Z 301:

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



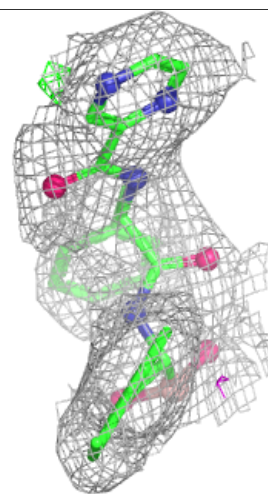
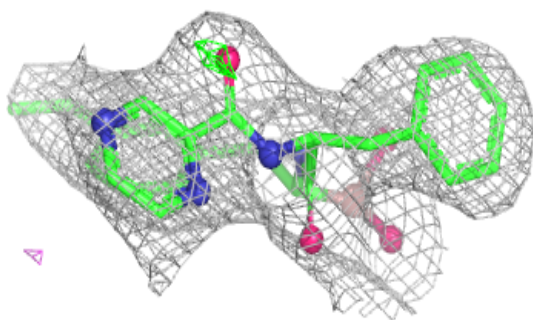
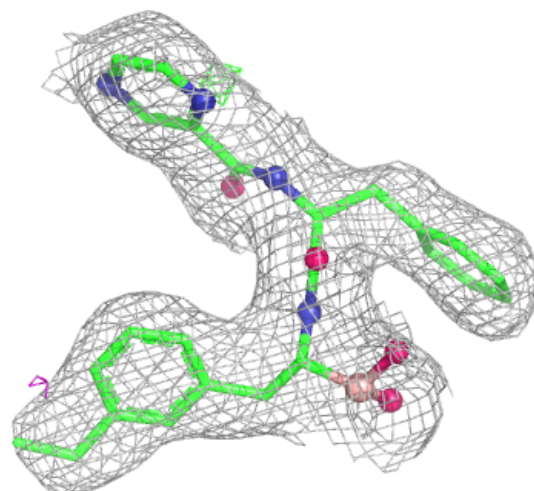
Electron density around SKN V 201:

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



Electron density around SKN L 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.