Full wwPDB X-ray Structure Validation Report ⓘ

May 25, 2020 – 08:33 am BST

PDB ID	:	4QLU
Title	:	yCP in complex with tripeptidic epoxyketone inhibitor 9
Authors	:	de Bruin, G.; Huber, E.; Xin, B.; van Rooden, E.; Al-Ayed, K.; Kim, K.; Kisselev, A.; Driessen, C.; van der Marel, G.; Groll, M.; Overkleeft, H.
Deposited on	:	2014-06-13
Resolution	:	2.80 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 following versions of software and data (see references ⓘ) were used in the production of this report:

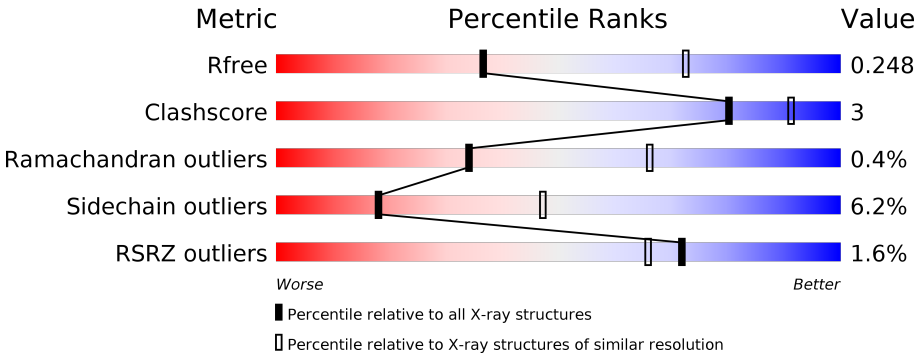
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

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 2.80 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}	130704	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)

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 on 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 <=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	2% 93% 7%
1	O	250	% 93% 7%
2	B	258	3% 83% 12% 5%
2	P	258	3% 82% 12% • 5%
3	C	254	4% 83% 10% • 6%
3	Q	254	5% 81% 12% • 6%

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Mol	Chain	Length	Quality of chain
4	D	260	2% 80% 10% 10%
4	R	260	2% 80% 10% 10%
5	E	234	2% 83% 14%
5	S	234	2% 82% 15%
6	F	288	2% 74% 9% 16%
6	T	288	2% 73% 10% 16%
7	G	252	2% 85% 10%
7	U	252	2% 85% 10%
8	H	232	2% 90% 6%
8	V	232	2% 90% 6%
9	I	205	88% 11%
9	W	205	2% 87% 12%
10	J	198	2% 87% 11%
10	X	198	2% 87% 11%
11	K	212	87% 12%
11	Y	212	2% 90% 8%
12	L	222	90% 9%
12	Z	222	91% 8%
13	M	246	2% 83% 11% 5%
13	a	246	88% 7% 5%
14	N	196	2% 90% 8%
14	b	196	2% 96%

2 Entry composition

There are 18 unique types of molecules in this entry. The entry contains 49665 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 (three-letter code: MG) (formula: Mg).

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

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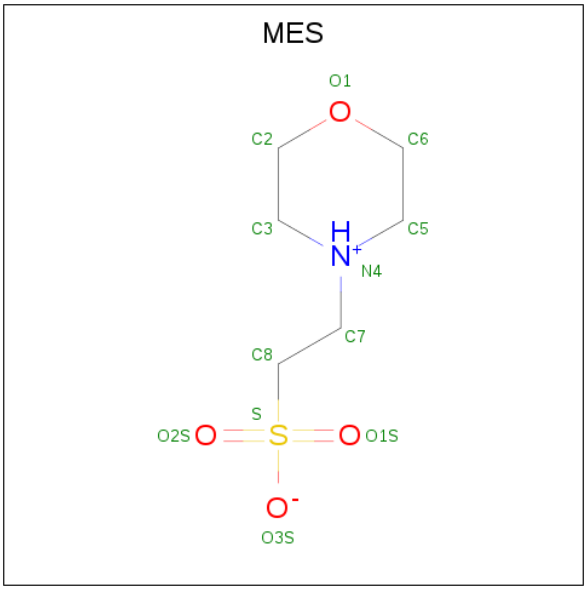
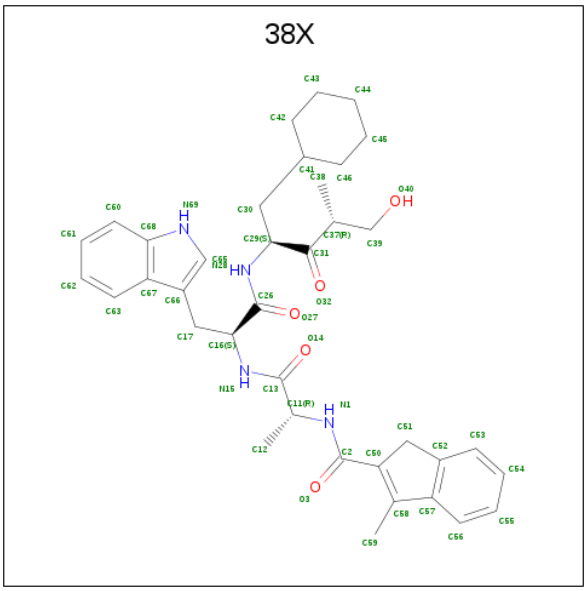
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
15	H	1	Total Mg 1 1	0	0
15	I	1	Total Mg 1 1	0	0
15	V	1	Total Mg 1 1	0	0
15	Z	1	Total Mg 1 1	0	0
15	N	1	Total Mg 1 1	0	0
15	Y	1	Total Mg 1 1	0	0

- Molecule 16 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (three-letter code: MES) (formula: $C_6H_{13}NO_4S$).



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

- Molecule 17 is N-[(3-methyl-1H-inden-2-yl)carbonyl]-D-alanyl-N-[(2S,4R)-1-cyclohexyl-5-hydroxy-4-methyl-3-oxopentan-2-yl]-L-tryptophanamide (three-letter code: 38X) (formula: $C_{37}H_{46}N_4O_5$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
17	K	1	Total C N O 46 37 4 5	0	0
17	Y	1	Total C N O 46 37 4 5	0	0

- Molecule 18 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
18	A	12	Total O 12 12	0	0
18	B	6	Total O 6 6	0	0
18	C	9	Total O 9 9	0	0
18	D	4	Total O 4 4	0	0
18	E	11	Total O 11 11	0	0
18	F	11	Total O 11 11	0	0
18	G	8	Total O 8 8	0	0
18	H	12	Total O 12 12	0	0
18	I	5	Total O 5 5	0	0
18	J	11	Total O 11 11	0	0

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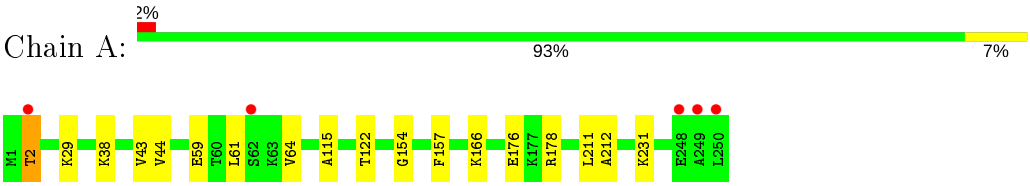
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
18	K	14	Total O 14 14	0	0
18	L	10	Total O 10 10	0	0
18	M	13	Total O 13 13	0	0
18	N	9	Total O 9 9	0	0
18	O	8	Total O 8 8	0	0
18	P	5	Total O 5 5	0	0
18	Q	5	Total O 5 5	0	0
18	R	5	Total O 5 5	0	0
18	S	5	Total O 5 5	0	0
18	T	6	Total O 6 6	0	0
18	U	11	Total O 11 11	0	0
18	V	6	Total O 6 6	0	0
18	W	6	Total O 6 6	0	0
18	X	12	Total O 12 12	0	0
18	Y	8	Total O 8 8	0	0
18	Z	12	Total O 12 12	0	0
18	a	10	Total O 10 10	0	0
18	b	11	Total O 11 11	0	0

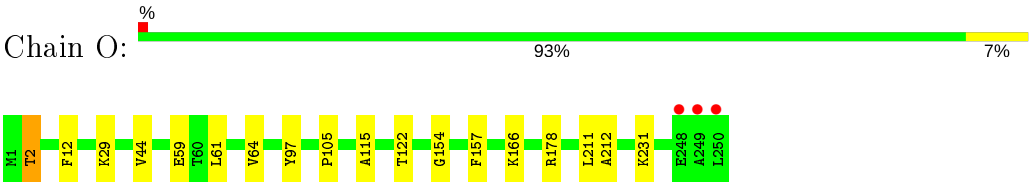
3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA 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.

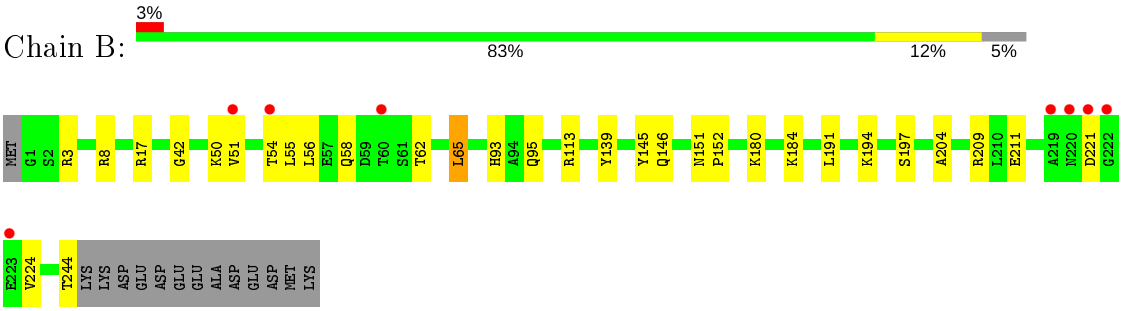
- Molecule 1: Proteasome subunit alpha type-2



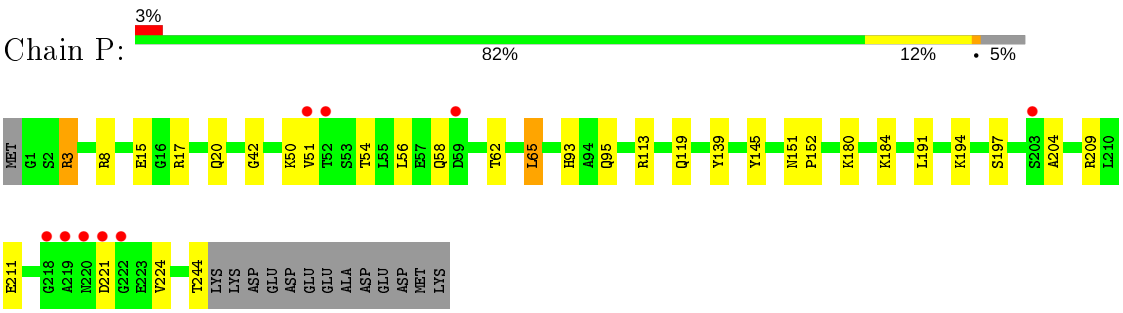
- Molecule 1: Proteasome subunit alpha type-2



- Molecule 2: Proteasome subunit alpha type-3

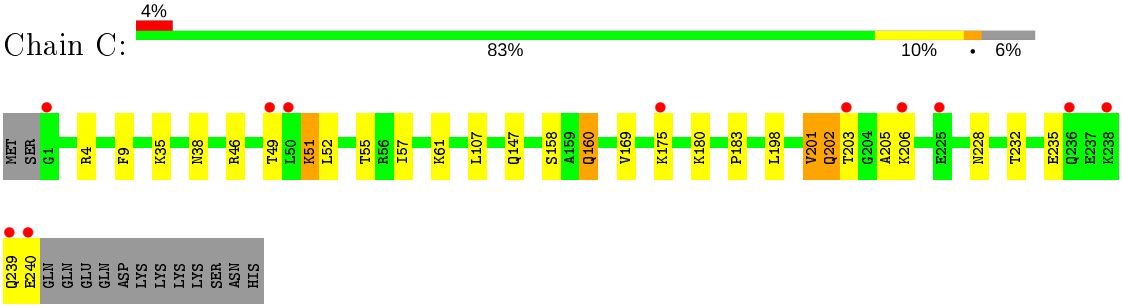


- Molecule 2: Proteasome subunit alpha type-3



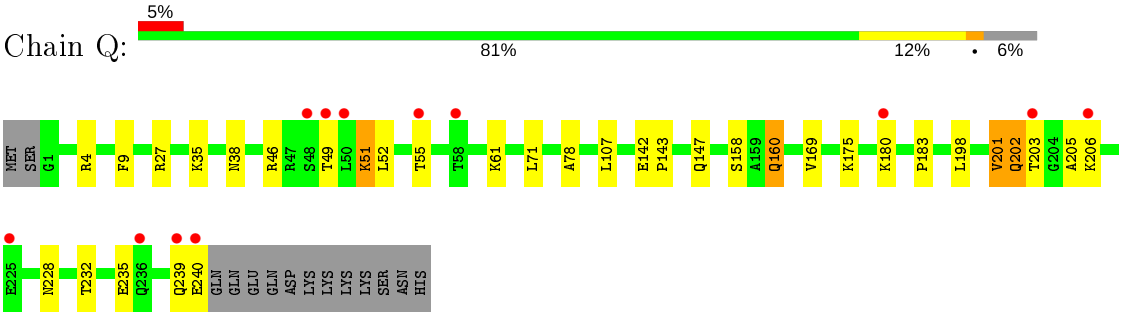
- Molecule 3: Proteasome subunit alpha type-4

Chain C:



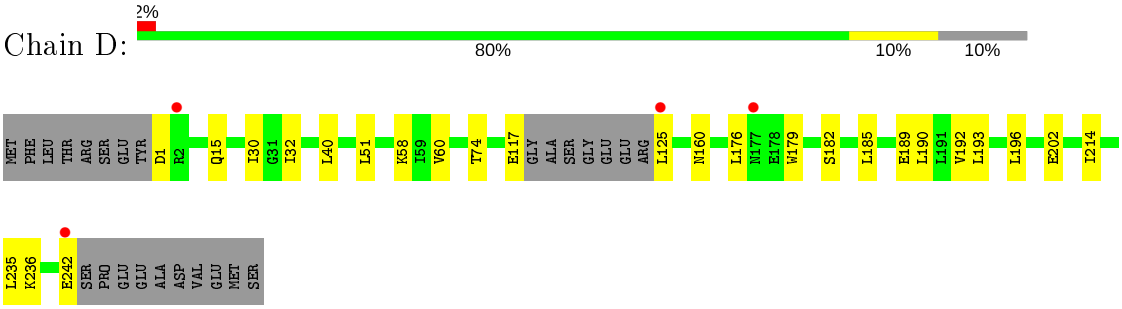
• Molecule 3: Proteasome subunit alpha type-4

Chain Q:



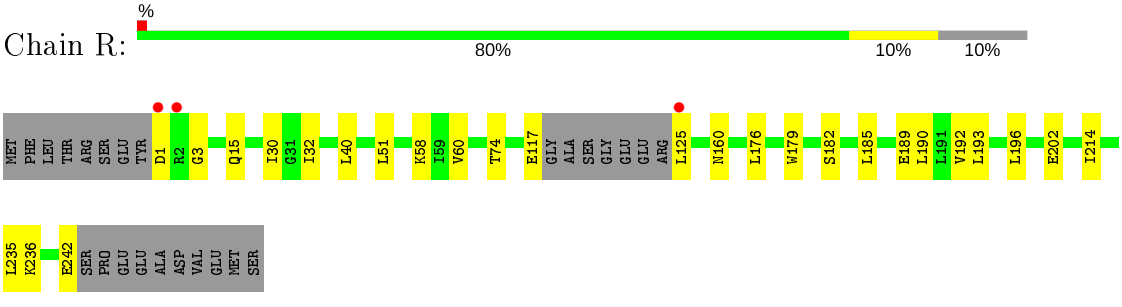
• Molecule 4: Proteasome subunit alpha type-5

Chain D:



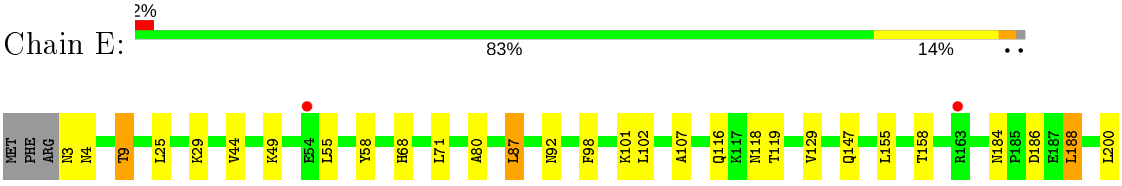
• Molecule 4: Proteasome subunit alpha type-5

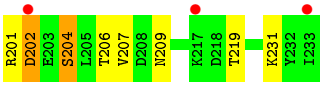
Chain R:



• Molecule 5: Proteasome subunit alpha type-6

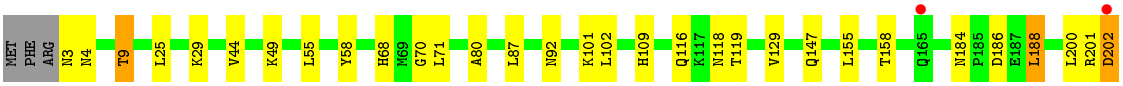
Chain E:

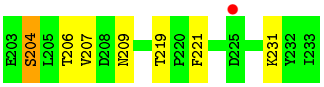




- Molecule 5: Proteasome subunit alpha type-6

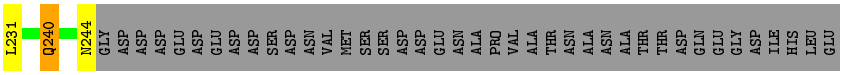
Chain S:





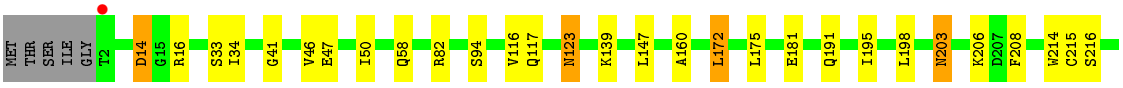
- Molecule 6: Probable proteasome subunit alpha type-7

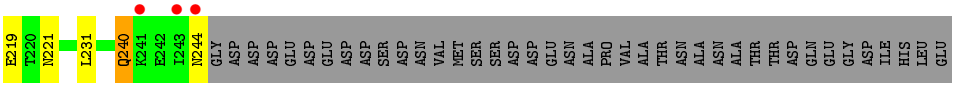
Chain F:



- Molecule 6: Probable proteasome subunit alpha type-7

Chain T:





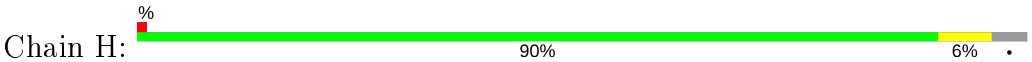
- Molecule 7: Proteasome subunit alpha type-1

Chain G:

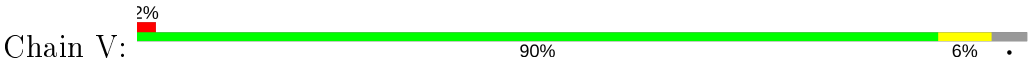
- Molecule 7: Proteasome subunit alpha type-1

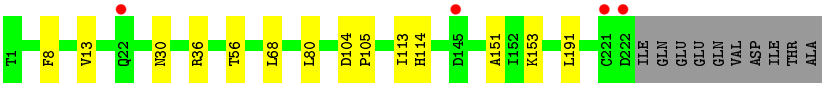
Chain U:

• Molecule 8: Proteasome subunit beta type-2

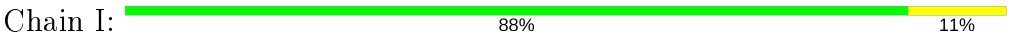


• Molecule 8: Proteasome subunit beta type-2

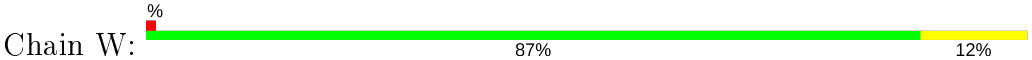


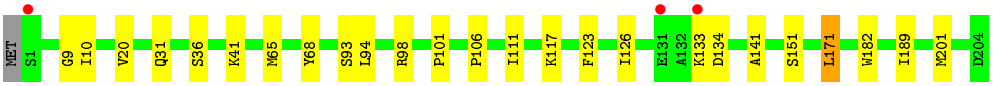


• Molecule 9: Proteasome subunit beta type-3

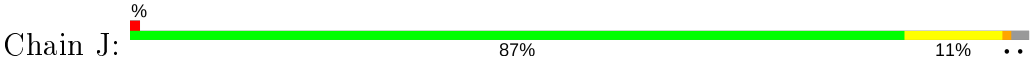


• Molecule 9: Proteasome subunit beta type-3

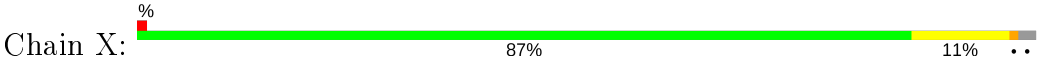




• Molecule 10: Proteasome subunit beta type-4

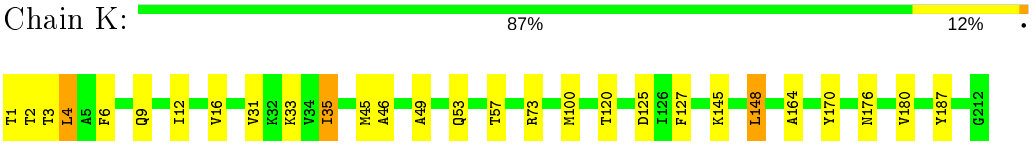


• Molecule 10: Proteasome subunit beta type-4



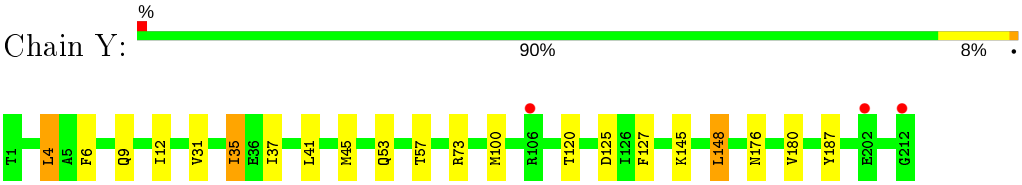
• Molecule 11: Proteasome subunit beta type-5

Chain K:



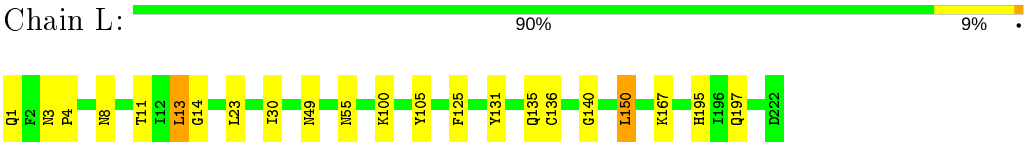
• Molecule 11: Proteasome subunit beta type-5

Chain Y:



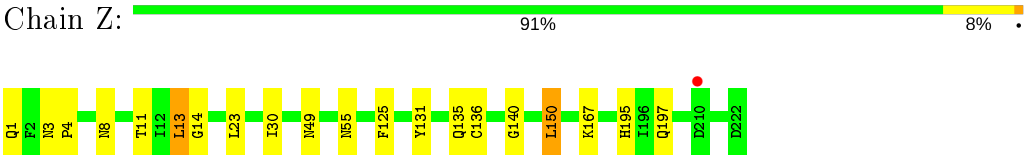
• Molecule 12: Proteasome subunit beta type-6

Chain L:



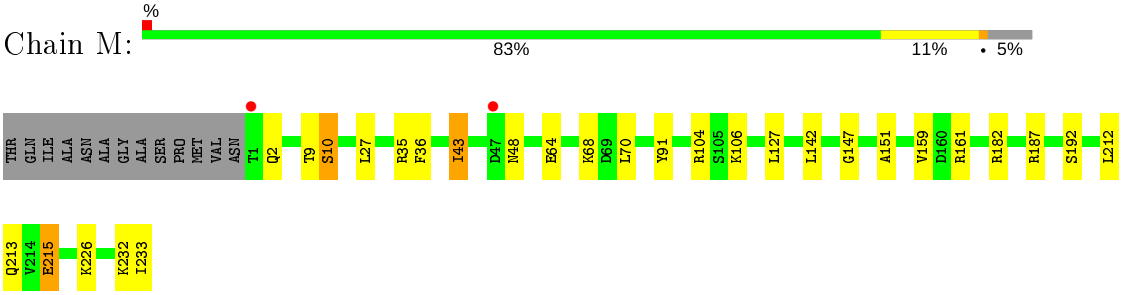
• Molecule 12: Proteasome subunit beta type-6

Chain Z:



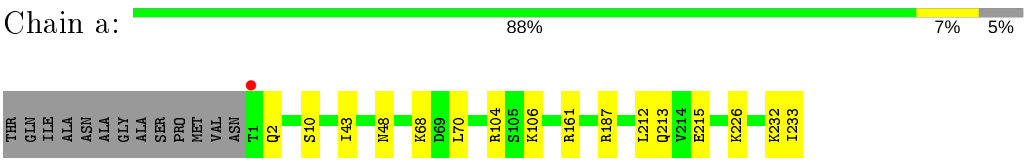
• Molecule 13: Proteasome subunit beta type-7

Chain M:



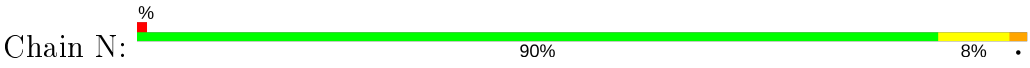
• Molecule 13: Proteasome subunit beta type-7

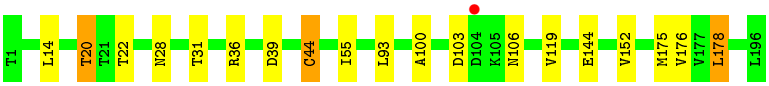
Chain a:



• Molecule 14: Proteasome subunit beta type-1

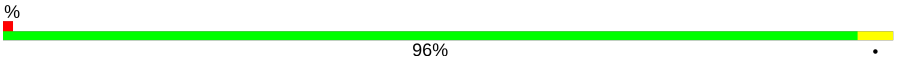
Chain N:

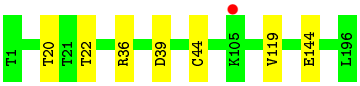




- Molecule 14: Proteasome subunit beta type-1

Chain b:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	134.88Å 299.38Å 144.83Å 90.00° 112.78° 90.00°	Depositor
Resolution (Å)	15.00 – 2.80 15.00 – 2.80	Depositor EDS
% Data completeness (in resolution range)	93.2 (15.00-2.80) 93.2 (15.00-2.80)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.21 (at 2.81Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.223 , 0.248 0.225 , 0.248	Depositor DCC
R_{free} test set	11995 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	56.1	Xtriage
Anisotropy	0.157	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 44.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.89	EDS
Total number of atoms	49665	wwPDB-VP
Average B, all atoms (Å^2)	55.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.75% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: 38X, MG, MES

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	A	0.28	0/1952	0.52	0/2642
1	O	0.28	0/1952	0.52	0/2642
2	B	0.29	0/1934	0.55	0/2618
2	P	0.29	0/1934	0.55	0/2618
3	C	0.30	0/1910	0.58	0/2586
3	Q	0.29	0/1910	0.57	0/2586
4	D	0.28	0/1837	0.55	0/2475
4	R	0.28	0/1837	0.55	0/2475
5	E	0.28	0/1800	0.53	0/2433
5	S	0.28	0/1800	0.53	0/2433
6	F	0.28	0/1932	0.51	0/2609
6	T	0.28	0/1932	0.51	0/2609
7	G	0.29	0/1945	0.54	0/2634
7	U	0.29	0/1945	0.53	0/2634
8	H	0.26	0/1715	0.51	0/2326
8	V	0.26	0/1715	0.51	0/2326
9	I	0.28	0/1611	0.53	0/2174
9	W	0.28	0/1611	0.53	0/2174
10	J	0.28	0/1589	0.53	0/2142
10	X	0.27	0/1589	0.53	0/2142
11	K	0.31	0/1681	0.54	1/2274 (0.0%)
11	Y	0.28	0/1681	0.54	1/2274 (0.0%)
12	L	0.28	0/1795	0.52	0/2420
12	Z	0.28	0/1795	0.52	0/2420
13	M	0.29	0/1855	0.56	0/2514
13	a	0.29	0/1855	0.56	0/2514
14	N	0.27	0/1541	0.50	0/2087
14	b	0.26	0/1541	0.50	0/2087
All	All	0.28	0/50194	0.53	2/67868 (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
12	L	0	1
12	Z	0	1
All	All	0	2

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	K	4	LEU	CA-CB-CG	5.22	127.30	115.30
11	Y	4	LEU	CA-CB-CG	5.13	127.11	115.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
12	L	135	GLN	Peptide
12	Z	135	GLN	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	5	0
1	O	1915	0	1929	5	0
2	B	1904	0	1904	9	0
2	P	1904	0	1904	11	0
3	C	1881	0	1895	15	0
3	Q	1881	0	1895	18	0
4	D	1813	0	1797	6	0
4	R	1813	0	1797	7	0
5	E	1773	0	1775	12	0
5	S	1773	0	1775	12	0
6	F	1892	0	1883	10	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	T	1892	0	1883	12	0
7	G	1907	0	1901	6	0
7	U	1907	0	1901	6	0
8	H	1684	0	1688	3	0
8	V	1684	0	1688	3	0
9	I	1581	0	1574	12	0
9	W	1581	0	1574	13	0
10	J	1561	0	1569	10	0
10	X	1561	0	1569	10	0
11	K	1644	0	1593	19	0
11	Y	1644	0	1593	11	0
12	L	1757	0	1711	9	0
12	Z	1757	0	1711	8	0
13	M	1824	0	1832	10	0
13	a	1824	0	1832	0	0
14	N	1512	0	1481	8	0
14	b	1512	0	1481	0	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	12	0	13	0	0
16	Y	12	0	13	0	0
17	K	46	0	45	8	0
17	Y	46	0	45	3	0
18	A	12	0	0	0	0
18	B	6	0	0	0	0
18	C	9	0	0	0	0
18	D	4	0	0	0	0
18	E	11	0	0	0	0
18	F	11	0	0	1	0
18	G	8	0	0	0	0
18	H	12	0	0	0	0
18	I	5	0	0	0	0
18	J	11	0	0	0	0
18	K	14	0	0	0	0
18	L	10	0	0	0	0
18	M	13	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
18	N	9	0	0	0	0
18	O	8	0	0	0	0
18	P	5	0	0	0	0
18	Q	5	0	0	0	0
18	R	5	0	0	0	0
18	S	5	0	0	0	0
18	T	6	0	0	0	0
18	U	11	0	0	0	0
18	V	6	0	0	0	0
18	W	6	0	0	0	0
18	X	12	0	0	0	0
18	Y	8	0	0	0	0
18	Z	12	0	0	0	0
18	a	10	0	0	0	0
18	b	11	0	0	0	0
All	All	49665	0	49180	240	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 3.

All (240) 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)
11:Y:100:MET:CE	11:Y:127:PHE:HB2	2.18	0.73
11:K:100:MET:CE	11:K:127:PHE:HB2	2.19	0.72
12:Z:13:LEU:HD13	12:Z:150:LEU:HD21	1.76	0.68
2:P:93:HIS:HB3	2:P:113:ARG:HH21	1.59	0.67
2:B:93:HIS:HB3	2:B:113:ARG:HH21	1.58	0.67
12:L:13:LEU:HD13	12:L:150:LEU:HD21	1.76	0.66
3:C:51:LYS:O	3:C:52:LEU:HB2	1.95	0.66
11:Y:100:MET:HE3	11:Y:127:PHE:HB2	1.77	0.65
10:J:23:ARG:NH2	11:K:120:THR:OG1	2.29	0.65
3:C:202:GLN:HG3	3:C:203:THR:H	1.63	0.64
3:Q:51:LYS:O	3:Q:52:LEU:HB2	1.96	0.64
11:K:100:MET:HE3	11:K:127:PHE:HB2	1.78	0.64
17:K:303:38X:O3	17:K:303:38X:H4	1.98	0.63
14:N:152:VAL:HA	14:N:175:MET:HE1	1.81	0.63
9:W:101:PRO:HB3	9:W:126:ILE:HD12	1.81	0.63
9:I:101:PRO:HB3	9:I:126:ILE:HD12	1.81	0.63
3:Q:198:LEU:HA	3:Q:201:VAL:HG12	1.81	0.62
3:Q:202:GLN:HG3	3:Q:203:THR:H	1.63	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:198:LEU:HA	3:C:201:VAL:HG12	1.81	0.61
17:Y:303:38X:H4	17:Y:303:38X:O3	1.99	0.61
3:Q:202:GLN:HG3	3:Q:203:THR:N	2.17	0.60
14:N:20:THR:HG22	14:N:31:THR:OG1	2.01	0.60
3:C:202:GLN:HG3	3:C:203:THR:N	2.16	0.59
3:Q:35:LYS:HG2	3:Q:158:SER:O	2.02	0.59
5:E:9:THR:HG21	5:E:119:THR:HA	1.85	0.59
5:S:9:THR:HG21	5:S:119:THR:HA	1.84	0.59
3:C:35:LYS:HG2	3:C:158:SER:O	2.03	0.58
6:F:172:LEU:CD1	6:F:195:ILE:HD13	2.33	0.58
10:X:23:ARG:NH2	11:Y:120:THR:OG1	2.36	0.58
6:T:172:LEU:CD1	6:T:195:ILE:HD13	2.33	0.58
12:L:8:ASN:HA	12:L:30:ILE:O	2.04	0.58
11:Y:53:GLN:O	11:Y:57:THR:HG23	2.03	0.57
11:K:53:GLN:O	11:K:57:THR:HG23	2.04	0.56
3:C:160:GLN:HE21	3:C:160:GLN:HA	1.70	0.56
12:Z:8:ASN:HA	12:Z:30:ILE:O	2.04	0.56
5:E:155:LEU:HD13	5:E:158:THR:HB	1.88	0.56
6:F:96:LYS:NZ	18:F:308:HOH:O	2.38	0.56
1:A:176:GLU:HG3	2:B:55:LEU:HD22	1.88	0.56
5:S:155:LEU:HD13	5:S:158:THR:HB	1.88	0.55
3:Q:160:GLN:HE21	3:Q:160:GLN:HA	1.70	0.55
3:C:46:ARG:NH1	3:C:55:THR:HG21	2.22	0.55
3:C:202:GLN:CG	3:C:203:THR:H	2.20	0.54
10:J:16:ALA:HB2	10:J:161:LEU:HD21	1.89	0.54
7:G:23:PHE:O	7:G:26:THR:HB	2.07	0.54
3:Q:46:ARG:NH1	3:Q:55:THR:HG21	2.22	0.54
7:U:23:PHE:O	7:U:26:THR:HB	2.07	0.54
10:J:174:MET:HA	10:X:174:MET:HA	1.90	0.54
9:I:36:SER:HB2	10:J:126:VAL:HG11	1.90	0.54
10:X:16:ALA:HB2	10:X:161:LEU:HD21	1.89	0.54
11:Y:100:MET:HE3	11:Y:127:PHE:CB	2.37	0.54
3:Q:202:GLN:CG	3:Q:203:THR:H	2.21	0.53
11:K:1:THR:HG22	11:K:2:THR:N	2.23	0.53
10:X:185:ASP:OD2	10:X:190:ARG:NH1	2.37	0.53
11:K:100:MET:HE3	11:K:127:PHE:CB	2.39	0.52
9:W:101:PRO:HB3	9:W:126:ILE:CD1	2.39	0.52
5:S:109:HIS:HB3	6:T:82:ARG:NH2	2.24	0.52
9:W:36:SER:HB2	10:X:126:VAL:HG11	1.91	0.52
4:R:32:ILE:HD12	4:R:192:VAL:HG23	1.91	0.52
4:D:160:ASN:HB3	4:D:179:TRP:CE2	2.46	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:101:PRO:HB3	9:I:126:ILE:CD1	2.40	0.51
10:J:185:ASP:OD2	10:J:190:ARG:NH1	2.37	0.51
10:J:1:MET:HA	10:J:34:LYS:HE3	1.93	0.51
3:Q:201:VAL:O	3:Q:202:GLN:CB	2.58	0.51
4:R:160:ASN:HB3	4:R:179:TRP:CE2	2.46	0.51
3:C:201:VAL:O	3:C:202:GLN:CB	2.59	0.51
4:D:32:ILE:HD12	4:D:192:VAL:HG23	1.92	0.51
17:K:303:38X:O3	17:K:303:38X:H16	2.10	0.51
10:X:1:MET:HA	10:X:34:LYS:HE3	1.92	0.51
3:C:201:VAL:HG13	3:C:202:GLN:N	2.26	0.50
6:F:216:SER:HB3	6:F:219:GLU:HB2	1.94	0.50
3:Q:201:VAL:HG13	3:Q:202:GLN:N	2.26	0.50
4:R:185:LEU:O	4:R:189:GLU:HG3	2.11	0.50
4:D:185:LEU:O	4:D:189:GLU:HG3	2.12	0.50
6:T:216:SER:HB3	6:T:219:GLU:HB2	1.94	0.50
10:J:36:ARG:NH1	10:J:58:GLU:OE2	2.45	0.49
5:S:68:HIS:CD2	5:S:101:LYS:HE2	2.48	0.49
5:E:68:HIS:CD2	5:E:101:LYS:HE2	2.48	0.49
1:O:115:ALA:HB1	1:O:154:GLY:O	2.13	0.49
12:Z:55:ASN:OD1	12:Z:140:GLY:HA3	2.13	0.49
14:N:176:VAL:HG12	14:N:178:LEU:HD13	1.94	0.48
10:X:36:ARG:NH1	10:X:58:GLU:OE2	2.46	0.48
2:P:15:GLU:O	3:Q:27:ARG:NH1	2.46	0.48
11:K:1:THR:HG21	11:K:46:ALA:HB2	1.96	0.48
8:H:104:ASP:HB2	8:H:105:PRO:HD2	1.95	0.47
12:L:55:ASN:OD1	12:L:140:GLY:HA3	2.14	0.47
8:V:104:ASP:HB2	8:V:105:PRO:HD2	1.95	0.47
13:M:127:LEU:HG	13:M:142:LEU:HD12	1.96	0.47
17:K:303:38X:O32	17:K:303:38X:O40	2.16	0.47
2:B:139:TYR:CD1	2:B:224:VAL:HG21	2.50	0.47
1:A:115:ALA:HB1	1:A:154:GLY:O	2.14	0.46
2:B:42:GLY:HA2	2:B:145:TYR:CE1	2.50	0.46
9:I:98:ARG:O	9:I:126:ILE:HD11	2.15	0.46
2:P:42:GLY:HA2	2:P:145:TYR:CE1	2.49	0.46
11:K:2:THR:HG21	11:K:164:ALA:CB	2.45	0.46
5:E:206:THR:OG1	5:E:209:ASN:HB2	2.15	0.46
5:S:206:THR:OG1	5:S:209:ASN:HB2	2.15	0.46
2:P:139:TYR:CD1	2:P:224:VAL:HG21	2.51	0.46
6:F:123:ASN:C	6:F:123:ASN:HD22	2.18	0.46
17:K:303:38X:H18	17:K:303:38X:H24	1.68	0.46
9:W:10:ILE:HG21	9:W:141:ALA:HB3	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:U:227:LEU:HB3	7:U:231:ASN:HB2	1.98	0.46
14:N:55:ILE:HD11	14:N:93:LEU:HD13	1.98	0.46
5:S:200:LEU:HD13	5:S:204:SER:HA	1.98	0.46
11:K:145:LYS:HB2	11:K:148:LEU:HD13	1.98	0.46
11:K:176:ASN:ND2	11:K:187:TYR:OH	2.49	0.46
13:M:43:ILE:HG12	13:M:43:ILE:O	2.16	0.46
3:C:46:ARG:NH1	3:C:206:LYS:HG2	2.31	0.45
5:E:68:HIS:HE1	5:E:102:LEU:O	1.97	0.45
8:H:8:PHE:HB3	8:H:151:ALA:HB2	1.98	0.45
12:L:13:LEU:HD12	12:L:14:GLY:N	2.31	0.45
14:N:103:ASP:HB2	14:N:106:ASN:HB2	1.98	0.45
5:S:68:HIS:HE1	5:S:102:LEU:O	1.98	0.45
11:Y:176:ASN:ND2	11:Y:187:TYR:OH	2.50	0.45
12:L:125:PHE:CD2	12:L:131:TYR:HB3	2.52	0.45
9:W:9:GLY:HA3	9:W:41:LYS:HE2	1.97	0.45
10:X:1:MET:HA	10:X:34:LYS:CE	2.47	0.45
9:I:10:ILE:HG21	9:I:141:ALA:HB3	1.98	0.45
9:I:9:GLY:HA3	9:I:41:LYS:HE2	1.97	0.45
11:K:170:TYR:O	17:K:303:38X:H41	2.17	0.45
11:K:49:ALA:HA	17:K:303:38X:H33	1.98	0.45
3:Q:202:GLN:CG	3:Q:203:THR:N	2.78	0.45
6:T:123:ASN:HD22	6:T:123:ASN:C	2.19	0.45
7:U:149:ASP:HB2	7:U:150:PRO:CD	2.47	0.45
5:E:200:LEU:HD13	5:E:204:SER:HA	1.98	0.45
11:K:12:ILE:HB	11:K:180:VAL:HB	1.99	0.45
4:R:58:LYS:HE2	4:R:74:THR:HG21	1.99	0.45
12:L:136:CYS:SG	12:L:150:LEU:HB3	2.56	0.45
14:N:14:LEU:HD11	14:N:100:ALA:HB3	1.99	0.45
8:V:8:PHE:HB3	8:V:151:ALA:HB2	1.99	0.45
12:Z:136:CYS:SG	12:Z:150:LEU:HB3	2.57	0.45
5:E:44:VAL:HG23	5:E:188:LEU:HD13	1.98	0.45
7:G:227:LEU:HB3	7:G:231:ASN:HB2	1.98	0.45
2:B:146:GLN:HG2	3:C:57:ILE:HG21	1.99	0.45
5:E:80:ALA:HB2	5:E:129:VAL:HG21	1.99	0.45
10:J:1:MET:HA	10:J:34:LYS:CE	2.47	0.45
9:W:171:LEU:HD11	9:W:201:MET:HB3	1.99	0.45
13:M:9:THR:OG1	13:M:10:SER:N	2.50	0.44
3:Q:46:ARG:NH1	3:Q:206:LYS:HG2	2.31	0.44
3:Q:9:PHE:H	4:R:15:GLN:HE22	1.65	0.44
12:Z:125:PHE:CD2	12:Z:131:TYR:HB3	2.52	0.44
7:G:149:ASP:HB2	7:G:150:PRO:CD	2.48	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:W:98:ARG:O	9:W:126:ILE:HD11	2.18	0.44
13:M:27:LEU:HB2	13:M:192:SER:HB3	1.99	0.44
12:Z:13:LEU:HD12	12:Z:14:GLY:N	2.32	0.44
9:I:94:LEU:HD11	9:I:106:PRO:HG2	2.00	0.44
9:I:111:ILE:HD12	9:I:189:ILE:HG22	2.00	0.44
6:F:50:ILE:HG13	6:F:208:PHE:HA	1.99	0.44
10:J:3:ILE:HD12	10:J:176:PHE:CG	2.53	0.44
6:T:50:ILE:HG13	6:T:208:PHE:HA	1.99	0.44
11:Y:145:LYS:HB2	11:Y:148:LEU:HD13	2.00	0.44
17:Y:303:38X:N28	17:Y:303:38X:H44	2.33	0.44
12:L:3:ASN:HD22	12:L:4:PRO:HD2	1.83	0.44
13:M:147:GLY:O	13:M:151:ALA:HB3	2.17	0.44
4:D:58:LYS:HE2	4:D:74:THR:HG21	1.99	0.43
14:N:20:THR:CG2	14:N:28:ASN:HB3	2.48	0.43
5:S:44:VAL:HG23	5:S:188:LEU:HD13	1.99	0.43
2:B:151:ASN:HB2	2:B:152:PRO:CD	2.48	0.43
11:K:33:LYS:NZ	17:K:303:38X:H42	2.33	0.43
5:E:98:PHE:O	13:M:91:TYR:HA	2.18	0.43
2:P:204:ALA:O	2:P:209:ARG:NH2	2.51	0.43
5:S:80:ALA:HB2	5:S:129:VAL:HG21	2.00	0.43
9:W:133:LYS:HG3	9:W:134:ASP:N	2.33	0.43
11:K:6:PHE:HA	11:K:125:ASP:O	2.18	0.43
11:Y:12:ILE:HB	11:Y:180:VAL:HB	1.99	0.43
17:Y:303:38X:H16	17:Y:303:38X:O3	2.18	0.43
9:I:133:LYS:HG3	9:I:134:ASP:N	2.34	0.43
9:I:171:LEU:HD11	9:I:201:MET:HB3	2.01	0.43
6:T:34:ILE:HG22	6:T:160:ALA:HB2	2.01	0.43
9:W:111:ILE:HD12	9:W:189:ILE:HG22	2.00	0.43
2:P:65:LEU:HD22	2:P:211:GLU:HB3	2.01	0.43
6:T:14:ASP:CB	6:T:16:ARG:HD3	2.48	0.43
2:B:204:ALA:O	2:B:209:ARG:NH2	2.51	0.43
3:C:9:PHE:H	4:D:15:GLN:HE22	1.67	0.43
1:O:64:VAL:HG11	1:O:212:ALA:HB3	2.01	0.43
3:C:202:GLN:CG	3:C:203:THR:N	2.78	0.43
11:K:1:THR:CG2	11:K:2:THR:N	2.82	0.43
11:K:35:ILE:HB	11:K:45:MET:CE	2.49	0.43
2:P:119:GLN:CG	3:Q:78:ALA:HB1	2.49	0.43
11:Y:6:PHE:HA	11:Y:125:ASP:O	2.19	0.43
13:M:159:VAL:HG23	13:M:159:VAL:O	2.19	0.43
9:W:94:LEU:HD11	9:W:106:PRO:HG2	2.00	0.43
2:B:65:LEU:HD22	2:B:211:GLU:HB3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:S:9:THR:CG2	5:S:119:THR:HA	2.49	0.42
4:D:30:ILE:HD12	4:D:196:LEU:HG	2.00	0.42
6:F:34:ILE:HG22	6:F:160:ALA:HB2	2.01	0.42
10:X:3:ILE:HD12	10:X:176:PHE:CG	2.54	0.42
4:R:30:ILE:HD12	4:R:196:LEU:HG	2.01	0.42
6:T:33:SER:HB3	6:T:46:VAL:HG23	2.01	0.42
2:P:95:GLN:HB3	9:W:68:TYR:CD2	2.54	0.42
5:E:49:LYS:HB3	5:E:58:TYR:HB3	2.01	0.42
1:A:38:LYS:HG3	1:A:43:VAL:HG22	2.02	0.42
2:B:95:GLN:HB3	9:I:68:TYR:CD2	2.54	0.42
6:F:116:VAL:HG21	6:F:147:LEU:HD21	2.01	0.42
1:A:64:VAL:HG11	1:A:212:ALA:HB3	2.02	0.42
9:I:65:MET:CE	9:I:93:SER:HB3	2.50	0.42
1:O:12:PHE:H	2:P:20:GLN:HE22	1.68	0.42
11:K:3:THR:HG22	11:K:16:VAL:HG12	2.01	0.42
13:M:35:ARG:HG3	13:M:36:PHE:CE1	2.55	0.42
6:F:14:ASP:CB	6:F:16:ARG:HD3	2.50	0.42
2:P:151:ASN:HB2	2:P:152:PRO:CD	2.49	0.42
14:N:14:LEU:HD23	14:N:44:CYS:SG	2.59	0.42
5:S:49:LYS:HB3	5:S:58:TYR:HB3	2.00	0.42
11:Y:35:ILE:HB	11:Y:45:MET:CE	2.50	0.42
7:U:73:VAL:HG12	7:U:133:THR:HB	2.02	0.41
10:X:147:HIS:HB3	10:X:160:LEU:HD11	2.02	0.41
8:V:80:LEU:HD12	8:V:113:ILE:HD11	2.01	0.41
8:H:80:LEU:HD12	8:H:113:ILE:HD11	2.02	0.41
10:J:147:HIS:HB3	10:J:160:LEU:HD11	2.02	0.41
5:S:70:GLY:HA3	5:S:221:PHE:CE2	2.55	0.41
6:F:240:GLN:HA	6:F:240:GLN:HE21	1.85	0.41
6:F:33:SER:HB3	6:F:46:VAL:HG23	2.01	0.41
12:L:100:LYS:HD3	12:L:105:TYR:CZ	2.55	0.41
3:C:51:LYS:CE	3:C:206:LYS:HD2	2.51	0.41
3:Q:71:LEU:HD23	3:Q:71:LEU:C	2.41	0.41
1:O:44:VAL:HG23	1:O:211:LEU:HD21	2.01	0.41
6:T:240:GLN:HA	6:T:240:GLN:HE21	1.85	0.41
9:W:20:VAL:HG23	9:W:189:ILE:HB	2.03	0.41
12:Z:3:ASN:HD22	12:Z:4:PRO:HD2	1.84	0.41
13:M:182:ARG:NH2	13:M:215:GLU:O	2.53	0.41
6:T:116:VAL:HG21	6:T:147:LEU:HD21	2.02	0.41
7:G:78:ILE:N	7:G:79:PRO:CD	2.84	0.41
6:T:41:GLY:HA3	6:T:215:CYS:O	2.21	0.41
12:L:195:HIS:HD2	12:L:197:GLN:H	1.69	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:43:ILE:HG21	13:M:64:GLU:HG2	2.02	0.41
2:P:3:ARG:NH2	4:R:3:GLY:HA2	2.36	0.41
3:Q:142:GLU:HA	3:Q:143:PRO:HD3	1.98	0.41
5:E:87:LEU:HD21	5:E:107:ALA:HB1	2.04	0.40
3:Q:51:LYS:CE	3:Q:206:LYS:HD2	2.51	0.40
7:U:239:ILE:O	7:U:242:GLN:HB3	2.21	0.40
11:Y:37:ILE:HB	11:Y:41:LEU:HB3	2.03	0.40
1:A:44:VAL:HG23	1:A:211:LEU:HD21	2.02	0.40
9:W:65:MET:CE	9:W:93:SER:HB3	2.51	0.40
12:Z:195:HIS:HD2	12:Z:197:GLN:H	1.69	0.40
5:E:9:THR:CG2	5:E:119:THR:HA	2.50	0.40
7:G:73:VAL:HG12	7:G:133:THR:HB	2.03	0.40
7:G:239:ILE:O	7:G:242:GLN:HB3	2.21	0.40
7:U:78:ILE:N	7:U:79:PRO:CD	2.84	0.40
11:K:33:LYS:HZ1	17:K:303:38X:H42	1.87	0.40
1:O:97:TYR:CE1	1:O:105:PRO:HA	2.57	0.40
6:T:175:LEU:HD11	6:T:191:GLN:HB3	2.04	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%)	240 (97%)	6 (2%)	2 (1%)	19	49
1	O	248/250 (99%)	240 (97%)	6 (2%)	2 (1%)	19	49
2	B	242/258 (94%)	232 (96%)	8 (3%)	2 (1%)	19	49
2	P	242/258 (94%)	232 (96%)	8 (3%)	2 (1%)	19	49
3	C	238/254 (94%)	225 (94%)	8 (3%)	5 (2%)	7	23
3	Q	238/254 (94%)	225 (94%)	8 (3%)	5 (2%)	7	23
4	D	231/260 (89%)	225 (97%)	6 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	R	231/260 (89%)	225 (97%)	6 (3%)	0	100	100
5	E	229/234 (98%)	215 (94%)	13 (6%)	1 (0%)	34	66
5	S	229/234 (98%)	215 (94%)	13 (6%)	1 (0%)	34	66
6	F	241/288 (84%)	233 (97%)	7 (3%)	1 (0%)	34	66
6	T	241/288 (84%)	233 (97%)	7 (3%)	1 (0%)	34	66
7	G	239/252 (95%)	233 (98%)	5 (2%)	1 (0%)	34	66
7	U	239/252 (95%)	233 (98%)	5 (2%)	1 (0%)	34	66
8	H	220/232 (95%)	211 (96%)	9 (4%)	0	100	100
8	V	220/232 (95%)	211 (96%)	9 (4%)	0	100	100
9	I	202/205 (98%)	195 (96%)	7 (4%)	0	100	100
9	W	202/205 (98%)	194 (96%)	8 (4%)	0	100	100
10	J	193/198 (98%)	188 (97%)	3 (2%)	2 (1%)	15	44
10	X	193/198 (98%)	188 (97%)	3 (2%)	2 (1%)	15	44
11	K	210/212 (99%)	203 (97%)	7 (3%)	0	100	100
11	Y	210/212 (99%)	203 (97%)	7 (3%)	0	100	100
12	L	220/222 (99%)	214 (97%)	6 (3%)	0	100	100
12	Z	220/222 (99%)	214 (97%)	6 (3%)	0	100	100
13	M	231/246 (94%)	222 (96%)	9 (4%)	0	100	100
13	a	231/246 (94%)	222 (96%)	9 (4%)	0	100	100
14	N	194/196 (99%)	185 (95%)	9 (5%)	0	100	100
14	b	194/196 (99%)	185 (95%)	9 (5%)	0	100	100
All	All	6276/6614 (95%)	6041 (96%)	207 (3%)	28 (0%)	34	66

All (28) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	202	GLN
3	Q	202	GLN
1	A	2	THR
3	C	205	ALA
6	F	203	ASN
1	O	2	THR
3	Q	205	ALA
6	T	203	ASN
1	A	166	LYS

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Mol	Chain	Res	Type
3	C	239	GLN
1	O	166	LYS
3	Q	239	GLN
2	B	221	ASP
10	J	2	ASP
2	P	221	ASP
5	S	202	ASP
10	X	2	ASP
2	B	51	VAL
5	E	202	ASP
10	J	9	VAL
2	P	51	VAL
10	X	9	VAL
7	G	51	PRO
7	U	51	PRO
3	C	201	VAL
3	Q	201	VAL
3	C	183	PRO
3	Q	183	PRO

5.3.2 Protein sidechains (i)

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%)	201 (96%)	8 (4%)	33	67
1	O	209/209 (100%)	201 (96%)	8 (4%)	33	67
2	B	203/216 (94%)	188 (93%)	15 (7%)	13	37
2	P	203/216 (94%)	188 (93%)	15 (7%)	13	37
3	C	212/226 (94%)	197 (93%)	15 (7%)	14	39
3	Q	212/226 (94%)	197 (93%)	15 (7%)	14	39
4	D	194/215 (90%)	179 (92%)	15 (8%)	13	35
4	R	194/215 (90%)	179 (92%)	15 (8%)	13	35
5	E	190/193 (98%)	169 (89%)	21 (11%)	6	19

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
5	S	190/193 (98%)	169 (89%)	21 (11%)	6 19
6	F	201/239 (84%)	184 (92%)	17 (8%)	10 31
6	T	201/239 (84%)	184 (92%)	17 (8%)	10 31
7	G	206/210 (98%)	192 (93%)	14 (7%)	16 42
7	U	206/210 (98%)	192 (93%)	14 (7%)	16 42
8	H	181/190 (95%)	173 (96%)	8 (4%)	28 61
8	V	181/190 (95%)	173 (96%)	8 (4%)	28 61
9	I	172/173 (99%)	166 (96%)	6 (4%)	36 70
9	W	172/173 (99%)	166 (96%)	6 (4%)	36 70
10	J	173/175 (99%)	165 (95%)	8 (5%)	27 60
10	X	173/175 (99%)	165 (95%)	8 (5%)	27 60
11	K	169/169 (100%)	163 (96%)	6 (4%)	35 69
11	Y	169/169 (100%)	163 (96%)	6 (4%)	35 69
12	L	185/185 (100%)	178 (96%)	7 (4%)	33 67
12	Z	185/185 (100%)	178 (96%)	7 (4%)	33 67
13	M	199/208 (96%)	183 (92%)	16 (8%)	12 34
13	a	199/208 (96%)	183 (92%)	16 (8%)	12 34
14	N	162/162 (100%)	154 (95%)	8 (5%)	25 57
14	b	162/162 (100%)	155 (96%)	7 (4%)	29 62
All	All	5312/5540 (96%)	4985 (94%)	327 (6%)	18 47

All (327) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	THR
1	A	29	LYS
1	A	59	GLU
1	A	61	LEU
1	A	122	THR
1	A	157	PHE
1	A	178	ARG
1	A	231	LYS
2	B	3	ARG
2	B	8	ARG
2	B	17	ARG

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Mol	Chain	Res	Type
2	B	50	LYS
2	B	54	THR
2	B	56	LEU
2	B	58	GLN
2	B	62	THR
2	B	65	LEU
2	B	180	LYS
2	B	184	LYS
2	B	191	LEU
2	B	194	LYS
2	B	197	SER
2	B	244	THR
3	C	4	ARG
3	C	38	ASN
3	C	49	THR
3	C	51	LYS
3	C	61	LYS
3	C	107	LEU
3	C	147	GLN
3	C	160	GLN
3	C	169	VAL
3	C	175	LYS
3	C	180	LYS
3	C	228	ASN
3	C	232	THR
3	C	235	GLU
3	C	240	GLU
4	D	1	ASP
4	D	40	LEU
4	D	51	LEU
4	D	60	VAL
4	D	117	GLU
4	D	125	LEU
4	D	176	LEU
4	D	182	SER
4	D	190	LEU
4	D	193	LEU
4	D	202	GLU
4	D	214	ILE
4	D	235	LEU
4	D	236	LYS
4	D	242	GLU

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Mol	Chain	Res	Type
5	E	3	ASN
5	E	4	ASN
5	E	9	THR
5	E	25	LEU
5	E	29	LYS
5	E	55	LEU
5	E	71	LEU
5	E	87	LEU
5	E	92	ASN
5	E	116	GLN
5	E	118	ASN
5	E	147	GLN
5	E	184	ASN
5	E	186	ASP
5	E	188	LEU
5	E	201	ARG
5	E	202	ASP
5	E	204	SER
5	E	207	VAL
5	E	219	THR
5	E	231	LYS
6	F	14	ASP
6	F	47	GLU
6	F	58	GLN
6	F	94	SER
6	F	117	GLN
6	F	123	ASN
6	F	139	LYS
6	F	172	LEU
6	F	181	GLU
6	F	198	LEU
6	F	203	ASN
6	F	206	LYS
6	F	214	TRP
6	F	221	ASN
6	F	231	LEU
6	F	240	GLN
6	F	244	ASN
7	G	26	THR
7	G	31	ILE
7	G	83	ASN
7	G	115	LEU

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Mol	Chain	Res	Type
7	G	117	GLN
7	G	122	ARG
7	G	166	GLN
7	G	171	THR
7	G	178	LYS
7	G	181	LYS
7	G	215	GLU
7	G	230	GLU
7	G	235	ARG
7	G	236	LEU
8	H	13	VAL
8	H	30	ASN
8	H	36	ARG
8	H	56	THR
8	H	68	LEU
8	H	114	HIS
8	H	153	LYS
8	H	191	LEU
9	I	31	GLN
9	I	117	LYS
9	I	123	PHE
9	I	151	SER
9	I	171	LEU
9	I	182	TRP
10	J	23	ARG
10	J	35	THR
10	J	75	LEU
10	J	78	GLN
10	J	91	SER
10	J	144	LEU
10	J	163	LEU
10	J	174	MET
11	K	4	LEU
11	K	9	GLN
11	K	31	VAL
11	K	35	ILE
11	K	73	ARG
11	K	148	LEU
12	L	1	GLN
12	L	11	THR
12	L	13	LEU
12	L	23	LEU

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Mol	Chain	Res	Type
12	L	49	ASN
12	L	150	LEU
12	L	167	LYS
13	M	2	GLN
13	M	10	SER
13	M	43	ILE
13	M	48	ASN
13	M	68	LYS
13	M	70	LEU
13	M	104	ARG
13	M	106	LYS
13	M	161	ARG
13	M	187	ARG
13	M	212	LEU
13	M	213	GLN
13	M	215	GLU
13	M	226	LYS
13	M	232	LYS
13	M	233	ILE
14	N	20	THR
14	N	22	THR
14	N	36	ARG
14	N	39	ASP
14	N	44	CYS
14	N	119	VAL
14	N	144	GLU
14	N	178	LEU
1	O	2	THR
1	O	29	LYS
1	O	59	GLU
1	O	61	LEU
1	O	122	THR
1	O	157	PHE
1	O	178	ARG
1	O	231	LYS
2	P	3	ARG
2	P	8	ARG
2	P	17	ARG
2	P	50	LYS
2	P	54	THR
2	P	56	LEU
2	P	58	GLN

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Mol	Chain	Res	Type
2	P	62	THR
2	P	65	LEU
2	P	180	LYS
2	P	184	LYS
2	P	191	LEU
2	P	194	LYS
2	P	197	SER
2	P	244	THR
3	Q	4	ARG
3	Q	38	ASN
3	Q	49	THR
3	Q	51	LYS
3	Q	61	LYS
3	Q	107	LEU
3	Q	147	GLN
3	Q	160	GLN
3	Q	169	VAL
3	Q	175	LYS
3	Q	180	LYS
3	Q	228	ASN
3	Q	232	THR
3	Q	235	GLU
3	Q	240	GLU
4	R	1	ASP
4	R	40	LEU
4	R	51	LEU
4	R	60	VAL
4	R	117	GLU
4	R	125	LEU
4	R	176	LEU
4	R	182	SER
4	R	190	LEU
4	R	193	LEU
4	R	202	GLU
4	R	214	ILE
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

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Mol	Chain	Res	Type
5	S	29	LYS
5	S	55	LEU
5	S	71	LEU
5	S	87	LEU
5	S	92	ASN
5	S	116	GLN
5	S	118	ASN
5	S	147	GLN
5	S	184	ASN
5	S	186	ASP
5	S	188	LEU
5	S	201	ARG
5	S	202	ASP
5	S	204	SER
5	S	207	VAL
5	S	219	THR
5	S	231	LYS
6	T	14	ASP
6	T	47	GLU
6	T	58	GLN
6	T	94	SER
6	T	117	GLN
6	T	123	ASN
6	T	139	LYS
6	T	172	LEU
6	T	181	GLU
6	T	198	LEU
6	T	203	ASN
6	T	206	LYS
6	T	214	TRP
6	T	221	ASN
6	T	231	LEU
6	T	240	GLN
6	T	244	ASN
7	U	26	THR
7	U	31	ILE
7	U	83	ASN
7	U	115	LEU
7	U	117	GLN
7	U	122	ARG
7	U	166	GLN
7	U	171	THR

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Mol	Chain	Res	Type
7	U	178	LYS
7	U	181	LYS
7	U	215	GLU
7	U	230	GLU
7	U	235	ARG
7	U	236	LEU
8	V	13	VAL
8	V	30	ASN
8	V	36	ARG
8	V	56	THR
8	V	68	LEU
8	V	114	HIS
8	V	153	LYS
8	V	191	LEU
9	W	31	GLN
9	W	117	LYS
9	W	123	PHE
9	W	151	SER
9	W	171	LEU
9	W	182	TRP
10	X	23	ARG
10	X	35	THR
10	X	75	LEU
10	X	78	GLN
10	X	91	SER
10	X	144	LEU
10	X	163	LEU
10	X	174	MET
11	Y	4	LEU
11	Y	9	GLN
11	Y	31	VAL
11	Y	35	ILE
11	Y	73	ARG
11	Y	148	LEU
12	Z	1	GLN
12	Z	11	THR
12	Z	13	LEU
12	Z	23	LEU
12	Z	49	ASN
12	Z	150	LEU
12	Z	167	LYS
13	a	2	GLN

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Mol	Chain	Res	Type
13	a	10	SER
13	a	43	ILE
13	a	48	ASN
13	a	68	LYS
13	a	70	LEU
13	a	104	ARG
13	a	106	LYS
13	a	161	ARG
13	a	187	ARG
13	a	212	LEU
13	a	213	GLN
13	a	215	GLU
13	a	226	LYS
13	a	232	LYS
13	a	233	ILE
14	b	20	THR
14	b	22	THR
14	b	36	ARG
14	b	39	ASP
14	b	44	CYS
14	b	119	VAL
14	b	144	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (98) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	94	HIS
2	B	20	GLN
2	B	95	GLN
2	B	119	GLN
2	B	123	GLN
2	B	155	ASN
3	C	38	ASN
3	C	77	ASN
3	C	147	GLN
3	C	160	GLN
4	D	15	GLN
4	D	91	HIS
4	D	100	ASN
4	D	146	GLN
5	E	68	HIS
5	E	116	GLN

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Mol	Chain	Res	Type
5	E	118	ASN
5	E	120	GLN
5	E	184	ASN
6	F	117	GLN
6	F	123	ASN
6	F	191	GLN
6	F	240	GLN
7	G	30	ASN
7	G	83	ASN
7	G	114	ASN
7	G	117	GLN
7	G	121	GLN
8	H	30	ASN
8	H	66	HIS
8	H	172	ASN
8	H	189	ASN
10	J	55	GLN
10	J	118	GLN
10	J	146	HIS
10	J	191	GLN
11	K	85	ASN
11	K	143	ASN
11	K	176	ASN
12	L	3	ASN
12	L	49	ASN
12	L	158	ASN
13	M	18	ASN
13	M	48	ASN
13	M	102	GLN
13	M	108	ASN
13	M	194	ASN
13	M	213	GLN
14	N	38	HIS
14	N	161	GLN
1	O	94	HIS
2	P	20	GLN
2	P	119	GLN
2	P	123	GLN
2	P	155	ASN
3	Q	38	ASN
3	Q	77	ASN
3	Q	147	GLN

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Mol	Chain	Res	Type
3	Q	160	GLN
4	R	15	GLN
4	R	100	ASN
4	R	146	GLN
5	S	68	HIS
5	S	116	GLN
5	S	118	ASN
5	S	120	GLN
5	S	184	ASN
6	T	117	GLN
6	T	123	ASN
6	T	191	GLN
6	T	240	GLN
7	U	30	ASN
7	U	83	ASN
7	U	114	ASN
7	U	117	GLN
7	U	121	GLN
8	V	30	ASN
8	V	66	HIS
8	V	172	ASN
8	V	189	ASN
10	X	55	GLN
10	X	63	ASN
10	X	146	HIS
10	X	147	HIS
10	X	191	GLN
11	Y	85	ASN
11	Y	176	ASN
12	Z	3	ASN
12	Z	49	ASN
12	Z	158	ASN
13	a	18	ASN
13	a	48	ASN
13	a	102	GLN
13	a	108	ASN
13	a	194	ASN
13	a	213	GLN
14	b	38	HIS
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

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

Of 12 ligands modelled in this entry, 8 are monoatomic - leaving 4 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
16	MES	Y	302	-	12,12,12	2.19	1 (8%)	14,16,16	1.29	2 (14%)
17	38X	Y	303	-	48,50,50	3.87	15 (31%)	56,70,70	1.94	16 (28%)
16	MES	K	302	-	12,12,12	2.22	1 (8%)	14,16,16	1.37	3 (21%)
17	38X	K	303	-	48,50,50	3.73	17 (35%)	56,70,70	2.15	15 (26%)

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	MES	Y	302	-	-	0/6/14/14	0/1/1/1
17	38X	Y	303	-	-	11/41/62/62	0/5/5/5
16	MES	K	302	-	-	0/6/14/14	0/1/1/1
17	38X	K	303	-	-	10/41/62/62	0/5/5/5

All (34) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	Y	303	38X	C51-C50	-12.47	1.34	1.51
17	Y	303	38X	C2-C50	-12.37	1.32	1.49
17	K	303	38X	C2-C50	-11.81	1.33	1.49
17	K	303	38X	C51-C50	-11.29	1.36	1.51
17	K	303	38X	O32-C31	8.46	1.35	1.21
17	K	303	38X	C51-C52	-7.63	1.38	1.50
17	Y	303	38X	O32-C31	7.61	1.33	1.21
16	K	302	MES	C8-S	-7.40	1.67	1.77
17	Y	303	38X	C51-C52	-7.29	1.39	1.50
16	Y	302	MES	C8-S	-7.28	1.67	1.77
17	Y	303	38X	C57-C58	-7.13	1.30	1.44
17	Y	303	38X	C60-C68	-6.72	1.30	1.41
17	Y	303	38X	C57-C52	-6.67	1.30	1.39
17	K	303	38X	C57-C52	-6.42	1.31	1.39
17	K	303	38X	C60-C68	-5.99	1.31	1.41
17	K	303	38X	C57-C58	-5.87	1.33	1.44
17	Y	303	38X	C56-C57	-5.63	1.30	1.39
17	Y	303	38X	C63-C67	-5.29	1.31	1.42
17	K	303	38X	C63-C67	-4.89	1.32	1.42
17	Y	303	38X	C53-C52	-4.77	1.31	1.39
17	K	303	38X	C56-C57	-4.69	1.32	1.39
17	K	303	38X	C67-C68	-4.30	1.31	1.42
17	K	303	38X	C53-C52	-4.20	1.32	1.39
17	Y	303	38X	C67-C68	-3.98	1.32	1.42
17	K	303	38X	C68-N69	-3.64	1.27	1.38
17	K	303	38X	C65-N69	-3.57	1.29	1.36
17	Y	303	38X	C68-N69	-3.11	1.29	1.38
17	Y	303	38X	C65-C66	-3.03	1.29	1.37
17	K	303	38X	C65-C66	-2.94	1.29	1.37
17	Y	303	38X	C65-N69	-2.60	1.31	1.36
17	K	303	38X	C50-C58	-2.43	1.31	1.36
17	K	303	38X	C29-C31	2.31	1.56	1.52
17	K	303	38X	C11-C13	-2.24	1.47	1.52
17	Y	303	38X	C50-C58	-2.13	1.32	1.36

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	K	303	38X	O32-C31-C37	-7.96	106.49	121.26
17	Y	303	38X	O32-C31-C37	-5.61	110.85	121.26
17	Y	303	38X	C17-C66-C65	-5.07	121.71	127.97
17	K	303	38X	C41-C30-C29	4.60	120.70	114.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	K	303	38X	C30-C29-N28	-4.52	100.16	110.58
17	Y	303	38X	C30-C29-N28	-4.36	100.53	110.58
17	K	303	38X	C52-C51-C50	4.30	105.96	102.67
17	K	303	38X	C17-C66-C65	-4.05	122.96	127.97
17	K	303	38X	C43-C42-C41	3.76	119.25	112.15
17	Y	303	38X	C43-C42-C41	3.41	118.59	112.15
17	K	303	38X	C17-C16-C26	3.18	118.51	110.25
17	Y	303	38X	C11-N1-C2	3.14	126.41	121.57
17	K	303	38X	C30-C41-C42	-3.12	104.96	111.73
17	Y	303	38X	C61-C60-C68	-3.04	115.71	120.08
17	Y	303	38X	C52-C51-C50	3.03	104.98	102.67
16	Y	302	MES	O3S-S-C8	3.03	110.66	105.77
17	K	303	38X	C62-C61-C60	-2.90	116.37	120.44
17	K	303	38X	C17-C66-C67	2.84	130.66	126.25
17	Y	303	38X	C63-C67-C68	2.80	121.89	118.17
16	K	302	MES	O3S-S-C8	2.73	110.18	105.77
17	Y	303	38X	C45-C46-C41	2.61	117.08	112.15
17	K	303	38X	C11-N1-C2	2.60	125.59	121.57
16	Y	302	MES	O2S-S-C8	2.60	110.04	106.92
17	Y	303	38X	C30-C41-C42	-2.58	106.12	111.73
17	K	303	38X	C45-C46-C41	2.55	116.97	112.15
17	Y	303	38X	C57-C58-C50	2.53	110.86	109.15
17	Y	303	38X	C60-C68-C67	2.31	124.98	120.76
17	K	303	38X	C60-C68-C67	2.31	124.98	120.76
17	Y	303	38X	C12-C11-N1	2.29	114.68	110.38
17	Y	303	38X	C62-C63-C67	-2.22	117.82	120.89
17	Y	303	38X	C41-C30-C29	2.15	117.41	114.52
16	K	302	MES	O1S-S-C8	2.14	109.50	106.92
17	K	303	38X	C44-C45-C46	2.07	115.63	111.42
17	K	303	38X	C55-C54-C53	-2.05	117.07	120.19
17	Y	303	38X	C44-C45-C46	2.04	115.58	111.42
16	K	302	MES	O2S-S-C8	2.02	109.35	106.92

There are no chirality outliers.

All (21) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
17	K	303	38X	O32-C31-C37-C38
17	Y	303	38X	N15-C16-C17-C66
17	Y	303	38X	C26-C16-C17-C66
17	Y	303	38X	N28-C29-C31-C37
17	Y	303	38X	O32-C31-C37-C38

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Mol	Chain	Res	Type	Atoms
17	K	303	38X	C12-C11-C13-O14
17	Y	303	38X	C12-C11-C13-O14
17	K	303	38X	C12-C11-C13-N15
17	Y	303	38X	C12-C11-C13-N15
17	K	303	38X	C26-C16-C17-C66
17	Y	303	38X	C12-C11-N1-C2
17	K	303	38X	N15-C16-C17-C66
17	K	303	38X	C12-C11-N1-C2
17	K	303	38X	N28-C29-C30-C41
17	Y	303	38X	N28-C29-C30-C41
17	K	303	38X	C31-C29-C30-C41
17	Y	303	38X	C31-C29-C30-C41
17	Y	303	38X	C29-C31-C37-C38
17	K	303	38X	C16-C17-C66-C65
17	Y	303	38X	C30-C29-C31-O32
17	K	303	38X	N28-C29-C31-C37

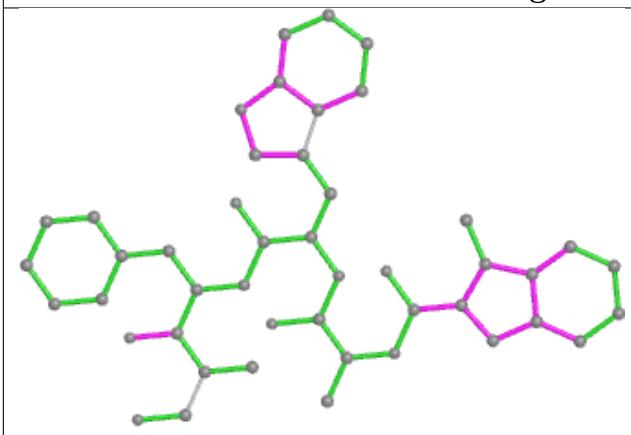
There are no ring outliers.

2 monomers are involved in 11 short contacts:

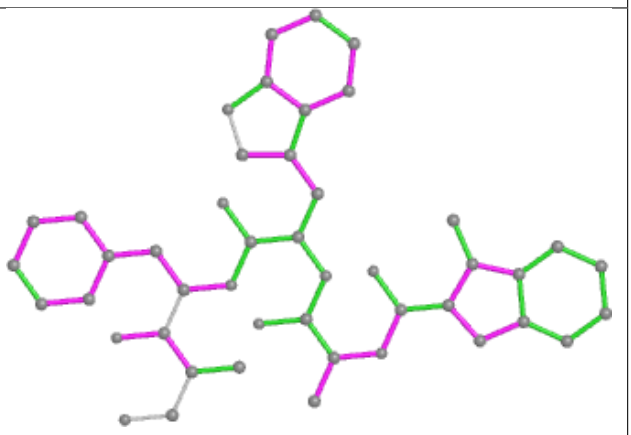
Mol	Chain	Res	Type	Clashes	Symm-Clashes
17	Y	303	38X	3	0
17	K	303	38X	8	0

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

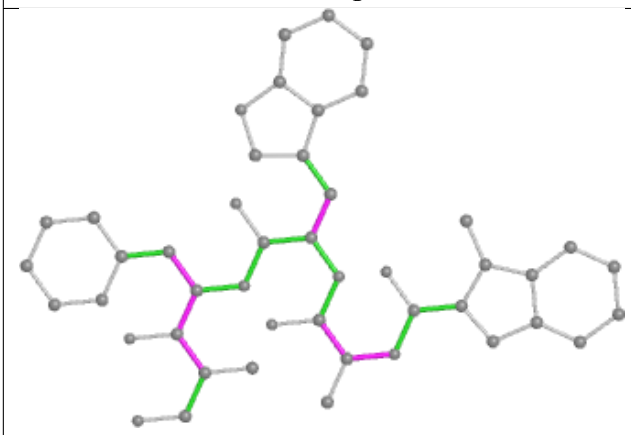
Ligand 38X Y 303



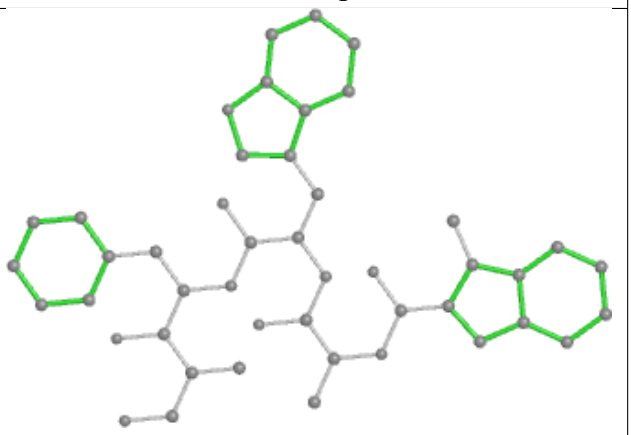
Bond lengths



Bond angles

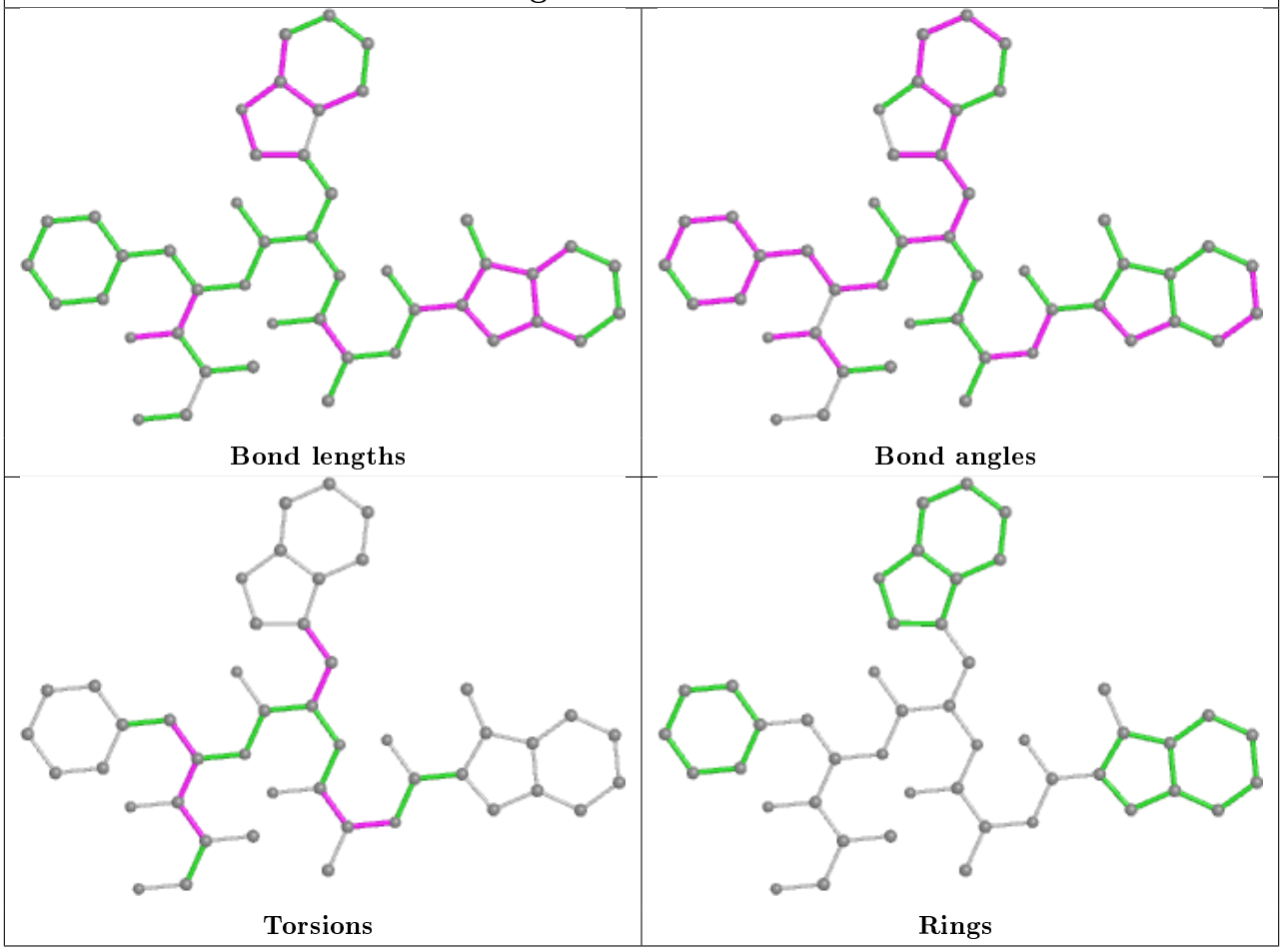


Torsions



Rings

Ligand 38X K 303



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, 95^{th} 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%)	-0.27	5 (2%)	65	56	31, 49, 83, 118	0
1	O	250/250 (100%)	-0.28	3 (1%)	79	73	33, 53, 88, 119	0
2	B	244/258 (94%)	-0.22	8 (3%)	46	36	31, 53, 93, 127	0
2	P	244/258 (94%)	-0.10	9 (3%)	41	31	32, 54, 100, 146	0
3	C	240/254 (94%)	-0.13	11 (4%)	32	22	32, 57, 113, 132	0
3	Q	240/254 (94%)	0.13	12 (5%)	28	19	37, 65, 123, 145	0
4	D	235/260 (90%)	-0.19	4 (1%)	70	63	34, 56, 87, 124	0
4	R	235/260 (90%)	-0.20	3 (1%)	77	72	37, 60, 91, 110	0
5	E	231/234 (98%)	-0.11	5 (2%)	62	52	39, 62, 96, 137	0
5	S	231/234 (98%)	-0.03	3 (1%)	77	72	38, 65, 96, 119	0
6	F	243/288 (84%)	-0.23	4 (1%)	72	66	34, 56, 96, 122	0
6	T	243/288 (84%)	-0.18	4 (1%)	72	66	36, 58, 95, 123	0
7	G	241/252 (95%)	-0.32	4 (1%)	70	63	31, 50, 86, 127	0
7	U	241/252 (95%)	-0.30	3 (1%)	79	73	33, 50, 78, 107	0
8	H	222/232 (95%)	-0.34	3 (1%)	75	70	29, 46, 69, 116	0
8	V	222/232 (95%)	-0.32	4 (1%)	68	61	32, 48, 72, 109	0
9	I	204/205 (99%)	-0.52	0	100	100	28, 44, 67, 108	0
9	W	204/205 (99%)	-0.50	3 (1%)	73	68	26, 44, 68, 102	0
10	J	195/198 (98%)	-0.48	2 (1%)	82	77	25, 44, 72, 109	0
10	X	195/198 (98%)	-0.41	1 (0%)	91	88	31, 47, 69, 129	0
11	K	212/212 (100%)	-0.45	0	100	100	31, 45, 67, 88	0
11	Y	212/212 (100%)	-0.41	3 (1%)	75	70	34, 47, 72, 98	0
12	L	222/222 (100%)	-0.44	0	100	100	32, 48, 71, 93	0
12	Z	222/222 (100%)	-0.43	1 (0%)	91	88	30, 48, 74, 90	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
13	M	233/246 (94%)	-0.44	2 (0%) 84 80	27, 48, 66, 83	0
13	a	233/246 (94%)	-0.46	1 (0%) 92 91	25, 45, 67, 82	0
14	N	196/196 (100%)	-0.46	1 (0%) 91 88	29, 44, 69, 89	0
14	b	196/196 (100%)	-0.41	1 (0%) 91 88	31, 44, 73, 86	0
All	All	6336/6614 (95%)	-0.30	100 (1%) 72 66	25, 51, 88, 146	0

All (100) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	Q	49	THR	7.0
2	P	218	GLY	5.9
2	P	222	GLY	5.8
2	P	219	ALA	5.7
3	C	206	LYS	5.4
2	B	223	GLU	5.0
8	V	222	ASP	4.9
5	E	202	ASP	4.8
3	Q	240	GLU	4.8
3	C	49	THR	4.5
3	Q	50	LEU	4.5
8	H	222	ASP	4.3
5	S	202	ASP	4.3
2	P	51	VAL	4.2
8	H	221	CYS	4.2
8	V	221	CYS	4.1
2	B	221	ASP	4.0
7	U	2	GLY	3.9
4	D	242	GLU	3.8
6	F	181	GLU	3.7
10	X	194	ASP	3.6
3	C	239	GLN	3.6
2	P	52	THR	3.6
3	Q	203	THR	3.5
2	P	59	ASP	3.3
2	B	222	GLY	3.3
2	B	51	VAL	3.3
6	T	243	ILE	3.1
1	A	2	THR	3.1
3	Q	180	LYS	3.1
2	P	220	ASN	3.1
2	P	221	ASP	3.1

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Mol	Chain	Res	Type	RSRZ
3	Q	236	GLN	3.0
3	Q	55	THR	3.0
2	B	219	ALA	3.0
6	T	244	ASN	3.0
3	Q	206	LYS	3.0
6	F	2	THR	2.9
4	R	125	LEU	2.8
9	W	1	SER	2.8
8	H	198	GLU	2.8
7	U	242	GLN	2.7
13	a	1	THR	2.7
10	J	194	ASP	2.7
9	W	133	LYS	2.7
13	M	47	ASP	2.7
7	G	242	GLN	2.7
1	A	249	ALA	2.6
3	C	240	GLU	2.6
2	P	203	SER	2.6
3	C	236	GLN	2.5
3	Q	225	GLU	2.5
3	Q	239	GLN	2.5
6	F	215	CYS	2.5
7	U	241	GLU	2.4
1	O	249	ALA	2.4
2	B	54	THR	2.4
5	S	165	GLN	2.4
9	W	131	GLU	2.4
11	Y	212	GLY	2.4
1	O	250	LEU	2.4
11	Y	106	ARG	2.4
6	T	241	LYS	2.4
11	Y	202	GLU	2.4
4	R	1	ASP	2.3
4	D	125	LEU	2.3
3	C	238	LYS	2.3
5	E	233	ILE	2.3
4	R	2	ARG	2.3
3	C	203	THR	2.3
1	A	62	SER	2.3
3	Q	48	SER	2.3
1	A	248	GLU	2.3
6	T	2	THR	2.3

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Mol	Chain	Res	Type	RSRZ
4	D	2	ARG	2.3
3	Q	58	THR	2.2
14	b	105	LYS	2.2
1	O	248	GLU	2.2
7	G	188	GLU	2.2
7	G	240	ALA	2.2
14	N	104	ASP	2.2
3	C	175	LYS	2.2
10	J	1	MET	2.2
4	D	177	ASN	2.2
7	G	2	GLY	2.1
12	Z	210	ASP	2.1
8	V	22	GLN	2.1
3	C	50	LEU	2.1
8	V	145	ASP	2.1
5	S	225	ASP	2.1
1	A	250	LEU	2.1
2	B	220	ASN	2.1
5	E	217	LYS	2.1
3	C	1	GLY	2.0
6	F	201	GLU	2.0
3	C	225	GLU	2.0
5	E	54	GLU	2.0
2	B	60	THR	2.0
5	E	163	ARG	2.0
13	M	1	THR	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 carbohydrates in this entry.

6.4 Ligands (i)

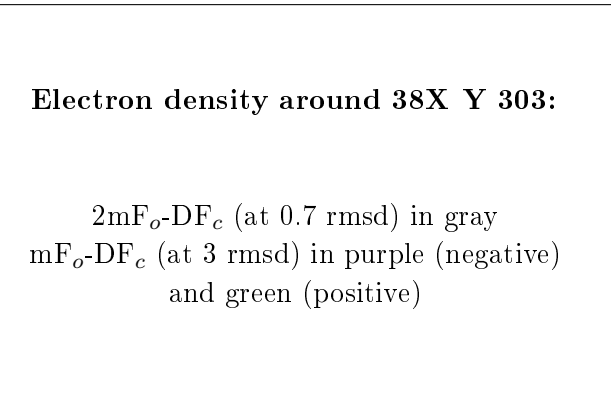
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

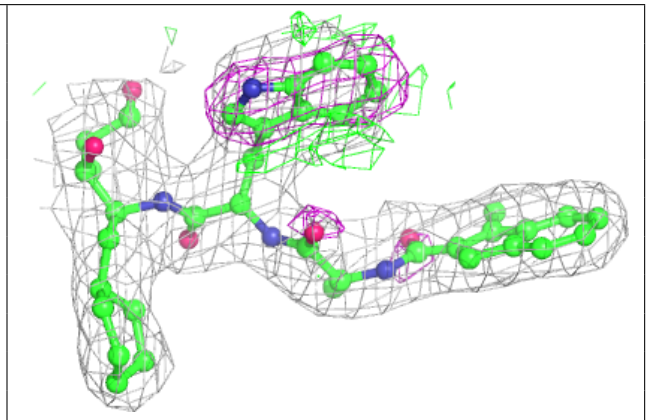
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
17	38X	Y	303	46/46	0.84	0.23	14,45,52,61	0
17	38X	K	303	46/46	0.87	0.21	12,40,48,49	0
15	MG	Z	301	1/1	0.88	0.48	71,71,71,71	0
15	MG	V	301	1/1	0.89	0.20	67,67,67,67	0
15	MG	H	301	1/1	0.92	0.24	64,64,64,64	0
16	MES	Y	302	12/12	0.92	0.21	63,66,72,72	0
15	MG	I	301	1/1	0.93	0.29	54,54,54,54	0
16	MES	K	302	12/12	0.93	0.21	55,58,65,70	0
15	MG	Y	301	1/1	0.94	0.15	36,36,36,36	0
15	MG	K	301	1/1	0.95	0.11	52,52,52,52	0
15	MG	N	201	1/1	0.97	0.13	38,38,38,38	0
15	MG	G	301	1/1	0.98	0.08	40,40,40,40	0

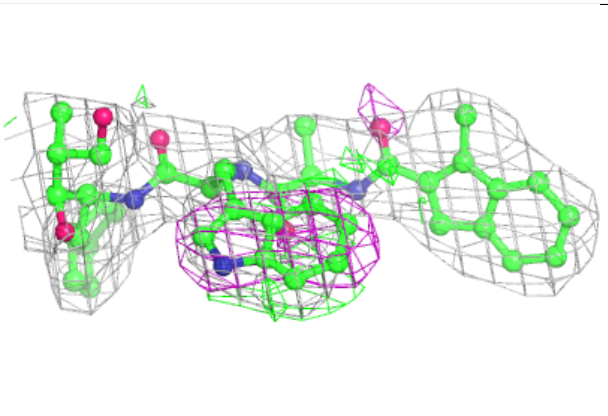
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

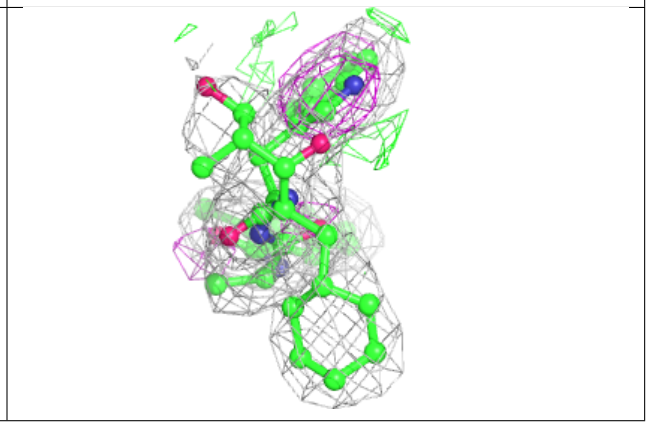
Electron density around 38X Y 303:

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



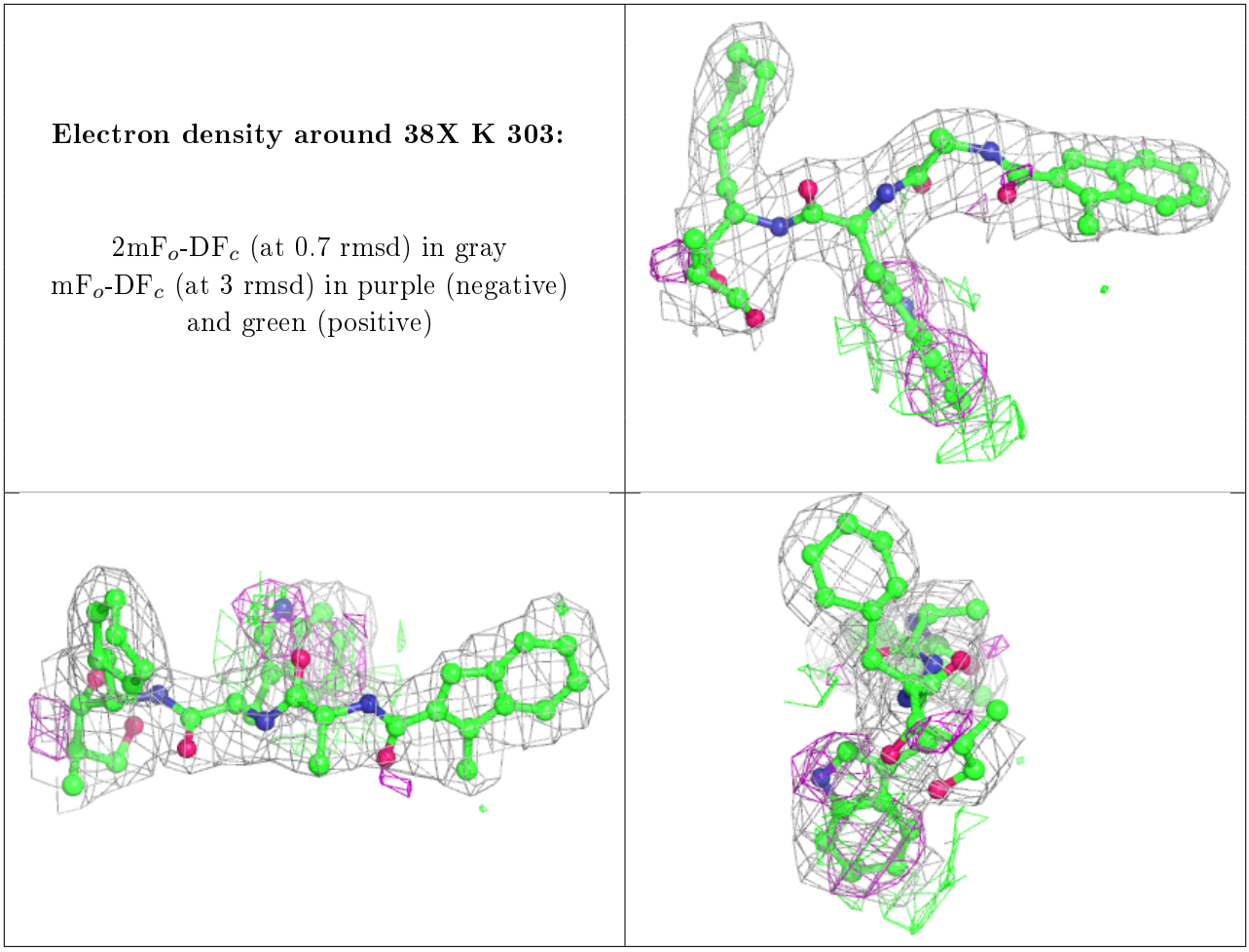






Electron density around 38X K 303:

$2mF_o$-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

There are no such residues in this entry.