



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 18, 2026 – 12:43 AM UTC

PDB ID : 4NO6 / pdb_00004no6
Title : yCP in complex with Z-Leu-Leu-Leu-vinylsulfone
Authors : Stein, M.L.; Cui, H.; Beck, P.; Dubiella, C.; Voss, C.; Krueger, A.; Schmidt, B.; Groll, M.
Deposited on : 2013-11-19
Resolution : 3.00 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

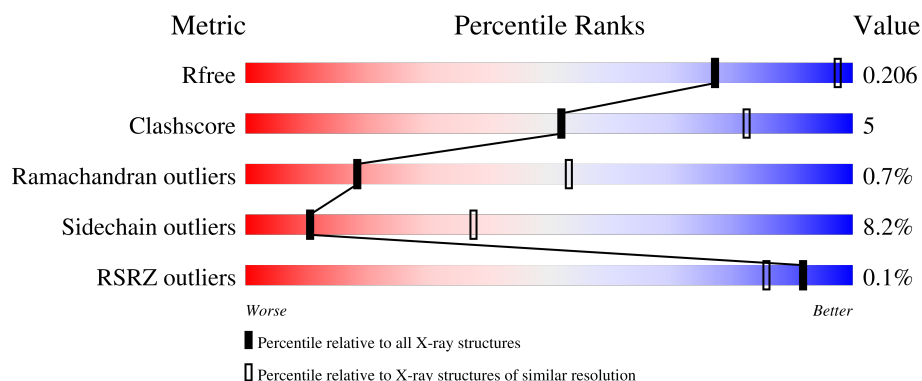
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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.



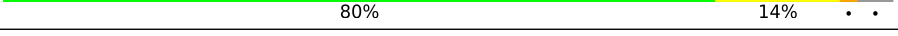
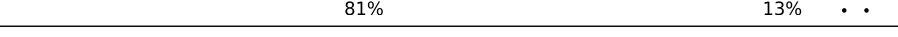
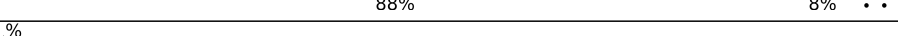
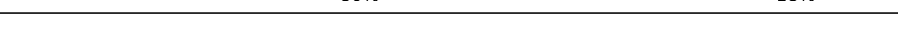
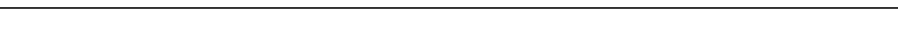
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	2672 (3.00-3.00)
Clashscore	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)
RSRZ outliers	180081	2671 (3.00-3.00)

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	90% 9% .
1	O	250	86% 12% .
2	B	258	71% 19% • • 5%
2	P	258	69% 21% • • 5%
3	C	254	75% 16% • 6%

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Mol	Chain	Length	Quality of chain
3	Q	254	 76%15%•6%
4	D	260	 72%16%•10%
4	R	260	 71%17%•10%
5	E	234	 78%19%••
5	S	234	 77%19%••
6	F	288	 68%15%•16%
6	T	288	 66%16%•16%
7	G	252	 81%13%••
7	U	252	 80%14%••
8	H	232	 80%13%••
8	V	232	 81%13%••
9	I	205	 85%13%•
9	W	205	 85%13%•
10	J	198	 88%8%••
10	X	198	 87%9%••
11	K	212	 85%12%•
11	Y	212	 84%14%•
12	L	222	 82%17%•
12	Z	222	 80%18%•
13	M	246	 80%13%•5%
13	a	246	 81%12%•5%
14	N	196	 88%12%•
14	b	196	 87%12%•

2 Entry composition

There are 17 unique types of molecules in this entry. The entry contains 49661 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 alpha type-2.

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 subunit alpha type-3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	244	Total	C	N	O	S	0	0	0
			1904	1201	321	379	3			
2	P	244	Total	C	N	O	S	0	0	0
			1904	1201	321	379	3			

- Molecule 3 is a protein called Proteasome subunit alpha type-4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	240	Total	C	N	O	S	0	0	0
			1881	1176	329	372	4			
3	Q	240	Total	C	N	O	S	0	0	0
			1881	1176	329	372	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	235	Total	C	N	O	S	0	0	0
			1813	1136	304	366	7			
4	R	235	Total	C	N	O	S	0	0	0
			1813	1136	304	366	7			

- Molecule 5 is a protein called Proteasome subunit alpha type-6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	231	Total	C	N	O	S	0	0	0
			1773	1114	307	348	4			
5	S	231	Total	C	N	O	S	0	0	0
			1773	1114	307	348	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	243	Total	C	N	O	S	0	0	0
			1892	1203	329	356	4			
6	T	243	Total	C	N	O	S	0	0	0
			1892	1203	329	356	4			

- Molecule 7 is a protein called Proteasome subunit alpha type-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	G	241	Total	C	N	O	S	0	0	0
			1907	1214	320	365	8			
7	U	241	Total	C	N	O	S	0	0	0
			1907	1214	320	365	8			

- Molecule 8 is a protein called Proteasome subunit beta type-2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	H	222	Total	C	N	O	S	0	0	0
			1684	1061	293	323	7			
8	V	222	Total	C	N	O	S	0	0	0
			1684	1061	293	323	7			

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

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 subunit beta type-4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	J	195	Total	C	N	O	S	0	0	0
			1561	992	264	299	6			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	X	195	Total	C	N	O	S	0	0	0
			1561	992	264	299	6			

- Molecule 11 is a protein called Proteasome subunit beta type-5.

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 subunit beta type-6.

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 subunit beta type-7.

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

- Molecule 14 is a protein called Proteasome subunit beta type-1.

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

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

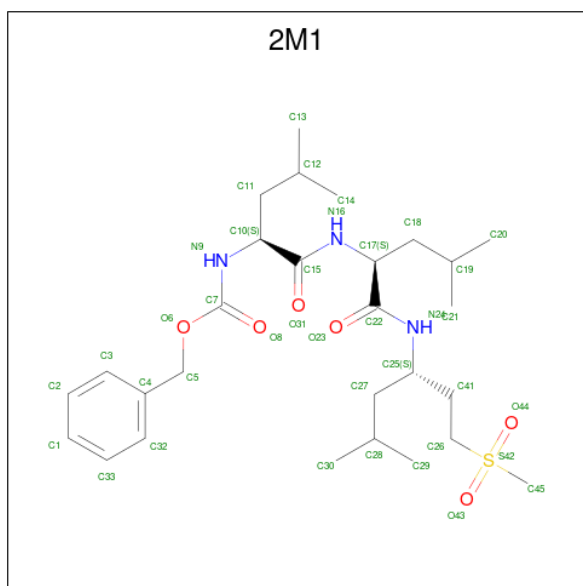
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
15	G	1	Total	Mg	0	0
			1	1		
15	H	1	Total	Mg	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
15	I	1	Total	Mg	0	0
			1	1		
15	K	1	Total	Mg	0	0
			1	1		
15	N	1	Total	Mg	0	0
			1	1		
15	V	1	Total	Mg	0	0
			1	1		
15	Y	1	Total	Mg	0	0
			1	1		
15	Z	1	Total	Mg	0	0
			1	1		

- Molecule 16 is N-[(benzyloxy)carbonyl]-L-leucyl-N-[(3S)-5-methyl-1-(methylsulfonyl)hexan-3-yl]-L-leucinamide (CCD ID: 2M1) (formula: $C_{28}H_{47}N_3O_6S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
16	K	1	Total	C	N	O	S	0	0
			38	28	3	6	1		
16	Y	1	Total	C	N	O	S	0	0
			38	28	3	6	1		

- Molecule 17 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
17	A	5	Total	O	0	0
			5	5		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
17	B	8	Total O 8 8	0	0
17	C	4	Total O 4 4	0	0
17	D	11	Total O 11 11	0	0
17	E	5	Total O 5 5	0	0
17	F	11	Total O 11 11	0	0
17	G	11	Total O 11 11	0	0
17	H	14	Total O 14 14	0	0
17	I	7	Total O 7 7	0	0
17	J	11	Total O 11 11	0	0
17	K	6	Total O 6 6	0	0
17	L	12	Total O 12 12	0	0
17	M	16	Total O 16 16	0	0
17	N	14	Total O 14 14	0	0
17	O	7	Total O 7 7	0	0
17	P	7	Total O 7 7	0	0
17	Q	8	Total O 8 8	0	0
17	R	7	Total O 7 7	0	0
17	S	8	Total O 8 8	0	0
17	T	9	Total O 9 9	0	0
17	U	10	Total O 10 10	0	0
17	V	14	Total O 14 14	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
17	W	11	Total 11	O 11	0	0
17	X	14	Total 14	O 14	0	0
17	Y	8	Total 8	O 8	0	0
17	Z	19	Total 19	O 19	0	0
17	a	13	Total 13	O 13	0	0
17	b	11	Total 11	O 11	0	0

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.

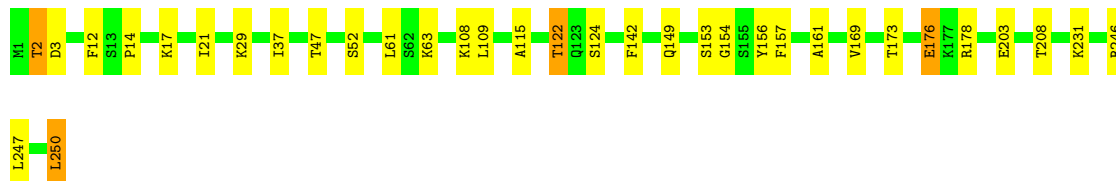
• Molecule 1: Proteasome subunit alpha type-2

Chain A:  90% 9% .



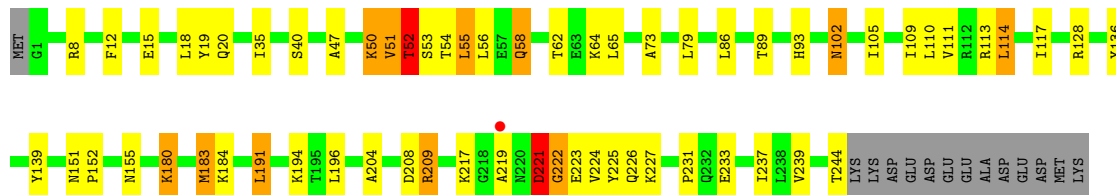
• Molecule 1: Proteasome subunit alpha type-2

Chain O:  86% 12% .



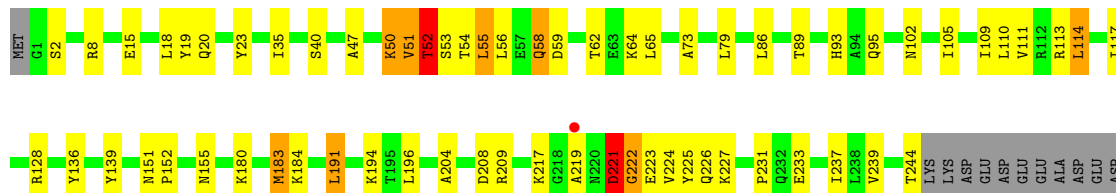
• Molecule 2: Proteasome subunit alpha type-3

Chain B:  71% 19% . . 5%



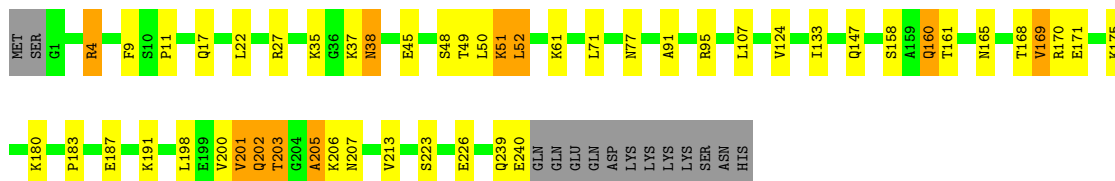
• Molecule 2: Proteasome subunit alpha type-3

Chain P:  69% 21% . . 5%

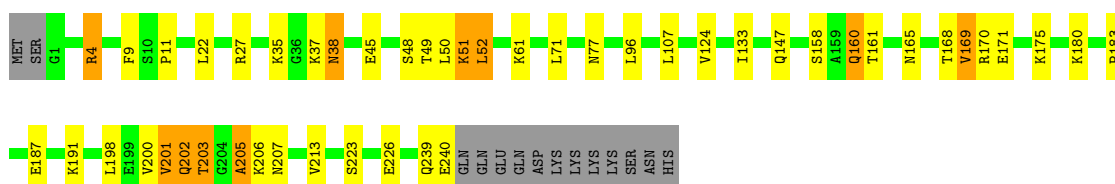


MET
LYS

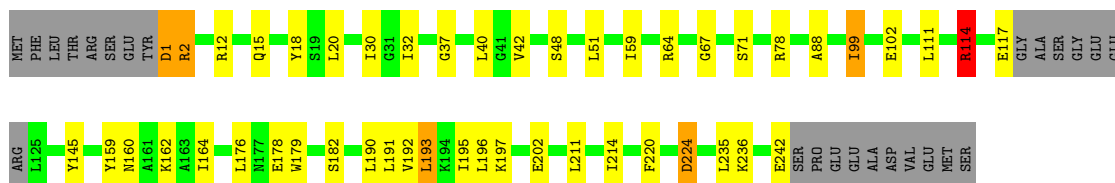
- Molecule 3: Proteasome subunit alpha type-4

Chain C:  75% 16% 6%

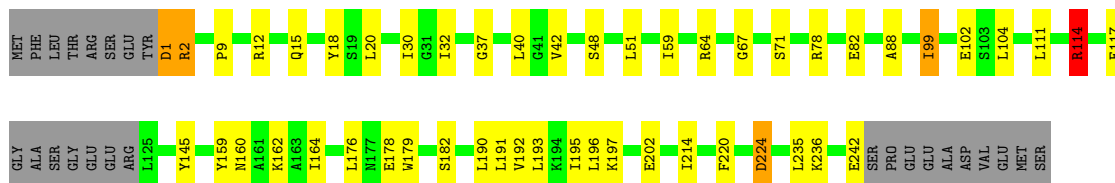
- Molecule 3: Proteasome subunit alpha type-4

Chain Q:  76% 15% 6%

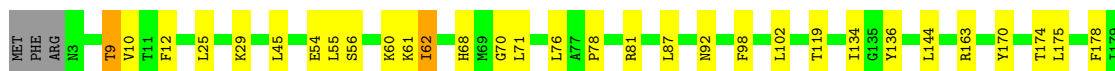
- Molecule 4: Proteasome subunit alpha type-5

Chain D:  72% 16% 10%

- Molecule 4: Proteasome subunit alpha type-5

Chain R:  71% 17% 10%

- Molecule 5: Proteasome subunit alpha type-6

Chain E:  78% 19% 2%



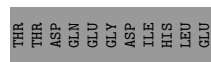
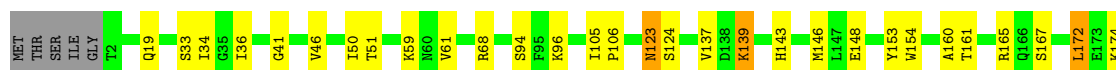
• Molecule 5: Proteasome subunit alpha type-6

Chain S: 77% 19% ..



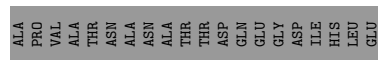
• Molecule 6: Probable proteasome subunit alpha type-7

Chain F: 68% 15% • 16%



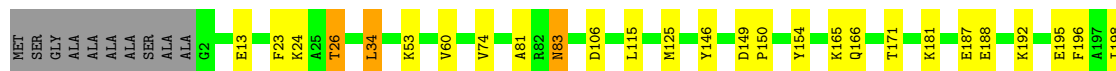
• Molecule 6: Probable proteasome subunit alpha type-7

Chain T: 66% 16% • 16%



• Molecule 7: Proteasome subunit alpha type-1

Chain G: 81% 13% • •



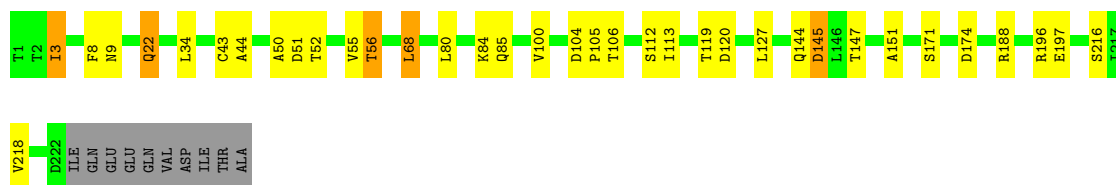
• Molecule 7: Proteasome subunit alpha type-1

Chain U:  80% 14% . .



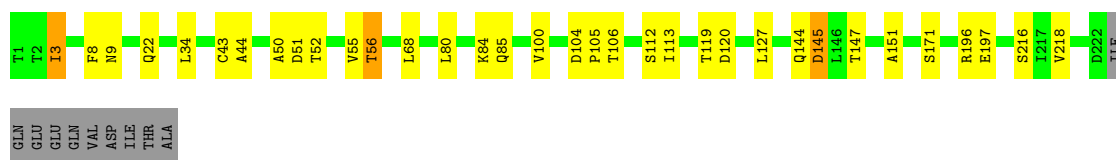
- Molecule 8: Proteasome subunit beta type-2

Chain H:  80% 13% . .



- Molecule 8: Proteasome subunit beta type-2

Chain V:  81% 13% . .



- Molecule 9: Proteasome subunit beta type-3

Chain I:  85% 13% .



- Molecule 9: Proteasome subunit beta type-3

Chain W:  85% 13% .

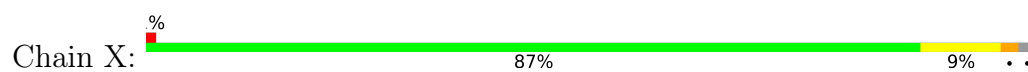


- Molecule 10: Proteasome subunit beta type-4

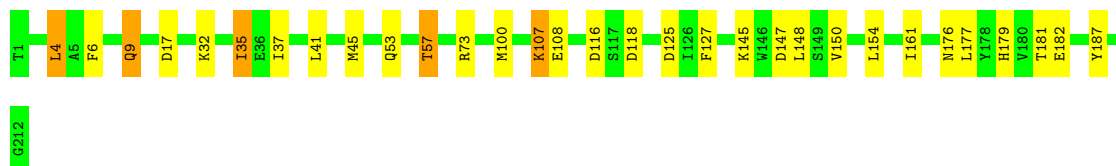
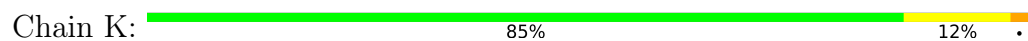
Chain J:  88% 8% . .



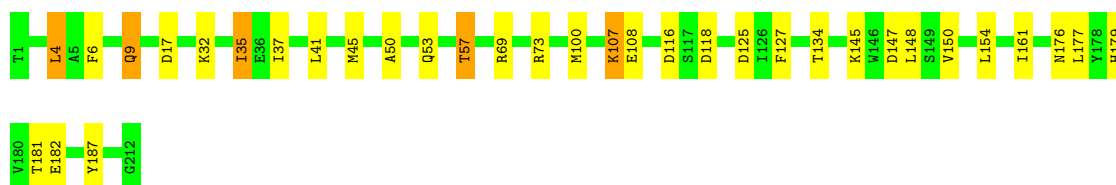
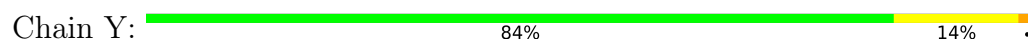
- Molecule 10: Proteasome subunit beta type-4



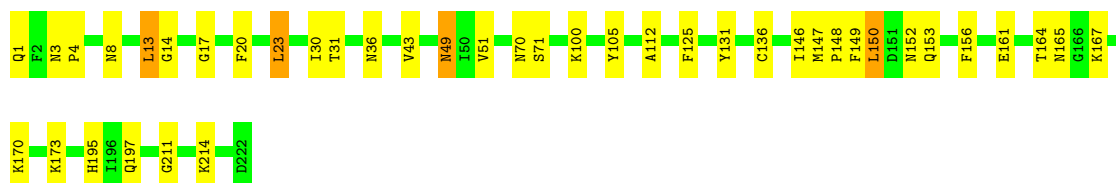
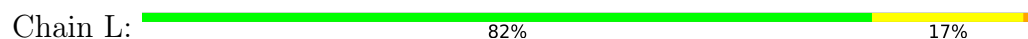
- Molecule 11: Proteasome subunit beta type-5



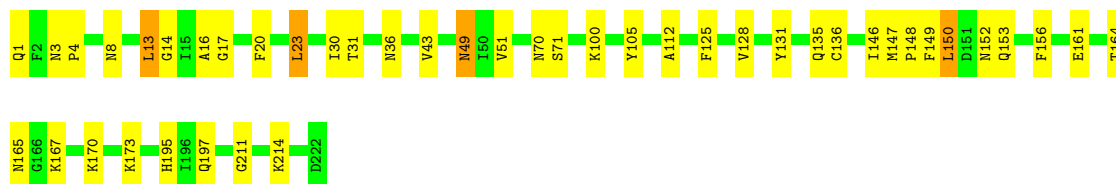
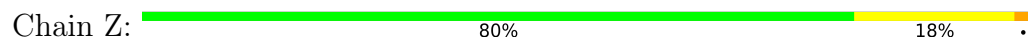
- Molecule 11: Proteasome subunit beta type-5



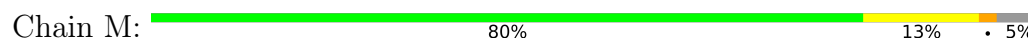
- Molecule 12: Proteasome subunit beta type-6

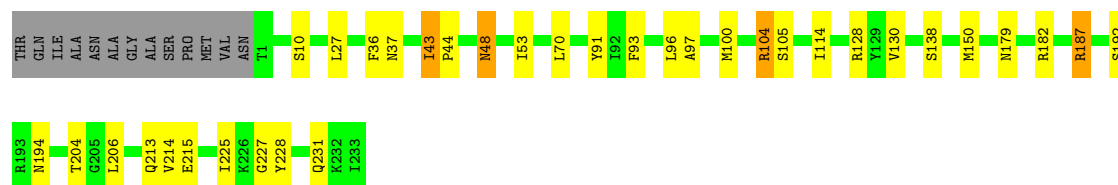


- Molecule 12: Proteasome subunit beta type-6



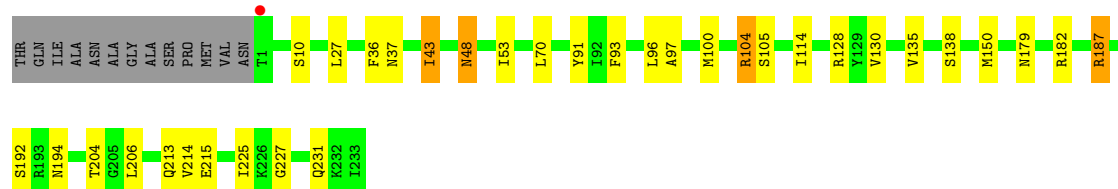
- Molecule 13: Proteasome subunit beta type-7





• Molecule 13: Proteasome subunit beta type-7

Chain a: 81% 12% 5%



• Molecule 14: Proteasome subunit beta type-1

Chain N: 88% 12% 0%



• Molecule 14: Proteasome subunit beta type-1

Chain b: 87% 12% 0%



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	134.45Å 299.75Å 144.52Å 90.00° 112.60° 90.00°	Depositor
Resolution (Å)	15.00 – 3.00 15.00 – 3.00	Depositor EDS
% Data completeness (in resolution range)	92.1 (15.00-3.00) 91.5 (15.00-3.00)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.98 (at 3.01Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.180 , 0.207 0.182 , 0.206	Depositor DCC
R_{free} test set	9609 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	59.2	Xtriage
Anisotropy	0.121	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 64.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	49661	wwPDB-VP
Average B, all atoms (Å ²)	59.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.61% 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: 2M1, MG

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.44	0/1952	0.80	0/2642
1	O	0.44	0/1952	0.80	0/2642
2	B	0.43	0/1934	0.81	0/2618
2	P	0.44	0/1934	0.81	0/2618
3	C	0.43	0/1910	0.82	0/2586
3	Q	0.43	0/1910	0.81	0/2586
4	D	0.43	0/1837	0.77	0/2475
4	R	0.43	0/1837	0.77	0/2475
5	E	0.41	0/1800	0.76	0/2433
5	S	0.41	0/1800	0.76	0/2433
6	F	0.42	0/1932	0.79	0/2609
6	T	0.42	0/1932	0.79	0/2609
7	G	0.43	0/1945	0.80	0/2634
7	U	0.43	0/1945	0.80	0/2634
8	H	0.43	0/1715	0.78	0/2326
8	V	0.43	0/1715	0.78	0/2326
9	I	0.42	0/1611	0.79	0/2174
9	W	0.42	0/1611	0.79	0/2174
10	J	0.40	0/1589	0.75	0/2142
10	X	0.40	0/1589	0.75	0/2142
11	K	0.42	0/1681	0.76	1/2274 (0.0%)
11	Y	0.42	0/1681	0.76	2/2274 (0.1%)
12	L	0.39	0/1795	0.75	0/2420
12	Z	0.40	0/1795	0.74	0/2420
13	M	0.41	0/1855	0.77	0/2514
13	a	0.41	0/1855	0.77	0/2514
14	N	0.39	0/1541	0.77	0/2087
14	b	0.39	0/1541	0.77	0/2087
All	All	0.42	0/50194	0.78	3/67868 (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
9	I	0	1
9	W	0	1
All	All	0	2

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	K	32	LYS	CA-CB-CG	-5.83	102.43	114.10
11	Y	32	LYS	CA-CB-CG	-5.58	102.95	114.10
11	Y	32	LYS	CG-CD-CE	-5.04	99.71	111.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
9	I	192	ASP	Peptide
9	W	192	ASP	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	1929	9	0
1	O	1915	0	1929	14	0
2	B	1904	0	1904	38	0
2	P	1904	0	1904	38	0
3	C	1881	0	1895	31	0
3	Q	1881	0	1895	28	0
4	D	1813	0	1797	19	0
4	R	1813	0	1797	21	0
5	E	1773	0	1775	23	0
5	S	1773	0	1775	23	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	F	1892	0	1883	21	0
6	T	1892	0	1883	24	0
7	G	1907	0	1901	18	0
7	U	1907	0	1901	20	0
8	H	1684	0	1688	16	0
8	V	1684	0	1688	13	0
9	I	1581	0	1574	15	0
9	W	1581	0	1574	17	0
10	J	1561	0	1569	10	0
10	X	1561	0	1569	13	0
11	K	1644	0	1594	15	0
11	Y	1644	0	1594	18	0
12	L	1757	0	1711	22	0
12	Z	1757	0	1711	26	0
13	M	1824	0	1832	18	0
13	a	1824	0	1832	17	0
14	N	1512	0	1481	12	0
14	b	1512	0	1481	14	0
15	G	1	0	0	0	0
15	H	1	0	0	0	0
15	I	1	0	0	0	0
15	K	1	0	0	0	0
15	N	1	0	0	0	0
15	V	1	0	0	0	0
15	Y	1	0	0	0	0
15	Z	1	0	0	0	0
16	K	38	0	46	0	0
16	Y	38	0	46	0	0
17	A	5	0	0	0	0
17	B	8	0	0	0	0
17	C	4	0	0	0	0
17	D	11	0	0	0	0
17	E	5	0	0	0	0
17	F	11	0	0	0	0
17	G	11	0	0	0	0
17	H	14	0	0	0	0
17	I	7	0	0	0	0
17	J	11	0	0	0	0
17	K	6	0	0	0	0
17	L	12	0	0	0	0
17	M	16	0	0	0	0
17	N	14	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
17	O	7	0	0	1	0
17	P	7	0	0	0	0
17	Q	8	0	0	0	0
17	R	7	0	0	0	0
17	S	8	0	0	0	0
17	T	9	0	0	0	0
17	U	10	0	0	0	0
17	V	14	0	0	0	0
17	W	11	0	0	0	0
17	X	14	0	0	0	0
17	Y	8	0	0	0	0
17	Z	19	0	0	0	0
17	a	13	0	0	0	0
17	b	11	0	0	0	0
All	All	49661	0	49158	498	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 (498) 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)
2:P:93:HIS:HB3	2:P:113:ARG:HH21	1.25	1.00
11:Y:100:MET:HE3	11:Y:127:PHE:HB2	1.43	0.99
11:K:100:MET:HE3	11:K:127:PHE:HB2	1.43	0.98
2:B:93:HIS:HB3	2:B:113:ARG:HH21	1.25	0.97
11:Y:100:MET:CE	11:Y:127:PHE:HB2	2.05	0.86
11:K:100:MET:CE	11:K:127:PHE:HB2	2.05	0.86
12:L:31:THR:HG23	12:L:36:ASN:HD21	1.43	0.82
12:Z:31:THR:HG23	12:Z:36:ASN:HD21	1.43	0.81
14:N:20:THR:HG22	14:N:31:THR:OG1	1.83	0.79
10:J:16:ALA:HB2	10:J:161:LEU:HD21	1.66	0.78
14:b:20:THR:HG22	14:b:31:THR:OG1	1.85	0.77
11:K:100:MET:HE3	11:K:127:PHE:CB	2.15	0.77
10:X:16:ALA:HB2	10:X:161:LEU:HD21	1.67	0.76
2:B:204:ALA:O	2:B:209:ARG:NH2	2.19	0.76
11:K:53:GLN:O	11:K:57:THR:HG23	1.85	0.76
2:P:204:ALA:O	2:P:209:ARG:NH2	2.19	0.76
11:Y:53:GLN:O	11:Y:57:THR:HG23	1.85	0.75
14:N:136:GLY:HA2	14:b:161:GLN:HE21	1.52	0.74
14:N:161:GLN:HE21	14:b:136:GLY:HA2	1.53	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:Y:100:MET:HE3	11:Y:127:PHE:CB	2.15	0.73
1:A:176:GLU:HG3	2:B:55:LEU:HD22	1.71	0.73
2:B:93:HIS:HB3	2:B:113:ARG:NH2	2.03	0.73
2:P:93:HIS:HB3	2:P:113:ARG:NH2	2.03	0.72
7:U:23:PHE:O	7:U:26:THR:HB	1.89	0.72
9:W:97:ARG:HG2	9:W:97:ARG:HH11	1.54	0.72
9:I:97:ARG:HH11	9:I:97:ARG:HG2	1.54	0.71
7:G:23:PHE:O	7:G:26:THR:HB	1.91	0.71
14:N:152:VAL:HA	14:N:175:MET:HE1	1.74	0.69
14:b:152:VAL:HA	14:b:175:MET:HE1	1.73	0.69
2:B:47:ALA:HB1	2:B:64:LYS:HD2	1.78	0.65
2:P:47:ALA:HB1	2:P:64:LYS:HD2	1.78	0.65
4:R:32:ILE:HD12	4:R:192:VAL:HG23	1.77	0.65
3:Q:51:LYS:O	3:Q:52:LEU:HB2	1.97	0.65
4:D:88:ALA:HA	4:D:99:ILE:HG21	1.79	0.64
4:D:32:ILE:HD12	4:D:192:VAL:HG23	1.78	0.64
4:R:88:ALA:HA	4:R:99:ILE:HG21	1.78	0.64
3:C:51:LYS:O	3:C:52:LEU:HB2	1.98	0.63
14:N:20:THR:CG2	14:N:31:THR:OG1	2.46	0.63
14:b:20:THR:CG2	14:b:31:THR:OG1	2.47	0.63
3:Q:51:LYS:HA	3:Q:51:LYS:HE3	1.83	0.61
8:H:113:ILE:HG12	8:H:119:THR:HG22	1.83	0.60
1:O:122:THR:HG22	2:P:128:ARG:HH21	1.66	0.60
3:C:51:LYS:HE3	3:C:51:LYS:HA	1.83	0.60
3:Q:160:GLN:HE21	3:Q:161:THR:H	1.50	0.60
12:Z:8:ASN:HA	12:Z:30:ILE:O	2.02	0.60
8:V:113:ILE:HG12	8:V:119:THR:HG22	1.83	0.60
3:C:160:GLN:HE21	3:C:161:THR:H	1.50	0.60
12:L:8:ASN:HA	12:L:30:ILE:O	2.02	0.59
5:S:92:ASN:HD21	12:Z:70:ASN:HD21	1.50	0.59
9:W:97:ARG:HG2	9:W:97:ARG:NH1	2.17	0.59
1:A:122:THR:HG22	2:B:128:ARG:HH21	1.68	0.59
2:P:15:GLU:O	3:Q:27:ARG:NH2	2.37	0.58
5:S:175:LEU:HA	5:S:178:PHE:CE2	2.39	0.58
2:B:217:LYS:HD3	2:B:222:GLY:HA2	1.85	0.58
8:V:104:ASP:OD1	8:V:106:THR:HB	2.03	0.58
2:P:217:LYS:HD3	2:P:222:GLY:HA2	1.86	0.58
14:N:13:ILE:HG21	14:N:175:MET:HE2	1.85	0.58
8:H:104:ASP:OD1	8:H:106:THR:HB	2.04	0.58
12:L:164:THR:O	12:L:165:ASN:HB3	2.04	0.58
5:E:175:LEU:HA	5:E:178:PHE:CE2	2.39	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:V:3:ILE:HG12	8:V:44:ALA:HB1	1.86	0.57
9:W:20:VAL:HG13	9:W:118:PRO:HB3	1.86	0.57
7:G:202:ILE:HG23	7:G:207:THR:O	2.04	0.57
3:C:201:VAL:O	3:C:202:GLN:HB2	2.05	0.57
9:I:20:VAL:HG13	9:I:118:PRO:HB3	1.86	0.57
3:Q:201:VAL:O	3:Q:202:GLN:HB2	2.03	0.57
12:Z:164:THR:O	12:Z:165:ASN:HB3	2.04	0.57
8:H:3:ILE:HG12	8:H:44:ALA:HB1	1.86	0.57
12:L:17:GLY:HA3	12:L:20:PHE:CE1	2.40	0.57
3:Q:160:GLN:HE21	3:Q:160:GLN:HA	1.70	0.57
12:Z:17:GLY:HA3	12:Z:20:PHE:CE1	2.40	0.57
14:b:13:ILE:HG21	14:b:175:MET:HE2	1.87	0.57
6:F:123:ASN:C	6:F:123:ASN:HD22	2.13	0.56
12:L:13:LEU:HD13	12:L:150:LEU:HD21	1.87	0.56
1:O:12:PHE:H	2:P:20:GLN:HE22	1.53	0.56
8:V:52:THR:O	8:V:56:THR:HB	2.06	0.56
11:K:35:ILE:HB	11:K:45:MET:HE3	1.88	0.56
6:T:33:SER:HB3	6:T:46:VAL:HG23	1.87	0.56
2:B:155:ASN:ND2	3:C:77:ASN:HB2	2.20	0.56
6:F:33:SER:HB3	6:F:46:VAL:HG23	1.87	0.56
12:Z:13:LEU:HD13	12:Z:150:LEU:HD21	1.88	0.56
3:C:160:GLN:HE21	3:C:160:GLN:HA	1.70	0.55
6:F:172:LEU:CD1	6:F:195:ILE:HD13	2.37	0.55
2:P:219:ALA:HB2	2:P:225:TYR:HB2	1.88	0.55
6:T:172:LEU:CD1	6:T:195:ILE:HD13	2.36	0.55
8:H:52:THR:O	8:H:56:THR:HB	2.06	0.55
10:J:1:MET:HA	10:J:34:LYS:HE3	1.89	0.55
5:E:9:THR:HG21	5:E:119:THR:HA	1.89	0.55
7:U:202:ILE:HG23	7:U:207:THR:O	2.07	0.55
6:T:123:ASN:C	6:T:123:ASN:HD22	2.15	0.55
3:C:201:VAL:HG13	3:C:202:GLN:N	2.23	0.54
3:Q:9:PHE:H	4:R:15:GLN:HE22	1.53	0.54
6:T:34:ILE:HG22	6:T:160:ALA:HB2	1.89	0.54
6:F:34:ILE:HG22	6:F:160:ALA:HB2	1.89	0.54
2:P:139:TYR:CD1	2:P:224:VAL:HG21	2.43	0.54
2:B:219:ALA:HB2	2:B:225:TYR:HB2	1.89	0.54
11:Y:35:ILE:HB	11:Y:45:MET:HE3	1.89	0.54
5:E:163:ARG:HD3	5:E:201:ARG:NH1	2.23	0.54
9:I:97:ARG:HG2	9:I:97:ARG:NH1	2.17	0.54
12:L:4:PRO:O	13:M:104:ARG:NH1	2.38	0.54
1:A:122:THR:CG2	2:B:128:ARG:HH21	2.20	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:71:LEU:HD12	3:C:133:ILE:HG12	1.90	0.53
2:B:139:TYR:CD1	2:B:224:VAL:HG21	2.43	0.53
4:R:30:ILE:HD12	4:R:196:LEU:HG	1.90	0.53
3:Q:201:VAL:HG13	3:Q:202:GLN:N	2.23	0.53
5:S:163:ARG:HD3	5:S:201:ARG:NH1	2.23	0.53
3:Q:71:LEU:HD12	3:Q:133:ILE:HG12	1.89	0.53
12:Z:146:ILE:HG22	12:Z:150:LEU:HD22	1.91	0.53
5:E:92:ASN:HD21	12:L:70:ASN:HD21	1.55	0.53
10:X:1:MET:HA	10:X:34:LYS:HE3	1.90	0.53
6:T:154:TRP:CZ3	7:U:60:VAL:HA	2.43	0.53
4:D:224:ASP:OD2	4:D:224:ASP:N	2.42	0.53
3:C:160:GLN:HE22	3:C:170:ARG:HE	1.56	0.53
12:L:161:GLU:HB3	12:L:164:THR:CG2	2.39	0.53
4:R:224:ASP:OD2	4:R:224:ASP:N	2.40	0.53
5:S:9:THR:HG21	5:S:119:THR:HA	1.90	0.53
4:D:30:ILE:HD12	4:D:196:LEU:HG	1.89	0.53
4:R:82:GLU:OE2	11:Y:69:ARG:NH1	2.42	0.52
1:O:122:THR:CG2	2:P:128:ARG:HH21	2.21	0.52
9:W:10:ILE:HG21	9:W:141:ALA:HB3	1.91	0.52
12:Z:3:ASN:HD22	12:Z:4:PRO:HD2	1.74	0.52
13:a:179:ASN:HD22	13:a:182:ARG:HH11	1.56	0.52
14:b:20:THR:HG23	14:b:28:ASN:HB3	1.90	0.52
9:I:10:ILE:HG21	9:I:141:ALA:HB3	1.91	0.52
12:L:3:ASN:HD22	12:L:4:PRO:HD2	1.74	0.52
12:L:146:ILE:HG22	12:L:150:LEU:HD22	1.91	0.52
13:M:179:ASN:HD22	13:M:182:ARG:HH11	1.56	0.52
3:Q:160:GLN:HE22	3:Q:170:ARG:HE	1.56	0.52
13:M:53:ILE:HG12	13:M:114:ILE:HG12	1.92	0.52
14:N:20:THR:HG23	14:N:28:ASN:HB3	1.90	0.52
12:L:161:GLU:HB3	12:L:164:THR:HG21	1.93	0.51
3:C:9:PHE:H	4:D:15:GLN:HE22	1.57	0.51
12:Z:161:GLU:HB3	12:Z:164:THR:CG2	2.39	0.51
12:Z:195:HIS:HD2	12:Z:197:GLN:H	1.58	0.51
9:W:27:ARG:HD3	9:W:179:LEU:O	2.10	0.51
12:Z:4:PRO:O	13:a:104:ARG:NH1	2.40	0.51
7:G:187:GLU:HG2	7:G:192:LYS:HB2	1.93	0.51
6:T:206:LYS:HE3	6:T:206:LYS:HA	1.92	0.51
12:Z:13:LEU:HD12	12:Z:14:GLY:N	2.26	0.51
12:Z:100:LYS:HD3	12:Z:105:TYR:CE2	2.46	0.51
12:Z:149:PHE:CE1	12:Z:153:GLN:HG3	2.45	0.51
3:C:35:LYS:HG2	3:C:158:SER:O	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:50:LYS:HE3	2:P:51:VAL:H	1.75	0.51
6:F:206:LYS:HE3	6:F:206:LYS:HA	1.92	0.51
1:O:149:GLN:O	1:O:156:TYR:HA	2.11	0.51
7:G:239:ILE:O	7:G:242:GLN:HB3	2.11	0.51
1:A:149:GLN:O	1:A:156:TYR:HA	2.10	0.50
7:G:188:GLU:OE2	7:G:188:GLU:HA	2.11	0.50
7:G:149:ASP:HB2	7:G:150:PRO:CD	2.42	0.50
12:L:100:LYS:HD3	12:L:105:TYR:CE2	2.46	0.50
7:U:187:GLU:HG2	7:U:192:LYS:HB2	1.93	0.50
9:W:98:ARG:O	9:W:126:ILE:HD11	2.12	0.50
2:B:50:LYS:HE3	2:B:51:VAL:H	1.76	0.50
2:B:86:LEU:HB3	2:B:114:LEU:HD21	1.93	0.50
7:G:34:LEU:C	7:G:34:LEU:HD23	2.37	0.50
12:L:195:HIS:HD2	12:L:197:GLN:H	1.59	0.50
14:N:136:GLY:HA2	14:b:161:GLN:NE2	2.24	0.50
5:E:70:GLY:HA3	5:E:221:PHE:CE2	2.46	0.50
12:L:149:PHE:CE1	12:L:153:GLN:HG3	2.47	0.50
2:P:86:LEU:HB3	2:P:114:LEU:HD21	1.93	0.50
3:Q:35:LYS:HG2	3:Q:158:SER:O	2.11	0.50
7:U:188:GLU:OE2	7:U:188:GLU:HA	2.11	0.50
2:P:151:ASN:HB2	2:P:152:PRO:HD2	1.94	0.50
5:S:70:GLY:HA3	5:S:221:PHE:CE2	2.46	0.50
7:U:239:ILE:O	7:U:242:GLN:HB3	2.11	0.50
9:I:27:ARG:HD3	9:I:179:LEU:O	2.12	0.50
7:U:149:ASP:HB2	7:U:150:PRO:CD	2.42	0.50
10:X:119:ILE:HA	10:X:124:THR:O	2.12	0.50
12:Z:161:GLU:HB3	12:Z:164:THR:HG21	1.93	0.50
14:N:161:GLN:NE2	14:b:136:GLY:HA2	2.26	0.50
2:P:183:MET:HE1	2:P:191:LEU:HD12	1.94	0.50
5:S:170:TYR:HB2	5:S:198:GLN:HG3	1.94	0.50
3:C:160:GLN:NE2	3:C:161:THR:H	2.10	0.49
3:Q:11:PRO:HA	4:R:18:TYR:CD1	2.47	0.49
3:Q:160:GLN:NE2	3:Q:161:THR:H	2.09	0.49
10:X:67:TYR:CE1	10:X:75:LEU:HD13	2.47	0.49
2:B:151:ASN:HB2	2:B:152:PRO:HD2	1.94	0.49
5:E:170:TYR:HB2	5:E:198:GLN:HG3	1.94	0.49
9:I:98:ARG:O	9:I:126:ILE:HD11	2.12	0.49
9:I:104:VAL:HG23	9:I:106:PRO:HD3	1.94	0.49
12:L:13:LEU:HD12	12:L:14:GLY:N	2.26	0.49
3:C:38:ASN:N	3:C:38:ASN:HD22	2.10	0.49
6:F:36:ILE:HD12	6:F:192:ALA:HB2	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:65:MET:HE1	9:I:93:SER:HB3	1.94	0.49
10:J:67:TYR:CE1	10:J:75:LEU:HD13	2.48	0.49
7:U:34:LEU:C	7:U:34:LEU:HD23	2.37	0.49
9:W:107:VAL:HG13	9:W:136:ILE:HG21	1.94	0.49
1:A:12:PHE:H	2:B:20:GLN:HE22	1.60	0.49
2:P:155:ASN:ND2	3:Q:77:ASN:HB2	2.28	0.49
2:P:227:LYS:NZ	2:P:233:GLU:OE2	2.46	0.49
2:B:8:ARG:HD2	3:C:4:ARG:CZ	2.43	0.48
4:D:159:TYR:CZ	4:D:162:LYS:HD3	2.48	0.48
10:J:119:ILE:HA	10:J:124:THR:O	2.12	0.48
3:Q:168:THR:O	3:Q:171:GLU:HB3	2.13	0.48
13:a:53:ILE:HG12	13:a:114:ILE:HG12	1.94	0.48
2:B:12:PHE:H	3:C:17:GLN:HE22	1.61	0.48
7:G:198:ILE:HG23	7:G:214:LEU:HD11	1.95	0.48
12:L:49:ASN:HD21	12:L:211:GLY:HA2	1.77	0.48
4:R:159:TYR:CZ	4:R:162:LYS:HD3	2.48	0.48
6:T:36:ILE:HD12	6:T:192:ALA:HB2	1.95	0.48
2:B:105:ILE:HD11	2:B:109:ILE:HG22	1.95	0.48
2:B:227:LYS:NZ	2:B:233:GLU:OE2	2.46	0.48
3:C:11:PRO:HA	4:D:18:TYR:CD1	2.49	0.48
2:P:105:ILE:HD11	2:P:109:ILE:HG22	1.96	0.48
8:H:50:ALA:CB	9:I:126:ILE:HG23	2.44	0.48
3:Q:38:ASN:N	3:Q:38:ASN:HD22	2.11	0.48
9:W:65:MET:HE1	9:W:93:SER:HB3	1.95	0.48
2:B:183:MET:HE1	2:B:191:LEU:HD12	1.94	0.48
8:V:51:ASP:O	8:V:55:VAL:HG12	2.14	0.48
8:V:104:ASP:HB2	8:V:105:PRO:HD2	1.96	0.48
12:Z:49:ASN:HD21	12:Z:211:GLY:HA2	1.77	0.48
9:W:104:VAL:HG23	9:W:106:PRO:HD3	1.94	0.48
13:a:182:ARG:HG3	13:a:214:VAL:CG1	2.44	0.48
5:E:12:PHE:H	6:F:19:GLN:HE22	1.61	0.48
11:K:6:PHE:HA	11:K:125:ASP:O	2.14	0.48
2:B:110:LEU:HD23	2:B:110:LEU:C	2.39	0.48
7:U:149:ASP:HB2	7:U:150:PRO:HD2	1.96	0.48
7:U:198:ILE:HG23	7:U:214:LEU:HD11	1.95	0.48
13:M:182:ARG:HG3	13:M:214:VAL:CG1	2.44	0.48
7:G:83:ASN:C	7:G:83:ASN:HD22	2.21	0.47
2:B:151:ASN:HB2	2:B:152:PRO:CD	2.44	0.47
8:H:104:ASP:HB2	8:H:105:PRO:HD2	1.95	0.47
2:P:89:THR:HG21	2:P:117:ILE:CD1	2.45	0.47
4:R:159:TYR:CE2	5:S:56:SER:HB3	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:89:THR:HG21	2:B:117:ILE:CD1	2.44	0.47
10:J:174:MET:HA	10:X:174:MET:HA	1.96	0.47
5:S:170:TYR:CD1	5:S:170:TYR:C	2.92	0.47
4:D:37:GLY:HA2	4:D:145:TYR:CE1	2.50	0.47
3:C:168:THR:O	3:C:171:GLU:HB3	2.14	0.47
2:B:8:ARG:HD2	3:C:4:ARG:NH2	2.30	0.47
2:B:58:GLN:HE22	2:B:231:PRO:HB3	1.80	0.47
4:R:67:GLY:HA3	4:R:220:PHE:CD1	2.50	0.47
11:Y:6:PHE:HA	11:Y:125:ASP:O	2.15	0.47
2:B:15:GLU:O	3:C:27:ARG:NH2	2.48	0.47
5:S:62:ILE:HG21	5:S:213:ALA:HB2	1.97	0.47
7:U:83:ASN:C	7:U:83:ASN:HD22	2.23	0.47
5:E:62:ILE:HG21	5:E:213:ALA:HB2	1.97	0.47
9:I:107:VAL:HG13	9:I:136:ILE:HG21	1.95	0.47
10:J:139:TYR:CE2	10:J:172:MET:HE2	2.50	0.47
4:R:78:ARG:HA	4:R:78:ARG:HD3	1.74	0.46
6:T:216:SER:HB3	6:T:219:GLU:HB2	1.97	0.46
8:V:80:LEU:HD12	8:V:113:ILE:HD11	1.97	0.46
4:D:67:GLY:HA3	4:D:220:PHE:CD1	2.50	0.46
2:P:110:LEU:C	2:P:110:LEU:HD23	2.40	0.46
2:P:151:ASN:HB2	2:P:152:PRO:CD	2.45	0.46
1:A:203:GLU:HB2	1:A:208:THR:HG21	1.97	0.46
3:C:51:LYS:HA	3:C:51:LYS:CE	2.44	0.46
6:F:216:SER:HB3	6:F:219:GLU:HB2	1.97	0.46
8:H:51:ASP:O	8:H:55:VAL:HG12	2.15	0.46
1:O:14:PRO:HA	2:P:23:TYR:CD1	2.51	0.46
3:Q:51:LYS:HA	3:Q:51:LYS:CE	2.45	0.46
5:S:68:HIS:HE1	5:S:102:LEU:O	1.99	0.46
4:D:71:SER:HB3	4:D:164:ILE:HD12	1.96	0.46
5:E:170:TYR:CD1	5:E:170:TYR:C	2.93	0.46
11:K:4:LEU:HD13	11:K:161:ILE:HD11	1.97	0.46
6:F:197:TYR:CD1	6:F:239:ALA:HB1	2.51	0.46
11:K:179:HIS:CE1	11:K:181:THR:CG2	2.99	0.46
4:R:37:GLY:HA2	4:R:145:TYR:CE1	2.50	0.46
7:G:149:ASP:HB2	7:G:150:PRO:HD2	1.96	0.46
1:O:203:GLU:HB2	1:O:208:THR:HG21	1.97	0.46
6:F:139:LYS:O	6:F:139:LYS:HG2	2.16	0.46
6:T:197:TYR:CD1	6:T:239:ALA:HB1	2.50	0.46
2:B:35:ILE:HD12	2:B:196:LEU:HG	1.98	0.46
11:Y:179:HIS:CE1	11:Y:181:THR:CG2	2.99	0.46
8:H:9:ASN:ND2	8:H:147:THR:HA	2.31	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:V:9:ASN:ND2	8:V:147:THR:HA	2.30	0.46
6:F:228:LYS:HB2	6:F:228:LYS:HE3	1.80	0.46
11:K:154:LEU:HD22	11:K:177:LEU:HD13	1.98	0.46
8:V:50:ALA:CB	9:W:126:ILE:HG23	2.46	0.46
5:E:186:ASP:OD2	5:E:231:LYS:HE2	2.16	0.45
4:R:71:SER:HB3	4:R:164:ILE:HD12	1.98	0.45
9:I:20:VAL:CG1	9:I:118:PRO:HB3	2.46	0.45
2:P:58:GLN:HE22	2:P:231:PRO:HB3	1.80	0.45
4:D:111:LEU:O	4:D:114:ARG:HB2	2.17	0.45
9:I:98:ARG:HD2	9:I:126:ILE:CG1	2.46	0.45
9:W:20:VAL:CG1	9:W:118:PRO:HB3	2.46	0.45
9:W:98:ARG:HD2	9:W:126:ILE:CG1	2.46	0.45
12:Z:23:LEU:HD13	12:Z:43:VAL:HG13	1.98	0.45
2:P:35:ILE:HD12	2:P:196:LEU:HG	1.99	0.45
10:X:139:TYR:CE2	10:X:172:MET:HE2	2.52	0.45
11:Y:37:ILE:HB	11:Y:41:LEU:HB3	1.99	0.45
13:a:97:ALA:HA	13:a:130:VAL:HG21	1.98	0.45
13:M:97:ALA:HA	13:M:130:VAL:HG21	1.99	0.45
2:P:95:GLN:HB3	9:W:68:TYR:CD2	2.52	0.45
5:E:68:HIS:HE1	5:E:102:LEU:O	1.99	0.45
6:F:154:TRP:CZ3	7:G:60:VAL:HA	2.52	0.45
11:K:37:ILE:HB	11:K:41:LEU:HB3	1.98	0.45
8:V:144:GLN:O	8:V:145:ASP:HB2	2.17	0.45
3:C:165:ASN:HB2	3:C:200:VAL:HG11	1.99	0.45
5:E:197:SER:HA	5:E:200:LEU:HD12	1.99	0.45
8:H:80:LEU:HD12	8:H:113:ILE:HD11	1.98	0.45
8:H:84:LYS:HG3	8:H:85:GLN:N	2.32	0.45
4:R:160:ASN:HB3	4:R:179:TRP:CE2	2.52	0.45
5:E:178:PHE:HA	5:E:181:ILE:HG13	1.99	0.45
12:L:23:LEU:HD13	12:L:43:VAL:HG13	1.98	0.45
4:D:160:ASN:HB3	4:D:179:TRP:CE2	2.52	0.45
2:P:73:ALA:HB2	2:P:226:GLN:NE2	2.32	0.45
7:U:83:ASN:C	7:U:83:ASN:ND2	2.75	0.45
11:Y:4:LEU:HD13	11:Y:161:ILE:HD11	1.98	0.45
11:Y:107:LYS:HE2	11:Y:108:GLU:HG2	1.99	0.44
13:a:194:ASN:ND2	13:a:213:GLN:HG2	2.32	0.44
3:C:161:THR:HG21	3:C:169:VAL:HG22	1.99	0.44
7:U:223:LYS:HB2	7:U:223:LYS:HE3	1.82	0.44
4:D:78:ARG:HA	4:D:78:ARG:HD3	1.74	0.44
13:M:194:ASN:ND2	13:M:213:GLN:HG2	2.33	0.44
3:C:198:LEU:HA	3:C:201:VAL:HG12	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:125:PHE:CD2	12:L:131:TYR:HB3	2.53	0.44
5:S:197:SER:HA	5:S:200:LEU:HD12	1.99	0.44
6:F:146:MET:CE	6:F:161:THR:HB	2.48	0.44
7:G:83:ASN:C	7:G:83:ASN:ND2	2.75	0.44
12:Z:51:VAL:HG23	12:Z:112:ALA:HB3	2.00	0.44
12:L:51:VAL:HG23	12:L:112:ALA:HB3	1.99	0.44
6:T:139:LYS:O	6:T:139:LYS:HG2	2.17	0.44
7:U:195:GLU:HG3	7:U:235:ARG:HG3	2.00	0.44
11:Y:107:LYS:HG3	11:Y:108:GLU:HG3	2.00	0.44
11:Y:154:LEU:HD22	11:Y:177:LEU:HD13	2.00	0.44
11:K:107:LYS:HG3	11:K:108:GLU:HG3	2.00	0.44
4:R:111:LEU:O	4:R:114:ARG:HB2	2.18	0.44
5:S:186:ASP:OD2	5:S:231:LYS:HE2	2.17	0.44
3:C:48:SER:C	3:C:50:LEU:H	2.26	0.44
7:G:195:GLU:HG3	7:G:235:ARG:HG3	2.00	0.44
7:G:223:LYS:HB2	7:G:223:LYS:HE3	1.82	0.44
3:Q:96:LEU:HD11	10:X:58:GLU:HB3	2.00	0.44
3:Q:198:LEU:HA	3:Q:201:VAL:HG12	2.00	0.44
4:R:191:LEU:O	4:R:195:ILE:HG13	2.18	0.44
13:a:96:LEU:O	13:a:100:MET:HG2	2.17	0.44
3:C:203:THR:C	3:C:205:ALA:H	2.26	0.43
11:K:176:ASN:ND2	11:K:187:TYR:OH	2.51	0.43
3:Q:165:ASN:HB2	3:Q:200:VAL:HG11	2.00	0.43
2:B:73:ALA:HB2	2:B:226:GLN:NE2	2.33	0.43
8:H:144:GLN:O	8:H:145:ASP:HB2	2.17	0.43
6:T:146:MET:CE	6:T:161:THR:HB	2.48	0.43
12:Z:125:PHE:CD2	12:Z:131:TYR:HB3	2.53	0.43
2:B:58:GLN:NE2	2:B:231:PRO:HB3	2.33	0.43
3:Q:161:THR:HG21	3:Q:169:VAL:HG22	2.00	0.43
3:Q:205:ALA:C	3:Q:207:ASN:H	2.25	0.43
5:S:178:PHE:HA	5:S:181:ILE:HG13	1.99	0.43
8:V:8:PHE:HB3	8:V:151:ALA:HB2	2.01	0.43
8:V:84:LYS:HG3	8:V:85:GLN:N	2.32	0.43
3:Q:48:SER:C	3:Q:50:LEU:H	2.26	0.43
12:Z:156:PHE:CG	12:Z:170:LYS:HD3	2.53	0.43
3:C:205:ALA:C	3:C:207:ASN:H	2.26	0.43
4:D:191:LEU:O	4:D:195:ILE:HG13	2.18	0.43
6:T:34:ILE:HG22	6:T:160:ALA:CB	2.48	0.43
2:B:111:VAL:HG22	2:B:136:TYR:CG	2.54	0.43
4:D:159:TYR:CE2	5:E:56:SER:HB3	2.53	0.43
11:K:107:LYS:HE2	11:K:108:GLU:HG2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:27:LEU:HB2	13:M:192:SER:HB3	2.00	0.43
9:I:163:PHE:CE1	9:I:197:ARG:HD2	2.53	0.43
9:W:163:PHE:CE1	9:W:197:ARG:HD2	2.54	0.43
3:C:51:LYS:HE3	3:C:52:LEU:H	1.84	0.43
2:P:58:GLN:NE2	2:P:231:PRO:HB3	2.34	0.43
4:D:42:VAL:HG22	4:D:59:ILE:HD11	2.01	0.43
5:E:98:PHE:O	13:M:91:TYR:HA	2.18	0.43
7:G:106:ASP:HB3	7:G:146:TYR:CZ	2.54	0.43
2:P:111:VAL:HG22	2:P:136:TYR:CG	2.54	0.43
5:S:112:CYS:SG	6:T:82:ARG:HD3	2.59	0.43
11:Y:145:LYS:HB2	11:Y:148:LEU:HD13	2.01	0.43
12:Z:152:ASN:O	12:Z:156:PHE:HA	2.19	0.43
2:B:52:THR:HG23	2:B:53:SER:O	2.19	0.42
8:H:8:PHE:HB3	8:H:151:ALA:HB2	2.00	0.42
10:J:36:ARG:HA	10:J:36:ARG:HD3	1.82	0.42
12:Z:147:MET:N	12:Z:148:PRO:HD2	2.34	0.42
14:b:35:THR:HG21	14:b:45:ARG:HE	1.84	0.42
5:E:134:ILE:HD12	5:E:215:VAL:HG12	2.01	0.42
6:F:153:TYR:CD1	6:F:153:TYR:C	2.97	0.42
10:J:173:PRO:HB3	10:X:22:THR:HG21	2.01	0.42
12:L:152:ASN:O	12:L:156:PHE:HA	2.19	0.42
13:a:27:LEU:HD12	13:a:36:PHE:O	2.19	0.42
11:K:145:LYS:HB2	11:K:148:LEU:HD13	2.01	0.42
1:O:176:GLU:HG3	2:P:55:LEU:HD22	2.01	0.42
2:P:58:GLN:NE2	2:P:208:ASP:HA	2.35	0.42
3:Q:203:THR:C	3:Q:205:ALA:H	2.27	0.42
4:R:178:GLU:HB2	4:R:191:LEU:HD21	2.01	0.42
10:X:25:ILE:HD11	11:Y:134:THR:HG21	2.00	0.42
2:B:89:THR:HG21	2:B:117:ILE:HD13	2.02	0.42
6:F:123:ASN:C	6:F:123:ASN:ND2	2.76	0.42
2:P:18:LEU:O	2:P:19:TYR:C	2.63	0.42
1:A:247:LEU:O	1:A:250:LEU:HB2	2.19	0.42
10:J:1:MET:HA	10:J:34:LYS:CE	2.49	0.42
1:O:247:LEU:O	1:O:250:LEU:HB2	2.19	0.42
10:X:1:MET:HA	10:X:34:LYS:CE	2.50	0.42
6:F:34:ILE:HG22	6:F:160:ALA:CB	2.48	0.42
12:L:147:MET:N	12:L:148:PRO:HD2	2.34	0.42
2:P:221:ASP:O	2:P:223:GLU:N	2.53	0.42
3:Q:51:LYS:HE3	3:Q:52:LEU:H	1.85	0.42
6:T:105:ILE:HG21	6:T:143:HIS:HB2	2.01	0.42
6:T:123:ASN:C	6:T:123:ASN:ND2	2.77	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:160:GLN:HE21	3:C:160:GLN:CA	2.33	0.42
6:F:172:LEU:HD12	6:F:195:ILE:HD13	2.01	0.42
7:G:74:VAL:HG11	7:G:81:ALA:CB	2.50	0.42
9:I:36:SER:HB2	10:J:126:VAL:HG11	2.01	0.42
1:O:142:PHE:CE2	9:W:114:LYS:HD3	2.55	0.42
4:R:42:VAL:HG22	4:R:59:ILE:HD11	2.01	0.42
10:X:162:LYS:HE2	10:X:162:LYS:HB3	1.87	0.42
11:Y:176:ASN:ND2	11:Y:187:TYR:OH	2.52	0.42
13:M:27:LEU:HD12	13:M:36:PHE:O	2.20	0.42
13:M:48:ASN:H	13:M:48:ASN:HD22	1.66	0.42
2:P:52:THR:HG23	2:P:53:SER:O	2.18	0.42
5:S:153:THR:HG21	6:T:55:LEU:CD2	2.49	0.42
6:T:155:GLY:HA3	7:U:59:THR:HG21	2.02	0.42
13:a:27:LEU:HB2	13:a:192:SER:HB3	2.01	0.42
13:a:43:ILE:HD11	13:a:53:ILE:HD12	2.01	0.42
5:S:45:LEU:HB2	5:S:213:ALA:HB3	2.02	0.42
5:S:136:TYR:CE1	5:S:217:LYS:HA	2.55	0.42
9:W:97:ARG:HH11	9:W:97:ARG:CG	2.30	0.42
13:M:96:LEU:O	13:M:100:MET:HG2	2.20	0.42
6:T:41:GLY:HA3	6:T:215:CYS:O	2.20	0.42
11:Y:116:ASP:OD1	11:Y:116:ASP:C	2.63	0.42
12:Z:164:THR:O	12:Z:165:ASN:CB	2.68	0.42
3:C:91:ALA:O	3:C:95:ARG:HG3	2.20	0.41
4:D:178:GLU:HB2	4:D:191:LEU:HD21	2.01	0.41
6:F:105:ILE:N	6:F:106:PRO:CD	2.83	0.41
12:L:156:PHE:CG	12:L:170:LYS:HD3	2.54	0.41
5:S:207:VAL:HG22	5:S:226:GLY:O	2.20	0.41
6:T:172:LEU:HD12	6:T:195:ILE:HD13	2.00	0.41
8:V:112:SER:OG	8:V:120:ASP:HB2	2.19	0.41
10:X:36:ARG:HD3	10:X:36:ARG:HA	1.83	0.41
2:B:221:ASP:O	2:B:223:GLU:N	2.53	0.41
5:E:78:PRO:O	5:E:81:ARG:HB3	2.20	0.41
5:E:136:TYR:CE1	5:E:217:LYS:HA	2.55	0.41
13:M:43:ILE:HD11	13:M:53:ILE:HD12	2.02	0.41
6:T:105:ILE:N	6:T:106:PRO:CD	2.83	0.41
6:F:105:ILE:HG21	6:F:143:HIS:HB2	2.01	0.41
11:K:116:ASP:OD1	11:K:116:ASP:C	2.63	0.41
2:B:102:ASN:ND2	9:I:67:ARG:HH12	2.18	0.41
2:B:180:LYS:O	2:B:183:MET:HB2	2.20	0.41
3:C:223:SER:OG	3:C:226:GLU:HG3	2.20	0.41
7:G:187:GLU:CG	7:G:192:LYS:HB2	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:90:ARG:HD3	8:H:68:LEU:HD23	2.02	0.41
13:M:93:PHE:CE2	13:M:128:ARG:HD3	2.56	0.41
1:O:37:ILE:HG23	1:O:161:ALA:HB2	2.02	0.41
7:U:106:ASP:HB3	7:U:146:TYR:CZ	2.55	0.41
7:U:196:PHE:CD1	7:U:196:PHE:C	2.97	0.41
9:W:36:SER:HB2	10:X:126:VAL:HG11	2.02	0.41
8:H:174:ASP:OD2	8:H:188:ARG:NH1	2.52	0.41
13:M:227:GLY:HA3	13:M:231:GLN:HB3	2.02	0.41
14:N:8:PHE:HB2	14:N:146:MET:O	2.21	0.41
1:O:21:ILE:HG21	1:O:153:SER:HB3	2.02	0.41
2:P:8:ARG:HD2	3:Q:4:ARG:NH2	2.36	0.41
11:Y:50:ALA:CB	12:Z:128:VAL:HG23	2.51	0.41
12:Z:16:ALA:O	12:Z:135:GLN:NE2	2.52	0.41
13:a:48:ASN:H	13:a:48:ASN:HD22	1.67	0.41
13:a:93:PHE:CE2	13:a:128:ARG:HD3	2.56	0.41
14:b:8:PHE:HB2	14:b:146:MET:O	2.20	0.41
14:b:103:ASP:HB3	14:b:106:ASN:H	1.86	0.41
5:E:207:VAL:HG22	5:E:226:GLY:O	2.20	0.41
14:N:67:THR:HA	14:N:71:GLY:O	2.21	0.41
4:R:9:PRO:HA	5:S:23:TYR:CG	2.56	0.41
5:S:78:PRO:O	5:S:81:ARG:HB3	2.21	0.41
5:S:134:ILE:HD12	5:S:215:VAL:HG12	2.01	0.41
2:B:58:GLN:NE2	2:B:208:ASP:HA	2.35	0.41
5:E:45:LEU:HB2	5:E:213:ALA:HB3	2.03	0.41
6:F:41:GLY:HA3	6:F:215:CYS:O	2.21	0.41
14:N:156:LYS:HE2	14:N:188:PHE:CD1	2.56	0.41
3:Q:223:SER:OG	3:Q:226:GLU:HG3	2.20	0.41
7:U:74:VAL:HG11	7:U:81:ALA:CB	2.50	0.41
13:a:130:VAL:HA	13:a:135:VAL:O	2.21	0.41
13:a:227:GLY:HA3	13:a:231:GLN:HB3	2.02	0.41
1:A:37:ILE:HG23	1:A:161:ALA:HB2	2.02	0.41
6:F:123:ASN:HD22	6:F:124:SER:N	2.19	0.41
7:G:196:PHE:CD1	7:G:196:PHE:C	2.98	0.41
8:H:22:GLN:HE21	8:H:22:GLN:HB2	1.72	0.41
13:M:43:ILE:HA	13:M:44:PRO:HD3	1.84	0.41
1:O:108:LYS:HG2	17:O:301:HOH:O	2.21	0.41
2:P:50:LYS:O	2:P:52:THR:N	2.54	0.41
2:P:59:ASP:HB3	2:P:231:PRO:HG2	2.03	0.41
2:P:93:HIS:CG	2:P:113:ARG:HE	2.39	0.41
4:R:1:ASP:O	4:R:2:ARG:CB	2.69	0.41
7:U:190:TRP:O	7:U:194:VAL:HG23	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:a:104:ARG:HG3	13:a:105:SER:N	2.36	0.41
5:E:180:LYS:HB2	5:E:180:LYS:HE3	1.92	0.41
13:M:150:MET:HE1	13:M:187:ARG:HG2	2.03	0.41
4:R:104:LEU:C	4:R:104:LEU:HD13	2.46	0.41
6:T:123:ASN:HD22	6:T:124:SER:N	2.19	0.41
3:C:45:GLU:HG3	3:C:201:VAL:HG23	2.04	0.40
13:M:104:ARG:HG3	13:M:105:SER:N	2.35	0.40
4:D:1:ASP:O	4:D:2:ARG:CB	2.69	0.40
5:E:197:SER:C	5:E:199:SER:H	2.29	0.40
5:S:98:PHE:O	13:a:91:TYR:HA	2.20	0.40
5:S:104:VAL:HG12	5:S:144:LEU:HD22	2.03	0.40
13:M:228:TYR:HE2	14:b:35:THR:HG21	1.87	0.40
2:P:89:THR:HG21	2:P:117:ILE:HD13	2.02	0.40
12:Z:147:MET:N	12:Z:148:PRO:CD	2.85	0.40
14:b:156:LYS:HE2	14:b:188:PHE:CD1	2.56	0.40
8:H:112:SER:OG	8:H:120:ASP:HB2	2.21	0.40
2:B:18:LEU:O	2:B:19:TYR:C	2.62	0.40
2:B:50:LYS:O	2:B:52:THR:N	2.54	0.40
4:D:193:LEU:HD22	4:D:211:LEU:HD11	2.04	0.40
5:E:197:SER:HA	5:E:200:LEU:CD1	2.52	0.40
1:O:47:THR:HG21	1:O:63:LYS:HE2	2.04	0.40
1:O:115:ALA:HB1	1:O:154:GLY:O	2.21	0.40
3:Q:45:GLU:HG3	3:Q:201:VAL:HG23	2.03	0.40
6:T:50:ILE:HD11	6:T:209:GLU:HB2	2.04	0.40
6:T:87:ARG:HG2	6:T:115:TYR:CD1	2.57	0.40
6:T:153:TYR:CD1	6:T:153:TYR:C	2.99	0.40
7:U:187:GLU:CG	7:U:192:LYS:HB2	2.51	0.40
13:a:150:MET:HE1	13:a:187:ARG:HG2	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%)	236 (95%)	11 (4%)	1 (0%)	30	65
1	O	248/250 (99%)	236 (95%)	11 (4%)	1 (0%)	30	65
2	B	242/258 (94%)	226 (93%)	11 (4%)	5 (2%)	5	27
2	P	242/258 (94%)	226 (93%)	11 (4%)	5 (2%)	5	27
3	C	238/254 (94%)	224 (94%)	8 (3%)	6 (2%)	4	23
3	Q	238/254 (94%)	224 (94%)	8 (3%)	6 (2%)	4	23
4	D	231/260 (89%)	225 (97%)	4 (2%)	2 (1%)	14	48
4	R	231/260 (89%)	225 (97%)	4 (2%)	2 (1%)	14	48
5	E	229/234 (98%)	210 (92%)	17 (7%)	2 (1%)	14	48
5	S	229/234 (98%)	210 (92%)	17 (7%)	2 (1%)	14	48
6	F	241/288 (84%)	230 (95%)	11 (5%)	0	100	100
6	T	241/288 (84%)	230 (95%)	11 (5%)	0	100	100
7	G	239/252 (95%)	231 (97%)	8 (3%)	0	100	100
7	U	239/252 (95%)	231 (97%)	8 (3%)	0	100	100
8	H	220/232 (95%)	208 (94%)	10 (4%)	2 (1%)	14	48
8	V	220/232 (95%)	208 (94%)	10 (4%)	2 (1%)	14	48
9	I	202/205 (98%)	196 (97%)	6 (3%)	0	100	100
9	W	202/205 (98%)	196 (97%)	6 (3%)	0	100	100
10	J	193/198 (98%)	188 (97%)	3 (2%)	2 (1%)	12	45
10	X	193/198 (98%)	188 (97%)	3 (2%)	2 (1%)	12	45
11	K	210/212 (99%)	203 (97%)	6 (3%)	1 (0%)	24	60
11	Y	210/212 (99%)	203 (97%)	6 (3%)	1 (0%)	24	60
12	L	220/222 (99%)	209 (95%)	11 (5%)	0	100	100
12	Z	220/222 (99%)	211 (96%)	9 (4%)	0	100	100
13	M	231/246 (94%)	219 (95%)	12 (5%)	0	100	100
13	a	231/246 (94%)	219 (95%)	12 (5%)	0	100	100
14	N	194/196 (99%)	187 (96%)	7 (4%)	0	100	100
14	b	194/196 (99%)	187 (96%)	7 (4%)	0	100	100
All	All	6276/6614 (95%)	5986 (95%)	248 (4%)	42 (1%)	18	53

All (42) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	2	THR
2	B	51	VAL
2	B	52	THR
2	B	183	MET
3	C	202	GLN
3	C	205	ALA
4	D	2	ARG
1	O	2	THR
2	P	51	VAL
2	P	52	THR
2	P	183	MET
3	Q	202	GLN
3	Q	205	ALA
4	R	2	ARG
2	B	222	GLY
4	D	114	ARG
5	E	231	LYS
10	J	2	ASP
2	P	222	GLY
4	R	114	ARG
5	S	231	LYS
10	X	2	ASP
3	C	49	THR
3	Q	49	THR
8	H	145	ASP
8	H	171	SER
11	K	9	GLN
8	V	145	ASP
8	V	171	SER
11	Y	9	GLN
2	B	221	ASP
3	C	183	PRO
2	P	221	ASP
3	Q	183	PRO
3	Q	206	LYS
3	C	206	LYS
3	C	201	VAL
3	Q	201	VAL
10	J	9	VAL
10	X	9	VAL
5	E	185	PRO
5	S	185	PRO

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%)	192 (92%)	17 (8%)	11	38
1	O	209/209 (100%)	192 (92%)	17 (8%)	11	38
2	B	203/216 (94%)	182 (90%)	21 (10%)	7	28
2	P	203/216 (94%)	182 (90%)	21 (10%)	7	28
3	C	212/226 (94%)	192 (91%)	20 (9%)	8	32
3	Q	212/226 (94%)	192 (91%)	20 (9%)	8	32
4	D	194/215 (90%)	172 (89%)	22 (11%)	5	24
4	R	194/215 (90%)	172 (89%)	22 (11%)	5	24
5	E	190/193 (98%)	172 (90%)	18 (10%)	8	31
5	S	190/193 (98%)	172 (90%)	18 (10%)	8	31
6	F	201/239 (84%)	176 (88%)	25 (12%)	4	20
6	T	201/239 (84%)	176 (88%)	25 (12%)	4	20
7	G	206/210 (98%)	188 (91%)	18 (9%)	9	35
7	U	206/210 (98%)	188 (91%)	18 (9%)	9	35
8	H	181/190 (95%)	169 (93%)	12 (7%)	15	46
8	V	181/190 (95%)	169 (93%)	12 (7%)	15	46
9	I	172/173 (99%)	160 (93%)	12 (7%)	14	44
9	W	172/173 (99%)	160 (93%)	12 (7%)	14	44
10	J	173/175 (99%)	165 (95%)	8 (5%)	24	58
10	X	173/175 (99%)	166 (96%)	7 (4%)	28	62
11	K	169/169 (100%)	158 (94%)	11 (6%)	15	47
11	Y	169/169 (100%)	158 (94%)	11 (6%)	15	47
12	L	185/185 (100%)	175 (95%)	10 (5%)	20	53
12	Z	185/185 (100%)	175 (95%)	10 (5%)	20	53
13	M	199/208 (96%)	187 (94%)	12 (6%)	17	50
13	a	199/208 (96%)	187 (94%)	12 (6%)	17	50

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
14	N	162/162 (100%)	151 (93%)	11 (7%)	14	45
14	b	162/162 (100%)	151 (93%)	11 (7%)	14	45
All	All	5312/5540 (96%)	4879 (92%)	433 (8%)	10	37

All (433) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	THR
1	A	3	ASP
1	A	17	LYS
1	A	29	LYS
1	A	52	SER
1	A	61	LEU
1	A	109	LEU
1	A	122	THR
1	A	124	SER
1	A	157	PHE
1	A	169	VAL
1	A	173	THR
1	A	176	GLU
1	A	178	ARG
1	A	231	LYS
1	A	246	ARG
1	A	250	LEU
2	B	40	SER
2	B	50	LYS
2	B	52	THR
2	B	54	THR
2	B	55	LEU
2	B	56	LEU
2	B	58	GLN
2	B	62	THR
2	B	65	LEU
2	B	79	LEU
2	B	102	ASN
2	B	114	LEU
2	B	180	LYS
2	B	184	LYS
2	B	191	LEU
2	B	194	LYS
2	B	209	ARG

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Mol	Chain	Res	Type
2	B	221	ASP
2	B	237	ILE
2	B	239	VAL
2	B	244	THR
3	C	4	ARG
3	C	22	LEU
3	C	37	LYS
3	C	38	ASN
3	C	51	LYS
3	C	52	LEU
3	C	61	LYS
3	C	107	LEU
3	C	124	VAL
3	C	147	GLN
3	C	160	GLN
3	C	169	VAL
3	C	175	LYS
3	C	180	LYS
3	C	187	GLU
3	C	191	LYS
3	C	203	THR
3	C	213	VAL
3	C	239	GLN
3	C	240	GLU
4	D	1	ASP
4	D	12	ARG
4	D	20	LEU
4	D	40	LEU
4	D	48	SER
4	D	51	LEU
4	D	64	ARG
4	D	99	ILE
4	D	102	GLU
4	D	114	ARG
4	D	117	GLU
4	D	176	LEU
4	D	182	SER
4	D	190	LEU
4	D	193	LEU
4	D	197	LYS
4	D	202	GLU
4	D	214	ILE

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Mol	Chain	Res	Type
4	D	224	ASP
4	D	235	LEU
4	D	236	LYS
4	D	242	GLU
5	E	9	THR
5	E	10	VAL
5	E	25	LEU
5	E	29	LYS
5	E	54	GLU
5	E	55	LEU
5	E	60	LYS
5	E	61	LYS
5	E	62	ILE
5	E	71	LEU
5	E	76	LEU
5	E	87	LEU
5	E	144	LEU
5	E	174	THR
5	E	188	LEU
5	E	207	VAL
5	E	211	SER
5	E	231	LYS
6	F	50	ILE
6	F	51	THR
6	F	59	LYS
6	F	61	VAL
6	F	68	ARG
6	F	94	SER
6	F	96	LYS
6	F	123	ASN
6	F	137	VAL
6	F	139	LYS
6	F	148	GLU
6	F	165	ARG
6	F	167	SER
6	F	172	LEU
6	F	174	LYS
6	F	181	GLU
6	F	186	ARG
6	F	187	GLU
6	F	203	ASN
6	F	206	LYS

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Mol	Chain	Res	Type
6	F	221	ASN
6	F	228	LYS
6	F	241	LYS
6	F	242	GLU
6	F	243	ILE
7	G	13	GLU
7	G	24	LYS
7	G	26	THR
7	G	34	LEU
7	G	53	LYS
7	G	83	ASN
7	G	115	LEU
7	G	125	MET
7	G	154	TYR
7	G	165	LYS
7	G	166	GLN
7	G	171	THR
7	G	181	LYS
7	G	201	MET
7	G	230	GLU
7	G	235	ARG
7	G	236	LEU
7	G	239	ILE
8	H	3	ILE
8	H	22	GLN
8	H	34	LEU
8	H	43	CYS
8	H	56	THR
8	H	68	LEU
8	H	100	VAL
8	H	127	LEU
8	H	196	ARG
8	H	197	GLU
8	H	216	SER
8	H	218	VAL
9	I	37	ASN
9	I	97	ARG
9	I	126	ILE
9	I	130	ASP
9	I	133	LYS
9	I	151	SER
9	I	159	PRO

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Mol	Chain	Res	Type
9	I	171	LEU
9	I	182	TRP
9	I	191	LYS
9	I	192	ASP
9	I	202	ARG
10	J	2	ASP
10	J	23	ARG
10	J	35	THR
10	J	36	ARG
10	J	69	ILE
10	J	75	LEU
10	J	144	LEU
10	J	174	MET
11	K	4	LEU
11	K	9	GLN
11	K	17	ASP
11	K	35	ILE
11	K	57	THR
11	K	73	ARG
11	K	107	LYS
11	K	118	ASP
11	K	147	ASP
11	K	150	VAL
11	K	182	GLU
12	L	1	GLN
12	L	13	LEU
12	L	23	LEU
12	L	49	ASN
12	L	71	SER
12	L	136	CYS
12	L	150	LEU
12	L	167	LYS
12	L	173	LYS
12	L	214	LYS
13	M	10	SER
13	M	37	ASN
13	M	43	ILE
13	M	48	ASN
13	M	70	LEU
13	M	104	ARG
13	M	138	SER
13	M	187	ARG

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Mol	Chain	Res	Type
13	M	204	THR
13	M	206	LEU
13	M	215	GLU
13	M	225	ILE
14	N	9	LYS
14	N	20	THR
14	N	22	THR
14	N	68	SER
14	N	103	ASP
14	N	104	ASP
14	N	105	LYS
14	N	115	LEU
14	N	119	VAL
14	N	144	GLU
14	N	178	LEU
1	O	2	THR
1	O	3	ASP
1	O	17	LYS
1	O	29	LYS
1	O	52	SER
1	O	61	LEU
1	O	109	LEU
1	O	122	THR
1	O	124	SER
1	O	157	PHE
1	O	169	VAL
1	O	173	THR
1	O	176	GLU
1	O	178	ARG
1	O	231	LYS
1	O	246	ARG
1	O	250	LEU
2	P	2	SER
2	P	40	SER
2	P	50	LYS
2	P	52	THR
2	P	54	THR
2	P	55	LEU
2	P	56	LEU
2	P	58	GLN
2	P	62	THR
2	P	65	LEU

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Mol	Chain	Res	Type
2	P	79	LEU
2	P	102	ASN
2	P	114	LEU
2	P	180	LYS
2	P	184	LYS
2	P	191	LEU
2	P	194	LYS
2	P	221	ASP
2	P	237	ILE
2	P	239	VAL
2	P	244	THR
3	Q	4	ARG
3	Q	22	LEU
3	Q	37	LYS
3	Q	38	ASN
3	Q	51	LYS
3	Q	52	LEU
3	Q	61	LYS
3	Q	107	LEU
3	Q	124	VAL
3	Q	147	GLN
3	Q	160	GLN
3	Q	169	VAL
3	Q	175	LYS
3	Q	180	LYS
3	Q	187	GLU
3	Q	191	LYS
3	Q	203	THR
3	Q	213	VAL
3	Q	239	GLN
3	Q	240	GLU
4	R	1	ASP
4	R	12	ARG
4	R	20	LEU
4	R	40	LEU
4	R	48	SER
4	R	51	LEU
4	R	64	ARG
4	R	99	ILE
4	R	102	GLU
4	R	114	ARG
4	R	117	GLU

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Mol	Chain	Res	Type
4	R	176	LEU
4	R	182	SER
4	R	190	LEU
4	R	193	LEU
4	R	197	LYS
4	R	202	GLU
4	R	214	ILE
4	R	224	ASP
4	R	235	LEU
4	R	236	LYS
4	R	242	GLU
5	S	9	THR
5	S	10	VAL
5	S	25	LEU
5	S	29	LYS
5	S	54	GLU
5	S	55	LEU
5	S	60	LYS
5	S	61	LYS
5	S	62	ILE
5	S	71	LEU
5	S	76	LEU
5	S	87	LEU
5	S	144	LEU
5	S	174	THR
5	S	188	LEU
5	S	207	VAL
5	S	211	SER
5	S	231	LYS
6	T	50	ILE
6	T	51	THR
6	T	59	LYS
6	T	61	VAL
6	T	68	ARG
6	T	94	SER
6	T	96	LYS
6	T	123	ASN
6	T	137	VAL
6	T	139	LYS
6	T	148	GLU
6	T	165	ARG
6	T	167	SER

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Mol	Chain	Res	Type
6	T	172	LEU
6	T	174	LYS
6	T	181	GLU
6	T	186	ARG
6	T	187	GLU
6	T	203	ASN
6	T	206	LYS
6	T	221	ASN
6	T	228	LYS
6	T	241	LYS
6	T	242	GLU
6	T	243	ILE
7	U	13	GLU
7	U	24	LYS
7	U	26	THR
7	U	34	LEU
7	U	53	LYS
7	U	83	ASN
7	U	115	LEU
7	U	125	MET
7	U	154	TYR
7	U	165	LYS
7	U	166	GLN
7	U	171	THR
7	U	181	LYS
7	U	201	MET
7	U	230	GLU
7	U	235	ARG
7	U	236	LEU
7	U	239	ILE
8	V	3	ILE
8	V	22	GLN
8	V	34	LEU
8	V	43	CYS
8	V	56	THR
8	V	68	LEU
8	V	100	VAL
8	V	127	LEU
8	V	196	ARG
8	V	197	GLU
8	V	216	SER
8	V	218	VAL

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Mol	Chain	Res	Type
9	W	37	ASN
9	W	97	ARG
9	W	126	ILE
9	W	130	ASP
9	W	133	LYS
9	W	151	SER
9	W	159	PRO
9	W	171	LEU
9	W	182	TRP
9	W	191	LYS
9	W	192	ASP
9	W	202	ARG
10	X	2	ASP
10	X	23	ARG
10	X	35	THR
10	X	36	ARG
10	X	75	LEU
10	X	144	LEU
10	X	174	MET
11	Y	4	LEU
11	Y	9	GLN
11	Y	17	ASP
11	Y	35	ILE
11	Y	57	THR
11	Y	73	ARG
11	Y	107	LYS
11	Y	118	ASP
11	Y	147	ASP
11	Y	150	VAL
11	Y	182	GLU
12	Z	1	GLN
12	Z	13	LEU
12	Z	23	LEU
12	Z	49	ASN
12	Z	71	SER
12	Z	136	CYS
12	Z	150	LEU
12	Z	167	LYS
12	Z	173	LYS
12	Z	214	LYS
13	a	10	SER
13	a	37	ASN

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Mol	Chain	Res	Type
13	a	43	ILE
13	a	48	ASN
13	a	70	LEU
13	a	104	ARG
13	a	138	SER
13	a	187	ARG
13	a	204	THR
13	a	206	LEU
13	a	215	GLU
13	a	225	ILE
14	b	9	LYS
14	b	20	THR
14	b	22	THR
14	b	68	SER
14	b	103	ASP
14	b	104	ASP
14	b	105	LYS
14	b	115	LEU
14	b	119	VAL
14	b	144	GLU
14	b	178	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (180) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	30	GLN
1	A	94	HIS
1	A	149	GLN
2	B	20	GLN
2	B	58	GLN
2	B	95	GLN
2	B	102	ASN
2	B	119	GLN
2	B	123	GLN
2	B	155	ASN
2	B	176	GLN
2	B	226	GLN
2	B	232	GLN
3	C	17	GLN
3	C	38	ASN
3	C	53	GLN
3	C	77	ASN

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Mol	Chain	Res	Type
3	C	147	GLN
3	C	160	GLN
3	C	165	ASN
3	C	233	GLN
4	D	15	GLN
4	D	100	ASN
4	D	106	GLN
4	D	146	GLN
4	D	225	ASN
5	E	4	ASN
5	E	59	GLN
5	E	68	HIS
5	E	92	ASN
5	E	99	ASN
5	E	116	GLN
5	E	120	GLN
5	E	147	GLN
5	E	151	ASN
5	E	209	ASN
6	F	19	GLN
6	F	86	ASN
6	F	117	GLN
6	F	123	ASN
6	F	191	GLN
6	F	224	HIS
6	F	240	GLN
7	G	83	ASN
7	G	114	ASN
7	G	117	GLN
7	G	121	GLN
7	G	166	GLN
7	G	167	GLN
7	G	175	ASN
7	G	184	HIS
7	G	186	ASN
8	H	9	ASN
8	H	22	GLN
8	H	30	ASN
8	H	66	HIS
8	H	172	ASN
8	H	189	ASN
8	H	200	GLN

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Mol	Chain	Res	Type
8	H	219	ASN
9	I	31	GLN
9	I	37	ASN
10	J	55	GLN
10	J	63	ASN
10	J	78	GLN
10	J	118	GLN
10	J	146	HIS
11	K	9	GLN
11	K	85	ASN
11	K	133	GLN
11	K	143	ASN
11	K	176	ASN
11	K	208	ASN
11	K	209	ASN
12	L	3	ASN
12	L	36	ASN
12	L	49	ASN
12	L	80	ASN
12	L	153	GLN
12	L	165	ASN
12	L	197	GLN
13	M	18	ASN
13	M	48	ASN
13	M	62	HIS
13	M	108	ASN
13	M	179	ASN
13	M	194	ASN
13	M	203	ASN
13	M	213	GLN
14	N	38	HIS
14	N	141	ASN
14	N	161	GLN
1	O	30	GLN
1	O	94	HIS
1	O	149	GLN
2	P	20	GLN
2	P	58	GLN
2	P	119	GLN
2	P	123	GLN
2	P	155	ASN
2	P	176	GLN

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Mol	Chain	Res	Type
2	P	226	GLN
2	P	232	GLN
3	Q	38	ASN
3	Q	77	ASN
3	Q	116	GLN
3	Q	120	GLN
3	Q	147	GLN
3	Q	160	GLN
3	Q	165	ASN
3	Q	233	GLN
4	R	15	GLN
4	R	91	HIS
4	R	100	ASN
4	R	106	GLN
4	R	146	GLN
4	R	225	ASN
5	S	4	ASN
5	S	68	HIS
5	S	92	ASN
5	S	99	ASN
5	S	116	GLN
5	S	120	GLN
5	S	147	GLN
5	S	151	ASN
5	S	209	ASN
6	T	19	GLN
6	T	58	GLN
6	T	86	ASN
6	T	117	GLN
6	T	123	ASN
6	T	191	GLN
6	T	224	HIS
7	U	83	ASN
7	U	114	ASN
7	U	117	GLN
7	U	121	GLN
7	U	166	GLN
7	U	167	GLN
7	U	175	ASN
7	U	186	ASN
8	V	22	GLN
8	V	66	HIS

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Mol	Chain	Res	Type
8	V	172	ASN
8	V	200	GLN
8	V	219	ASN
9	W	31	GLN
9	W	37	ASN
9	W	203	GLN
10	X	55	GLN
10	X	61	GLN
10	X	63	ASN
10	X	86	GLN
10	X	118	GLN
10	X	146	HIS
11	Y	9	GLN
11	Y	85	ASN
11	Y	133	GLN
11	Y	143	ASN
11	Y	176	ASN
11	Y	208	ASN
11	Y	209	ASN
12	Z	3	ASN
12	Z	36	ASN
12	Z	49	ASN
12	Z	79	HIS
12	Z	80	ASN
12	Z	153	GLN
12	Z	165	ASN
12	Z	197	GLN
13	a	18	ASN
13	a	48	ASN
13	a	102	GLN
13	a	108	ASN
13	a	179	ASN
13	a	194	ASN
13	a	213	GLN
14	b	38	HIS
14	b	141	ASN
14	b	161	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 10 ligands modelled in this entry, 8 are monoatomic - leaving 2 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
16	2M1	Y	301	11	38,38,38	1.52	5 (13%)	49,51,51	1.36	6 (12%)
16	2M1	K	301	11	38,38,38	1.60	5 (13%)	49,51,51	1.34	5 (10%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
16	2M1	Y	301	11	-	5/43/43/43	0/1/1/1
16	2M1	K	301	11	-	6/43/43/43	0/1/1/1

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	K	301	2M1	O43-S42	4.67	1.53	1.44
16	K	301	2M1	C26-S42	4.42	1.84	1.78
16	Y	301	2M1	O43-S42	4.40	1.53	1.44
16	K	301	2M1	O44-S42	4.37	1.52	1.44
16	Y	301	2M1	O44-S42	4.33	1.52	1.44
16	Y	301	2M1	C5-C4	-4.03	1.41	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	K	301	2M1	C5-C4	-3.92	1.41	1.50
16	Y	301	2M1	C26-S42	3.79	1.83	1.78
16	K	301	2M1	C41-C26	2.72	1.55	1.52
16	Y	301	2M1	C41-C26	2.43	1.55	1.52

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	Y	301	2M1	O6-C7-N9	4.60	120.29	110.45
16	Y	301	2M1	O44-S42-O43	-4.34	109.09	117.22
16	K	301	2M1	O6-C7-N9	4.29	119.62	110.45
16	K	301	2M1	O44-S42-O43	-3.99	109.72	117.22
16	K	301	2M1	O43-S42-C26	3.61	110.93	108.33
16	Y	301	2M1	O43-S42-C26	2.94	110.45	108.33
16	Y	301	2M1	O8-C7-N9	-2.68	120.47	124.86
16	Y	301	2M1	O6-C7-O8	-2.62	119.25	124.26
16	K	301	2M1	O8-C7-N9	-2.57	120.65	124.86
16	Y	301	2M1	C5-O6-C7	-2.48	110.34	115.93
16	K	301	2M1	O6-C7-O8	-2.37	119.72	124.26

There are no chirality outliers.

All (11) torsion outliers are listed below:

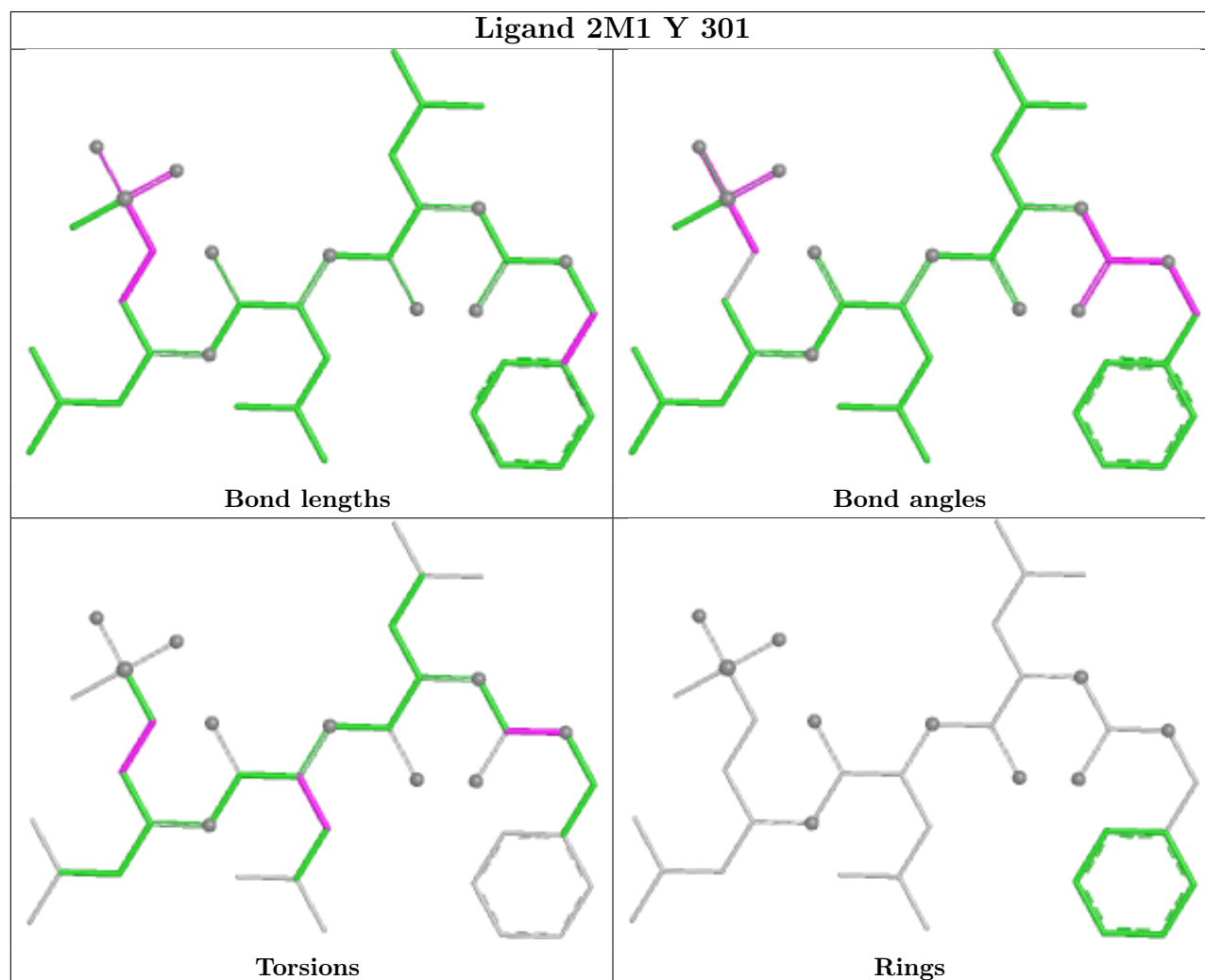
Mol	Chain	Res	Type	Atoms
16	K	301	2M1	O8-C7-O6-C5
16	Y	301	2M1	N9-C7-O6-C5
16	Y	301	2M1	O8-C7-O6-C5
16	K	301	2M1	N9-C7-O6-C5
16	K	301	2M1	N16-C17-C18-C19
16	Y	301	2M1	N16-C17-C18-C19
16	K	301	2M1	C22-C17-C18-C19
16	Y	301	2M1	C22-C17-C18-C19
16	K	301	2M1	S42-C26-C41-C25
16	Y	301	2M1	S42-C26-C41-C25
16	K	301	2M1	C17-C18-C19-C20

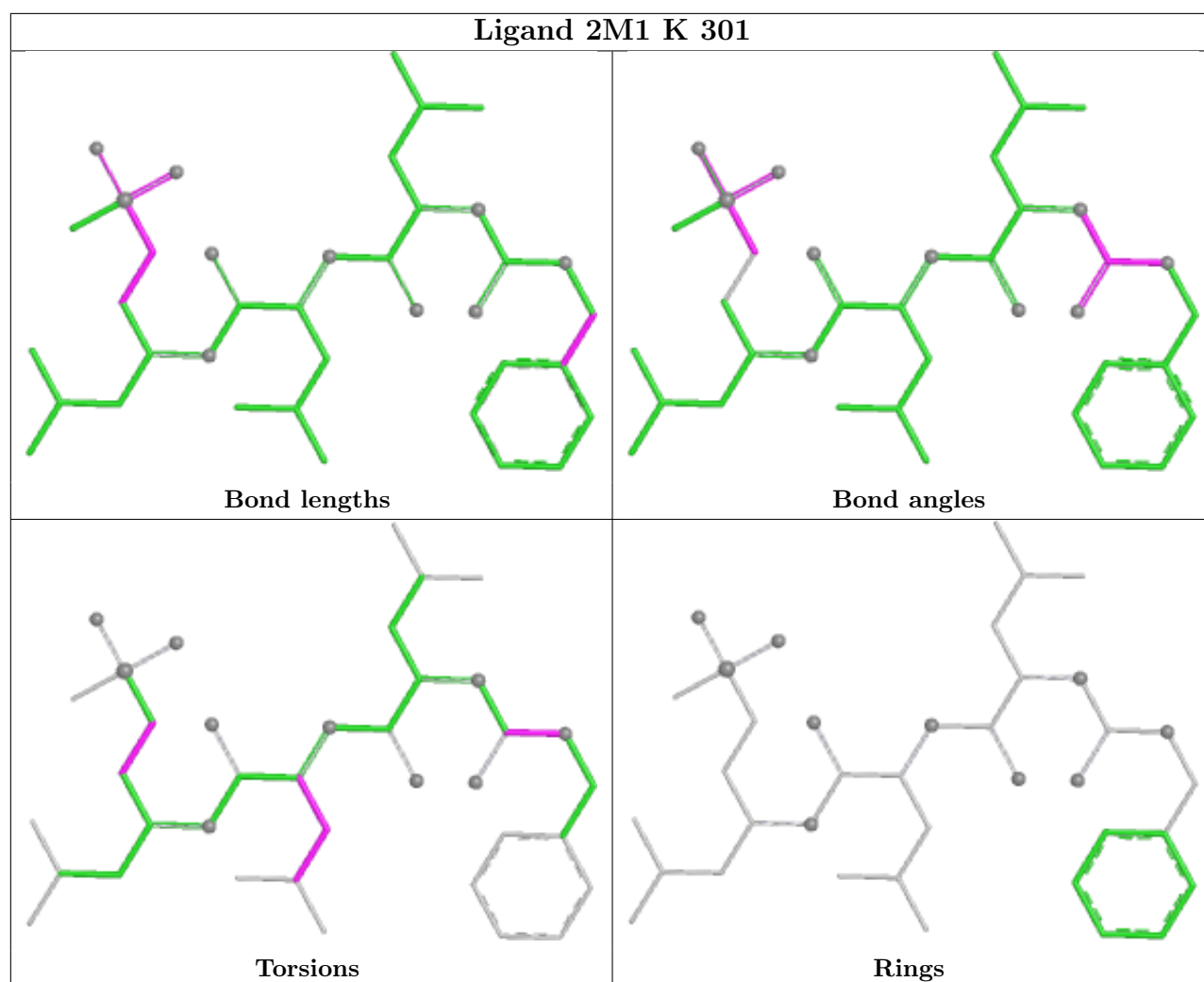
There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will

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





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	250/250 (100%)	-0.72	1 (0%) 88 76	34, 54, 89, 118	0
1	O	250/250 (100%)	-0.63	0 100 100	38, 59, 93, 121	0
2	B	244/258 (94%)	-0.57	1 (0%) 88 76	34, 59, 100, 154	0
2	P	244/258 (94%)	-0.53	1 (0%) 88 76	41, 59, 107, 156	0
3	C	240/254 (94%)	-0.54	0 100 100	38, 60, 112, 142	0
3	Q	240/254 (94%)	-0.52	0 100 100	38, 69, 123, 149	0
4	D	235/260 (90%)	-0.62	0 100 100	35, 60, 87, 108	0
4	R	235/260 (90%)	-0.53	0 100 100	38, 65, 100, 117	0
5	E	231/234 (98%)	-0.56	0 100 100	37, 65, 94, 130	0
5	S	231/234 (98%)	-0.52	0 100 100	41, 67, 99, 128	0
6	F	243/288 (84%)	-0.60	0 100 100	38, 59, 101, 134	0
6	T	243/288 (84%)	-0.57	0 100 100	40, 58, 96, 115	0
7	G	241/252 (95%)	-0.66	0 100 100	34, 54, 84, 140	0
7	U	241/252 (95%)	-0.68	0 100 100	36, 54, 87, 127	0
8	H	222/232 (95%)	-0.75	0 100 100	31, 50, 70, 130	0
8	V	222/232 (95%)	-0.75	0 100 100	35, 53, 74, 130	0
9	I	204/205 (99%)	-0.87	0 100 100	33, 51, 74, 101	0
9	W	204/205 (99%)	-0.81	0 100 100	35, 51, 76, 97	0
10	J	195/198 (98%)	-0.80	0 100 100	33, 49, 80, 119	0
10	X	195/198 (98%)	-0.78	1 (0%) 87 72	34, 51, 74, 135	0
11	K	212/212 (100%)	-0.71	0 100 100	31, 50, 74, 87	0
11	Y	212/212 (100%)	-0.73	0 100 100	32, 54, 80, 99	0
12	L	222/222 (100%)	-0.82	0 100 100	30, 53, 73, 95	0
12	Z	222/222 (100%)	-0.81	0 100 100	30, 53, 76, 93	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	M	233/246 (94%)	-0.80	0 100 100	34, 52, 71, 82	0
13	a	233/246 (94%)	-0.79	1 (0%) 88 76	31, 49, 69, 80	0
14	N	196/196 (100%)	-0.79	0 100 100	31, 47, 70, 94	0
14	b	196/196 (100%)	-0.77	0 100 100	34, 48, 71, 98	0
All	All	6336/6614 (95%)	-0.68	5 (0%) 92 86	30, 55, 92, 156	0

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
10	X	1	MET	3.1
2	P	219	ALA	3.0
1	A	2	THR	2.8
13	a	1	THR	2.7
2	B	219	ALA	2.3

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

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

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
16	2M1	K	301	38/38	0.94	0.11	54,64,80,81	0
16	2M1	Y	301	38/38	0.95	0.10	55,65,78,80	0
15	MG	K	302	1/1	0.97	0.06	53,53,53,53	0
15	MG	V	301	1/1	0.98	0.06	59,59,59,59	0
15	MG	I	301	1/1	0.98	0.06	45,45,45,45	0
15	MG	H	301	1/1	0.98	0.13	38,38,38,38	0
15	MG	Y	302	1/1	0.99	0.03	42,42,42,42	0

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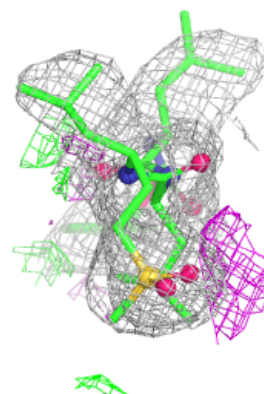
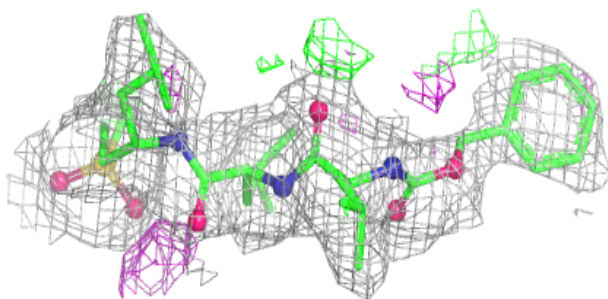
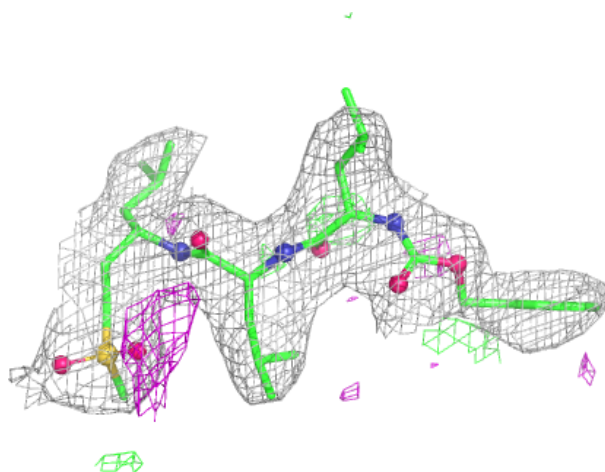
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
15	MG	Z	301	1/1	0.99	0.04	54,54,54,54	0
15	MG	N	201	1/1	0.99	0.03	43,43,43,43	0
15	MG	G	301	1/1	0.99	0.02	64,64,64,64	0

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.

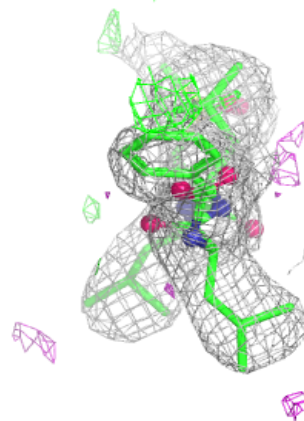
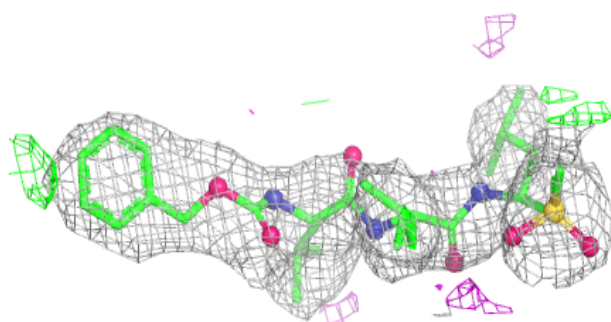
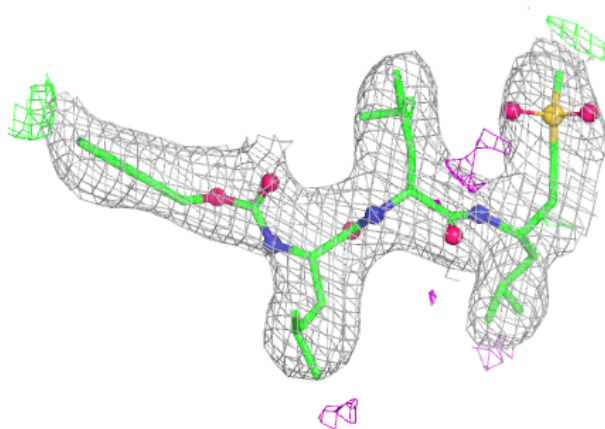
Electron density around 2M1 K 301:

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 2M1 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.