



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 11:28 AM UTC

PDB ID : 4R17 / pdb_00004r17
Title : Ligand-induced aziridine-formation at subunit beta5 of the yeast 20S proteasome
Authors : Dubiella, C.; Cui, H.; Gersch, M.; Brouwer, A.J.; Sieber, S.A.; Krueger, A.; Liskamp, R.; Groll, M.
Deposited on : 2014-08-04
Resolution : 2.10 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:

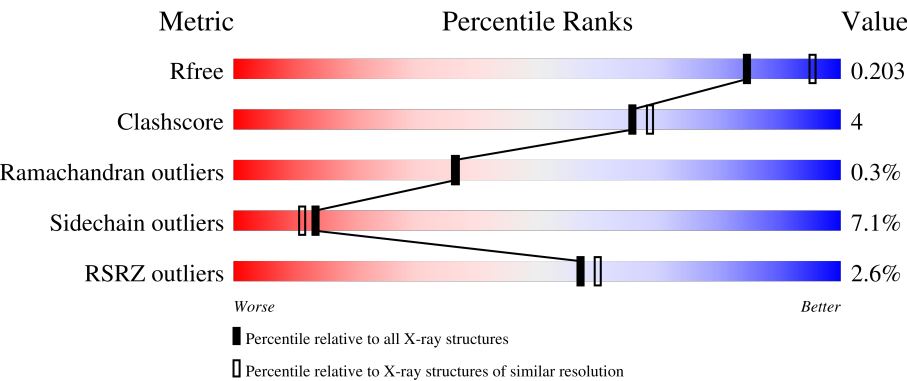
MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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	6658 (2.10-2.10)
Clashscore	190562	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)
RSRZ outliers	180081	6662 (2.10-2.10)

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

Mol	Chain	Length	Quality of chain
1	A	250	3% 94%
1	O	250	3% 94%
2	B	258	3% 79% 13% 5%
2	P	258	5% 81% 11% 5%
3	C	254	6% 77% 13% 6%

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Mol	Chain	Length	Quality of chain
3	Q	254	
4	D	260	
4	R	260	
5	E	234	
5	S	234	
6	F	288	
6	T	288	
7	G	252	
7	U	252	
8	H	232	
8	V	232	
9	I	205	
9	W	205	
10	J	198	
10	X	198	
11	K	212	
11	Y	212	
12	L	222	
12	Z	222	
13	M	246	
13	a	246	
14	N	196	
14	b	196	

2 Entry composition

There are 17 unique types of molecules in this entry. The entry contains 52831 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	249	Total	C	N	O	S	0	0	0
			1907	1214	314	376	3			
1	O	249	Total	C	N	O	S	0	0	0
			1907	1214	314	376	3			

- 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 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	226	Total	C	N	O	S	0	0	0
			1719	1082	298	332	7			
8	V	226	Total	C	N	O	S	0	0	0
			1719	1082	298	332	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	211	Total	C	N	O	S	0	0	0
			1637	1041	279	310	7			
11	Y	211	Total	C	N	O	S	0	0	0
			1637	1041	279	310	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).

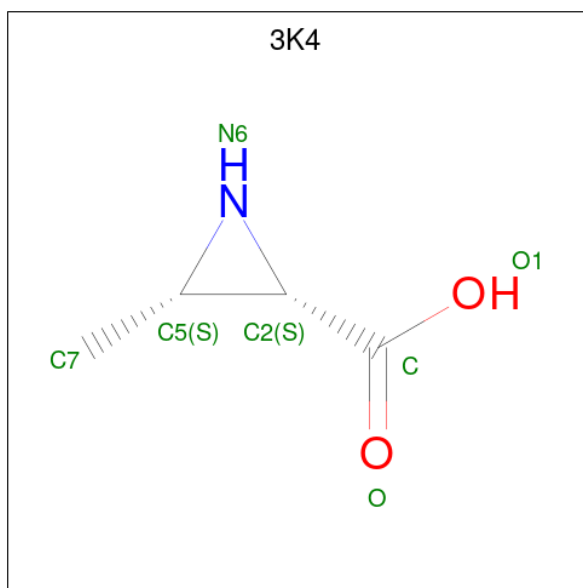
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
15	G	1	Total	Mg	0	0
			1	1		
15	H	1	Total	Mg	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
15	I	2	Total 2	Mg 2	0	0
15	J	1	Total 1	Mg 1	0	0
15	K	2	Total 2	Mg 2	0	0
15	N	1	Total 1	Mg 1	0	0
15	V	1	Total 1	Mg 1	0	0
15	Y	1	Total 1	Mg 1	0	0
15	Z	1	Total 1	Mg 1	0	0

- Molecule 16 is (2S,3S)-3-methylaziridine-2-carboxylic acid (CCD ID: 3K4) (formula: $C_4H_7NO_2$).



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

- Molecule 17 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
17	A	167	Total O 167 167	0	0
17	B	115	Total O 115 115	0	0
17	C	105	Total O 105 105	0	0
17	D	123	Total O 123 123	0	0
17	E	69	Total O 69 69	0	0
17	F	117	Total O 117 117	0	0
17	G	158	Total O 158 158	0	0
17	H	135	Total O 135 135	0	0
17	I	140	Total O 140 140	0	0
17	J	123	Total O 123 123	0	0
17	K	152	Total O 152 152	0	0
17	L	158	Total O 158 158	0	0
17	M	168	Total O 168 168	0	0
17	N	112	Total O 112 112	0	0
17	O	118	Total O 118 118	0	0
17	P	91	Total O 91 91	0	0
17	Q	79	Total O 79 79	0	0
17	R	107	Total O 107 107	0	0
17	S	55	Total O 55 55	0	0
17	T	94	Total O 94 94	0	0
17	U	133	Total O 133 133	0	0
17	V	111	Total O 111 111	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
17	W	128	Total 128	O 128	0	0
17	X	118	Total 118	O 118	0	0
17	Y	148	Total 148	O 148	0	0
17	Z	166	Total 166	O 166	0	0
17	a	165	Total 165	O 165	0	0
17	b	117	Total 117	O 117	0	0

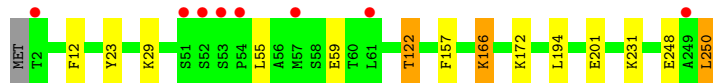
3 Residue-property plots [i](#)

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.

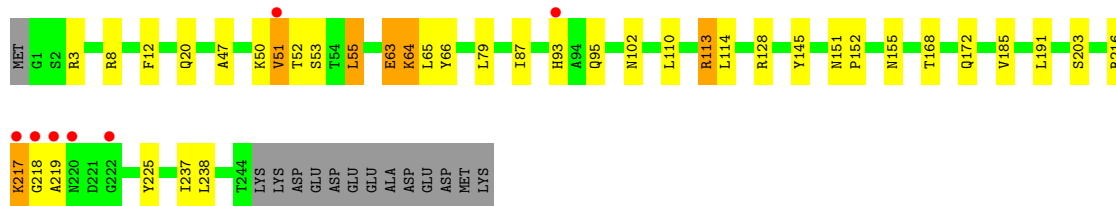
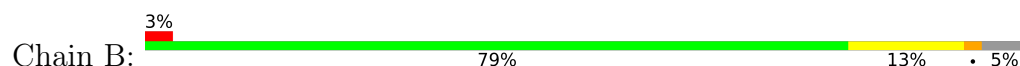
- Molecule 1: Proteasome subunit alpha type-2



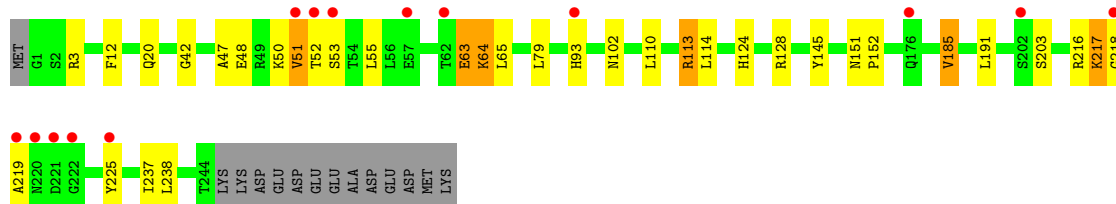
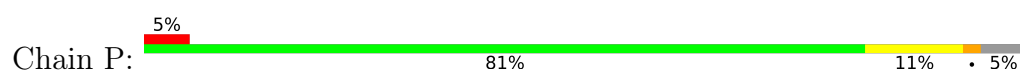
- Molecule 1: Proteasome subunit alpha type-2



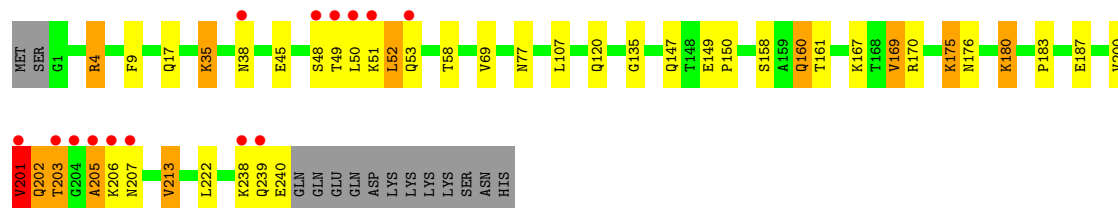
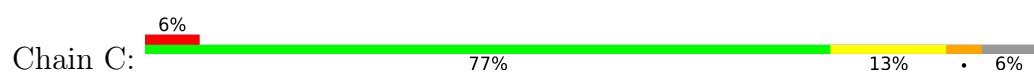
- Molecule 2: Proteasome subunit alpha type-3



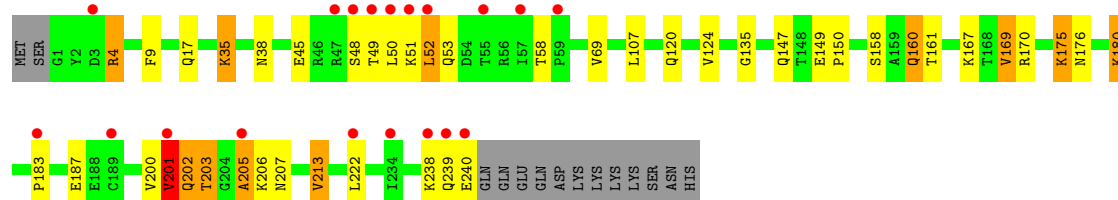
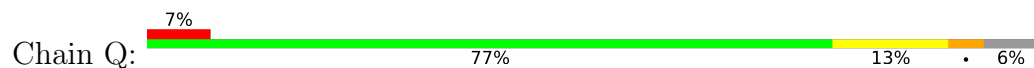
- Molecule 2: Proteasome subunit alpha type-3



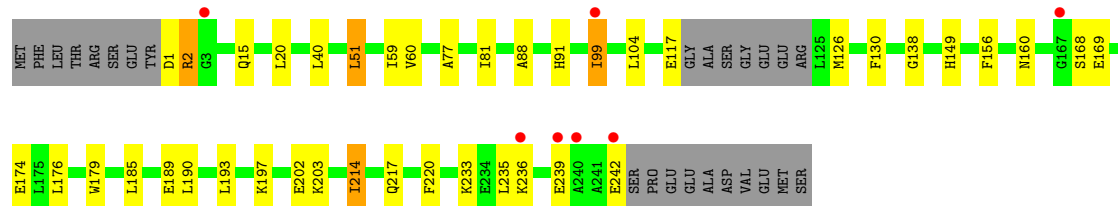
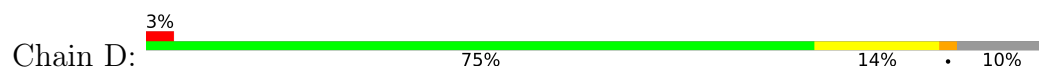
- Molecule 3: Proteasome subunit alpha type-4



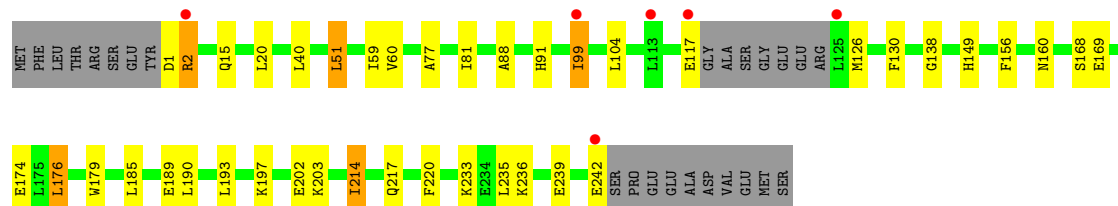
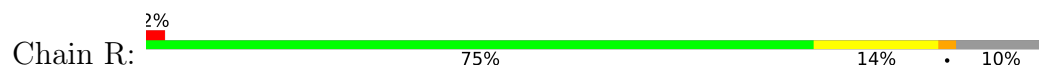
- Molecule 3: Proteasome subunit alpha type-4



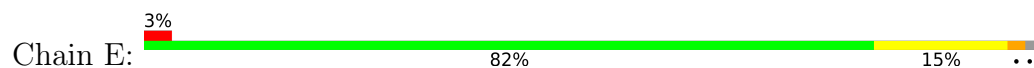
- Molecule 4: Proteasome subunit alpha type-5



- Molecule 4: Proteasome subunit alpha type-5

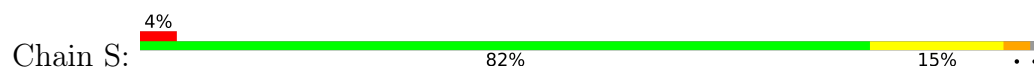


- Molecule 5: Proteasome subunit alpha type-6

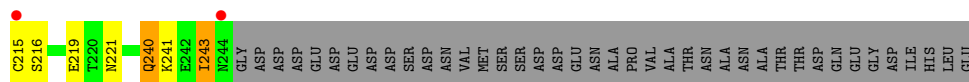




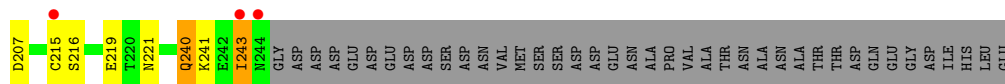
• Molecule 5: Proteasome subunit alpha type-6



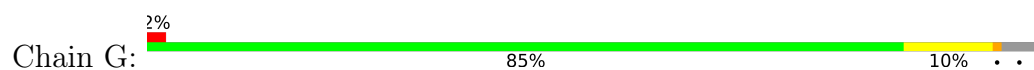
• Molecule 6: Proteasome subunit alpha type-7



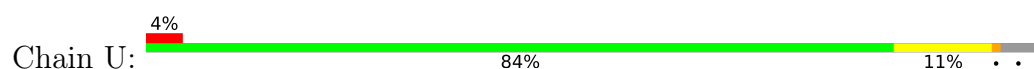
• Molecule 6: Proteasome subunit alpha type-7

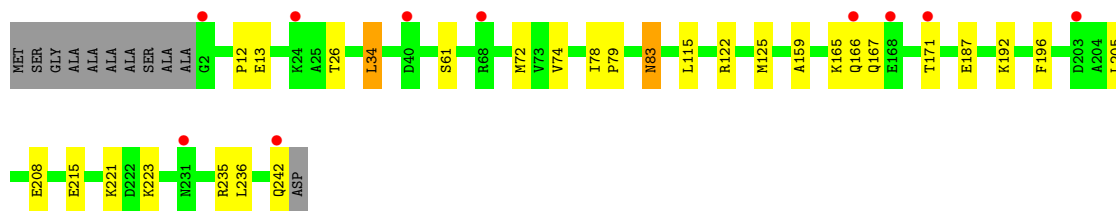


• Molecule 7: Proteasome subunit alpha type-1

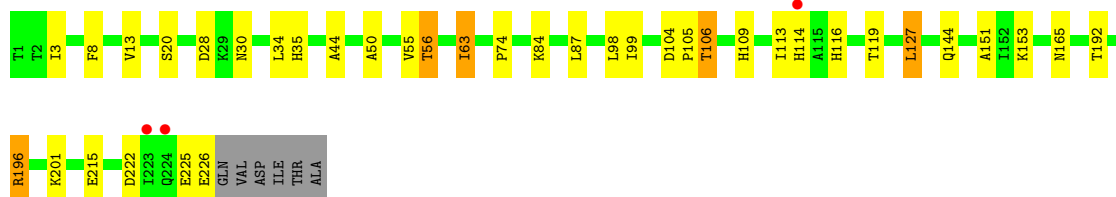
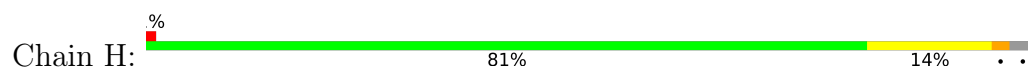


• Molecule 7: Proteasome subunit alpha type-1

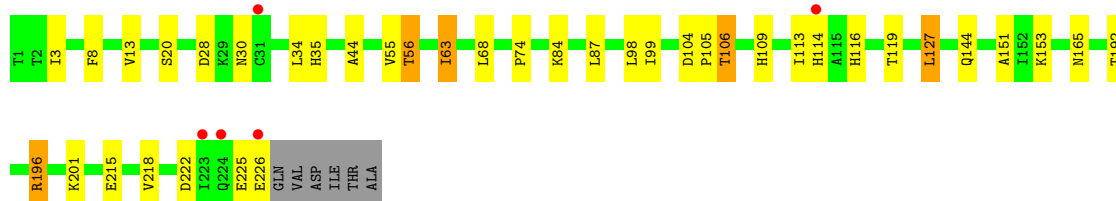
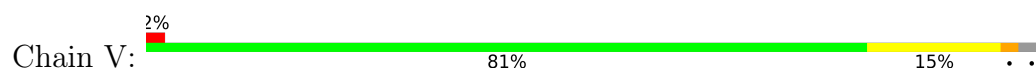




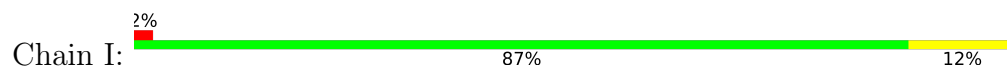
• Molecule 8: Proteasome subunit beta type-2



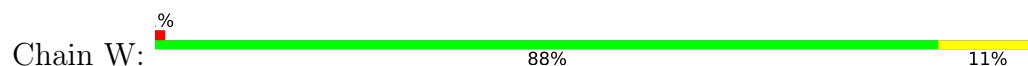
• Molecule 8: Proteasome subunit beta type-2



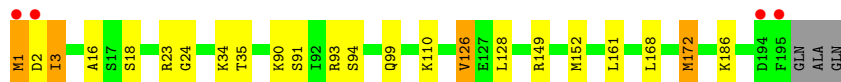
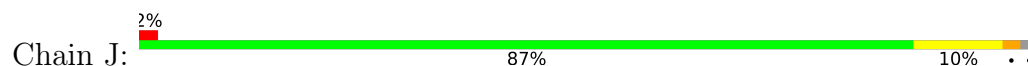
• Molecule 9: Proteasome subunit beta type-3



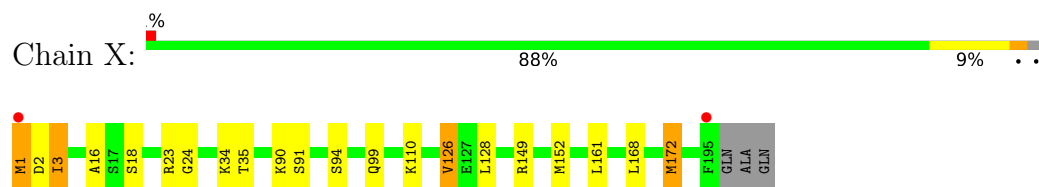
• Molecule 9: Proteasome subunit beta type-3



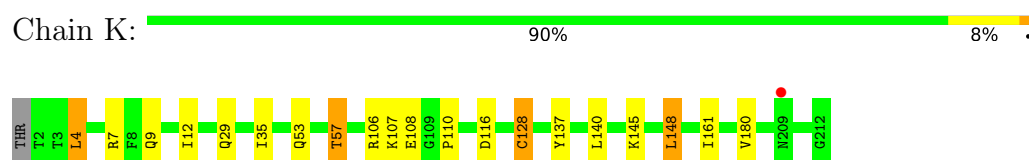
• Molecule 10: Proteasome subunit beta type-4



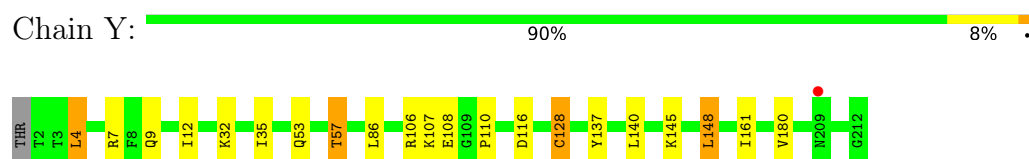
• Molecule 10: Proteasome subunit beta type-4



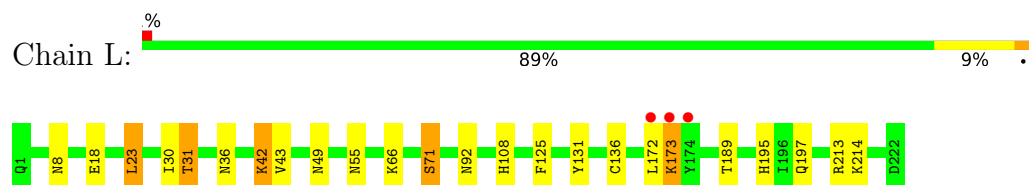
• Molecule 11: Proteasome subunit beta type-5



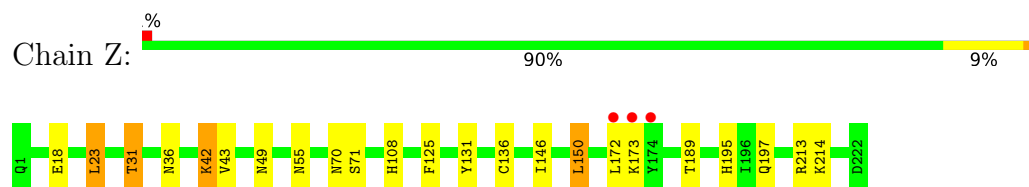
• Molecule 11: Proteasome subunit beta type-5



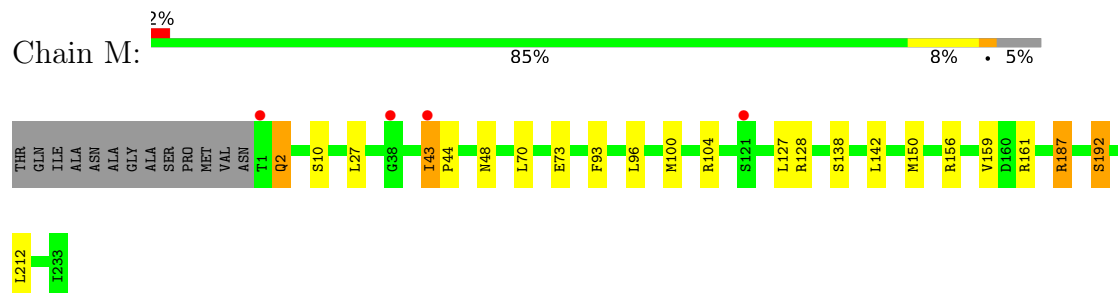
• Molecule 12: Proteasome subunit beta type-6



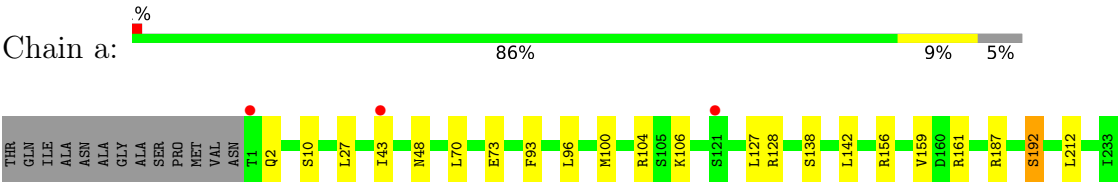
• Molecule 12: Proteasome subunit beta type-6



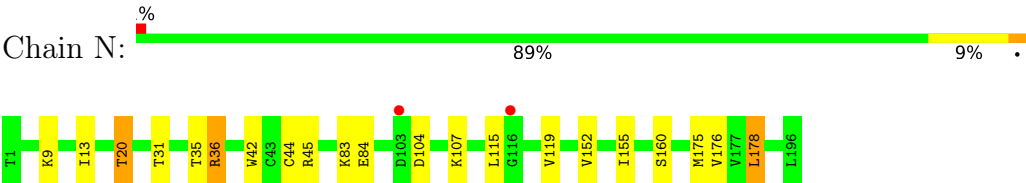
• Molecule 13: Proteasome subunit beta type-7



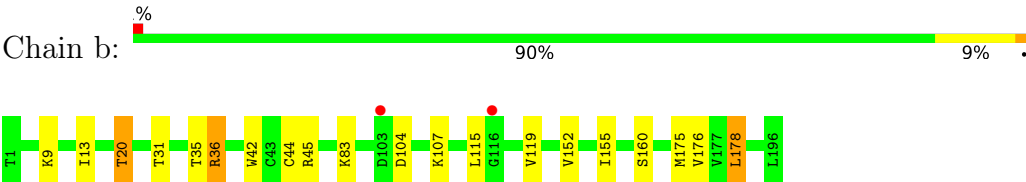
• Molecule 13: Proteasome subunit beta type-7



• Molecule 14: Proteasome subunit beta type-1



• Molecule 14: Proteasome subunit beta type-1



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	134.72Å 301.36Å 144.74Å 90.00° 112.81° 90.00°	Depositor
Resolution (Å)	15.00 – 2.10 15.00 – 2.10	Depositor EDS
% Data completeness (in resolution range)	98.9 (15.00-2.10) 98.6 (15.00-2.10)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.04 (at 2.10Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.185 , 0.198 0.191 , 0.203	Depositor DCC
R_{free} test set	30359 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	38.1	Xtriage
Anisotropy	0.086	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 57.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	52831	wwPDB-VP
Average B, all atoms (Å ²)	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.30% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: 3K4, 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	0.41	0/1944	0.74	0/2632
1	O	0.40	0/1944	0.73	0/2632
2	B	0.44	0/1934	0.75	0/2618
2	P	0.44	0/1934	0.75	0/2618
3	C	0.42	0/1910	0.76	1/2586 (0.0%)
3	Q	0.42	0/1910	0.76	1/2586 (0.0%)
4	D	0.39	0/1837	0.73	1/2475 (0.0%)
4	R	0.39	0/1837	0.73	1/2475 (0.0%)
5	E	0.40	0/1800	0.71	0/2433
5	S	0.40	0/1800	0.71	0/2433
6	F	0.40	0/1932	0.72	0/2609
6	T	0.40	0/1932	0.72	0/2609
7	G	0.40	0/1945	0.72	1/2634 (0.0%)
7	U	0.39	0/1945	0.72	1/2634 (0.0%)
8	H	0.45	0/1750	0.72	0/2373
8	V	0.38	0/1750	0.72	0/2373
9	I	0.38	0/1611	0.70	0/2174
9	W	0.38	0/1611	0.70	0/2174
10	J	0.40	0/1589	0.68	0/2142
10	X	0.40	0/1589	0.68	0/2142
11	K	0.38	0/1674	0.72	0/2264
11	Y	0.38	0/1674	0.72	0/2264
12	L	0.50	0/1795	0.72	0/2420
12	Z	0.39	0/1795	0.71	0/2420
13	M	0.51	0/1855	0.74	1/2514 (0.0%)
13	a	0.46	0/1855	0.73	1/2514 (0.0%)
14	N	0.37	0/1541	0.69	0/2087
14	b	0.37	0/1541	0.69	0/2087
All	All	0.41	0/50234	0.72	8/67922 (0.0%)

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	Q	201	VAL	N-CA-C	6.77	116.90	110.74
3	C	201	VAL	N-CA-C	6.73	116.86	110.74
4	R	168	SER	N-CA-C	6.33	118.26	111.36
4	D	168	SER	N-CA-C	6.30	118.23	111.36
7	U	223	LYS	N-CA-C	6.12	118.42	108.76
7	G	223	LYS	N-CA-C	6.11	118.42	108.76
13	M	10	SER	N-CA-C	5.46	117.33	110.24
13	a	10	SER	N-CA-C	5.45	117.32	110.24

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	A	1907	0	1917	6	0
1	O	1907	0	1917	6	0
2	B	1904	0	1904	28	0
2	P	1904	0	1904	20	0
3	C	1881	0	1895	21	0
3	Q	1881	0	1895	20	0
4	D	1813	0	1797	16	0
4	R	1813	0	1797	17	0
5	E	1773	0	1775	15	0
5	S	1773	0	1775	19	0
6	F	1892	0	1883	20	0
6	T	1892	0	1883	21	0
7	G	1907	0	1901	11	0
7	U	1907	0	1901	14	0
8	H	1719	0	1719	26	0
8	V	1719	0	1719	27	0
9	I	1581	0	1574	16	0
9	W	1581	0	1574	14	0
10	J	1561	0	1569	14	0
10	X	1561	0	1569	13	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
11	K	1637	0	1585	9	0
11	Y	1637	0	1585	10	0
12	L	1757	0	1711	11	0
12	Z	1757	0	1711	10	0
13	M	1824	0	1832	9	0
13	a	1824	0	1832	6	0
14	N	1512	0	1481	13	0
14	b	1512	0	1481	13	0
15	G	1	0	0	0	0
15	H	1	0	0	0	0
15	I	2	0	0	0	0
15	J	1	0	0	0	0
15	K	2	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	6	0	5	0	0
16	Y	6	0	5	0	0
17	A	167	0	0	0	0
17	B	115	0	0	0	0
17	C	105	0	0	1	0
17	D	123	0	0	0	0
17	E	69	0	0	0	0
17	F	117	0	0	0	0
17	G	158	0	0	0	0
17	H	135	0	0	0	0
17	I	140	0	0	0	0
17	J	123	0	0	1	0
17	K	152	0	0	1	0
17	L	158	0	0	0	0
17	M	168	0	0	1	0
17	N	112	0	0	0	0
17	O	118	0	0	0	0
17	P	91	0	0	0	0
17	Q	79	0	0	1	0
17	R	107	0	0	0	0
17	S	55	0	0	0	0
17	T	94	0	0	0	0
17	U	133	0	0	0	0
17	V	111	0	0	0	0
17	W	128	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
17	X	118	0	0	0	0
17	Y	148	0	0	0	0
17	Z	166	0	0	0	0
17	a	165	0	0	0	0
17	b	117	0	0	1	0
All	All	52831	0	49096	378	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 4.

All (378) 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:B:52:THR:HG22	2:B:53:SER:H	1.22	1.03
14:N:35:THR:HG21	14:N:45:ARG:HE	1.36	0.90
2:B:52:THR:HG22	2:B:53:SER:N	1.80	0.90
14:b:35:THR:HG21	14:b:45:ARG:HE	1.36	0.90
2:P:52:THR:HG22	2:P:53:SER:N	1.88	0.89
2:P:52:THR:CG2	2:P:53:SER:N	2.39	0.86
6:F:146:MET:CE	6:F:161:THR:HB	2.09	0.83
6:T:146:MET:CE	6:T:161:THR:HB	2.10	0.81
2:P:52:THR:CG2	2:P:53:SER:H	1.93	0.80
2:B:52:THR:CG2	2:B:53:SER:H	1.94	0.80
6:T:146:MET:HE1	6:T:161:THR:HB	1.69	0.74
2:B:12:PHE:H	3:C:17:GLN:HE22	1.34	0.74
6:F:146:MET:HE1	6:F:161:THR:HB	1.69	0.73
11:K:53:GLN:O	11:K:57:THR:HG23	1.89	0.73
11:Y:53:GLN:O	11:Y:57:THR:HG23	1.88	0.72
14:N:13:ILE:HG21	14:N:175:MET:HE2	1.73	0.70
2:B:219:ALA:HB2	2:B:225:TYR:HB2	1.73	0.69
14:b:13:ILE:HG21	14:b:175:MET:HE2	1.73	0.69
14:N:83:LYS:HG3	14:N:119:VAL:CG2	2.23	0.69
2:P:219:ALA:HB2	2:P:225:TYR:HB2	1.73	0.68
6:T:240:GLN:HE21	6:T:240:GLN:HA	1.59	0.68
6:F:240:GLN:HE21	6:F:240:GLN:HA	1.59	0.67
14:b:83:LYS:HG3	14:b:119:VAL:CG2	2.24	0.67
10:J:126:VAL:HG12	10:J:128:LEU:HG	1.77	0.66
2:B:3:ARG:HB3	5:E:122:TYR:OH	1.95	0.66
10:J:3:ILE:HG23	10:J:18:SER:HB3	1.76	0.66
10:X:3:ILE:HG23	10:X:18:SER:HB3	1.76	0.65
10:X:126:VAL:HG12	10:X:128:LEU:HG	1.77	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:R:176:LEU:HD11	5:S:54:GLU:HB2	1.81	0.63
14:N:35:THR:CG2	14:N:45:ARG:HE	2.12	0.62
1:O:12:PHE:H	2:P:20:GLN:HE22	1.47	0.62
8:H:3:ILE:HG22	8:H:99:ILE:HD12	1.82	0.62
3:Q:51:LYS:O	3:Q:52:LEU:HB2	2.00	0.61
12:Z:42:LYS:HD2	12:Z:55:ASN:HD22	1.65	0.61
8:V:3:ILE:HG22	8:V:99:ILE:HD12	1.82	0.61
2:B:52:THR:HG22	2:B:53:SER:O	2.01	0.60
12:L:42:LYS:HD2	12:L:55:ASN:HD22	1.65	0.60
3:C:51:LYS:O	3:C:52:LEU:HB2	1.99	0.60
2:P:12:PHE:H	3:Q:17:GLN:HE22	1.47	0.60
10:X:1:MET:CB	10:X:34:LYS:HE3	2.32	0.60
14:b:35:THR:CG2	14:b:45:ARG:HE	2.12	0.60
5:E:12:PHE:H	6:F:19:GLN:HE22	1.50	0.60
2:P:52:THR:HG23	2:P:53:SER:H	1.64	0.60
5:S:12:PHE:H	6:T:19:GLN:HE22	1.48	0.60
6:F:172:LEU:HD13	6:F:195:ILE:HD13	1.84	0.60
6:T:172:LEU:HD13	6:T:195:ILE:HD13	1.84	0.59
10:J:1:MET:CB	10:J:34:LYS:HE3	2.32	0.59
4:D:91:HIS:HB3	4:D:99:ILE:HG22	1.85	0.59
4:R:197:LYS:NZ	4:R:239:GLU:OE2	2.35	0.59
4:D:197:LYS:NZ	4:D:239:GLU:OE2	2.35	0.58
7:G:34:LEU:C	7:G:34:LEU:HD23	2.28	0.58
7:G:165:LYS:HD2	7:G:205:LEU:HD22	1.86	0.58
1:A:12:PHE:H	2:B:20:GLN:HE22	1.52	0.58
4:D:88:ALA:HA	4:D:99:ILE:HG21	1.86	0.58
2:P:216:ARG:HB3	2:P:218:GLY:H	1.69	0.58
4:R:91:HIS:HB3	4:R:99:ILE:HG22	1.85	0.58
4:R:88:ALA:HA	4:R:99:ILE:HG21	1.86	0.57
7:U:34:LEU:C	7:U:34:LEU:HD23	2.28	0.57
11:Y:145:LYS:HB2	11:Y:148:LEU:HD13	1.87	0.57
2:P:217:LYS:C	2:P:219:ALA:H	2.12	0.57
3:C:201:VAL:O	3:C:202:GLN:CB	2.53	0.57
7:U:165:LYS:HD2	7:U:205:LEU:HD22	1.85	0.57
3:Q:9:PHE:H	4:R:15:GLN:HE22	1.51	0.57
2:B:216:ARG:HB3	2:B:218:GLY:H	1.69	0.57
11:K:145:LYS:HB2	11:K:148:LEU:HD13	1.87	0.57
14:N:35:THR:HG21	14:N:45:ARG:NE	2.16	0.56
2:B:217:LYS:C	2:B:219:ALA:H	2.12	0.56
3:C:9:PHE:H	4:D:15:GLN:HE22	1.52	0.56
5:E:206:THR:C	5:E:233:ILE:HD11	2.30	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:114:HIS:HD2	8:H:116:HIS:H	1.54	0.56
11:K:107:LYS:HG3	11:K:108:GLU:HG3	1.87	0.56
11:Y:107:LYS:HG3	11:Y:108:GLU:HG3	1.87	0.56
3:Q:201:VAL:O	3:Q:202:GLN:CB	2.53	0.56
4:D:91:HIS:HB3	4:D:99:ILE:CG2	2.36	0.56
3:Q:203:THR:C	3:Q:205:ALA:H	2.14	0.56
5:S:206:THR:C	5:S:233:ILE:HD11	2.30	0.56
5:S:87:LEU:HD21	5:S:107:ALA:HB1	1.87	0.56
2:B:110:LEU:HD23	2:B:110:LEU:C	2.31	0.56
4:R:91:HIS:HB3	4:R:99:ILE:CG2	2.36	0.56
14:b:35:THR:HG21	14:b:45:ARG:NE	2.16	0.56
2:P:110:LEU:C	2:P:110:LEU:HD23	2.31	0.56
11:K:106:ARG:HG2	11:K:106:ARG:HH11	1.72	0.55
11:Y:106:ARG:HH11	11:Y:106:ARG:HG2	1.71	0.55
6:T:172:LEU:HD13	6:T:195:ILE:CD1	2.37	0.55
10:X:1:MET:HG2	10:X:34:LYS:HE3	1.88	0.55
8:V:114:HIS:HD2	8:V:116:HIS:H	1.54	0.55
10:J:1:MET:HG2	10:J:34:LYS:HE3	1.89	0.55
9:W:170:LEU:C	9:W:170:LEU:HD23	2.32	0.55
3:C:203:THR:C	3:C:205:ALA:H	2.14	0.54
8:V:3:ILE:HG21	8:V:44:ALA:HB3	1.90	0.54
14:b:20:THR:CG2	14:b:31:THR:OG1	2.55	0.54
14:N:20:THR:CG2	14:N:31:THR:OG1	2.55	0.54
8:H:3:ILE:HG21	8:H:44:ALA:HB3	1.89	0.54
1:O:122:THR:CG2	2:P:128:ARG:HH21	2.20	0.54
7:U:187:GLU:HG2	7:U:192:LYS:CB	2.37	0.54
2:B:155:ASN:ND2	3:C:77:ASN:HB2	2.23	0.54
6:F:172:LEU:HD13	6:F:195:ILE:CD1	2.37	0.54
5:E:87:LEU:HD21	5:E:107:ALA:HB1	1.88	0.54
9:I:170:LEU:C	9:I:170:LEU:HD23	2.33	0.54
10:J:1:MET:HB3	10:J:34:LYS:HE3	1.90	0.54
10:X:1:MET:CG	10:X:34:LYS:HE3	2.39	0.53
4:R:138:GLY:HA2	4:R:214:ILE:HG12	1.91	0.53
7:G:187:GLU:HG2	7:G:192:LYS:CB	2.37	0.53
10:X:1:MET:HB3	10:X:34:LYS:HE3	1.89	0.53
4:R:99:ILE:HD11	4:R:104:LEU:HB2	1.90	0.53
10:J:168:LEU:O	10:J:172:MET:HB2	2.09	0.53
4:D:138:GLY:HA2	4:D:214:ILE:HG12	1.90	0.53
12:Z:146:ILE:HG22	12:Z:150:LEU:HD22	1.90	0.53
4:D:99:ILE:HD11	4:D:104:LEU:HB2	1.91	0.53
1:A:122:THR:CG2	2:B:128:ARG:HH21	2.22	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:176:GLU:HG3	2:B:55:LEU:HD22	1.92	0.52
6:F:123:ASN:C	6:F:123:ASN:HD22	2.17	0.52
12:L:189:THR:HG22	8:V:196:ARG:HH11	1.74	0.52
9:I:10:ILE:HG21	9:I:141:ALA:HB3	1.92	0.52
6:T:123:ASN:C	6:T:123:ASN:HD22	2.17	0.52
3:C:175:LYS:HG3	3:C:176:ASN:ND2	2.25	0.52
3:C:201:VAL:O	3:C:202:GLN:HB2	2.09	0.52
10:J:1:MET:CG	10:J:34:LYS:HE3	2.39	0.52
14:N:13:ILE:CG2	14:N:175:MET:HE2	2.39	0.52
10:X:168:LEU:O	10:X:172:MET:HB2	2.09	0.52
9:W:98:ARG:HD2	9:W:126:ILE:HG12	1.93	0.51
3:Q:175:LYS:HG3	3:Q:176:ASN:ND2	2.25	0.51
14:b:176:VAL:HG12	14:b:178:LEU:HD13	1.93	0.51
3:Q:201:VAL:O	3:Q:202:GLN:HB2	2.09	0.51
5:E:9:THR:HG21	5:E:119:THR:HA	1.92	0.51
9:I:101:PRO:HB3	9:I:126:ILE:HD12	1.93	0.51
14:N:176:VAL:HG12	14:N:178:LEU:HD13	1.93	0.51
5:S:9:THR:HG21	5:S:119:THR:HA	1.92	0.51
9:W:101:PRO:HB3	9:W:126:ILE:HD12	1.93	0.51
8:V:63:ILE:HG23	8:V:74:PRO:HB3	1.93	0.50
9:W:10:ILE:HG21	9:W:141:ALA:HB3	1.92	0.50
14:N:83:LYS:HG3	14:N:119:VAL:HG23	1.93	0.50
9:W:187:TYR:OH	9:W:196:LYS:HE3	2.11	0.50
12:L:189:THR:HG22	8:V:196:ARG:NH1	2.26	0.50
9:I:98:ARG:HD2	9:I:126:ILE:HG12	1.93	0.50
11:K:29:GLN:NE2	17:K:476:HOH:O	2.30	0.50
3:C:4:ARG:HG2	4:D:117:GLU:OE1	2.11	0.50
8:V:215:GLU:HG2	9:W:197:ARG:HG2	1.93	0.50
14:b:83:LYS:HG3	14:b:119:VAL:HG23	1.93	0.50
8:H:63:ILE:HG23	8:H:74:PRO:HB3	1.93	0.49
8:H:196:ARG:HH11	12:Z:189:THR:HG22	1.77	0.49
2:B:63:GLU:HG2	2:B:64:LYS:HG2	1.94	0.49
3:C:160:GLN:HE22	3:C:170:ARG:HE	1.60	0.49
8:V:222:ASP:OD1	9:W:74:LYS:NZ	2.45	0.49
2:P:63:GLU:HG2	2:P:64:LYS:HG2	1.94	0.49
1:A:122:THR:HG23	2:B:128:ARG:HH21	1.78	0.49
10:X:16:ALA:HB2	10:X:161:LEU:HD21	1.94	0.49
3:C:205:ALA:C	3:C:207:ASN:H	2.21	0.49
6:F:198:LEU:HD12	6:F:243:ILE:HG22	1.93	0.49
9:I:187:TYR:OH	9:I:196:LYS:HE3	2.12	0.49
8:H:222:ASP:OD1	9:I:74:LYS:NZ	2.45	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Q:205:ALA:C	3:Q:207:ASN:H	2.21	0.49
3:Q:160:GLN:HE22	3:Q:170:ARG:HE	1.60	0.49
9:I:65:MET:HE1	9:I:93:SER:HB3	1.95	0.49
3:C:202:GLN:HG3	3:C:203:THR:H	1.78	0.48
10:J:16:ALA:HB2	10:J:161:LEU:HD21	1.94	0.48
10:X:1:MET:HB3	10:X:34:LYS:CE	2.43	0.48
8:H:215:GLU:HG2	9:I:197:ARG:HG2	1.95	0.48
14:b:13:ILE:CG2	14:b:175:MET:HE2	2.40	0.48
10:J:1:MET:HB3	10:J:34:LYS:CE	2.44	0.48
3:Q:202:GLN:HG3	3:Q:203:THR:H	1.78	0.48
6:T:198:LEU:HD12	6:T:243:ILE:HG22	1.93	0.48
6:T:202:ASP:OD1	6:T:202:ASP:N	2.44	0.48
7:G:167:GLN:HE21	7:G:171:THR:HG23	1.78	0.48
10:J:93:ARG:NH1	17:J:407:HOH:O	2.43	0.48
8:H:196:ARG:NH1	12:Z:189:THR:HG22	2.29	0.48
13:M:2:GLN:NE2	17:M:459:HOH:O	2.47	0.48
6:F:202:ASP:OD1	6:F:202:ASP:N	2.43	0.48
7:U:187:GLU:HG2	7:U:192:LYS:HB2	1.96	0.48
7:G:187:GLU:HG2	7:G:192:LYS:HB2	1.96	0.47
9:W:65:MET:HE1	9:W:93:SER:HB3	1.95	0.47
7:U:187:GLU:HG2	7:U:192:LYS:HB3	1.96	0.47
11:Y:32:LYS:HB3	11:Y:32:LYS:HE2	1.72	0.47
5:E:170:TYR:CD1	5:E:170:TYR:C	2.93	0.47
11:K:128:CYS:HB2	11:K:137:TYR:CZ	2.50	0.47
5:S:170:TYR:CD1	5:S:170:TYR:C	2.93	0.47
7:U:167:GLN:HE21	7:U:171:THR:HG23	1.80	0.47
7:G:187:GLU:HG2	7:G:192:LYS:HB3	1.96	0.47
10:J:91:SER:O	10:J:94:SER:HB2	2.15	0.47
8:H:196:ARG:NH2	9:I:150:GLU:HG3	2.29	0.47
2:P:151:ASN:HB2	2:P:152:PRO:CD	2.45	0.47
9:W:26:LEU:HD21	9:W:185:VAL:HG23	1.96	0.47
8:V:35:HIS:HB3	8:V:56:THR:HG21	1.97	0.47
10:X:149:ARG:O	10:X:152:MET:HG3	2.15	0.47
8:V:35:HIS:CB	8:V:56:THR:HG21	2.45	0.46
3:C:120:GLN:NE2	17:C:323:HOH:O	2.47	0.46
9:I:26:LEU:HD21	9:I:185:VAL:HG23	1.96	0.46
11:Y:128:CYS:HB2	11:Y:137:TYR:CZ	2.50	0.46
2:B:151:ASN:HB2	2:B:152:PRO:CD	2.45	0.46
8:H:35:HIS:CB	8:H:56:THR:HG21	2.45	0.46
4:D:160:ASN:HB3	4:D:179:TRP:CE2	2.51	0.46
8:H:35:HIS:HB3	8:H:56:THR:HG21	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:R:160:ASN:HB3	4:R:179:TRP:CE2	2.51	0.46
10:J:149:ARG:O	10:J:152:MET:HG3	2.16	0.46
10:X:91:SER:O	10:X:94:SER:HB2	2.15	0.46
1:A:176:GLU:CG	2:B:55:LEU:HD22	2.46	0.45
3:Q:45:GLU:HG3	3:Q:201:VAL:HG23	1.99	0.45
5:E:68:HIS:HE1	5:E:102:LEU:O	1.99	0.45
8:H:192:THR:O	8:H:192:THR:HG22	2.16	0.45
9:I:20:VAL:HG13	9:I:118:PRO:HB3	1.98	0.45
4:R:1:ASP:O	4:R:2:ARG:HB2	2.16	0.45
5:E:178:PHE:HA	5:E:181:ILE:HG13	1.99	0.45
6:F:216:SER:HB3	6:F:219:GLU:HB2	1.97	0.45
5:S:68:HIS:HE1	5:S:102:LEU:O	1.99	0.45
8:H:84:LYS:HA	8:H:113:ILE:HD11	1.99	0.45
4:R:59:ILE:HG22	4:R:220:PHE:HZ	1.81	0.45
5:S:153:THR:HG21	6:T:55:LEU:CD2	2.47	0.45
2:B:95:GLN:HE22	9:I:71:ASN:HD22	1.63	0.45
5:S:42:HIS:HB2	5:S:188:LEU:HD12	1.99	0.45
5:S:178:PHE:HA	5:S:181:ILE:HG13	1.99	0.45
6:T:216:SER:HB3	6:T:219:GLU:HB2	1.97	0.45
9:W:20:VAL:HG13	9:W:118:PRO:HB3	1.99	0.45
3:C:45:GLU:HG3	3:C:201:VAL:HG23	1.99	0.45
6:F:97:LYS:NZ	14:N:84:GLU:OE1	2.48	0.45
8:V:192:THR:HG22	8:V:192:THR:O	2.16	0.45
6:F:146:MET:HE3	6:F:161:THR:HB	1.95	0.44
8:H:104:ASP:HB2	8:H:105:PRO:CD	2.47	0.44
2:P:3:ARG:HB3	5:S:122:TYR:OH	2.17	0.44
6:T:2:THR:HA	6:T:4:TYR:CD2	2.52	0.44
12:Z:31:THR:CG2	12:Z:36:ASN:HD21	2.31	0.44
4:D:59:ILE:HG22	4:D:220:PHE:HZ	1.82	0.44
13:M:127:LEU:HG	13:M:142:LEU:HD12	1.99	0.44
6:T:240:GLN:HE21	6:T:240:GLN:CA	2.28	0.44
8:V:104:ASP:HB2	8:V:105:PRO:CD	2.47	0.44
13:M:93:PHE:CZ	13:M:128:ARG:HG2	2.52	0.44
2:P:145:TYR:OH	2:P:217:LYS:N	2.50	0.44
6:T:146:MET:HE3	6:T:161:THR:HB	1.95	0.44
7:U:61:SER:OG	7:U:215:GLU:OE2	2.28	0.44
14:b:36:ARG:HG3	14:b:42:TRP:CE2	2.53	0.44
8:H:98:LEU:HB2	8:H:113:ILE:CG2	2.48	0.44
2:B:52:THR:CG2	2:B:53:SER:N	2.49	0.44
12:L:31:THR:CG2	12:L:36:ASN:HD21	2.31	0.44
10:X:1:MET:CB	10:X:34:LYS:CE	2.95	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:1:ASP:O	4:D:2:ARG:HB2	2.16	0.44
8:V:98:LEU:HB2	8:V:113:ILE:CG2	2.48	0.44
10:J:1:MET:CB	10:J:34:LYS:CE	2.95	0.44
5:S:226:GLY:O	5:S:229:VAL:HG22	2.18	0.44
12:L:125:PHE:CD2	12:L:131:TYR:HB3	2.53	0.44
14:N:36:ARG:HG3	14:N:42:TRP:CE2	2.53	0.44
13:a:159:VAL:HG23	13:a:159:VAL:O	2.18	0.44
8:V:106:THR:HG22	8:V:109:HIS:NE2	2.33	0.43
8:V:196:ARG:NH2	9:W:150:GLU:HG3	2.32	0.43
13:a:93:PHE:CZ	13:a:128:ARG:HG2	2.53	0.43
3:C:135:GLY:HA2	3:C:213:VAL:HG21	2.01	0.43
5:E:42:HIS:HB2	5:E:188:LEU:HD12	1.99	0.43
3:Q:135:GLY:HA2	3:Q:213:VAL:HG21	2.00	0.43
12:Z:125:PHE:CD2	12:Z:131:TYR:HB3	2.54	0.43
13:a:127:LEU:HG	13:a:142:LEU:HD12	1.99	0.43
1:O:23:TYR:CD1	7:U:12:PRO:HA	2.53	0.43
8:V:84:LYS:HA	8:V:113:ILE:HD11	1.99	0.43
6:F:240:GLN:HE21	6:F:240:GLN:CA	2.28	0.43
1:O:122:THR:HG23	2:P:128:ARG:HH21	1.82	0.43
3:Q:120:GLN:NE2	17:Q:330:HOH:O	2.51	0.43
6:F:2:THR:HA	6:F:4:TYR:CD2	2.53	0.43
8:H:106:THR:HG22	8:H:109:HIS:NE2	2.33	0.43
5:S:28:ILE:HD11	5:S:148:PRO:CD	2.48	0.43
2:B:8:ARG:HD2	3:C:4:ARG:NH2	2.33	0.43
2:B:145:TYR:OH	2:B:217:LYS:N	2.50	0.43
8:H:196:ARG:NH2	9:I:150:GLU:O	2.52	0.43
1:O:55:LEU:HB3	7:U:159:ALA:O	2.19	0.43
7:U:72:MET:HE3	7:U:74:VAL:CG2	2.49	0.43
8:V:99:ILE:HG13	8:V:127:LEU:HD22	2.01	0.43
14:N:152:VAL:HA	14:N:175:MET:HE1	2.00	0.43
8:V:114:HIS:CD2	8:V:116:HIS:H	2.35	0.43
14:b:152:VAL:HA	14:b:175:MET:HE1	2.00	0.43
8:H:225:GLU:O	8:H:226:GLU:HB2	2.19	0.43
8:H:84:LYS:HE2	8:H:119:THR:HG23	2.01	0.43
12:Z:23:LEU:HD13	12:Z:43:VAL:HG13	2.01	0.43
12:L:71:SER:OG	12:L:92:ASN:OD1	2.32	0.42
5:E:226:GLY:O	5:E:229:VAL:HG22	2.18	0.42
7:G:72:MET:HE3	7:G:74:VAL:CG2	2.49	0.42
8:H:165:ASN:HD22	13:a:156:ARG:HH11	1.67	0.42
13:M:159:VAL:HG23	13:M:159:VAL:O	2.18	0.42
7:G:78:ILE:N	7:G:79:PRO:CD	2.82	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:156:ARG:HH11	8:V:165:ASN:HD22	1.66	0.42
3:Q:180:LYS:NZ	3:Q:180:LYS:HB2	2.34	0.42
4:R:51:LEU:C	4:R:51:LEU:HD12	2.45	0.42
8:H:99:ILE:HG13	8:H:127:LEU:HD22	2.01	0.42
11:Y:12:ILE:HB	11:Y:180:VAL:HB	2.02	0.42
3:C:149:GLU:HB2	3:C:150:PRO:HD2	2.01	0.42
13:M:27:LEU:HB2	13:M:192:SER:HB3	2.02	0.42
13:M:43:ILE:HA	13:M:44:PRO:HD3	1.93	0.42
3:Q:4:ARG:HG2	4:R:117:GLU:OE1	2.19	0.42
2:B:217:LYS:C	2:B:219:ALA:N	2.77	0.42
3:C:35:LYS:HG2	3:C:158:SER:O	2.19	0.42
6:F:165:ARG:HE	6:F:165:ARG:HB3	1.61	0.42
7:G:61:SER:OG	7:G:215:GLU:OE2	2.28	0.42
7:U:78:ILE:N	7:U:79:PRO:CD	2.82	0.42
5:E:28:ILE:HD11	5:E:148:PRO:CD	2.49	0.42
3:Q:35:LYS:HG2	3:Q:158:SER:O	2.19	0.42
5:S:174:THR:O	5:S:175:LEU:C	2.62	0.42
7:U:34:LEU:C	7:U:34:LEU:CD2	2.93	0.42
7:G:34:LEU:C	7:G:34:LEU:CD2	2.92	0.42
10:J:3:ILE:HD12	10:J:168:LEU:HD13	2.02	0.42
11:K:7:ARG:HD2	11:K:110:PRO:O	2.20	0.42
6:T:198:LEU:CD1	6:T:243:ILE:HG22	2.50	0.42
14:b:35:THR:HG22	17:b:203:HOH:O	2.19	0.42
8:H:50:ALA:CB	9:I:126:ILE:HG23	2.49	0.42
11:K:12:ILE:HB	11:K:180:VAL:HB	2.02	0.42
5:S:210:LEU:HD23	5:S:229:VAL:HB	2.02	0.42
3:C:180:LYS:HB2	3:C:180:LYS:NZ	2.34	0.42
2:P:124:HIS:HB3	3:Q:124:VAL:HG12	2.02	0.42
4:R:185:LEU:O	4:R:189:GLU:HG3	2.19	0.42
4:D:185:LEU:O	4:D:189:GLU:HG3	2.20	0.41
5:E:71:LEU:C	5:E:71:LEU:CD2	2.93	0.41
5:E:210:LEU:HD23	5:E:229:VAL:HB	2.02	0.41
8:H:87:LEU:HD12	8:H:113:ILE:HD11	2.02	0.41
4:R:77:ALA:O	4:R:81:ILE:HG12	2.20	0.41
8:V:84:LYS:HE2	8:V:119:THR:HG23	2.02	0.41
8:V:196:ARG:NH2	9:W:150:GLU:O	2.53	0.41
11:Y:7:ARG:HD2	11:Y:110:PRO:O	2.20	0.41
1:A:194:LEU:HD23	1:A:250:LEU:HD13	2.03	0.41
4:D:149:HIS:O	4:D:156:PHE:HA	2.20	0.41
6:F:198:LEU:CD1	6:F:243:ILE:HG22	2.50	0.41
8:H:87:LEU:HD12	8:H:113:ILE:CD1	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:S:71:LEU:C	5:S:71:LEU:CD2	2.93	0.41
5:S:92:ASN:HD21	12:Z:70:ASN:HD21	1.68	0.41
8:V:87:LEU:HD12	8:V:113:ILE:CD1	2.50	0.41
13:a:27:LEU:HB2	13:a:192:SER:HB3	2.01	0.41
7:G:83:ASN:C	7:G:83:ASN:HD22	2.29	0.41
12:L:23:LEU:HD13	12:L:43:VAL:HG13	2.02	0.41
4:R:149:HIS:O	4:R:156:PHE:HA	2.20	0.41
5:S:155:LEU:HD13	5:S:158:THR:HB	2.03	0.41
12:Z:195:HIS:HD2	12:Z:197:GLN:H	1.67	0.41
13:M:96:LEU:O	13:M:100:MET:HG2	2.21	0.41
3:Q:149:GLU:HB2	3:Q:150:PRO:HD2	2.01	0.41
8:V:20:SER:OG	8:V:28:ASP:HB3	2.20	0.41
13:M:150:MET:HE1	13:M:187:ARG:HG2	2.03	0.41
2:P:93:HIS:CE1	2:P:113:ARG:HG2	2.55	0.41
6:T:99:TYR:O	6:T:100:LYS:HB3	2.20	0.41
4:D:77:ALA:O	4:D:81:ILE:HG12	2.20	0.41
5:E:174:THR:O	5:E:175:LEU:C	2.62	0.41
6:T:169:LYS:O	6:T:173:GLU:HG3	2.21	0.41
7:U:83:ASN:C	7:U:83:ASN:HD22	2.29	0.41
7:U:196:PHE:CD1	7:U:196:PHE:C	2.99	0.41
4:D:126:MET:HE1	4:D:130:PHE:CE2	2.56	0.41
5:E:153:THR:HG21	6:F:55:LEU:CD2	2.50	0.41
6:F:99:TYR:O	6:F:100:LYS:HB3	2.20	0.41
8:H:20:SER:OG	8:H:28:ASP:HB3	2.20	0.41
11:K:4:LEU:HD13	11:K:161:ILE:HD11	2.03	0.41
12:L:8:ASN:HA	12:L:30:ILE:O	2.21	0.41
12:L:195:HIS:HD2	12:L:197:GLN:H	1.68	0.41
2:P:42:GLY:HA3	2:P:185:VAL:HG21	2.03	0.41
4:R:126:MET:HE1	4:R:130:PHE:CE2	2.56	0.41
8:V:225:GLU:O	8:V:226:GLU:HB2	2.19	0.41
9:W:94:LEU:HD11	9:W:106:PRO:HG2	2.03	0.41
10:X:3:ILE:HD12	10:X:168:LEU:HD13	2.02	0.41
6:F:169:LYS:O	6:F:173:GLU:HG3	2.20	0.41
9:I:20:VAL:HG23	9:I:189:ILE:HB	2.03	0.41
2:P:47:ALA:HB1	2:P:64:LYS:HD3	2.03	0.41
3:Q:161:THR:HG21	3:Q:169:VAL:HG22	2.03	0.41
2:B:47:ALA:HB1	2:B:64:LYS:HD3	2.04	0.40
2:B:93:HIS:CE1	2:B:113:ARG:HG2	2.56	0.40
6:T:48:LYS:HG2	6:T:62:LYS:HD2	2.03	0.40
12:Z:213:ARG:HG2	12:Z:214:LYS:N	2.36	0.40
12:L:173:LYS:HA	12:L:173:LYS:HD3	1.89	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:213:ARG:HG2	12:L:214:LYS:N	2.36	0.40
5:S:153:THR:CG2	6:T:55:LEU:CD2	3.00	0.40
6:T:78:ILE:HB	6:T:79:PRO:HD3	2.04	0.40
6:T:200:HIS:O	6:T:200:HIS:CG	2.74	0.40
11:Y:86:LEU:HD13	11:Y:86:LEU:C	2.47	0.40
2:B:66:TYR:CG	2:B:87:ILE:HD13	2.56	0.40
2:B:168:THR:O	2:B:172:GLN:HB2	2.21	0.40
4:D:51:LEU:HD12	4:D:51:LEU:C	2.45	0.40
6:F:48:LYS:HG2	6:F:62:LYS:HD2	2.03	0.40
8:V:8:PHE:HB3	8:V:151:ALA:HB2	2.03	0.40
2:B:12:PHE:N	3:C:17:GLN:HE22	2.11	0.40
3:C:161:THR:HG21	3:C:169:VAL:HG22	2.03	0.40
9:I:94:LEU:HD11	9:I:106:PRO:HG2	2.03	0.40
14:N:155:ILE:HG21	14:N:175:MET:HE3	2.03	0.40
1:O:194:LEU:HD23	1:O:250:LEU:HD13	2.03	0.40
3:Q:149:GLU:HB2	3:Q:150:PRO:CD	2.51	0.40
8:V:87:LEU:HD12	8:V:113:ILE:HD11	2.02	0.40
8:V:218:VAL:CG2	9:W:196:LYS:HB2	2.52	0.40
11:Y:4:LEU:HD13	11:Y:161:ILE:HD11	2.03	0.40
13:a:96:LEU:O	13:a:100:MET:HG2	2.21	0.40
14:b:155:ILE:HG21	14:b:175:MET:HE3	2.03	0.40
8:H:8:PHE:HB3	8:H:151:ALA:HB2	2.03	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	247/250 (99%)	241 (98%)	5 (2%)	1 (0%)	30	28
1	O	247/250 (99%)	240 (97%)	6 (2%)	1 (0%)	30	28
2	B	242/258 (94%)	232 (96%)	9 (4%)	1 (0%)	30	28

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	P	242/258 (94%)	232 (96%)	9 (4%)	1 (0%)	30	28
3	C	238/254 (94%)	228 (96%)	6 (2%)	4 (2%)	7	3
3	Q	238/254 (94%)	228 (96%)	6 (2%)	4 (2%)	7	3
4	D	231/260 (89%)	230 (100%)	0	1 (0%)	30	28
4	R	231/260 (89%)	230 (100%)	0	1 (0%)	30	28
5	E	229/234 (98%)	218 (95%)	11 (5%)	0	100	100
5	S	229/234 (98%)	218 (95%)	11 (5%)	0	100	100
6	F	241/288 (84%)	234 (97%)	7 (3%)	0	100	100
6	T	241/288 (84%)	233 (97%)	8 (3%)	0	100	100
7	G	239/252 (95%)	238 (100%)	1 (0%)	0	100	100
7	U	239/252 (95%)	238 (100%)	1 (0%)	0	100	100
8	H	224/232 (97%)	218 (97%)	6 (3%)	0	100	100
8	V	224/232 (97%)	218 (97%)	6 (3%)	0	100	100
9	I	202/205 (98%)	197 (98%)	5 (2%)	0	100	100
9	W	202/205 (98%)	197 (98%)	5 (2%)	0	100	100
10	J	193/198 (98%)	187 (97%)	5 (3%)	1 (0%)	24	22
10	X	193/198 (98%)	187 (97%)	5 (3%)	1 (0%)	24	22
11	K	209/212 (99%)	206 (99%)	3 (1%)	0	100	100
11	Y	209/212 (99%)	206 (99%)	3 (1%)	0	100	100
12	L	220/222 (99%)	215 (98%)	5 (2%)	0	100	100
12	Z	220/222 (99%)	215 (98%)	5 (2%)	0	100	100
13	M	231/246 (94%)	220 (95%)	11 (5%)	0	100	100
13	a	231/246 (94%)	221 (96%)	10 (4%)	0	100	100
14	N	194/196 (99%)	189 (97%)	5 (3%)	0	100	100
14	b	194/196 (99%)	189 (97%)	5 (3%)	0	100	100
All	All	6280/6614 (95%)	6105 (97%)	159 (2%)	16 (0%)	36	36

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	202	GLN
3	C	205	ALA
3	Q	202	GLN

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Mol	Chain	Res	Type
3	Q	205	ALA
2	B	51	VAL
4	D	2	ARG
2	P	51	VAL
4	R	2	ARG
3	C	239	GLN
3	Q	239	GLN
1	A	166	LYS
1	O	166	LYS
10	J	24	GLY
10	X	24	GLY
3	C	183	PRO
3	Q	183	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	208/209 (100%)	198 (95%)	10 (5%)	23	23
1	O	208/209 (100%)	198 (95%)	10 (5%)	23	23
2	B	203/216 (94%)	187 (92%)	16 (8%)	11	9
2	P	203/216 (94%)	186 (92%)	17 (8%)	10	7
3	C	212/226 (94%)	186 (88%)	26 (12%)	4	2
3	Q	212/226 (94%)	186 (88%)	26 (12%)	4	2
4	D	194/215 (90%)	176 (91%)	18 (9%)	8	6
4	R	194/215 (90%)	176 (91%)	18 (9%)	8	6
5	E	190/193 (98%)	172 (90%)	18 (10%)	8	5
5	S	190/193 (98%)	172 (90%)	18 (10%)	8	5
6	F	201/239 (84%)	183 (91%)	18 (9%)	9	6
6	T	201/239 (84%)	183 (91%)	18 (9%)	9	6
7	G	206/210 (98%)	193 (94%)	13 (6%)	16	14
7	U	206/210 (98%)	193 (94%)	13 (6%)	16	14

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
8	H	185/190 (97%)	173 (94%)	12 (6%)	15	13
8	V	185/190 (97%)	172 (93%)	13 (7%)	14	11
9	I	172/173 (99%)	166 (96%)	6 (4%)	32	35
9	W	172/173 (99%)	166 (96%)	6 (4%)	32	35
10	J	173/175 (99%)	162 (94%)	11 (6%)	16	14
10	X	173/175 (99%)	163 (94%)	10 (6%)	18	16
11	K	168/169 (99%)	160 (95%)	8 (5%)	23	23
11	Y	168/169 (99%)	160 (95%)	8 (5%)	23	23
12	L	185/185 (100%)	174 (94%)	11 (6%)	18	16
12	Z	185/185 (100%)	174 (94%)	11 (6%)	18	16
13	M	199/208 (96%)	188 (94%)	11 (6%)	19	18
13	a	199/208 (96%)	187 (94%)	12 (6%)	17	15
14	N	162/162 (100%)	153 (94%)	9 (6%)	19	18
14	b	162/162 (100%)	153 (94%)	9 (6%)	19	18
All	All	5316/5540 (96%)	4940 (93%)	376 (7%)	13	11

All (376) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	29	LYS
1	A	59	GLU
1	A	122	THR
1	A	157	PHE
1	A	166	LYS
1	A	172	LYS
1	A	201	GLU
1	A	231	LYS
1	A	248	GLU
1	A	250	LEU
2	B	50	LYS
2	B	51	VAL
2	B	55	LEU
2	B	63	GLU
2	B	64	LYS
2	B	65	LEU
2	B	79	LEU
2	B	102	ASN

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Mol	Chain	Res	Type
2	B	113	ARG
2	B	114	LEU
2	B	185	VAL
2	B	191	LEU
2	B	203	SER
2	B	217	LYS
2	B	237	ILE
2	B	238	LEU
3	C	4	ARG
3	C	35	LYS
3	C	38	ASN
3	C	48	SER
3	C	49	THR
3	C	50	LEU
3	C	52	LEU
3	C	53	GLN
3	C	58	THR
3	C	69	VAL
3	C	107	LEU
3	C	147	GLN
3	C	160	GLN
3	C	167	LYS
3	C	169	VAL
3	C	175	LYS
3	C	180	LYS
3	C	187	GLU
3	C	200	VAL
3	C	201	VAL
3	C	203	THR
3	C	206	LYS
3	C	213	VAL
3	C	222	LEU
3	C	238	LYS
3	C	240	GLU
4	D	20	LEU
4	D	40	LEU
4	D	51	LEU
4	D	60	VAL
4	D	99	ILE
4	D	169	GLU
4	D	174	GLU
4	D	176	LEU

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Mol	Chain	Res	Type
4	D	190	LEU
4	D	193	LEU
4	D	202	GLU
4	D	203	LYS
4	D	214	ILE
4	D	217	GLN
4	D	233	LYS
4	D	235	LEU
4	D	236	LYS
4	D	242	GLU
5	E	3	ASN
5	E	4	ASN
5	E	9	THR
5	E	25	LEU
5	E	29	LYS
5	E	54	GLU
5	E	55	LEU
5	E	71	LEU
5	E	92	ASN
5	E	106	ARG
5	E	144	LEU
5	E	188	LEU
5	E	207	VAL
5	E	208	ASP
5	E	217	LYS
5	E	222	THR
5	E	231	LYS
5	E	233	ILE
6	F	68	ARG
6	F	94	SER
6	F	117	GLN
6	F	123	ASN
6	F	139	LYS
6	F	165	ARG
6	F	171	GLU
6	F	172	LEU
6	F	181	GLU
6	F	201	GLU
6	F	202	ASP
6	F	206	LYS
6	F	207	ASP
6	F	215	CYS

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Mol	Chain	Res	Type
6	F	221	ASN
6	F	240	GLN
6	F	241	LYS
6	F	243	ILE
7	G	13	GLU
7	G	26	THR
7	G	34	LEU
7	G	83	ASN
7	G	115	LEU
7	G	122	ARG
7	G	125	MET
7	G	166	GLN
7	G	208	GLU
7	G	221	LYS
7	G	235	ARG
7	G	236	LEU
7	G	242	GLN
8	H	13	VAL
8	H	30	ASN
8	H	34	LEU
8	H	55	VAL
8	H	56	THR
8	H	63	ILE
8	H	106	THR
8	H	127	LEU
8	H	144	GLN
8	H	153	LYS
8	H	196	ARG
8	H	201	LYS
9	I	37	ASN
9	I	96	GLU
9	I	114	LYS
9	I	126	ILE
9	I	133	LYS
9	I	171	LEU
10	J	1	MET
10	J	2	ASP
10	J	3	ILE
10	J	23	ARG
10	J	35	THR
10	J	90	LYS
10	J	99	GLN

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Mol	Chain	Res	Type
10	J	110	LYS
10	J	126	VAL
10	J	172	MET
10	J	186	LYS
11	K	4	LEU
11	K	9	GLN
11	K	35	ILE
11	K	57	THR
11	K	116	ASP
11	K	128	CYS
11	K	140	LEU
11	K	148	LEU
12	L	18	GLU
12	L	23	LEU
12	L	31	THR
12	L	42	LYS
12	L	49	ASN
12	L	66	LYS
12	L	71	SER
12	L	108	HIS
12	L	136	CYS
12	L	172	LEU
12	L	173	LYS
13	M	2	GLN
13	M	43	ILE
13	M	48	ASN
13	M	70	LEU
13	M	73	GLU
13	M	104	ARG
13	M	138	SER
13	M	161	ARG
13	M	187	ARG
13	M	192	SER
13	M	212	LEU
14	N	9	LYS
14	N	20	THR
14	N	36	ARG
14	N	44	CYS
14	N	104	ASP
14	N	107	LYS
14	N	115	LEU
14	N	160	SER

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Mol	Chain	Res	Type
14	N	178	LEU
1	O	29	LYS
1	O	59	GLU
1	O	122	THR
1	O	157	PHE
1	O	166	LYS
1	O	172	LYS
1	O	201	GLU
1	O	231	LYS
1	O	248	GLU
1	O	250	LEU
2	P	48	GLU
2	P	50	LYS
2	P	51	VAL
2	P	55	LEU
2	P	63	GLU
2	P	64	LYS
2	P	65	LEU
2	P	79	LEU
2	P	102	ASN
2	P	113	ARG
2	P	114	LEU
2	P	185	VAL
2	P	191	LEU
2	P	203	SER
2	P	217	LYS
2	P	237	ILE
2	P	238	LEU
3	Q	4	ARG
3	Q	35	LYS
3	Q	38	ASN
3	Q	48	SER
3	Q	49	THR
3	Q	50	LEU
3	Q	52	LEU
3	Q	53	GLN
3	Q	58	THR
3	Q	69	VAL
3	Q	107	LEU
3	Q	147	GLN
3	Q	160	GLN
3	Q	167	LYS

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Mol	Chain	Res	Type
3	Q	169	VAL
3	Q	175	LYS
3	Q	180	LYS
3	Q	187	GLU
3	Q	200	VAL
3	Q	201	VAL
3	Q	203	THR
3	Q	206	LYS
3	Q	213	VAL
3	Q	222	LEU
3	Q	238	LYS
3	Q	240	GLU
4	R	20	LEU
4	R	40	LEU
4	R	51	LEU
4	R	60	VAL
4	R	99	ILE
4	R	169	GLU
4	R	174	GLU
4	R	176	LEU
4	R	190	LEU
4	R	193	LEU
4	R	202	GLU
4	R	203	LYS
4	R	214	ILE
4	R	217	GLN
4	R	233	LYS
4	R	235	LEU
4	R	236	LYS
4	R	242	GLU
5	S	3	ASN
5	S	4	ASN
5	S	9	THR
5	S	25	LEU
5	S	29	LYS
5	S	54	GLU
5	S	55	LEU
5	S	71	LEU
5	S	92	ASN
5	S	106	ARG
5	S	144	LEU
5	S	188	LEU

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Mol	Chain	Res	Type
5	S	207	VAL
5	S	208	ASP
5	S	217	LYS
5	S	222	THR
5	S	231	LYS
5	S	233	ILE
6	T	68	ARG
6	T	94	SER
6	T	117	GLN
6	T	123	ASN
6	T	139	LYS
6	T	165	ARG
6	T	171	GLU
6	T	172	LEU
6	T	181	GLU
6	T	201	GLU
6	T	202	ASP
6	T	206	LYS
6	T	207	ASP
6	T	215	CYS
6	T	221	ASN
6	T	240	GLN
6	T	241	LYS
6	T	243	ILE
7	U	13	GLU
7	U	26	THR
7	U	34	LEU
7	U	83	ASN
7	U	115	LEU
7	U	122	ARG
7	U	125	MET
7	U	166	GLN
7	U	208	GLU
7	U	221	LYS
7	U	235	ARG
7	U	236	LEU
7	U	242	GLN
8	V	13	VAL
8	V	30	ASN
8	V	34	LEU
8	V	55	VAL
8	V	56	THR

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Mol	Chain	Res	Type
8	V	63	ILE
8	V	68	LEU
8	V	106	THR
8	V	127	LEU
8	V	144	GLN
8	V	153	LYS
8	V	196	ARG
8	V	201	LYS
9	W	37	ASN
9	W	96	GLU
9	W	114	LYS
9	W	126	ILE
9	W	133	LYS
9	W	171	LEU
10	X	1	MET
10	X	2	ASP
10	X	3	ILE
10	X	23	ARG
10	X	35	THR
10	X	90	LYS
10	X	99	GLN
10	X	110	LYS
10	X	126	VAL
10	X	172	MET
11	Y	4	LEU
11	Y	9	GLN
11	Y	35	ILE
11	Y	57	THR
11	Y	116	ASP
11	Y	128	CYS
11	Y	140	LEU
11	Y	148	LEU
12	Z	18	GLU
12	Z	23	LEU
12	Z	31	THR
12	Z	42	LYS
12	Z	49	ASN
12	Z	71	SER
12	Z	108	HIS
12	Z	136	CYS
12	Z	150	LEU
12	Z	172	LEU

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Mol	Chain	Res	Type
12	Z	173	LYS
13	a	2	GLN
13	a	43	ILE
13	a	48	ASN
13	a	70	LEU
13	a	73	GLU
13	a	104	ARG
13	a	106	LYS
13	a	138	SER
13	a	161	ARG
13	a	187	ARG
13	a	192	SER
13	a	212	LEU
14	b	9	LYS
14	b	20	THR
14	b	36	ARG
14	b	44	CYS
14	b	104	ASP
14	b	107	LYS
14	b	115	LEU
14	b	160	SER
14	b	178	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (157) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	30	GLN
1	A	94	HIS
2	B	20	GLN
2	B	95	GLN
2	B	119	GLN
2	B	123	GLN
2	B	155	ASN
2	B	176	GLN
3	C	17	GLN
3	C	38	ASN
3	C	53	GLN
3	C	77	ASN
3	C	116	GLN
3	C	120	GLN
3	C	147	GLN
3	C	160	GLN

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Mol	Chain	Res	Type
4	D	15	GLN
4	D	91	HIS
4	D	100	ASN
4	D	106	GLN
4	D	207	ASN
4	D	225	ASN
5	E	68	HIS
5	E	99	ASN
5	E	116	GLN
5	E	118	ASN
5	E	120	GLN
5	E	151	ASN
6	F	19	GLN
6	F	86	ASN
6	F	117	GLN
6	F	123	ASN
6	F	191	GLN
6	F	203	ASN
6	F	240	GLN
7	G	30	ASN
7	G	83	ASN
7	G	114	ASN
7	G	117	GLN
7	G	121	GLN
7	G	167	GLN
7	G	175	ASN
8	H	30	ASN
8	H	66	HIS
8	H	86	HIS
8	H	114	HIS
8	H	116	HIS
8	H	165	ASN
8	H	172	ASN
8	H	189	ASN
8	H	194	ASN
9	I	37	ASN
9	I	63	ASN
10	J	37	GLN
10	J	55	GLN
10	J	63	ASN
10	J	112	ASN
11	K	85	ASN

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Mol	Chain	Res	Type
11	K	176	ASN
11	K	208	ASN
12	L	3	ASN
12	L	49	ASN
12	L	55	ASN
12	L	70	ASN
12	L	79	HIS
12	L	80	ASN
12	L	153	GLN
12	L	197	GLN
13	M	48	ASN
13	M	62	HIS
13	M	102	GLN
13	M	108	ASN
13	M	149	HIS
13	M	179	ASN
13	M	194	ASN
13	M	213	GLN
14	N	38	HIS
14	N	60	GLN
14	N	141	ASN
14	N	161	GLN
1	O	30	GLN
1	O	94	HIS
2	P	20	GLN
2	P	95	GLN
2	P	119	GLN
2	P	123	GLN
2	P	176	GLN
3	Q	17	GLN
3	Q	38	ASN
3	Q	53	GLN
3	Q	116	GLN
3	Q	120	GLN
3	Q	147	GLN
3	Q	160	GLN
4	R	15	GLN
4	R	100	ASN
4	R	106	GLN
4	R	146	GLN
4	R	207	ASN
4	R	225	ASN

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Mol	Chain	Res	Type
5	S	68	HIS
5	S	99	ASN
5	S	116	GLN
5	S	118	ASN
5	S	120	GLN
5	S	151	ASN
6	T	19	GLN
6	T	86	ASN
6	T	117	GLN
6	T	123	ASN
6	T	191	GLN
6	T	203	ASN
6	T	240	GLN
7	U	30	ASN
7	U	83	ASN
7	U	114	ASN
7	U	117	GLN
7	U	121	GLN
7	U	167	GLN
7	U	175	ASN
8	V	30	ASN
8	V	66	HIS
8	V	86	HIS
8	V	114	HIS
8	V	116	HIS
8	V	165	ASN
8	V	172	ASN
8	V	189	ASN
8	V	194	ASN
9	W	37	ASN
9	W	63	ASN
10	X	55	GLN
10	X	63	ASN
10	X	86	GLN
10	X	112	ASN
10	X	146	HIS
11	Y	85	ASN
11	Y	176	ASN
11	Y	208	ASN
12	Z	3	ASN
12	Z	49	ASN
12	Z	55	ASN

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Mol	Chain	Res	Type
12	Z	70	ASN
12	Z	79	HIS
12	Z	80	ASN
12	Z	153	GLN
12	Z	197	GLN
13	a	18	ASN
13	a	48	ASN
13	a	102	GLN
13	a	108	ASN
13	a	149	HIS
13	a	194	ASN
13	a	213	GLN
14	b	38	HIS
14	b	141	ASN
14	b	161	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 13 ligands modelled in this entry, 11 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	3K4	Y	301	-	5,6,7	4.20	4 (80%)	4,8,10	4.38	3 (75%)
16	3K4	K	301	-	5,6,7	4.46	4 (80%)	4,8,10	4.41	3 (75%)

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	3K4	Y	301	-	-	0/1/7/9	0/1/1/1
16	3K4	K	301	-	-	0/1/7/9	0/1/1/1

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	K	301	3K4	C5-N6	-8.03	1.42	1.48
16	Y	301	3K4	C5-N6	-7.31	1.42	1.48
16	Y	301	3K4	C2-C5	-3.91	1.40	1.48
16	K	301	3K4	C2-C5	-3.87	1.40	1.48
16	K	301	3K4	C7-C5	-3.68	1.45	1.52
16	Y	301	3K4	C7-C5	-3.62	1.45	1.52
16	Y	301	3K4	C2-N6	-2.36	1.43	1.47
16	K	301	3K4	C2-N6	-2.33	1.43	1.47

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	Y	301	3K4	C7-C5-C2	7.88	136.03	122.56
16	K	301	3K4	C7-C5-C2	7.79	135.88	122.56
16	K	301	3K4	C2-C5-N6	2.84	60.93	59.83
16	K	301	3K4	C7-C5-N6	2.61	125.40	117.83
16	Y	301	3K4	C7-C5-N6	2.54	125.18	117.83
16	Y	301	3K4	C2-C5-N6	2.49	60.79	59.83

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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	249/250 (99%)	-0.15	7 (2%) 55 57	28, 38, 67, 111	0
1	O	249/250 (99%)	-0.03	8 (3%) 50 53	31, 44, 82, 118	0
2	B	244/258 (94%)	0.07	7 (2%) 53 56	26, 43, 80, 140	0
2	P	244/258 (94%)	0.18	14 (5%) 29 31	31, 46, 84, 131	0
3	C	240/254 (94%)	0.09	14 (5%) 29 30	27, 46, 102, 122	0
3	Q	240/254 (94%)	0.38	19 (7%) 18 20	31, 53, 120, 146	0
4	D	235/260 (90%)	0.06	7 (2%) 52 55	31, 46, 75, 110	0
4	R	235/260 (90%)	0.08	6 (2%) 57 60	32, 49, 79, 110	0
5	E	231/234 (98%)	0.06	7 (3%) 52 55	35, 48, 80, 126	0
5	S	231/234 (98%)	0.37	9 (3%) 43 45	35, 57, 90, 137	0
6	F	243/288 (84%)	-0.10	7 (2%) 53 56	29, 45, 85, 113	0
6	T	243/288 (84%)	0.13	8 (3%) 49 51	30, 50, 94, 118	0
7	G	241/252 (95%)	-0.12	5 (2%) 63 66	24, 38, 68, 115	0
7	U	241/252 (95%)	0.04	10 (4%) 41 43	31, 43, 69, 102	0
8	H	226/232 (97%)	-0.24	3 (1%) 75 77	26, 38, 64, 116	0
8	V	226/232 (97%)	-0.15	5 (2%) 62 65	30, 42, 66, 124	0
9	I	204/205 (99%)	-0.50	4 (1%) 65 67	25, 35, 60, 82	0
9	W	204/205 (99%)	-0.40	3 (1%) 72 74	26, 36, 63, 92	0
10	J	195/198 (98%)	-0.30	4 (2%) 63 66	25, 38, 62, 129	0
10	X	195/198 (98%)	-0.30	2 (1%) 79 81	25, 39, 63, 125	0
11	K	211/212 (99%)	-0.38	1 (0%) 87 88	26, 36, 55, 71	0
11	Y	211/212 (99%)	-0.37	1 (0%) 87 88	29, 38, 57, 74	0
12	L	222/222 (100%)	-0.39	3 (1%) 73 75	27, 39, 61, 95	0
12	Z	222/222 (100%)	-0.38	3 (1%) 73 75	27, 38, 61, 96	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å ²)	Q<0.9
13	M	233/246 (94%)	-0.38	4 (1%)	69 71	25, 39, 59, 77	0
13	a	233/246 (94%)	-0.36	3 (1%)	75 77	25, 37, 54, 72	0
14	N	196/196 (100%)	-0.41	2 (1%)	79 81	26, 36, 62, 88	0
14	b	196/196 (100%)	-0.31	2 (1%)	79 81	28, 37, 61, 95	0
All	All	6340/6614 (95%)	-0.12	168 (2%)	57 60	24, 42, 78, 146	0

All (168) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
10	X	1	MET	7.2
2	B	218	GLY	7.2
3	Q	50	LEU	6.6
10	J	1	MET	6.3
2	P	218	GLY	6.2
1	O	53	SER	6.1
2	B	219	ALA	5.9
8	V	223	ILE	5.0
13	M	1	THR	4.6
2	P	51	VAL	4.5
14	b	103	ASP	4.2
1	O	249	ALA	4.2
2	P	219	ALA	4.2
1	A	62	SER	3.9
7	U	242	GLN	3.9
8	H	223	ILE	3.8
13	a	1	THR	3.8
2	B	51	VAL	3.7
3	C	203	THR	3.6
5	E	122	TYR	3.6
3	C	49	THR	3.5
6	T	2	THR	3.5
6	T	182	GLY	3.4
12	L	174	TYR	3.4
6	F	215	CYS	3.4
3	Q	51	LYS	3.4
1	O	54	PRO	3.4
5	S	209	ASN	3.3
5	S	52	ALA	3.3
7	U	68	ARG	3.3
5	S	58	TYR	3.3
4	R	113	LEU	3.3

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Mol	Chain	Res	Type	RSRZ
14	N	103	ASP	3.2
6	T	206	LYS	3.2
9	I	1	SER	3.1
3	Q	49	THR	3.1
1	A	2	THR	3.1
6	F	202	ASP	3.1
7	U	203	ASP	3.1
3	C	205	ALA	3.1
3	C	51	LYS	3.1
6	F	244	ASN	3.0
3	Q	234	ILE	3.0
2	P	52	THR	3.0
7	G	166	GLN	2.9
4	R	99	ILE	2.9
14	b	116	GLY	2.9
3	C	50	LEU	2.8
9	W	133	LYS	2.8
8	V	224	GLN	2.8
2	P	202	SER	2.8
3	Q	205	ALA	2.8
1	O	52	SER	2.8
2	P	53	SER	2.8
3	Q	55	THR	2.8
5	S	233	ILE	2.8
6	T	203	ASN	2.7
10	X	195	PHE	2.7
1	O	61	LEU	2.7
2	P	220	ASN	2.7
3	Q	201	VAL	2.7
7	G	68	ARG	2.7
6	F	2	THR	2.7
5	S	3	ASN	2.7
6	T	243	ILE	2.7
3	Q	189	CYS	2.7
2	B	217	LYS	2.7
3	C	206	LYS	2.7
2	P	93	HIS	2.6
3	Q	52	LEU	2.6
6	T	215	CYS	2.6
3	Q	240	GLU	2.6
2	B	93	HIS	2.6
5	E	209	ASN	2.6

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Mol	Chain	Res	Type	RSRZ
5	S	122	TYR	2.6
4	D	242	GLU	2.6
4	R	2	ARG	2.6
5	E	202	ASP	2.6
3	C	48	SER	2.6
4	R	125	LEU	2.6
13	M	121	SER	2.6
3	Q	48	SER	2.5
7	U	168	GLU	2.5
3	C	238	LYS	2.5
12	Z	174	TYR	2.5
1	O	2	THR	2.5
7	G	242	GLN	2.5
4	R	117	GLU	2.5
9	I	131	GLU	2.5
3	Q	222	LEU	2.5
11	K	209	ASN	2.5
6	F	204	LYS	2.4
8	V	114	HIS	2.4
2	P	222	GLY	2.4
6	T	244	ASN	2.4
1	A	201	GLU	2.4
8	V	226	GLU	2.4
12	L	172	LEU	2.4
14	N	116	GLY	2.4
6	F	203	ASN	2.4
7	G	3	TYR	2.4
6	T	178	HIS	2.4
2	P	176	GLN	2.4
3	C	204	GLY	2.4
5	S	51	ASN	2.4
7	U	2	GLY	2.4
3	Q	59	PRO	2.4
2	P	57	GLU	2.3
12	Z	172	LEU	2.3
7	U	24	LYS	2.3
3	Q	57	ILE	2.3
5	S	207	VAL	2.3
8	H	224	GLN	2.3
1	A	249	ALA	2.3
7	U	231	ASN	2.3
1	A	61	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
3	C	201	VAL	2.3
5	E	3	ASN	2.3
11	Y	209	ASN	2.3
4	D	240	ALA	2.3
4	D	167	GLY	2.3
12	Z	173	LYS	2.3
4	D	239	GLU	2.2
3	Q	239	GLN	2.2
13	M	43	ILE	2.2
1	A	54	PRO	2.2
9	I	133	LYS	2.2
2	B	222	GLY	2.2
4	D	3	GLY	2.2
5	E	123	GLY	2.2
3	C	239	GLN	2.2
10	J	195	PHE	2.2
2	P	221	ASP	2.2
3	Q	47	ARG	2.2
3	Q	183	PRO	2.1
5	E	54	GLU	2.1
7	U	166	GLN	2.1
13	M	38	GLY	2.1
5	E	173	ARG	2.1
13	a	121	SER	2.1
3	C	38	ASN	2.1
10	J	194	ASP	2.1
7	U	171	THR	2.1
4	D	99	ILE	2.1
9	W	1	SER	2.1
1	O	57	MET	2.1
2	B	220	ASN	2.1
4	R	242	GLU	2.1
7	U	40	ASP	2.1
8	H	114	HIS	2.1
13	a	43	ILE	2.1
6	F	39	ASN	2.1
3	C	53	GLN	2.1
1	O	51	SER	2.1
3	C	207	ASN	2.0
3	Q	3	ASP	2.0
8	V	31	CYS	2.0
2	P	62	THR	2.0

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Mol	Chain	Res	Type	RSRZ
4	D	236	LYS	2.0
1	A	203	GLU	2.0
7	G	168	GLU	2.0
9	W	96	GLU	2.0
9	I	192	ASP	2.0
10	J	2	ASP	2.0
5	S	173	ARG	2.0
3	Q	238	LYS	2.0
12	L	173	LYS	2.0
2	P	225	TYR	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
15	MG	H	301	1/1	0.82	0.09	53,53,53,53	0
15	MG	I	302	1/1	0.92	0.36	59,59,59,59	0
16	3K4	K	301	6/7	0.92	0.12	36,41,45,48	0
16	3K4	Y	301	6/7	0.94	0.11	41,47,50,54	0
15	MG	V	301	1/1	0.97	0.11	38,38,38,38	0
15	MG	J	201	1/1	0.97	0.11	37,37,37,37	0
15	MG	N	201	1/1	0.97	0.05	40,40,40,40	0
15	MG	K	303	1/1	0.98	0.11	41,41,41,41	0
15	MG	Y	302	1/1	0.98	0.12	31,31,31,31	0
15	MG	G	301	1/1	0.99	0.08	31,31,31,31	0
15	MG	Z	301	1/1	0.99	0.10	40,40,40,40	0
15	MG	I	301	1/1	0.99	0.08	34,34,34,34	0
15	MG	K	302	1/1	0.99	0.06	29,29,29,29	0

6.5 Other polymers [i](#)

There are no such residues in this entry.