Full wwPDB X-ray Structure Validation Report (i)

Jan 7, 2024 – 07:57 pm GMT

PDB ID	:	6G8M
Title	:	Yeast 20S proteasome in complex with Cystargolide B Derivative 1
Authors	:	Groll, M.; Tello-Aburto, R.
Deposited on	:	2018-04-09
Resolution	:	2.70 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) 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 (i)) were used in the production of this report:

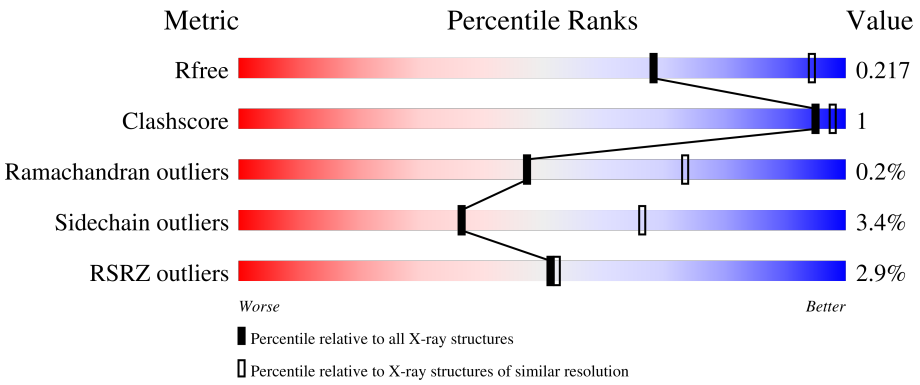
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.70 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (2.70-2.70)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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% 98% •
1	O	250	3% 98% •
2	B	258	3% 89% 6% 5%
2	P	258	6% 89% 5% 5%
3	C	254	6% 87% 6% • 6%

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Mol	Chain	Length	Quality of chain
3	Q	254	8% 88% 6% 6%
4	D	260	2% 86% 10%
4	R	260	4% 86% 10%
5	E	234	3% 94% 5%
5	S	234	5% 94% 5%
6	F	288	3% 81% 16%
6	T	288	3% 81% 16%
7	G	252	4% 89% 6%
7	U	252	3% 89% 6%
8	H	232	3% 90% 6%
8	V	232	4% 90% 6%
9	I	205	95%
9	W	205	% 95% 5%
10	J	198	2% 94% 5%
10	X	198	2% 95%
11	K	212	94% 5%
11	Y	212	92% 7%
12	L	222	95%
12	Z	222	% 95% 5%
13	M	246	2% 89% 7%
13	a	246	% 91% 6%
14	N	196	% 94% 6%
14	b	196	% 97%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
17	EQE	b	201	-	-	-	X

2 Entry composition (i)

There are 18 unique types of molecules in this entry. The entry contains 49780 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
			Total	C	N	O	S			
1	A	250	1915	1219	315	377	4	0	0	0
1	O	250	1915	1219	315	377	4	0	0	0

- Molecule 2 is a protein called Proteasome subunit alpha type-3.

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
8	H	226	1719	1082	298	332	7	0	0	0
8	V	226	1719	1082	298	332	7	0	0	0

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

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

- Molecule 10 is a protein called Proteasome subunit beta type-4.

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

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
11	K	212	1644	1045	280	312	7	0	0	0
			Total	C	N	O	S			
11	Y	212	1644	1045	280	312	7	0	0	0

- Molecule 12 is a protein called Proteasome subunit beta type-6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
12	L	222	1757	1115	303	335	4	0	0	0
			Total	C	N	O	S			
12	Z	222	1757	1115	303	335	4	0	0	0

- Molecule 13 is a protein called Proteasome subunit beta type-7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
13	M	229	1790	1133	306	344	7	0	0	0
			Total	C	N	O	S			
13	a	232	1815	1148	311	349	7	0	0	0

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

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

- Molecule 15 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

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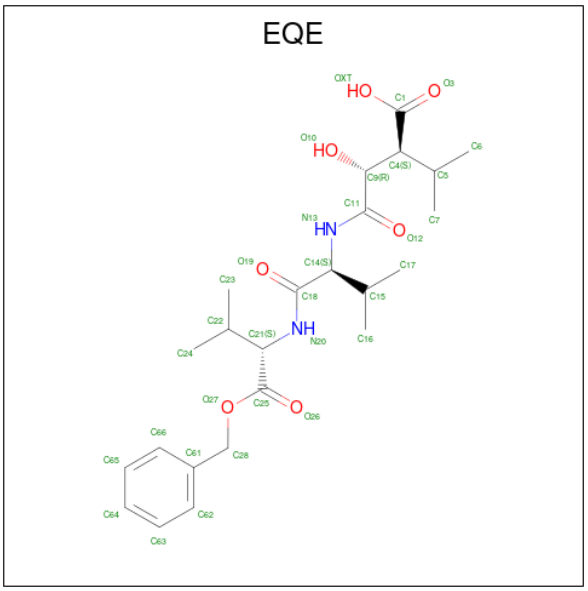
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
15	K	1	Total Mg 1 1	0	0
15	N	1	Total Mg 1 1	0	0
15	V	1	Total Mg 1 1	0	0
15	W	1	Total Mg 1 1	0	0
15	Y	1	Total Mg 1 1	0	0
15	Z	1	Total Mg 1 1	0	0

- Molecule 16 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
16	G	1	Total Cl 1 1	0	0
16	U	1	Total Cl 1 1	0	0

- Molecule 17 is (2 {S},3 {R})-4-[[(2 {S})-3-methyl-1-[[(2 {S})-3-methyl-1-oxidanylidene-1-phenylmethoxy-butan-2-yl]amino]-1-oxidanylidene-butan-2-yl]amino]-3-oxidanyl-4-oxidanylidene-2-propan-2-yl-butanoic acid (three-letter code: EQE) (formula: $C_{24}H_{36}N_2O_7$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
17	H	1	32	24	2	6	0	0
17	K	1	32	24	2	6	0	0
17	N	1	32	24	2	6	0	0
17	V	1	32	24	2	6	0	0
17	Y	1	32	24	2	6	0	0
17	b	1	32	24	2	6	0	0

- Molecule 18 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
18	A	14	14	14	0	0
18	B	8	8	8	0	0
18	C	10	10	10	0	0
18	D	6	6	6	0	0
18	E	6	6	6	0	0
18	F	12	12	12	0	0
18	G	9	9	9	0	0
18	H	11	11	11	0	0
18	I	9	9	9	0	0
18	J	10	10	10	0	0
18	K	14	14	14	0	0
18	L	13	13	13	0	0
18	M	13	13	13	0	0
18	N	5	5	5	0	0

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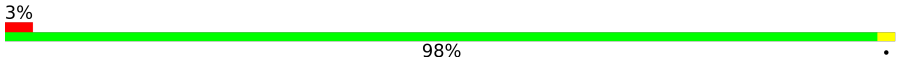
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
18	O	4	4	4	0	0
			Total	O		
18	P	8	8	8	0	0
			Total	O		
18	Q	12	12	12	0	0
			Total	O		
18	R	4	4	4	0	0
			Total	O		
18	S	5	5	5	0	0
			Total	O		
18	T	9	9	9	0	0
			Total	O		
18	U	7	7	7	0	0
			Total	O		
18	V	7	7	7	0	0
			Total	O		
18	W	4	4	4	0	0
			Total	O		
18	X	8	8	8	0	0
			Total	O		
18	Y	12	12	12	0	0
			Total	O		
18	Z	13	13	13	0	0
			Total	O		
18	a	15	15	15	0	0
			Total	O		
18	b	7	7	7	0	0

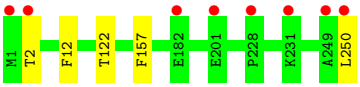
3 Residue-property plots (i)

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

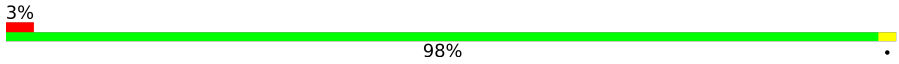
Chain A:





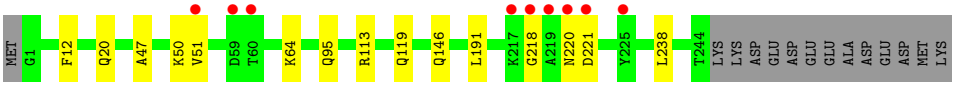
• Molecule 1: Proteasome subunit alpha type-2

Chain O:



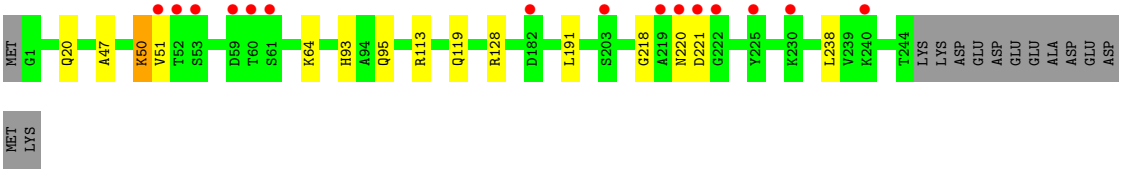
• Molecule 2: Proteasome subunit alpha type-3

Chain B:



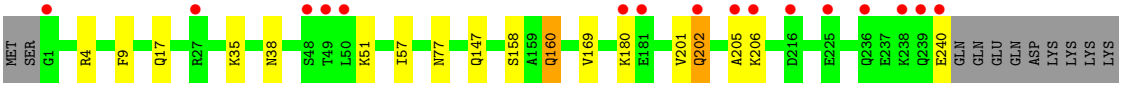
• Molecule 2: Proteasome subunit alpha type-3

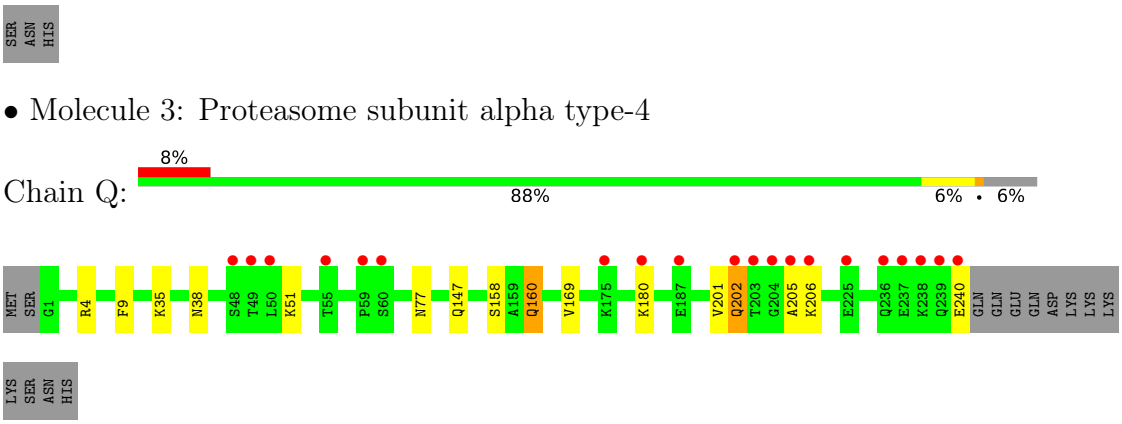
Chain P:

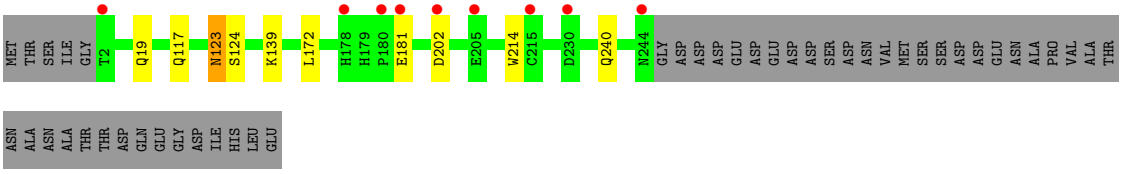


• Molecule 3: Proteasome subunit alpha type-4

Chain C:

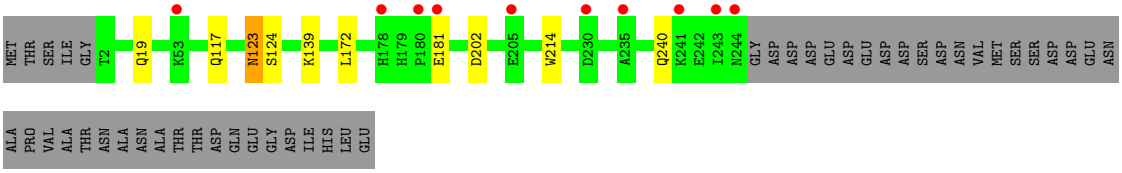



SER
ASN
HIS
• Molecule 3: Proteasome subunit alpha type-4
Chain Q:
8%
88%
6%
6%
MET SER G1 R4 F9 K35 N38 S48 T49 L50 K51 T55 P59 S60 N77 Q147 S158 A159 Q160 V169 K175 K180 E187 V201 Q202 T203 G204 A205 K206 E225 Q236 E237 K238 Q239 E240 GLN GLN GLU GLN ASP LYS LYS LYS
LYS
SER
ASN
HIS
• Molecule 4: Proteasome subunit alpha type-5
Chain D:
2%
86%
10%
MET PHE LEU THR ARG SER GLU TYR D1 Q15 A88 H91 I99 E117 GLY ALA SER GLY GLU GLU ARG L125 D143 L176 L193 I214 Q217 L235 K236 A241 E242 SER PRO GLU GLU ALA ASP VAL GLU MET SER
• Molecule 4: Proteasome subunit alpha type-5
Chain R:
4%
86%
10%
MET PHE LEU THR ARG SER GLU TYR D1 R2 Q15 H91 I99 E117 GLY ALA SER GLY GLU GLU ARG L125 A141 D142 D143 Y159 L176 L193 I214 Q217 D224 N225 E226 E230 L235 K236 A241 E242 SER PRO GLU GLU ALA ASP VAL GLU
MET
SER
• Molecule 5: Proteasome subunit alpha type-6
Chain E:
3%
94%
5%
MET PHE ARG N3 T9 F12 K29 E54 L71 L87 A107 Q116 R173 N184 L188 R201 D202 E203 K231 Y232 I233
• Molecule 5: Proteasome subunit alpha type-6
Chain S:
5%
94%
5%
MET PHE ARG N3 T9 F12 K29 Q30 E54 L55 S56 S57 Y58 L71 L87 A107 Q116 R173 K180 N184 E187 L188 E194 D202 E203 S204 E227 K231 Y232 I233
• Molecule 6: Probable proteasome subunit alpha type-7
Chain F:
3%
81%
16%



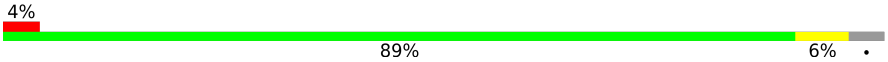
• Molecule 6: Probable proteasome subunit alpha type-7

Chain T:



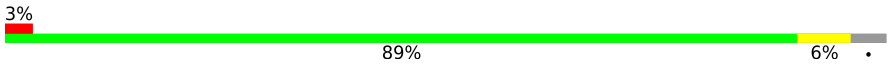
• Molecule 7: Proteasome subunit alpha type-1

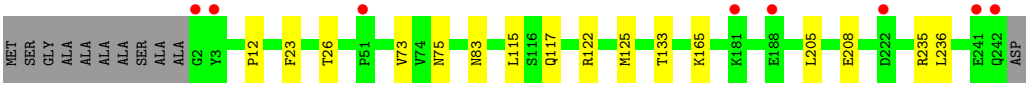
Chain G:



• Molecule 7: Proteasome subunit alpha type-1

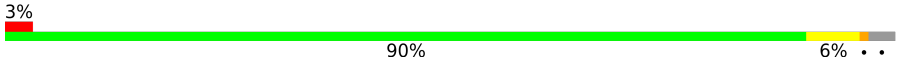
Chain U:

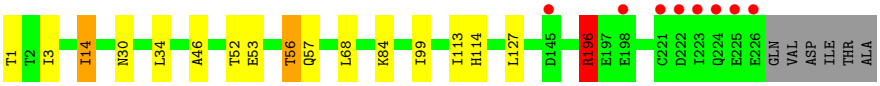




• Molecule 8: Proteasome subunit beta type-2

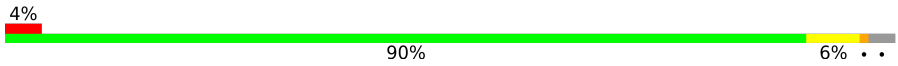
Chain H:





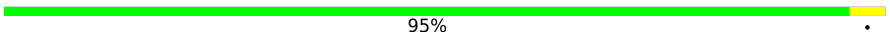
• Molecule 8: Proteasome subunit beta type-2

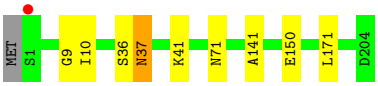
Chain V:



• Molecule 9: Proteasome subunit beta type-3

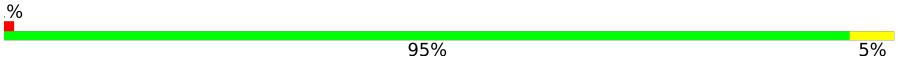
Chain I:





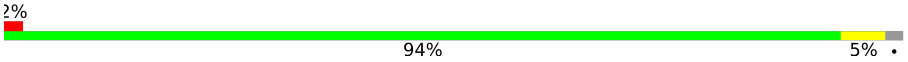
• Molecule 9: Proteasome subunit beta type-3

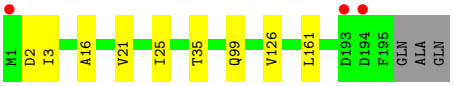
Chain W:



• Molecule 10: Proteasome subunit beta type-4

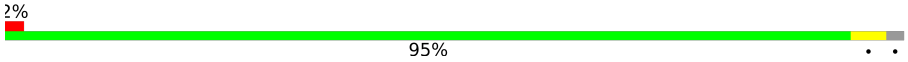
Chain J:

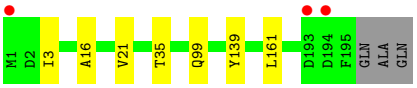




• Molecule 10: Proteasome subunit beta type-4

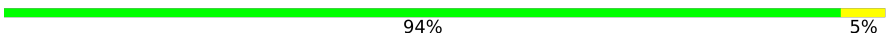
Chain X:





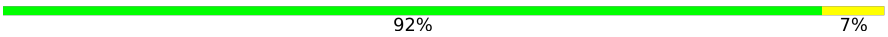
• Molecule 11: Proteasome subunit beta type-5

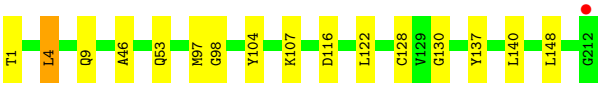
Chain K:



• Molecule 11: Proteasome subunit beta type-5

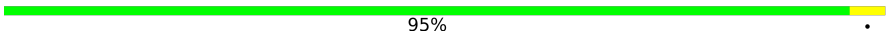
Chain Y:

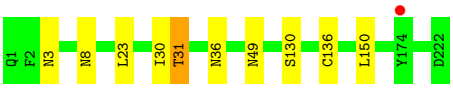




• Molecule 12: Proteasome subunit beta type-6

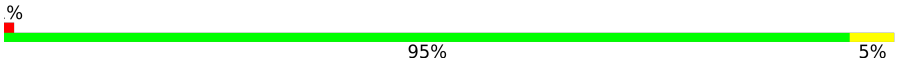
Chain L:

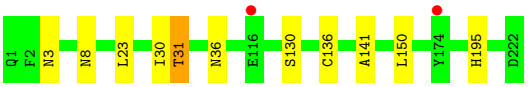




• Molecule 12: Proteasome subunit beta type-6

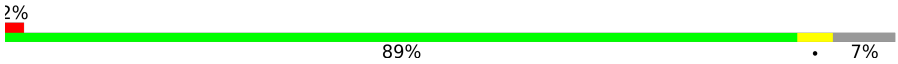
Chain Z:

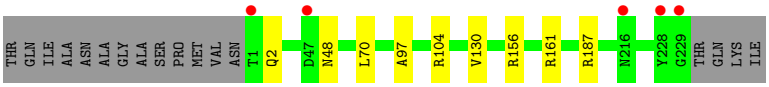




• Molecule 13: Proteasome subunit beta type-7

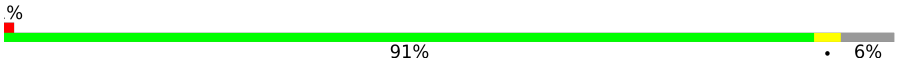
Chain M:

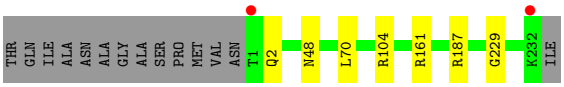




• Molecule 13: Proteasome subunit beta type-7

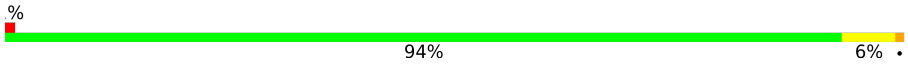
Chain a:

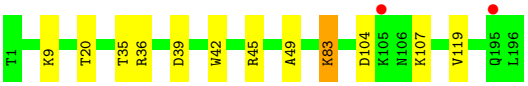




• Molecule 14: Proteasome subunit beta type-1

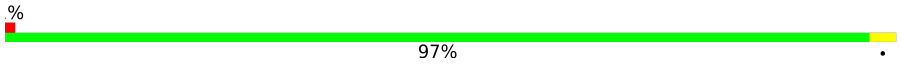
Chain N:

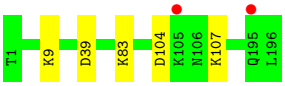




• Molecule 14: Proteasome subunit beta type-1

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	136.75Å 301.02Å 145.46Å 90.00° 113.64° 90.00°	Depositor
Resolution (Å)	15.00 – 2.70 15.00 – 2.70	Depositor EDS
% Data completeness (in resolution range)	97.3 (15.00-2.70) 97.9 (15.00-2.70)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.70 (at 2.69Å)	Xtriage
Refinement program	REFMAC 5.8.0158	Depositor
R, R_{free}	0.179 , 0.214 0.185 , 0.217	Depositor DCC
R_{free} test set	14294 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	61.6	Xtriage
Anisotropy	0.279	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 32.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	49780	wwPDB-VP
Average B, all atoms (Å^2)	73.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.56% 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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: CL, MG, EQE

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	0.35	0/1952	0.55	0/2642
1	O	0.35	0/1952	0.55	0/2642
2	B	0.36	0/1934	0.59	0/2618
2	P	0.35	0/1934	0.59	0/2618
3	C	0.35	0/1910	0.61	0/2586
3	Q	0.35	0/1910	0.61	0/2586
4	D	0.34	0/1837	0.57	0/2475
4	R	0.34	0/1837	0.57	0/2475
5	E	0.34	0/1800	0.57	0/2433
5	S	0.34	0/1800	0.56	0/2433
6	F	0.34	0/1932	0.54	0/2609
6	T	0.34	0/1932	0.54	0/2609
7	G	0.35	0/1945	0.55	0/2634
7	U	0.35	0/1945	0.55	0/2634
8	H	0.34	0/1750	0.59	1/2373 (0.0%)
8	V	0.33	0/1750	0.58	1/2373 (0.0%)
9	I	0.34	0/1611	0.57	0/2174
9	W	0.34	0/1611	0.57	0/2174
10	J	0.34	0/1589	0.59	0/2142
10	X	0.34	0/1589	0.59	0/2142
11	K	0.33	0/1681	0.59	1/2274 (0.0%)
11	Y	0.34	0/1681	0.59	1/2274 (0.0%)
12	L	0.34	0/1795	0.57	0/2420
12	Z	0.35	0/1795	0.57	0/2420
13	M	0.35	0/1821	0.62	0/2470
13	a	0.35	0/1846	0.61	0/2503
14	N	0.36	0/1541	0.59	0/2087
14	b	0.36	0/1541	0.58	0/2087
All	All	0.35	0/50221	0.58	4/67907 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	K	4	LEU	CA-CB-CG	5.62	128.22	115.30
11	Y	4	LEU	CA-CB-CG	5.60	128.18	115.30
8	H	196	ARG	NE-CZ-NH1	5.21	122.91	120.30
8	V	196	ARG	NE-CZ-NH1	5.20	122.90	120.30

There are no chirality outliers.

There are no planarity outliers.

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	1	0
1	O	1915	0	1929	3	0
2	B	1904	0	1904	5	0
2	P	1904	0	1904	6	0
3	C	1881	0	1895	6	0
3	Q	1881	0	1895	4	0
4	D	1813	0	1797	4	0
4	R	1813	0	1797	3	0
5	E	1773	0	1775	2	0
5	S	1773	0	1775	3	0
6	F	1892	0	1883	3	0
6	T	1892	0	1883	3	0
7	G	1907	0	1901	4	0
7	U	1907	0	1901	4	0
8	H	1719	0	1718	10	0
8	V	1719	0	1718	8	0
9	I	1581	0	1574	6	0
9	W	1581	0	1574	5	0
10	J	1561	0	1569	4	0
10	X	1561	0	1569	3	0
11	K	1644	0	1594	3	0
11	Y	1644	0	1594	6	0
12	L	1757	0	1711	2	0
12	Z	1757	0	1711	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
13	M	1790	0	1793	2	0
13	a	1815	0	1821	0	0
14	N	1512	0	1480	9	0
14	b	1512	0	1480	0	0
15	G	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	W	1	0	0	0	0
15	Y	1	0	0	0	0
15	Z	1	0	0	0	0
16	G	1	0	0	0	0
16	U	1	0	0	0	0
17	H	32	0	0	4	0
17	K	32	0	0	1	0
17	N	32	0	0	8	0
17	V	32	0	0	2	0
17	Y	32	0	0	1	0
17	b	32	0	0	0	0
18	A	14	0	0	0	0
18	B	8	0	0	0	0
18	C	10	0	0	0	0
18	D	6	0	0	0	0
18	E	6	0	0	0	0
18	F	12	0	0	0	0
18	G	9	0	0	0	0
18	H	11	0	0	4	0
18	I	9	0	0	0	0
18	J	10	0	0	0	0
18	K	14	0	0	0	0
18	L	13	0	0	0	0
18	M	13	0	0	0	0
18	N	5	0	0	0	0
18	O	4	0	0	0	0
18	P	8	0	0	1	0
18	Q	12	0	0	0	0
18	R	4	0	0	0	0
18	S	5	0	0	0	0
18	T	9	0	0	0	0
18	U	7	0	0	0	0
18	V	7	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
18	W	4	0	0	0	0
18	X	8	0	0	0	0
18	Y	12	0	0	0	0
18	Z	13	0	0	0	0
18	a	15	0	0	0	0
18	b	7	0	0	0	0
All	All	49780	0	49074	98	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 1.

All (98) 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)
14:N:49:ALA:HB3	17:N:201:EQE:C24	1.92	1.00
14:N:49:ALA:CB	17:N:201:EQE:C24	2.60	0.79
14:N:20:THR:CG2	17:N:201:EQE:C23	2.62	0.77
8:H:52:THR:O	8:H:56:THR:OG1	2.07	0.73
8:V:52:THR:O	8:V:56:THR:OG1	2.07	0.72
3:C:160:GLN:HE21	3:C:160:GLN:HA	1.62	0.64
3:Q:160:GLN:HE21	3:Q:160:GLN:HA	1.63	0.62
17:H:301:EQE:C66	18:H:405:HOH:O	2.47	0.62
8:H:53:GLU:OE1	8:H:57:GLN:NE2	2.33	0.62
8:H:1:THR:OG1	17:H:301:EQE:O10	2.19	0.60
8:V:53:GLU:OE1	8:V:57:GLN:NE2	2.35	0.59
2:B:12:PHE:H	3:C:17:GLN:HE22	1.54	0.56
7:G:23:PHE:O	7:G:26:THR:HB	2.05	0.56
7:U:23:PHE:O	7:U:26:THR:HB	2.05	0.56
14:N:20:THR:HG23	17:N:201:EQE:C23	2.37	0.55
2:P:93:HIS:HB3	18:P:301:HOH:O	2.07	0.55
5:E:12:PHE:H	6:F:19:GLN:HE22	1.54	0.55
17:N:201:EQE:C7	17:N:201:EQE:C11	2.85	0.54
8:H:3:ILE:HG13	8:H:99:ILE:HD12	1.89	0.54
5:S:12:PHE:H	6:T:19:GLN:HE22	1.58	0.52
17:H:301:EQE:C65	18:H:405:HOH:O	2.58	0.51
1:O:12:PHE:H	2:P:20:GLN:HE22	1.58	0.51
8:V:80:LEU:HD13	8:V:119:THR:HG21	1.91	0.51
1:A:12:PHE:H	2:B:20:GLN:HE22	1.57	0.51
8:H:114:HIS:HB3	18:H:410:HOH:O	2.10	0.51
10:J:16:ALA:HB2	10:J:161:LEU:HD21	1.93	0.51
4:R:159:TYR:CE2	5:S:56:SER:HB3	2.45	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:21:VAL:HG11	11:K:122:LEU:HD11	1.93	0.50
10:X:21:VAL:HG11	11:Y:122:LEU:HD11	1.94	0.50
11:K:128:CYS:HB2	11:K:137:TYR:CZ	2.47	0.50
11:Y:128:CYS:HB2	11:Y:137:TYR:CZ	2.47	0.50
9:I:9:GLY:HA3	9:I:41:LYS:HE2	1.94	0.49
9:I:10:ILE:HG21	9:I:141:ALA:HB3	1.95	0.48
12:Z:31:THR:HG23	12:Z:36:ASN:HD21	1.78	0.48
9:W:9:GLY:HA3	9:W:41:LYS:HE2	1.95	0.48
2:B:146:GLN:HG2	3:C:57:ILE:HG21	1.94	0.48
10:X:16:ALA:HB2	10:X:161:LEU:HD21	1.95	0.48
9:W:10:ILE:HG21	9:W:141:ALA:HB3	1.95	0.48
4:R:91:HIS:CD2	4:R:99:ILE:HG22	2.49	0.47
12:L:31:THR:HG23	12:L:36:ASN:HD21	1.79	0.47
9:I:36:SER:HB2	10:J:126:VAL:HG11	1.96	0.47
6:F:123:ASN:C	6:F:123:ASN:HD22	2.18	0.47
8:H:196:ARG:NH2	9:I:150:GLU:O	2.48	0.46
6:F:123:ASN:HD22	6:F:124:SER:N	2.13	0.46
8:V:84:LYS:HA	8:V:113:ILE:HD11	1.98	0.46
8:H:3:ILE:HD11	8:H:127:LEU:HB3	1.98	0.46
2:B:95:GLN:HE22	9:I:71:ASN:HD22	1.62	0.46
7:G:68:ARG:HH12	14:N:36:ARG:HH22	1.63	0.46
2:P:95:GLN:HE22	9:W:71:ASN:HD22	1.63	0.46
1:O:23:TYR:CD1	7:U:12:PRO:HA	2.51	0.45
18:H:407:HOH:O	17:N:201:EQE:C66	2.63	0.45
8:V:1:THR:OG1	17:V:301:EQE:O10	2.31	0.45
8:H:84:LYS:HA	8:H:113:ILE:HD11	1.98	0.45
11:Y:1:THR:HG21	17:Y:301:EQE:O3	2.16	0.45
4:D:91:HIS:CD2	4:D:99:ILE:HG22	2.52	0.45
6:T:123:ASN:C	6:T:123:ASN:HD22	2.20	0.45
8:H:46:ALA:HA	17:H:301:EQE:O3	2.17	0.44
6:T:123:ASN:HD22	6:T:124:SER:N	2.15	0.44
8:V:218:VAL:CG2	9:W:196:LYS:HB2	2.48	0.44
13:M:156:ARG:HH11	8:V:165:ASN:HD22	1.65	0.44
3:Q:9:PHE:H	4:R:15:GLN:HE22	1.66	0.44
5:S:87:LEU:HD21	5:S:107:ALA:HB1	1.99	0.44
11:K:128:CYS:HB2	11:K:137:TYR:CE2	2.53	0.44
8:H:14:ILE:HG21	8:H:14:ILE:HD13	1.82	0.43
11:Y:128:CYS:HB2	11:Y:137:TYR:CE2	2.53	0.43
2:P:47:ALA:HB1	2:P:64:LYS:HD2	2.00	0.43
2:B:47:ALA:HB1	2:B:64:LYS:HD2	2.01	0.43
8:V:46:ALA:HA	17:V:301:EQE:O3	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:87:LEU:HD21	5:E:107:ALA:HB1	2.00	0.43
3:C:201:VAL:O	3:C:202:GLN:CB	2.67	0.43
11:Y:1:THR:O	11:Y:130:GLY:HA3	2.18	0.42
12:Z:141:ALA:HB1	12:Z:195:HIS:NE2	2.34	0.42
3:C:35:LYS:HG2	3:C:158:SER:O	2.19	0.42
3:C:9:PHE:H	4:D:15:GLN:HE22	1.67	0.42
2:P:50:LYS:HD3	2:P:50:LYS:HA	1.92	0.42
3:Q:201:VAL:O	3:Q:202:GLN:CB	2.67	0.42
14:N:83:LYS:HG3	14:N:119:VAL:CG2	2.50	0.41
12:L:8:ASN:HA	12:L:30:ILE:O	2.20	0.41
14:N:35:THR:HG21	14:N:45:ARG:HE	1.85	0.41
7:U:73:VAL:HG12	7:U:133:THR:HB	2.01	0.41
14:N:36:ARG:HG3	14:N:42:TRP:CE2	2.55	0.41
9:I:37:ASN:HD22	9:I:37:ASN:C	2.24	0.41
17:N:201:EQE:C24	17:N:201:EQE:O19	2.69	0.41
1:O:122:THR:HG22	2:P:128:ARG:HH21	1.84	0.41
7:G:165:LYS:HD2	7:G:205:LEU:HD22	2.03	0.41
13:M:97:ALA:HA	13:M:130:VAL:HG21	2.03	0.41
3:Q:35:LYS:HG2	3:Q:158:SER:O	2.21	0.41
9:W:20:VAL:HG13	9:W:118:PRO:HB3	2.03	0.41
7:U:165:LYS:HD2	7:U:205:LEU:HD22	2.03	0.41
12:Z:8:ASN:HA	12:Z:30:ILE:O	2.21	0.41
4:D:88:ALA:HA	4:D:99:ILE:HG21	2.03	0.40
10:J:25:ILE:O	10:X:139:TYR:OH	2.39	0.40
17:K:301:EQE:O26	17:K:301:EQE:C24	2.69	0.40
12:Z:31:THR:CG2	12:Z:36:ASN:HD21	2.34	0.40
7:G:73:VAL:HG12	7:G:133:THR:HB	2.02	0.40
14:N:20:THR:HG21	17:N:201:EQE:C23	2.48	0.40
11:Y:46:ALA:HB3	11:Y:98:GLY:O	2.21	0.40
4:D:91:HIS:HB3	4:D:99:ILE:CG2	2.52	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%)	241 (97%)	6 (2%)	1 (0%)	34	60
1	O	248/250 (99%)	240 (97%)	7 (3%)	1 (0%)	34	60
2	B	242/258 (94%)	235 (97%)	3 (1%)	4 (2%)	9	23
2	P	242/258 (94%)	235 (97%)	3 (1%)	4 (2%)	9	23
3	C	238/254 (94%)	232 (98%)	4 (2%)	2 (1%)	19	43
3	Q	238/254 (94%)	232 (98%)	4 (2%)	2 (1%)	19	43
4	D	231/260 (89%)	227 (98%)	4 (2%)	0	100	100
4	R	231/260 (89%)	228 (99%)	3 (1%)	0	100	100
5	E	229/234 (98%)	221 (96%)	8 (4%)	0	100	100
5	S	229/234 (98%)	222 (97%)	7 (3%)	0	100	100
6	F	241/288 (84%)	237 (98%)	4 (2%)	0	100	100
6	T	241/288 (84%)	237 (98%)	4 (2%)	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%)	219 (98%)	5 (2%)	0	100	100
9	I	202/205 (98%)	194 (96%)	8 (4%)	0	100	100
9	W	202/205 (98%)	194 (96%)	8 (4%)	0	100	100
10	J	193/198 (98%)	187 (97%)	6 (3%)	0	100	100
10	X	193/198 (98%)	188 (97%)	5 (3%)	0	100	100
11	K	210/212 (99%)	205 (98%)	5 (2%)	0	100	100
11	Y	210/212 (99%)	205 (98%)	5 (2%)	0	100	100
12	L	220/222 (99%)	215 (98%)	5 (2%)	0	100	100
12	Z	220/222 (99%)	216 (98%)	4 (2%)	0	100	100
13	M	227/246 (92%)	221 (97%)	6 (3%)	0	100	100
13	a	230/246 (94%)	223 (97%)	6 (3%)	1 (0%)	34	60
14	N	194/196 (99%)	189 (97%)	5 (3%)	0	100	100
14	b	194/196 (99%)	190 (98%)	4 (2%)	0	100	100
All	All	6279/6614 (95%)	6127 (98%)	137 (2%)	15 (0%)	47	73

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	51	VAL
2	B	221	ASP
3	C	202	GLN
2	P	51	VAL
2	P	221	ASP
3	Q	202	GLN
1	A	2	THR
2	B	218	GLY
2	B	220	ASN
1	O	2	THR
2	P	218	GLY
2	P	220	ASN
3	C	205	ALA
3	Q	205	ALA
13	a	229	GLY

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%)	206 (99%)	3 (1%)	67	86
1	O	209/209 (100%)	206 (99%)	3 (1%)	67	86
2	B	203/216 (94%)	198 (98%)	5 (2%)	47	76
2	P	203/216 (94%)	198 (98%)	5 (2%)	47	76
3	C	212/226 (94%)	202 (95%)	10 (5%)	26	54
3	Q	212/226 (94%)	202 (95%)	10 (5%)	26	54
4	D	194/215 (90%)	185 (95%)	9 (5%)	27	54
4	R	194/215 (90%)	185 (95%)	9 (5%)	27	54
5	E	190/193 (98%)	182 (96%)	8 (4%)	30	58
5	S	190/193 (98%)	182 (96%)	8 (4%)	30	58
6	F	201/239 (84%)	193 (96%)	8 (4%)	31	60
6	T	201/239 (84%)	193 (96%)	8 (4%)	31	60
7	G	206/210 (98%)	197 (96%)	9 (4%)	28	56

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
7	U	206/210 (98%)	197 (96%)	9 (4%)	28	56
8	H	185/190 (97%)	179 (97%)	6 (3%)	39	68
8	V	185/190 (97%)	177 (96%)	8 (4%)	29	57
9	I	172/173 (99%)	170 (99%)	2 (1%)	71	88
9	W	172/173 (99%)	170 (99%)	2 (1%)	71	88
10	J	173/175 (99%)	169 (98%)	4 (2%)	50	78
10	X	173/175 (99%)	170 (98%)	3 (2%)	60	84
11	K	169/169 (100%)	160 (95%)	9 (5%)	22	48
11	Y	169/169 (100%)	160 (95%)	9 (5%)	22	48
12	L	185/185 (100%)	178 (96%)	7 (4%)	33	62
12	Z	185/185 (100%)	179 (97%)	6 (3%)	39	68
13	M	195/208 (94%)	189 (97%)	6 (3%)	40	69
13	a	198/208 (95%)	192 (97%)	6 (3%)	41	70
14	N	162/162 (100%)	157 (97%)	5 (3%)	40	69
14	b	162/162 (100%)	157 (97%)	5 (3%)	40	69
All	All	5315/5540 (96%)	5133 (97%)	182 (3%)	37	66

All (182) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	122	THR
1	A	157	PHE
1	A	250	LEU
2	B	50	LYS
2	B	113	ARG
2	B	119	GLN
2	B	191	LEU
2	B	238	LEU
3	C	4	ARG
3	C	38	ASN
3	C	51	LYS
3	C	77	ASN
3	C	147	GLN
3	C	160	GLN
3	C	169	VAL
3	C	180	LYS
3	C	206	LYS

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Mol	Chain	Res	Type
3	C	240	GLU
4	D	99	ILE
4	D	125	LEU
4	D	143	ASP
4	D	176	LEU
4	D	193	LEU
4	D	214	ILE
4	D	235	LEU
4	D	236	LYS
4	D	242	GLU
5	E	9	THR
5	E	29	LYS
5	E	71	LEU
5	E	116	GLN
5	E	184	ASN
5	E	188	LEU
5	E	202	ASP
5	E	231	LYS
6	F	117	GLN
6	F	123	ASN
6	F	139	LYS
6	F	172	LEU
6	F	181	GLU
6	F	202	ASP
6	F	214	TRP
6	F	240	GLN
7	G	75	ASN
7	G	83	ASN
7	G	115	LEU
7	G	117	GLN
7	G	122	ARG
7	G	125	MET
7	G	208	GLU
7	G	235	ARG
7	G	236	LEU
8	H	14	ILE
8	H	30	ASN
8	H	34	LEU
8	H	56	THR
8	H	68	LEU
8	H	196	ARG
9	I	37	ASN

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Mol	Chain	Res	Type
9	I	171	LEU
10	J	2	ASP
10	J	3	ILE
10	J	35	THR
10	J	99	GLN
11	K	4	LEU
11	K	9	GLN
11	K	53	GLN
11	K	97	MET
11	K	104	TYR
11	K	107	LYS
11	K	116	ASP
11	K	140	LEU
11	K	148	LEU
12	L	3	ASN
12	L	23	LEU
12	L	31	THR
12	L	49	ASN
12	L	130	SER
12	L	136	CYS
12	L	150	LEU
13	M	2	GLN
13	M	48	ASN
13	M	70	LEU
13	M	104	ARG
13	M	161	ARG
13	M	187	ARG
14	N	9	LYS
14	N	39	ASP
14	N	83	LYS
14	N	104	ASP
14	N	107	LYS
1	O	122	THR
1	O	157	PHE
1	O	250	LEU
2	P	50	LYS
2	P	113	ARG
2	P	119	GLN
2	P	191	LEU
2	P	238	LEU
3	Q	4	ARG
3	Q	38	ASN

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Mol	Chain	Res	Type
3	Q	51	LYS
3	Q	77	ASN
3	Q	147	GLN
3	Q	160	GLN
3	Q	169	VAL
3	Q	180	LYS
3	Q	206	LYS
3	Q	240	GLU
4	R	99	ILE
4	R	125	LEU
4	R	143	ASP
4	R	176	LEU
4	R	193	LEU
4	R	214	ILE
4	R	235	LEU
4	R	236	LYS
4	R	242	GLU
5	S	9	THR
5	S	29	LYS
5	S	71	LEU
5	S	116	GLN
5	S	184	ASN
5	S	188	LEU
5	S	202	ASP
5	S	231	LYS
6	T	117	GLN
6	T	123	ASN
6	T	139	LYS
6	T	172	LEU
6	T	181	GLU
6	T	202	ASP
6	T	214	TRP
6	T	240	GLN
7	U	75	ASN
7	U	83	ASN
7	U	115	LEU
7	U	117	GLN
7	U	122	ARG
7	U	125	MET
7	U	208	GLU
7	U	235	ARG
7	U	236	LEU

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Mol	Chain	Res	Type
8	V	14	ILE
8	V	22	GLN
8	V	30	ASN
8	V	34	LEU
8	V	56	THR
8	V	68	LEU
8	V	80	LEU
8	V	196	ARG
9	W	37	ASN
9	W	171	LEU
10	X	3	ILE
10	X	35	THR
10	X	99	GLN
11	Y	4	LEU
11	Y	9	GLN
11	Y	53	GLN
11	Y	97	MET
11	Y	104	TYR
11	Y	107	LYS
11	Y	116	ASP
11	Y	140	LEU
11	Y	148	LEU
12	Z	3	ASN
12	Z	23	LEU
12	Z	31	THR
12	Z	130	SER
12	Z	136	CYS
12	Z	150	LEU
13	a	2	GLN
13	a	48	ASN
13	a	70	LEU
13	a	104	ARG
13	a	161	ARG
13	a	187	ARG
14	b	9	LYS
14	b	39	ASP
14	b	83	LYS
14	b	104	ASP
14	b	107	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (120) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	94	HIS
2	B	20	GLN
2	B	58	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	77	ASN
3	C	116	GLN
3	C	120	GLN
3	C	147	GLN
3	C	160	GLN
4	D	15	GLN
4	D	100	ASN
4	D	225	ASN
5	E	68	HIS
5	E	92	ASN
5	E	99	ASN
5	E	116	GLN
5	E	118	ASN
5	E	120	GLN
5	E	151	ASN
5	E	184	ASN
6	F	19	GLN
6	F	86	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
7	G	166	GLN
7	G	167	GLN
7	G	175	ASN
8	H	30	ASN
8	H	35	HIS
8	H	57	GLN

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Mol	Chain	Res	Type
8	H	66	HIS
8	H	165	ASN
8	H	189	ASN
9	I	37	ASN
10	J	55	GLN
11	K	85	ASN
11	K	176	ASN
11	K	208	ASN
12	L	3	ASN
12	L	49	ASN
12	L	70	ASN
13	M	18	ASN
13	M	48	ASN
13	M	102	GLN
13	M	179	ASN
13	M	194	ASN
13	M	213	GLN
14	N	161	GLN
2	P	20	GLN
2	P	58	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	77	ASN
3	Q	116	GLN
3	Q	120	GLN
3	Q	147	GLN
3	Q	160	GLN
4	R	15	GLN
4	R	91	HIS
4	R	100	ASN
4	R	225	ASN
5	S	68	HIS
5	S	92	ASN
5	S	99	ASN
5	S	116	GLN
5	S	118	ASN
5	S	120	GLN
5	S	151	ASN

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Mol	Chain	Res	Type
5	S	184	ASN
6	T	19	GLN
6	T	86	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
7	U	166	GLN
7	U	167	GLN
7	U	175	ASN
8	V	30	ASN
8	V	35	HIS
8	V	57	GLN
8	V	165	ASN
8	V	189	ASN
9	W	37	ASN
10	X	55	GLN
11	Y	85	ASN
11	Y	176	ASN
11	Y	208	ASN
12	Z	3	ASN
12	Z	49	ASN
12	Z	70	ASN
12	Z	158	ASN
13	a	18	ASN
13	a	48	ASN
13	a	102	GLN
13	a	179	ASN
13	a	194	ASN
13	a	213	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 16 ligands modelled in this entry, 10 are monoatomic - leaving 6 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
17	EQE	V	301	8	32,32,33	2.49	6 (18%)	40,43,45	1.52	6 (15%)
17	EQE	H	301	8	32,32,33	2.56	5 (15%)	40,43,45	1.48	6 (15%)
17	EQE	K	301	11	32,32,33	2.34	5 (15%)	40,43,45	1.80	6 (15%)
17	EQE	b	201	14	32,32,33	2.17	4 (12%)	40,43,45	1.83	7 (17%)
17	EQE	N	201	14	32,32,33	2.12	4 (12%)	40,43,45	2.23	7 (17%)
17	EQE	Y	301	11	32,32,33	2.42	5 (15%)	40,43,45	1.65	6 (15%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
17	EQE	V	301	8	-	0/43/43/45	0/1/1/1
17	EQE	H	301	8	-	0/43/43/45	0/1/1/1
17	EQE	K	301	11	-	2/43/43/45	0/1/1/1
17	EQE	b	201	14	-	4/43/43/45	0/1/1/1
17	EQE	N	201	14	-	6/43/43/45	0/1/1/1
17	EQE	Y	301	11	-	4/43/43/45	0/1/1/1

All (29) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	H	301	EQE	O27-C28	-10.64	1.23	1.45
17	Y	301	EQE	O27-C28	-10.45	1.24	1.45
17	V	301	EQE	O27-C28	-10.39	1.24	1.45
17	K	301	EQE	O27-C28	-10.21	1.24	1.45
17	b	201	EQE	O27-C28	-9.86	1.25	1.45
17	N	201	EQE	O27-C28	-9.54	1.26	1.45
17	Y	301	EQE	C28-C61	-5.35	1.38	1.50
17	K	301	EQE	C28-C61	-5.22	1.38	1.50
17	V	301	EQE	C28-C61	-5.07	1.38	1.50
17	H	301	EQE	C28-C61	-4.93	1.39	1.50
17	H	301	EQE	O27-C25	-4.74	1.23	1.33
17	b	201	EQE	C28-C61	-4.47	1.40	1.50
17	H	301	EQE	C4-C9	-4.46	1.50	1.54
17	V	301	EQE	C4-C9	-4.41	1.50	1.54
17	N	201	EQE	C28-C61	-4.39	1.40	1.50
17	V	301	EQE	O27-C25	-4.15	1.24	1.33
17	K	301	EQE	O27-C25	-4.12	1.24	1.33
17	Y	301	EQE	O27-C25	-4.09	1.24	1.33
17	b	201	EQE	O27-C25	-3.80	1.25	1.33
17	H	301	EQE	C4-C5	-3.71	1.49	1.55
17	V	301	EQE	C4-C5	-3.62	1.49	1.55
17	K	301	EQE	C4-C5	-3.51	1.49	1.55
17	N	201	EQE	O27-C25	-3.29	1.26	1.33
17	N	201	EQE	C4-C9	-3.23	1.51	1.54
17	Y	301	EQE	C4-C5	-3.06	1.50	1.55
17	b	201	EQE	C4-C9	-3.01	1.51	1.54
17	Y	301	EQE	C4-C9	-2.89	1.51	1.54
17	V	301	EQE	O10-C9	-2.06	1.38	1.42
17	K	301	EQE	C4-C9	-2.01	1.52	1.54

All (38) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	N	201	EQE	O27-C28-C61	9.96	133.32	109.39
17	b	201	EQE	O27-C28-C61	7.80	128.14	109.39
17	K	301	EQE	O27-C28-C61	6.28	124.47	109.39
17	V	301	EQE	O27-C28-C61	6.03	123.88	109.39
17	Y	301	EQE	O27-C28-C61	6.00	123.82	109.39
17	H	301	EQE	O27-C28-C61	4.99	121.39	109.39
17	K	301	EQE	O27-C25-C21	4.88	119.17	111.32
17	N	201	EQE	O27-C25-C21	4.68	118.86	111.32
17	Y	301	EQE	O27-C25-C21	4.04	117.83	111.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	b	201	EQE	O27-C25-C21	3.80	117.44	111.32
17	Y	301	EQE	C6-C5-C4	-3.32	105.57	111.74
17	N	201	EQE	O26-C25-C21	-3.30	115.02	124.42
17	K	301	EQE	O26-C25-C21	-3.20	115.31	124.42
17	H	301	EQE	C28-O27-C25	3.20	121.97	116.32
17	V	301	EQE	O27-C25-C21	3.18	116.45	111.32
17	b	201	EQE	O26-C25-C21	-2.82	116.39	124.42
17	V	301	EQE	O26-C25-C21	-2.80	116.46	124.42
17	K	301	EQE	C23-C22-C24	-2.74	102.94	110.59
17	H	301	EQE	C6-C5-C4	-2.73	106.67	111.74
17	Y	301	EQE	O26-C25-C21	-2.72	116.67	124.42
17	H	301	EQE	O27-C25-C21	2.65	115.58	111.32
17	N	201	EQE	O3-C1-C4	-2.60	118.67	125.23
17	K	301	EQE	C6-C5-C4	-2.58	106.95	111.74
17	b	201	EQE	C15-C14-N13	-2.51	105.22	111.43
17	Y	301	EQE	C28-O27-C25	2.47	120.68	116.32
17	b	201	EQE	O3-C1-C4	-2.46	119.02	125.23
17	K	301	EQE	C28-O27-C25	2.45	120.66	116.32
17	b	201	EQE	C9-C4-C1	-2.43	105.62	110.65
17	V	301	EQE	C7-C5-C4	-2.34	107.39	111.74
17	V	301	EQE	C6-C5-C4	-2.28	107.51	111.74
17	H	301	EQE	O26-C25-C21	-2.28	117.94	124.42
17	Y	301	EQE	C22-C21-N20	-2.26	105.84	111.43
17	N	201	EQE	C9-C4-C1	-2.22	106.03	110.65
17	H	301	EQE	C7-C5-C4	-2.21	107.64	111.74
17	V	301	EQE	C28-O27-C25	2.13	120.08	116.32
17	N	201	EQE	C28-C61-C66	-2.09	115.74	120.66
17	N	201	EQE	C6-C5-C4	-2.03	107.97	111.74
17	b	201	EQE	C7-C5-C6	-2.03	104.92	110.59

There are no chirality outliers.

All (16) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
17	N	201	EQE	C25-C21-N20-C18
17	N	201	EQE	C22-C21-N20-C18
17	b	201	EQE	C25-C21-N20-C18
17	b	201	EQE	C22-C21-N20-C18
17	b	201	EQE	C22-C21-C25-O26
17	b	201	EQE	C22-C21-C25-O27
17	Y	301	EQE	C22-C21-C25-O27
17	N	201	EQE	N20-C21-C25-O26

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Mol	Chain	Res	Type	Atoms
17	Y	301	EQE	N20-C21-C25-O26
17	Y	301	EQE	C22-C21-C25-O26
17	N	201	EQE	N20-C21-C25-O27
17	N	201	EQE	C22-C21-C25-O26
17	Y	301	EQE	N20-C21-C25-O27
17	N	201	EQE	C22-C21-C25-O27
17	K	301	EQE	C22-C21-C25-O27
17	K	301	EQE	C22-C21-C25-O26

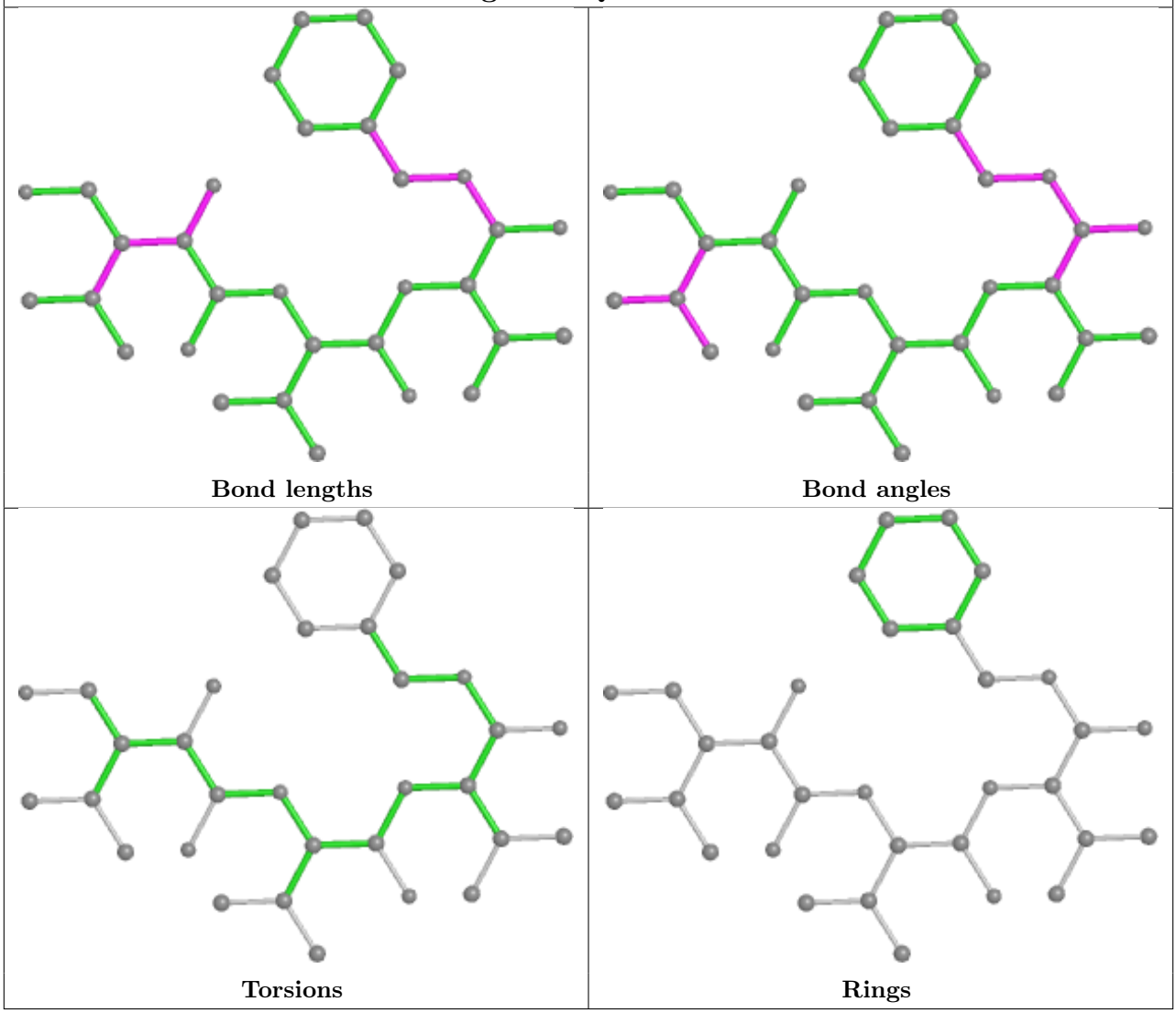
There are no ring outliers.

5 monomers are involved in 16 short contacts:

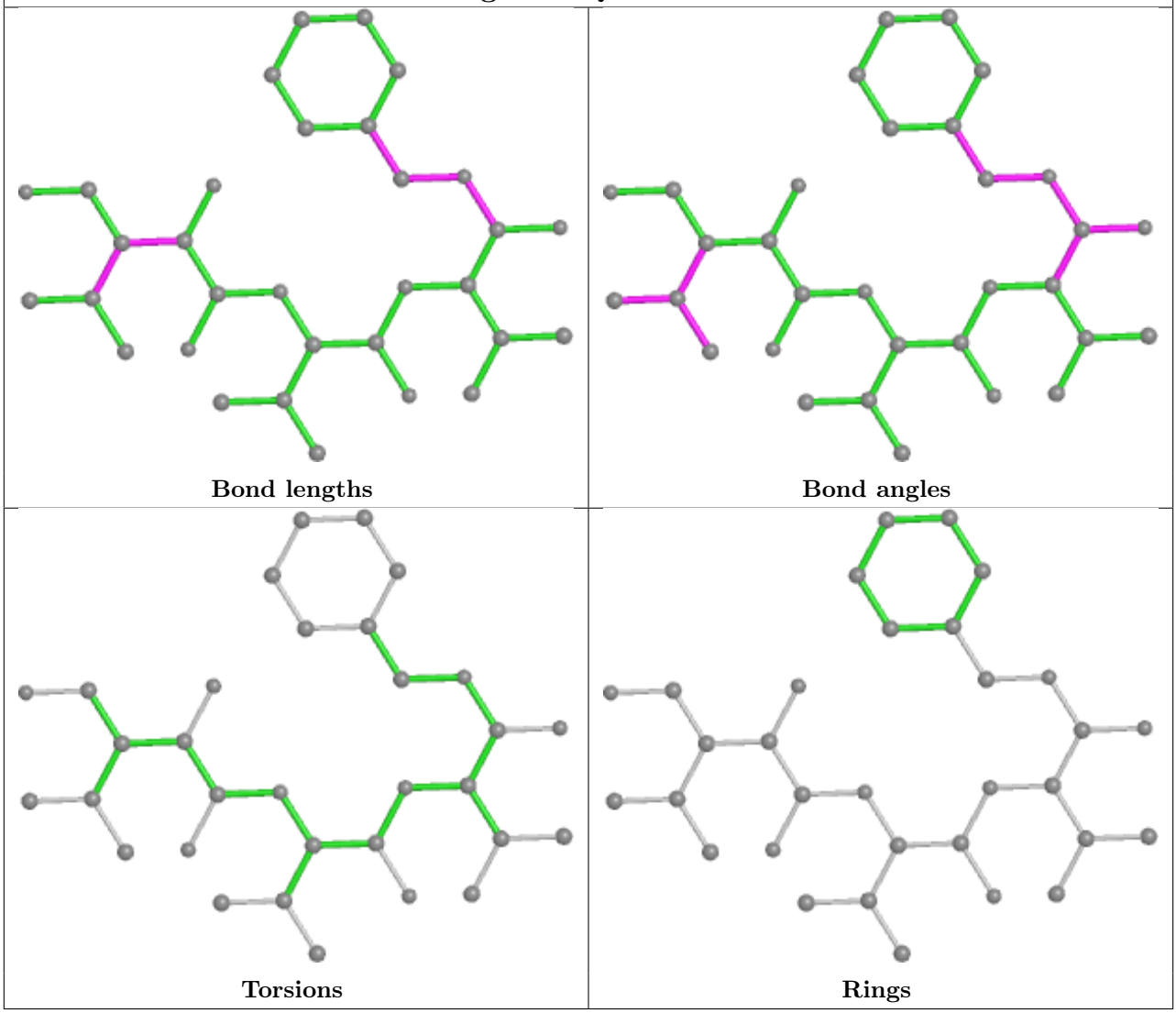
Mol	Chain	Res	Type	Clashes	Symm-Clashes
17	V	301	EQE	2	0
17	H	301	EQE	4	0
17	K	301	EQE	1	0
17	N	201	EQE	8	0
17	Y	301	EQE	1	0

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

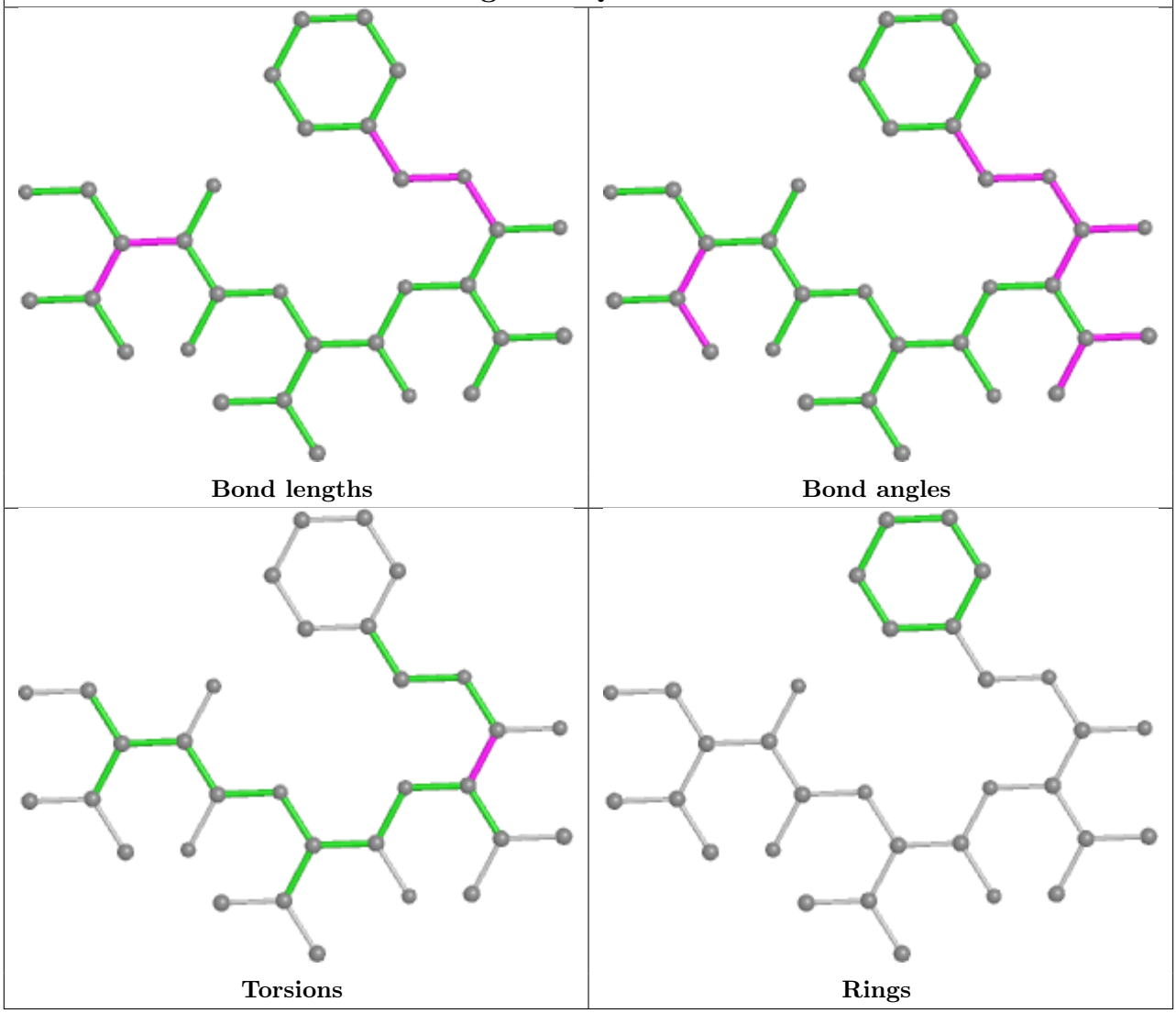
Ligand EQE V 301



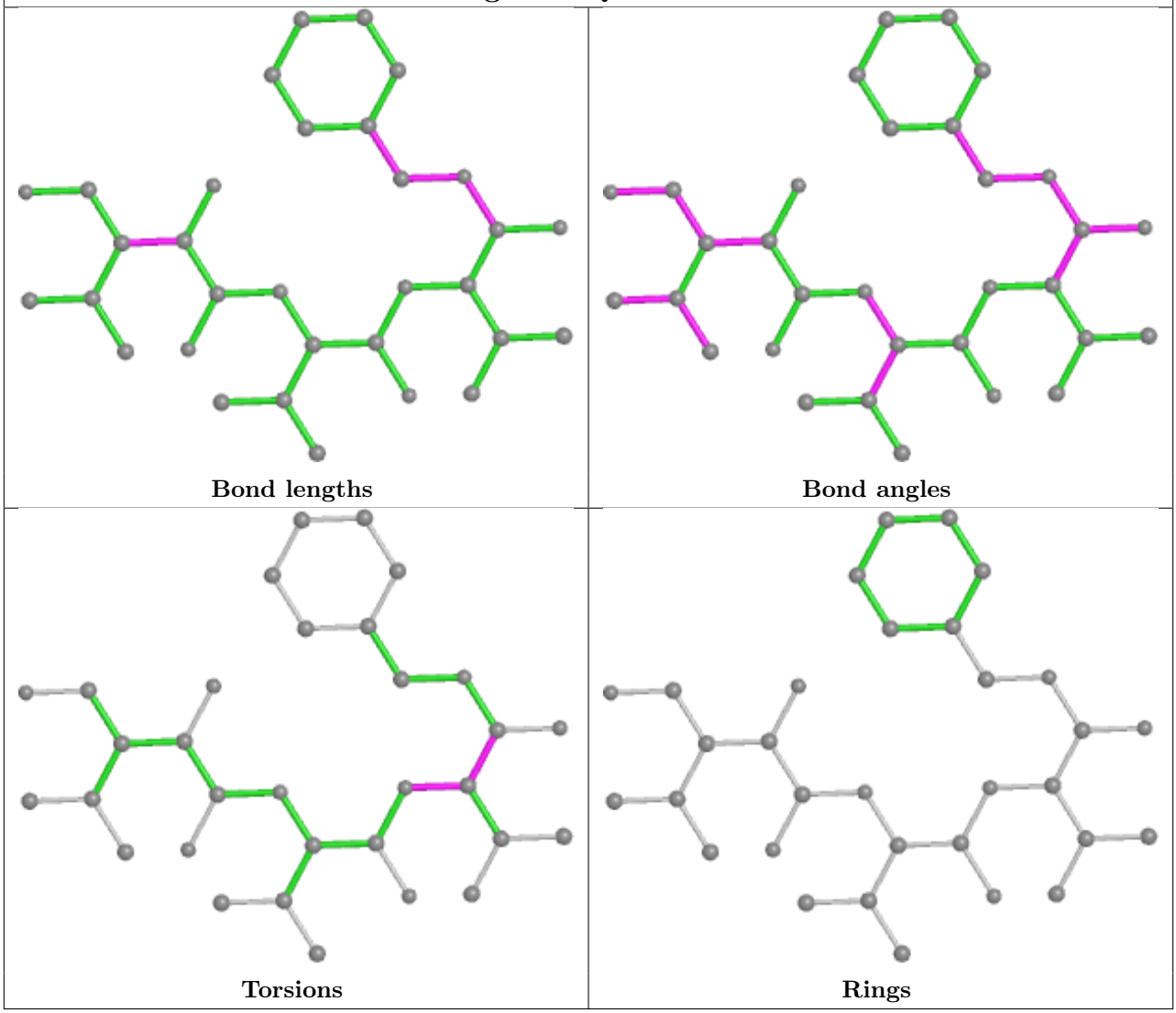
Ligand EQE H 301



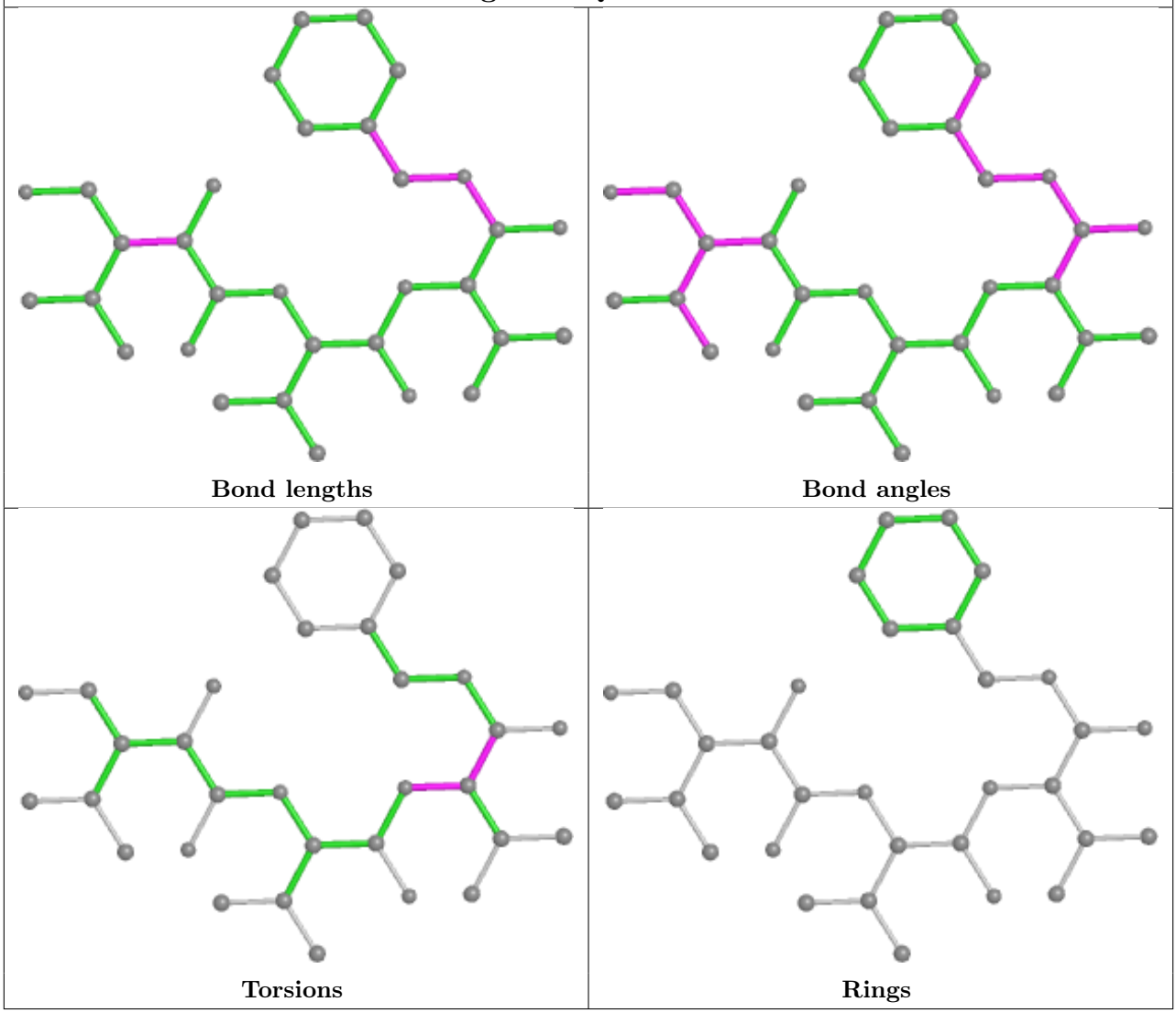
Ligand EQE K 301



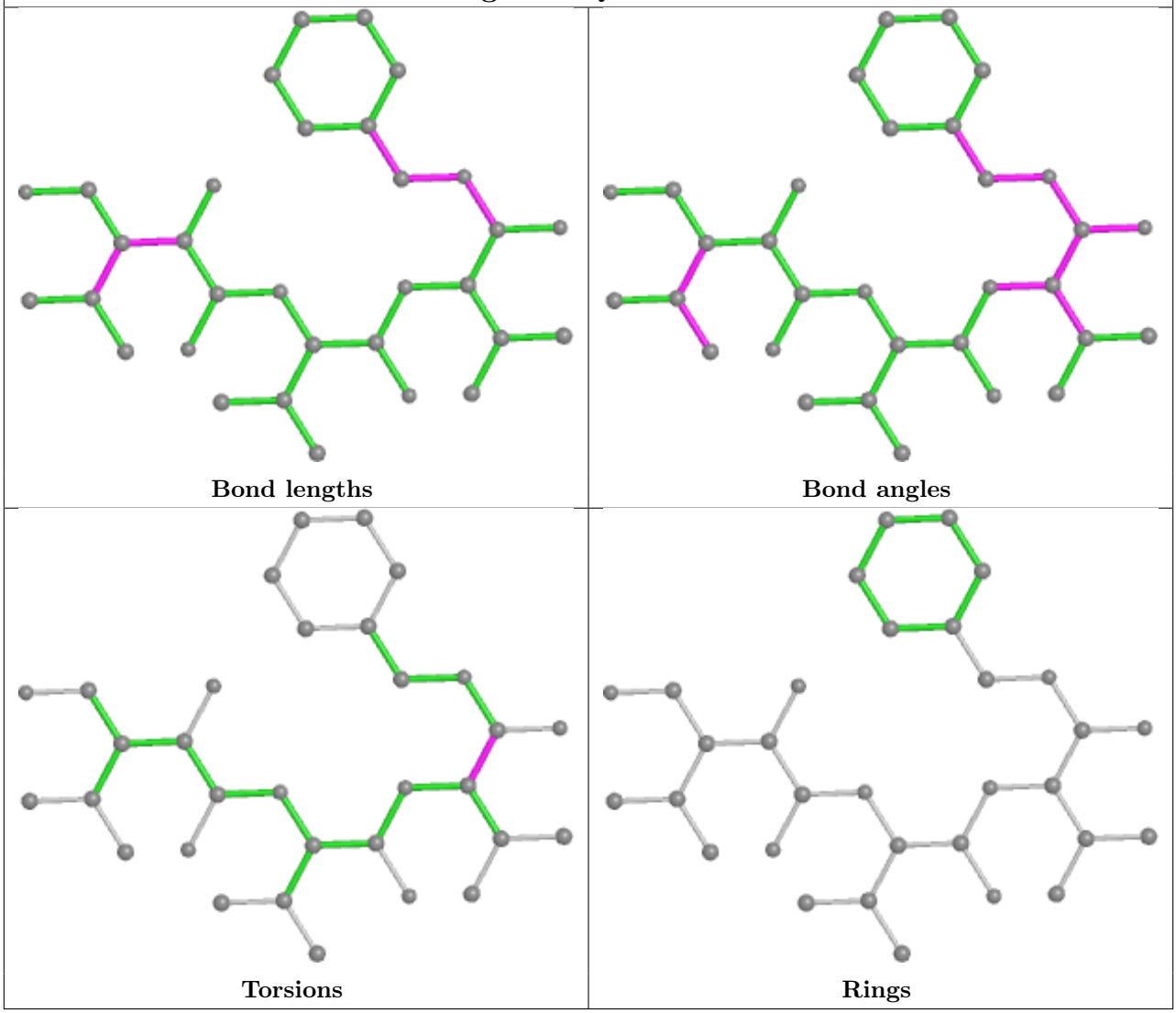
Ligand EQE b 201



Ligand EQE N 201



Ligand EQE Y 301



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 (i)

6.1 Protein, DNA and RNA chains (i)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	250/250 (100%)	-0.29	8 (3%)	47	48	48, 63, 99, 141	0
1	O	250/250 (100%)	-0.22	8 (3%)	47	48	53, 71, 116, 150	0
2	B	244/258 (94%)	-0.15	9 (3%)	41	41	50, 71, 121, 172	0
2	P	244/258 (94%)	0.03	15 (6%)	21	20	54, 74, 123, 170	0
3	C	240/254 (94%)	-0.03	16 (6%)	17	16	50, 74, 138, 167	0
3	Q	240/254 (94%)	0.11	20 (8%)	11	9	55, 86, 166, 197	0
4	D	235/260 (90%)	-0.30	4 (1%)	70	72	54, 77, 111, 155	0
4	R	235/260 (90%)	-0.16	10 (4%)	35	33	56, 81, 121, 158	0
5	E	231/234 (98%)	-0.16	6 (2%)	56	57	56, 77, 118, 158	0
5	S	231/234 (98%)	-0.04	12 (5%)	27	25	57, 84, 130, 171	0
6	F	243/288 (84%)	-0.27	9 (3%)	41	41	48, 68, 124, 147	0
6	T	243/288 (84%)	-0.25	10 (4%)	37	36	49, 76, 136, 166	0
7	G	241/252 (95%)	-0.42	9 (3%)	41	41	45, 62, 97, 145	0
7	U	241/252 (95%)	-0.32	8 (3%)	46	46	51, 67, 101, 141	0
8	H	226/232 (97%)	-0.25	8 (3%)	44	44	47, 60, 98, 169	0
8	V	226/232 (97%)	-0.15	9 (3%)	38	37	50, 65, 101, 180	0
9	I	204/205 (99%)	-0.60	1 (0%)	91	92	44, 60, 89, 114	0
9	W	204/205 (99%)	-0.52	2 (0%)	82	83	47, 61, 93, 118	0
10	J	195/198 (98%)	-0.42	3 (1%)	73	76	47, 64, 92, 144	0
10	X	195/198 (98%)	-0.38	3 (1%)	73	76	49, 66, 94, 154	0
11	K	212/212 (100%)	-0.46	1 (0%)	91	92	45, 62, 86, 107	0
11	Y	212/212 (100%)	-0.50	1 (0%)	91	92	50, 63, 90, 108	0
12	L	222/222 (100%)	-0.44	1 (0%)	91	92	47, 63, 95, 130	0
12	Z	222/222 (100%)	-0.41	2 (0%)	84	85	47, 63, 97, 131	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
13	M	229/246 (93%)	-0.44	5 (2%)	62	63	44, 63, 89, 105	0
13	a	232/246 (94%)	-0.47	2 (0%)	84	85	43, 61, 86, 98	0
14	N	196/196 (100%)	-0.50	2 (1%)	82	83	44, 57, 87, 116	0
14	b	196/196 (100%)	-0.48	2 (1%)	82	83	45, 59, 89, 124	0
All	All	6339/6614 (95%)	-0.29	186 (2%)	51	52	43, 67, 115, 197	0

All (186) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
8	V	224	GLN	10.4
2	P	219	ALA	10.0
8	V	223	ILE	8.8
2	B	221	ASP	8.3
2	P	220	ASN	8.1
2	P	59	ASP	8.0
3	Q	49	THR	7.6
8	H	223	ILE	7.5
3	Q	50	LEU	7.5
8	V	225	GLU	7.3
8	H	224	GLN	7.3
10	X	1	MET	7.3
8	V	221	CYS	7.0
8	V	222	ASP	6.8
8	V	226	GLU	6.5
8	H	226	GLU	6.0
4	R	241	ALA	5.9
8	H	222	ASP	5.6
2	P	51	VAL	5.6
2	B	219	ALA	5.5
3	Q	206	LYS	5.4
2	P	221	ASP	5.3
8	H	221	CYS	5.2
1	A	249	ALA	5.2
3	C	206	LYS	5.1
8	H	225	GLU	4.9
2	B	51	VAL	4.9
2	B	220	ASN	4.8
3	C	205	ALA	4.8
5	S	202	ASP	4.7
2	P	60	THR	4.6
10	J	1	MET	4.5

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Mol	Chain	Res	Type	RSRZ
5	S	54	GLU	4.5
3	Q	236	GLN	4.5
3	C	236	GLN	4.5
6	T	178	HIS	4.4
3	C	238	LYS	4.3
3	Q	180	LYS	4.2
5	E	202	ASP	4.2
10	X	194	ASP	4.2
2	P	225	TYR	4.2
11	Y	212	GLY	4.1
12	L	174	TYR	4.1
1	A	1	MET	4.1
13	a	1	THR	4.0
3	C	49	THR	3.9
3	Q	238	LYS	3.9
3	Q	239	GLN	3.8
2	B	59	ASP	3.8
2	B	217	LYS	3.8
10	J	194	ASP	3.7
1	A	2	THR	3.7
3	C	50	LEU	3.7
3	Q	202	GLN	3.7
2	B	218	GLY	3.6
6	F	181	GLU	3.6
1	O	249	ALA	3.6
3	Q	205	ALA	3.6
14	b	195	GLN	3.5
7	U	242	GLN	3.5
4	D	241	ALA	3.4
2	B	60	THR	3.4
4	R	217	GLN	3.4
6	F	202	ASP	3.4
6	T	181	GLU	3.4
7	U	188	GLU	3.4
10	X	193	ASP	3.3
14	N	195	GLN	3.3
1	O	201	GLU	3.3
3	Q	55	THR	3.3
13	M	216	ASN	3.3
6	T	180	PRO	3.3
9	W	1	SER	3.3
7	G	188	GLU	3.2

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Mol	Chain	Res	Type	RSRZ
7	G	179	LYS	3.2
9	W	192	ASP	3.2
3	Q	240	GLU	3.2
11	K	212	GLY	3.2
1	A	182	GLU	3.2
3	C	225	GLU	3.1
3	C	239	GLN	3.1
7	U	2	GLY	3.1
7	U	222	ASP	3.1
6	T	230	ASP	3.1
2	P	182	ASP	3.0
5	E	54	GLU	3.0
3	Q	204	GLY	3.0
3	C	216	ASP	3.0
6	F	2	THR	3.0
6	F	244	ASN	2.9
5	S	227	GLU	2.9
3	Q	187	GLU	2.9
1	O	1	MET	2.9
5	E	233	ILE	2.9
6	T	241	LYS	2.9
4	R	125	LEU	2.9
3	C	240	GLU	2.9
1	A	231	LYS	2.9
10	J	193	ASP	2.9
6	T	243	ILE	2.8
7	G	240	ALA	2.8
1	A	228	PRO	2.8
2	P	203	SER	2.8
3	C	202	GLN	2.8
1	A	250	LEU	2.7
6	T	244	ASN	2.7
6	F	205	GLU	2.7
2	P	52	THR	2.7
3	C	27	ARG	2.7
2	P	222	GLY	2.7
3	Q	175	LYS	2.7
3	Q	237	GLU	2.7
4	R	242	GLU	2.6
5	S	180	LYS	2.6
3	Q	48	SER	2.6
5	S	233	ILE	2.6

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Mol	Chain	Res	Type	RSRZ
8	V	145	ASP	2.6
7	G	241	GLU	2.6
7	U	241	GLU	2.6
5	E	173	ARG	2.6
4	R	1	ASP	2.6
2	B	225	TYR	2.6
5	S	173	ARG	2.6
1	O	2	THR	2.6
7	G	3	TYR	2.6
6	T	205	GLU	2.6
1	O	228	PRO	2.5
13	a	232	LYS	2.5
8	V	215	GLU	2.5
3	Q	203	THR	2.5
1	A	201	GLU	2.5
4	D	242	GLU	2.5
2	P	230	LYS	2.5
14	b	105	LYS	2.5
4	R	2	ARG	2.5
7	U	3	TYR	2.5
6	F	178	HIS	2.4
7	G	242	GLN	2.4
1	O	50	LYS	2.4
9	I	1	SER	2.4
12	Z	174	TYR	2.4
5	S	194	GLU	2.4
1	O	250	LEU	2.4
6	F	215	CYS	2.4
14	N	105	LYS	2.4
3	C	48	SER	2.4
2	P	240	LYS	2.3
13	M	1	THR	2.3
3	Q	225	GLU	2.3
3	C	181	GLU	2.3
7	U	51	PRO	2.3
1	O	203	GLU	2.3
7	G	68	ARG	2.3
2	P	61	SER	2.3
5	S	204	SER	2.3
7	G	222	ASP	2.3
4	R	224	ASP	2.2
4	R	141	ALA	2.2

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Mol	Chain	Res	Type	RSRZ
3	C	180	LYS	2.2
13	M	229	GLY	2.2
5	E	203	GLU	2.2
13	M	47	ASP	2.2
6	T	53	LYS	2.2
13	M	228	TYR	2.2
5	S	187	GLU	2.2
5	S	203	GLU	2.1
5	S	30	GLN	2.1
7	U	181	LYS	2.1
6	T	235	ALA	2.1
2	P	53	SER	2.1
6	F	230	ASP	2.1
7	G	2	GLY	2.1
8	H	198	GLU	2.1
8	V	219	ASN	2.1
6	F	180	PRO	2.1
8	H	145	ASP	2.1
4	D	125	LEU	2.1
12	Z	116	GLU	2.1
5	E	201	ARG	2.1
3	C	1	GLY	2.1
4	D	217	GLN	2.1
3	Q	59	PRO	2.0
4	R	226	GLU	2.0
5	S	58	TYR	2.0
3	Q	60	SER	2.0
4	R	230	GLU	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 monosaccharides 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,

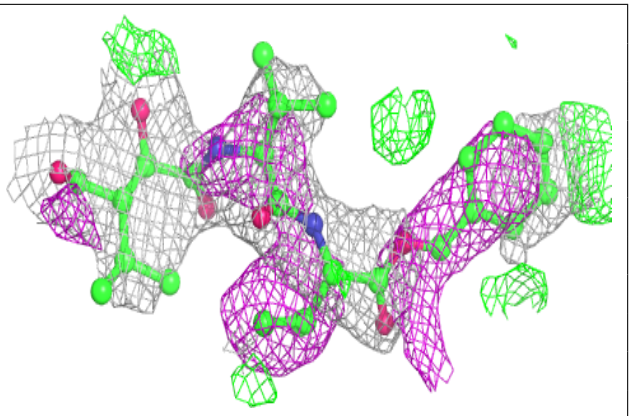
median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

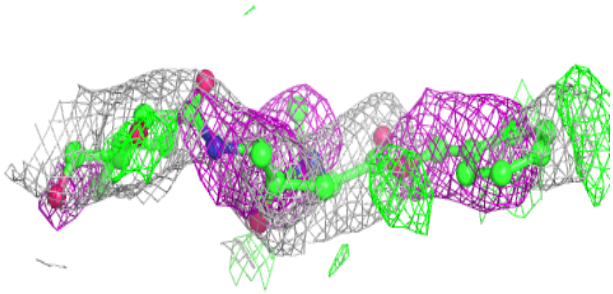
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
17	EQE	b	201	32/33	0.78	0.42	63,76,94,96	0
17	EQE	N	201	32/33	0.83	0.36	62,73,91,92	0
17	EQE	Y	301	32/33	0.89	0.27	63,70,87,90	0
17	EQE	K	301	32/33	0.89	0.27	57,71,86,88	0
17	EQE	V	301	32/33	0.94	0.17	54,61,82,85	0
15	MG	Z	301	1/1	0.94	0.34	70,70,70,70	0
17	EQE	H	301	32/33	0.94	0.18	55,62,80,81	0
15	MG	W	301	1/1	0.95	0.29	71,71,71,71	0
15	MG	V	302	1/1	0.97	0.11	85,85,85,85	0
15	MG	I	301	1/1	0.97	0.20	65,65,65,65	0
15	MG	N	202	1/1	0.97	0.09	59,59,59,59	0
15	MG	Y	302	1/1	0.99	0.09	71,71,71,71	0
15	MG	K	302	1/1	0.99	0.04	66,66,66,66	0
16	CL	G	302	1/1	0.99	0.15	54,54,54,54	0
16	CL	U	301	1/1	0.99	0.19	58,58,58,58	0
15	MG	G	301	1/1	0.99	0.06	61,61,61,61	0

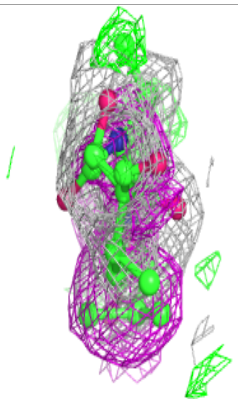
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around EQE b 201:

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

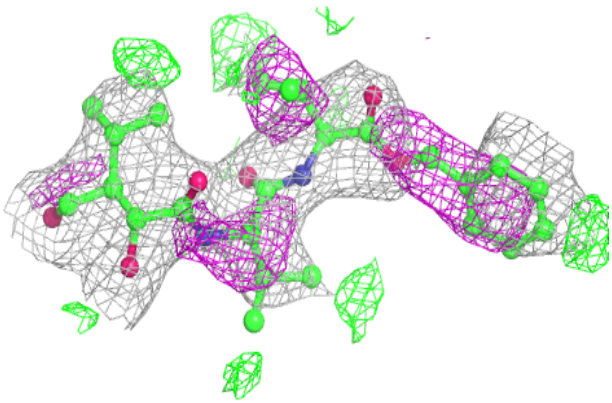


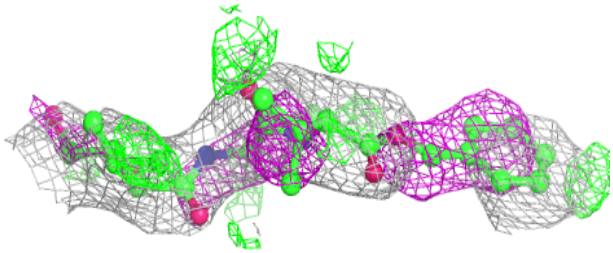


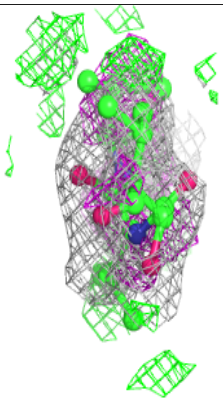


Electron density around EQE N 201:

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

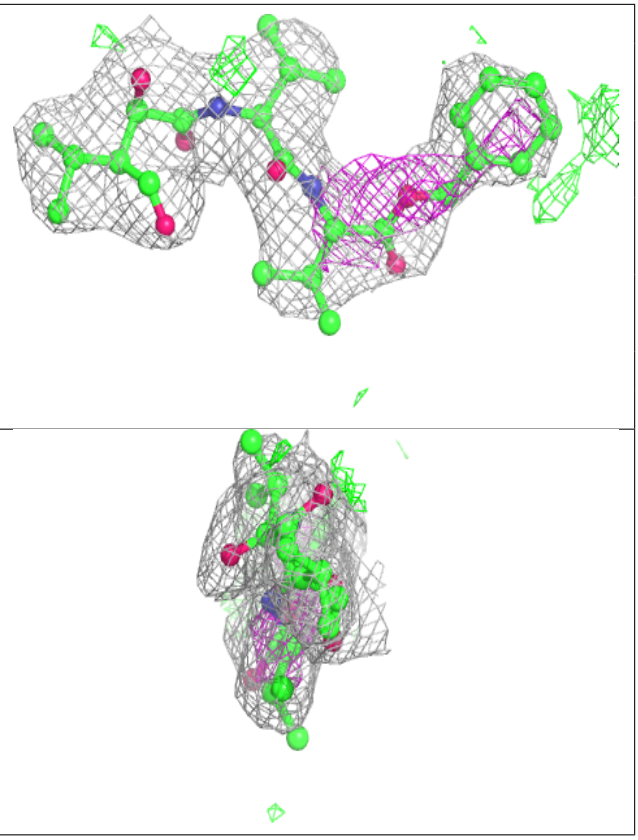






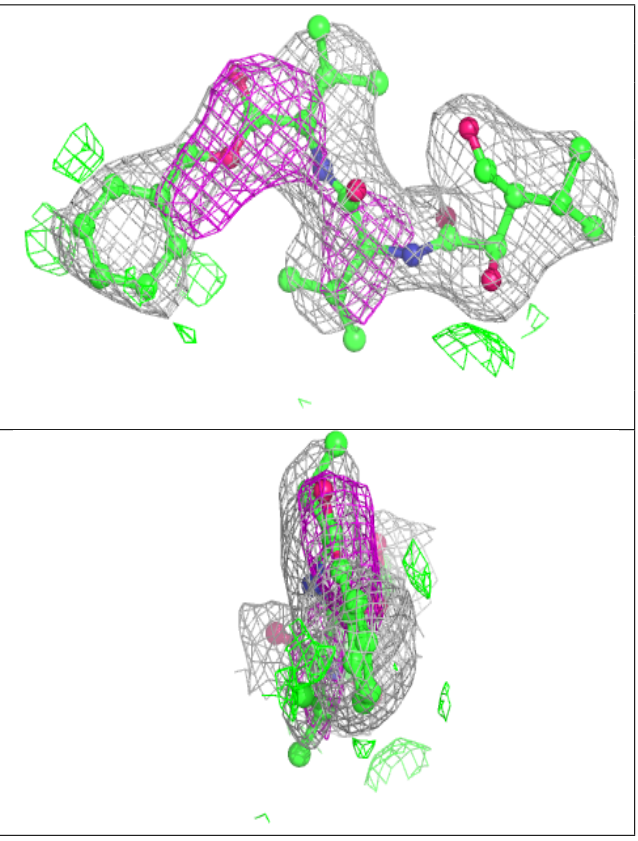
Electron density around EQE Y 301:

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



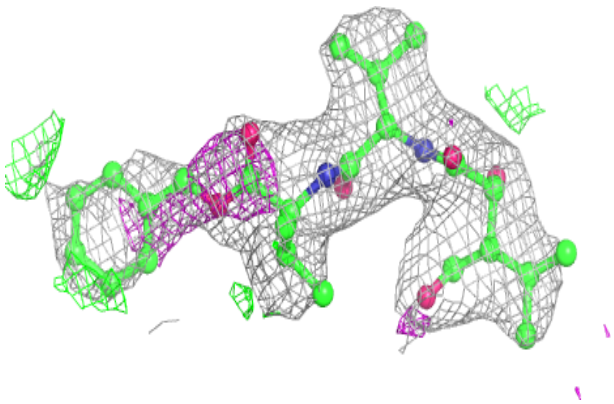
Electron density around EQE K 301:

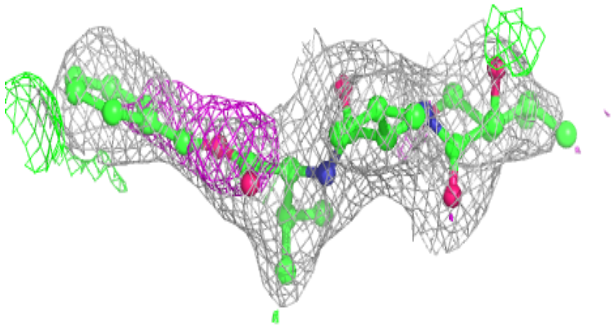
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

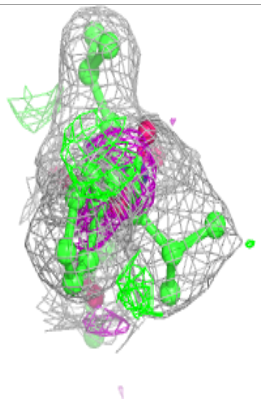


Electron density around EQE V 301:

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

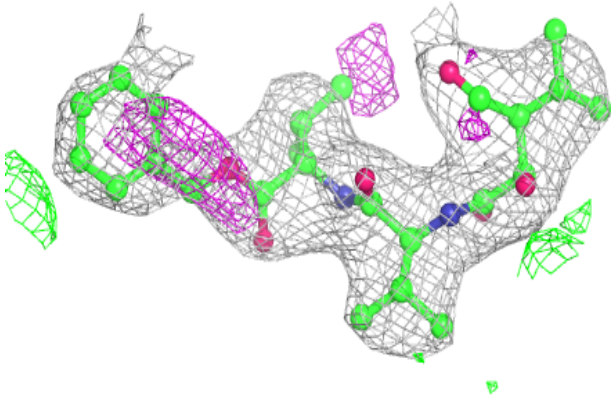


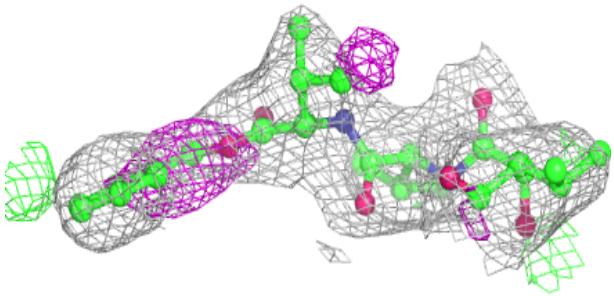


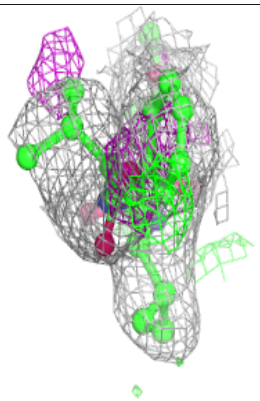


Electron density around EQE H 301:

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







6.5 Other polymers (i)

There are no such residues in this entry.