



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 19, 2026 – 12:20 AM UTC

PDB ID : 5LF3 / pdb_00005lf3
Title : Human 20S proteasome complex with Bortezomib at 2.1 Angstrom
Authors : Schrader, J.; Henneberg, F.; Mata, R.; Tittmann, K.; Schneider, T.R.; Stark, H.; Bourenkov, G.; Chari, A.
Deposited on : 2016-06-30
Resolution : 2.10 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

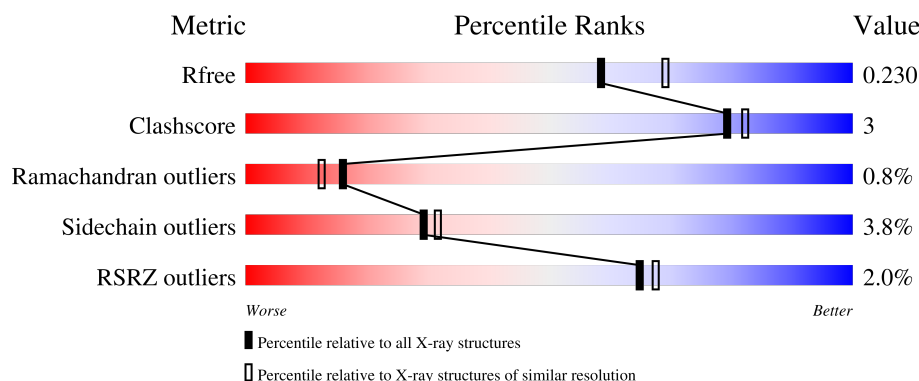
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	6658 (2.10-2.10)
Clashscore	190562	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)
RSRZ outliers	180081	6662 (2.10-2.10)

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

Mol	Chain	Length	Quality of chain
1	A	234	2% 87% 9% ..
1	O	234	6% 91% 6% ..
2	B	261	2% 87% 7% 5%
2	P	261	3% 84% 9% 5%
3	C	248	2% 85% 8% ..

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Mol	Chain	Length	Quality of chain
3	Q	248	
4	D	241	
4	R	241	
5	E	263	
5	S	263	
6	F	255	
6	T	255	
7	G	246	
7	U	246	
8	H	234	
8	V	234	
9	I	205	
9	W	205	
10	J	201	
10	X	201	
11	K	204	
11	Y	204	
12	L	213	
12	Z	213	
13	M	219	
13	a	219	
14	N	205	
14	b	205	

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
7	6V1	U	47	X	-	-	-

2 Entry composition

There are 20 unique types of molecules in this entry. The entry contains 52211 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	230	Total	C	N	O	S	0	3	0
			1788	1145	301	336	6			
1	O	230	Total	C	N	O	S	0	0	0
			1741	1111	293	331	6			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	248	Total	C	N	O	S	0	2	0
			1926	1220	332	363	11			
2	P	248	Total	C	N	O	S	0	2	0
			1909	1206	325	367	11			

- Molecule 3 is a protein called Proteasome subunit alpha type-7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	237	Total	C	N	O	S	0	2	0
			1798	1121	320	352	5			
3	Q	239	Total	C	N	O	S	0	0	0
			1820	1136	320	359	5			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	233	Total	C	N	O	S	0	1	0
			1762	1105	290	356	11			
4	R	233	Total	C	N	O	S	0	1	0
			1753	1103	293	346	11			

- Molecule 5 is a protein called Proteasome subunit alpha type-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	234	Total	C	N	O	S	0	1	0
			1822	1144	325	342	11			
5	S	238	Total	C	N	O	S	0	3	0
			1875	1175	340	349	11			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	148	6V1	CYS	engineered mutation	UNP P25786
S	148	6V1	CYS	engineered mutation	UNP P25786

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	239	Total	C	N	O	S	0	4	0
			1888	1198	325	353	12			
6	T	240	Total	C	N	O	S	0	1	0
			1856	1178	315	351	12			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	G	244	Total	C	N	O	S	0	2	0
			1912	1214	321	364	13			
7	U	238	Total	C	N	O	S	0	1	0
			1815	1147	304	350	14			

- Molecule 8 is a protein called Proteasome subunit beta type-7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	H	220	Total	C	N	O	S	0	2	0
			1664	1047	284	320	13			
8	V	220	Total	C	N	O	S	0	2	0
			1622	1023	269	318	12			

- 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	3	0
			1613	1028	270	295	20			
9	W	204	Total	C	N	O	S	0	2	0
			1599	1018	267	295	19			

- Molecule 10 is a protein called Proteasome subunit beta type-2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	J	196	Total	C	N	O	S	0	3	0
			1590	1021	271	288	10			
10	X	196	Total	C	N	O	S	0	2	0
			1574	1012	267	285	10			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	K	200	Total	C	N	O	S	0	1	0
			1550	978	269	293	10			
11	Y	201	Total	C	N	O	S	0	3	0
			1580	996	280	294	10			

- Molecule 12 is a protein called Proteasome subunit beta type-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	L	213	Total	C	N	O	S	0	2	0
			1636	1038	277	310	11			
12	Z	213	Total	C	N	O	S	0	1	0
			1642	1041	280	310	11			

- Molecule 13 is a protein called Proteasome subunit beta type-4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	M	216	Total	C	N	O	S	0	1	0
			1692	1067	291	322	12			
13	a	216	Total	C	N	O	S	0	2	0
			1688	1064	291	321	12			

- Molecule 14 is a protein called Proteasome subunit beta type-6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	N	202	Total	C	N	O	S	0	1	0
			1519	953	258	295	13			
14	b	203	Total	C	N	O	S	0	1	0
			1524	956	259	296	13			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
N	1	THR	-	expression tag	UNP P28072

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Chain	Residue	Modelled	Actual	Comment	Reference
b	1	THR	-	expression tag	UNP P28072

- Molecule 15 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
15	A	4	Total Cl 4 4	0	0
15	B	2	Total Cl 2 2	0	0
15	C	2	Total Cl 2 2	0	0
15	D	2	Total Cl 2 2	0	0
15	E	3	Total Cl 3 3	0	0
15	F	1	Total Cl 1 1	0	0
15	G	2	Total Cl 2 2	0	0
15	H	1	Total Cl 1 1	0	0
15	I	1	Total Cl 1 1	0	0
15	K	3	Total Cl 3 3	0	0
15	M	4	Total Cl 4 4	0	0
15	N	2	Total Cl 2 2	0	0
15	O	4	Total Cl 4 4	0	0
15	P	1	Total Cl 1 1	0	0
15	Q	2	Total Cl 2 2	0	0
15	R	2	Total Cl 2 2	0	0
15	S	3	Total Cl 3 3	0	0
15	U	1	Total Cl 1 1	0	0
15	V	1	Total Cl 1 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
15	W	1	Total 1	Cl 1	0	0
15	Y	4	Total 4	Cl 4	0	0
15	a	3	Total 3	Cl 3	0	0
15	b	2	Total 2	Cl 2	0	0

- Molecule 16 is POTASSIUM ION (CCD ID: K) (formula: K).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
16	G	1	Total 1	K 1	0	0
16	L	1	Total 1	K 1	0	0
16	N	1	Total 1	K 1	0	0
16	U	1	Total 1	K 1	0	0
16	Z	1	Total 1	K 1	0	0
16	b	1	Total 1	K 1	0	0

- Molecule 17 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

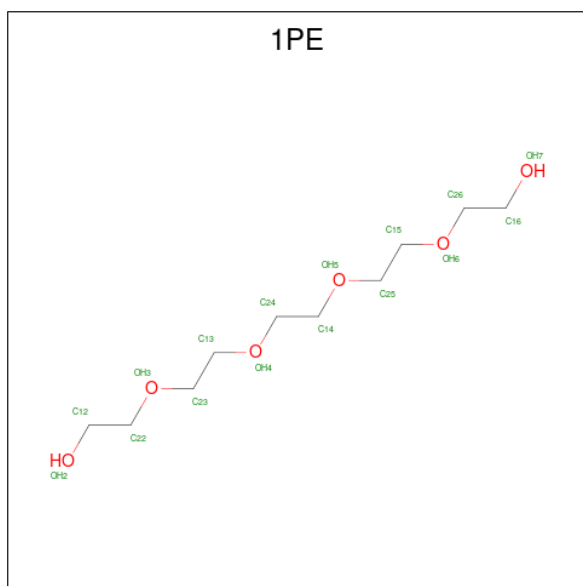
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
17	H	2	Total 2	Mg 2	0	0
17	I	2	Total 2	Mg 2	0	0
17	J	1	Total 1	Mg 1	0	0
17	K	1	Total 1	Mg 1	0	0
17	L	1	Total 1	Mg 1	0	0
17	V	1	Total 1	Mg 1	0	0
17	W	1	Total 1	Mg 1	0	0

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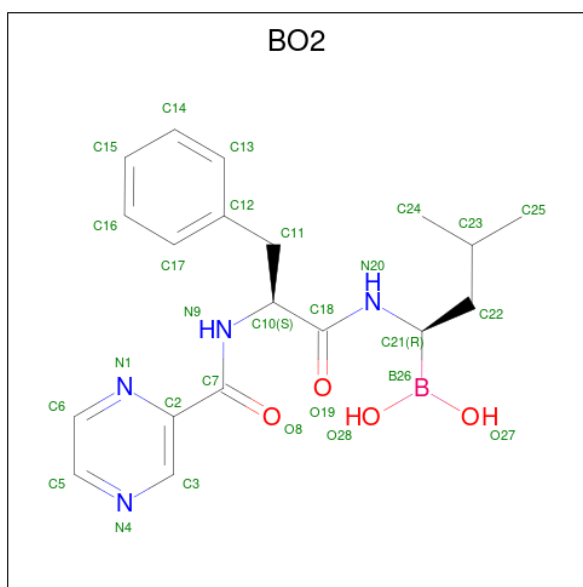
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
17	X	1	Total	Mg	0	0
			1	1		

- Molecule 18 is PENTAETHYLENE GLYCOL (CCD ID: 1PE) (formula: $C_{10}H_{22}O_6$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
18	H	1	Total	C	O	0	0
			16	10	6		
18	H	1	Total	C	O	0	0
			16	10	6		
18	I	1	Total	C	O	0	0
			16	10	6		
18	I	1	Total	C	O	0	0
			16	10	6		
18	L	1	Total	C	O	0	0
			16	10	6		
18	M	1	Total	C	O	0	0
			16	10	6		
18	W	1	Total	C	O	0	0
			16	10	6		
18	Z	1	Total	C	O	0	0
			16	10	6		
18	b	1	Total	C	O	0	0
			16	10	6		

- Molecule 19 is N-[(1R)-1-(DIHYDROXYBORYL)-3-METHYLBUTYL]-N-(PYRAZIN-2-YLCARBONYL)-L-PHENYLALANINAMIDE (CCD ID: BO2) (formula: $C_{19}H_{25}BN_4O_4$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
19	H	1	Total	B	C	N	O	0	0
			28	1	19	4	4		
19	K	1	Total	B	C	N	O	0	0
			28	1	19	4	4		
19	N	1	Total	B	C	N	O	0	0
			28	1	19	4	4		
19	V	1	Total	B	C	N	O	0	0
			28	1	19	4	4		
19	Y	1	Total	B	C	N	O	0	0
			28	1	19	4	4		
19	b	1	Total	B	C	N	O	0	0
			28	1	19	4	4		

- Molecule 20 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
20	A	115	Total	O	0	0
			115	115		
20	B	131	Total	O	0	0
			131	131		
20	C	75	Total	O	0	0
			75	75		
20	D	95	Total	O	0	0
			95	95		
20	E	147	Total	O	0	0
			147	147		
20	F	186	Total	O	0	0
			186	186		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
20	G	196	Total 196	O 196	0	0
20	H	159	Total 159	O 159	0	0
20	I	157	Total 157	O 157	0	0
20	J	138	Total 138	O 138	0	0
20	K	105	Total 105	O 105	0	0
20	L	125	Total 125	O 125	0	0
20	M	147	Total 147	O 147	0	0
20	N	162	Total 162	O 162	0	0
20	O	95	Total 95	O 95	0	0
20	P	125	Total 125	O 125	0	0
20	Q	75	Total 75	O 75	0	0
20	R	132	Total 132	O 132	0	0
20	S	130	Total 130	O 130	0	0
20	T	100	Total 100	O 100	0	0
20	U	107	Total 107	O 107	0	0
20	V	120	Total 120	O 120	0	0
20	W	118	Total 118	O 118	0	0
20	X	125	Total 125	O 125	0	0
20	Y	142	Total 142	O 142	0	0
20	Z	169	Total 169	O 169	0	0
20	a	174	Total 174	O 174	0	0

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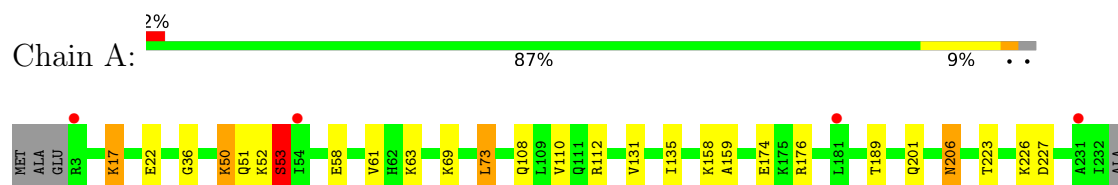
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
20	b	124	Total 124	O 124	0	0

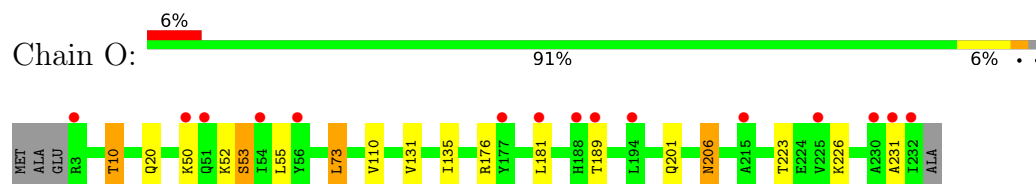
3 Residue-property plots [i](#)

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

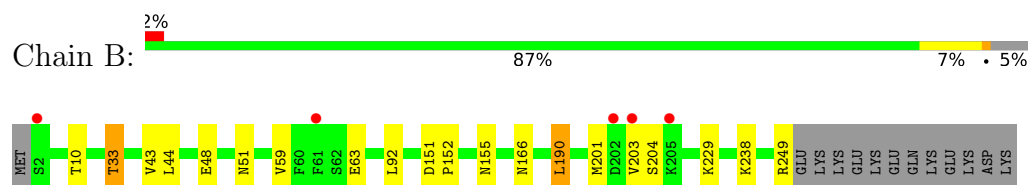
- Molecule 1: Proteasome subunit alpha type-2



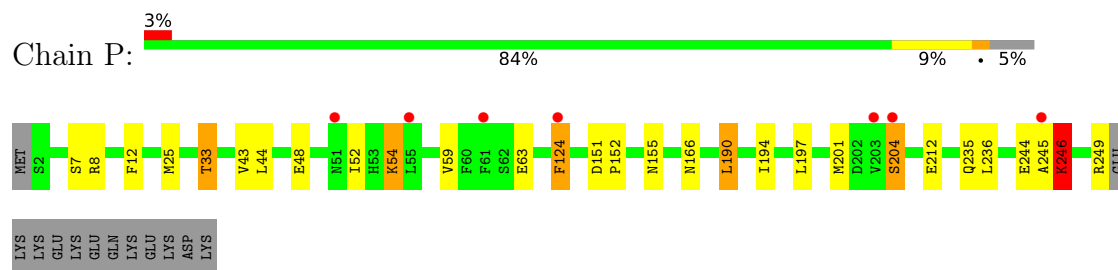
- Molecule 1: Proteasome subunit alpha type-2



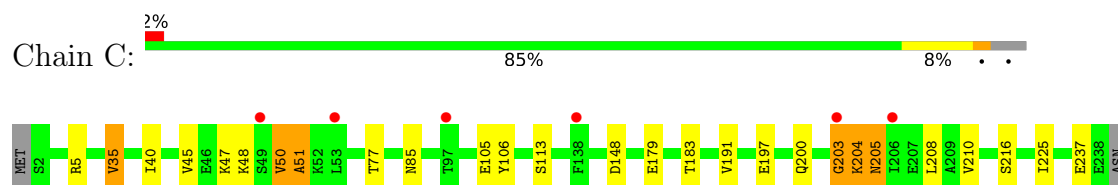
- Molecule 2: Proteasome subunit alpha type-4



- Molecule 2: Proteasome subunit alpha type-4



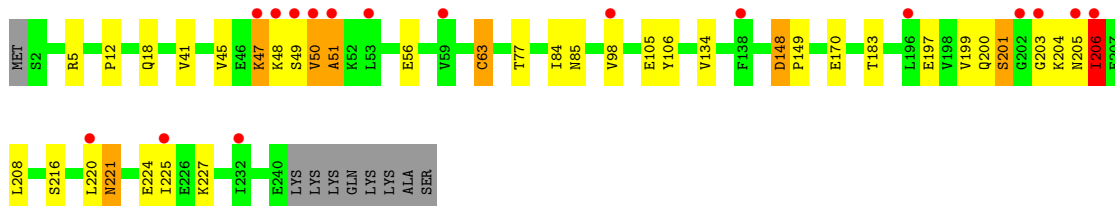
- Molecule 3: Proteasome subunit alpha type-7



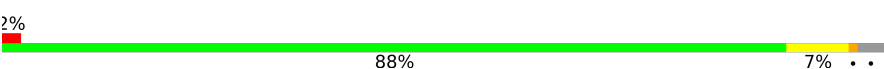
GLU
LYS
LYS
LYS
GLN
LYS
LYS
ALA
SER

• Molecule 3: Proteasome subunit alpha type-7

Chain Q: 

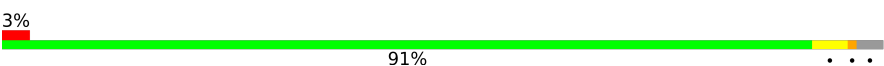


• Molecule 4: Proteasome subunit alpha type-5

Chain D: 



• Molecule 4: Proteasome subunit alpha type-5

Chain R: 



• Molecule 5: Proteasome subunit alpha type-1

Chain E: 



GLU
PRO
ALA
GLU
LYS
ALA
ASP
GLU
PRO
MET
GLU
HIS

• Molecule 5: Proteasome subunit alpha type-1

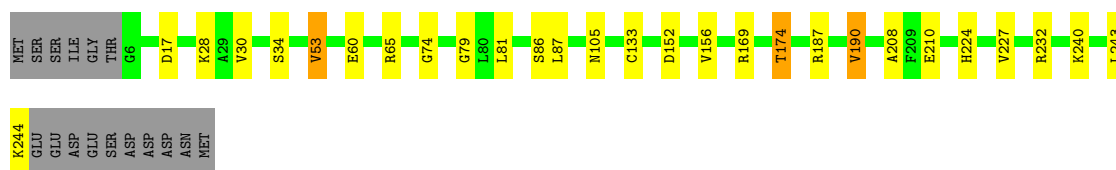
Chain S: 



GLN
ARG
LYS
ALA
GLN
PRO
ALA
GLN
PRO
ALA
ASP
GLU
ALA
LYS
GLU
ASP
GLU
PRO
MET
GLU
HIS

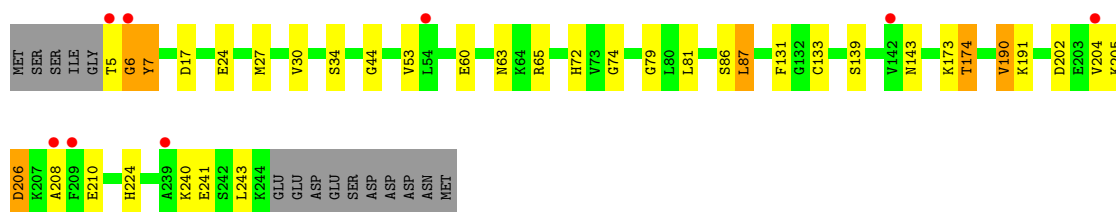
• Molecule 6: Proteasome subunit alpha type-3

Chain F:  83% 10% • 6%

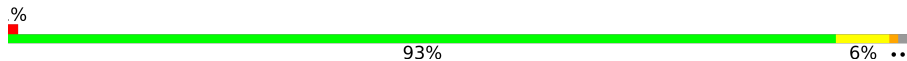


- Molecule 6: Proteasome subunit alpha type-3

Chain T:  80% 12% • 6%



- Molecule 7: Proteasome subunit alpha type-6

Chain G:  93% 6% ••



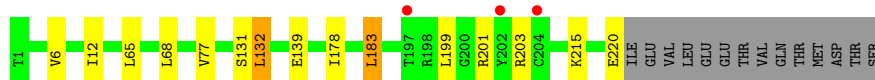
- Molecule 7: Proteasome subunit alpha type-6

Chain U:  87% 9% ••



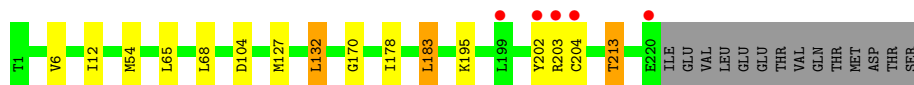
- Molecule 8: Proteasome subunit beta type-7

Chain H:  88% 6% • 6%

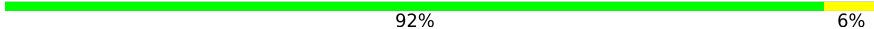


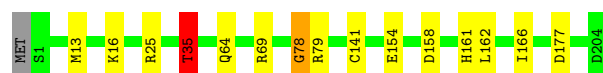
- Molecule 8: Proteasome subunit beta type-7

Chain V:  87% 6% • 6%



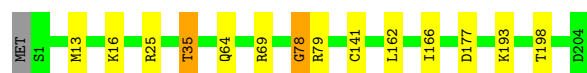
- Molecule 9: Proteasome subunit beta type-3

Chain I:  92% 6%



- Molecule 9: Proteasome subunit beta type-3

Chain W:  93% 6%



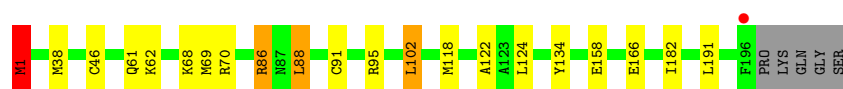
- Molecule 10: Proteasome subunit beta type-2

Chain J:  85% 11% ..



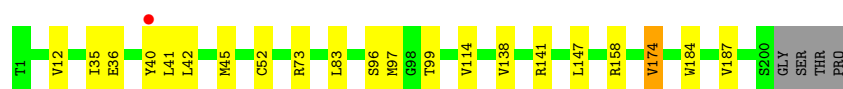
- Molecule 10: Proteasome subunit beta type-2

Chain X:  87% 8% ..



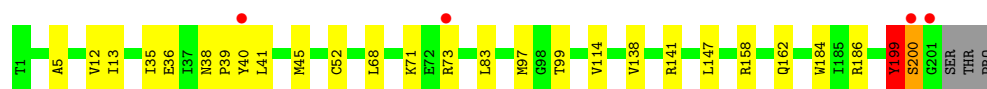
- Molecule 11: Proteasome subunit beta type-5

Chain K:  88% 10% .



- Molecule 11: Proteasome subunit beta type-5

Chain Y:  85% 12% .

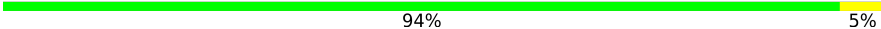


- Molecule 12: Proteasome subunit beta type-1

Chain L:  92% 8%

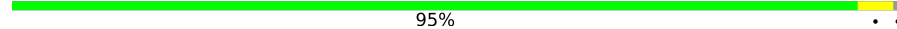


- Molecule 12: Proteasome subunit beta type-1

Chain Z:  94% 5%

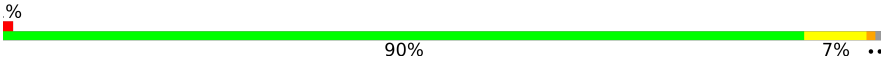


- Molecule 13: Proteasome subunit beta type-4

Chain M:  95% ..

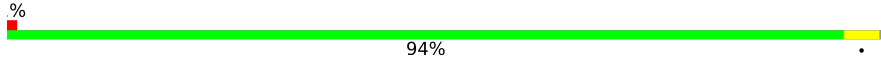


- Molecule 13: Proteasome subunit beta type-4

Chain a:  90% 7% ..

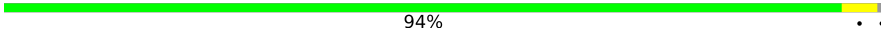


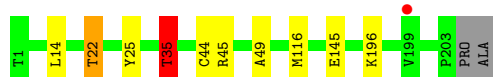
- Molecule 14: Proteasome subunit beta type-6

Chain N:  94% ..



- Molecule 14: Proteasome subunit beta type-6

Chain b:  94% ..



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	113.37Å 202.72Å 314.90Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	170.45 – 2.10 170.45 – 2.10	Depositor EDS
% Data completeness (in resolution range)	98.6 (170.45-2.10) 98.6 (170.45-2.10)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.15 (at 2.10Å)	Xtriage
Refinement program	REFMAC 5.8.0103	Depositor
R, R_{free}	0.184 , 0.226 0.191 , 0.230	Depositor DCC
R_{free} test set	20644 reflections (4.92%)	wwPDB-VP
Wilson B-factor (Å ²)	40.7	Xtriage
Anisotropy	0.168	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 50.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	52211	wwPDB-VP
Average B, all atoms (Å ²)	52.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.75% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: 1PE, K, CL, BO2, YCM, 6V1, MG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	0.92	0/1833	0.99	1/2489 (0.0%)
1	O	0.84	0/1778	0.97	0/2419
2	B	0.91	0/1962	0.98	0/2649
2	P	0.90	0/1945	1.00	2/2631 (0.1%)
3	C	0.90	0/1818	1.08	1/2469 (0.0%)
3	Q	0.93	1/1834 (0.1%)	1.12	8/2490 (0.3%)
4	D	0.92	1/1789 (0.1%)	1.01	2/2424 (0.1%)
4	R	0.98	0/1780	1.04	3/2408 (0.1%)
5	E	0.97	0/1842	1.02	2/2493 (0.1%)
5	S	0.93	0/1901	1.03	3/2571 (0.1%)
6	F	1.02	1/1935 (0.1%)	1.05	3/2605 (0.1%)
6	T	0.91	2/1894 (0.1%)	1.07	10/2556 (0.4%)
7	G	0.99	0/1909	1.02	4/2579 (0.2%)
7	U	0.88	1/1804 (0.1%)	0.95	0/2441
8	H	1.08	0/1697	1.03	0/2299
8	V	0.91	0/1655	0.98	1/2251 (0.0%)
9	I	0.96	0/1648	1.10	7/2219 (0.3%)
9	W	0.86	0/1630	1.02	6/2197 (0.3%)
10	J	0.94	0/1613	0.96	2/2180 (0.1%)
10	X	0.95	0/1597	0.98	2/2160 (0.1%)
11	K	0.94	0/1584	0.98	1/2141 (0.0%)
11	Y	1.00	0/1620	1.02	3/2185 (0.1%)
12	L	0.94	1/1672 (0.1%)	1.00	1/2257 (0.0%)
12	Z	1.01	0/1675	1.01	0/2257
13	M	0.96	1/1728 (0.1%)	0.97	0/2339
13	a	0.98	0/1724	0.99	1/2336 (0.0%)
14	N	1.04	1/1548 (0.1%)	1.02	2/2095 (0.1%)
14	b	0.92	0/1554	1.01	2/2104 (0.1%)
All	All	0.95	9/48969 (0.0%)	1.02	67/66244 (0.1%)

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
2	P	0	3
3	C	0	1
3	Q	0	2
4	D	0	4
4	R	0	2
5	E	0	1
6	T	0	1
7	U	1	0
9	I	0	1
9	W	0	1
10	J	0	2
10	X	0	1
11	Y	0	1
13	a	0	1
All	All	1	21

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	N	104	ASP	N-CA	6.17	1.51	1.45
6	F	79	GLY	C-O	-5.50	1.20	1.24
6	T	7	TYR	N-CA	5.49	1.56	1.46
13	M	3	ASN	C-O	-5.42	1.20	1.25
3	Q	206	ILE	CA-C	5.32	1.59	1.52
7	U	155	ASP	N-CA	5.21	1.49	1.46
6	T	79	GLY	C-O	-5.20	1.20	1.24
4	D	126	GLU	N-CA	5.09	1.52	1.46
12	L	140	SER	C-O	-5.03	1.18	1.24

All (67) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	I	16[A]	LYS	CA-C-N	9.43	135.94	122.08
9	I	16[A]	LYS	C-N-CA	9.43	135.94	122.08
9	I	16[B]	LYS	CA-C-N	9.43	135.94	122.08
9	I	16[B]	LYS	C-N-CA	9.43	135.94	122.08
7	G	183	VAL	CB-CA-C	-8.79	100.28	112.14
6	F	190	VAL	CB-CA-C	-8.74	100.58	112.04
6	T	190	VAL	CB-CA-C	-8.49	100.92	112.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	J	86	ARG	NE-CZ-NH2	-7.88	112.11	119.20
6	T	6	GLY	CA-C-N	7.87	135.87	121.70
6	T	6	GLY	C-N-CA	7.87	135.87	121.70
10	X	86	ARG	NE-CZ-NH2	-7.62	112.34	119.20
4	R	120[A]	ALA	N-CA-C	-7.59	97.70	109.76
4	R	120[B]	ALA	N-CA-C	-7.59	97.70	109.76
2	P	246	LYS	N-CA-C	7.42	121.59	112.54
9	I	78	GLY	N-CA-C	7.09	122.47	114.67
7	G	183	VAL	N-CA-CB	7.02	120.09	110.54
3	Q	220	LEU	CA-C-N	6.97	134.25	121.70
3	Q	220	LEU	C-N-CA	6.97	134.25	121.70
4	D	120	ALA	N-CA-C	6.81	119.33	111.02
14	b	22	THR	CB-CA-C	-6.73	99.91	110.74
7	G	183	VAL	N-CA-C	6.67	117.42	110.62
3	Q	220	LEU	N-CA-C	-6.63	99.78	110.32
6	T	143	ASN	N-CA-C	6.40	118.34	111.36
4	R	31	ILE	CB-CA-C	-6.09	103.92	112.14
11	K	174	VAL	CB-CA-C	6.08	119.31	110.98
14	N	35	THR	CB-CA-C	6.06	116.62	109.47
11	Y	199	TYR	N-CA-C	5.99	118.26	110.53
3	Q	12	PRO	N-CA-C	5.99	122.68	113.75
9	W	16[A]	LYS	CA-C-N	5.96	134.39	123.13
9	W	16[A]	LYS	C-N-CA	5.96	134.39	123.13
9	W	16[B]	LYS	CA-C-N	5.96	134.39	123.13
9	W	16[B]	LYS	C-N-CA	5.96	134.39	123.13
6	F	190	VAL	N-CA-CB	5.88	117.82	110.47
3	C	197	GLU	N-CA-C	5.84	118.59	111.82
2	P	124	PHE	CA-CB-CG	5.84	119.64	113.80
9	W	79	ARG	N-CA-C	5.83	117.12	108.60
6	T	7	TYR	N-CA-CB	5.76	120.29	110.50
3	Q	220	LEU	CA-C-O	-5.75	114.46	121.36
9	I	79	ARG	N-CA-C	5.70	117.20	108.42
10	J	86	ARG	NE-CZ-NH1	5.68	127.18	121.50
6	T	190	VAL	N-CA-CB	5.67	117.56	110.47
5	E	58	ALA	N-CA-C	5.62	118.13	111.33
14	b	35	THR	CB-CA-C	5.62	116.11	109.47
5	E	236	LEU	N-CA-C	-5.59	98.82	108.56
5	S	58	ALA	N-CA-C	-5.59	103.14	110.53
9	I	35	THR	N-CA-CB	-5.58	102.33	111.66
14	N	22	THR	CB-CA-C	-5.55	101.80	110.74
3	Q	12	PRO	CA-C-N	-5.53	114.41	122.86
3	Q	12	PRO	C-N-CA	-5.53	114.41	122.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	F	174	THR	N-CA-CB	5.51	118.23	110.12
12	L	2	PHE	CA-C-O	-5.50	115.71	120.88
6	T	44	GLY	N-CA-C	5.46	117.55	110.45
3	Q	220	LEU	O-C-N	-5.45	116.95	123.06
8	V	170	GLY	N-CA-C	5.44	118.47	110.80
11	Y	199	TYR	CA-C-N	5.42	131.46	121.70
11	Y	199	TYR	C-N-CA	5.42	131.46	121.70
4	D	125	GLU	N-CA-C	5.42	119.46	112.41
10	X	86	ARG	NE-CZ-NH1	5.39	126.89	121.50
5	S	114	SER	CB-CA-C	-5.19	102.73	110.88
6	T	6	GLY	N-CA-C	5.18	125.47	113.18
13	a	71	VAL	N-CA-CB	5.18	118.35	110.58
9	W	78	GLY	N-CA-C	5.17	120.36	114.67
7	G	244	GLU	N-CA-C	5.14	116.95	109.71
1	A	53	SER	N-CA-C	5.12	121.71	110.80
5	S	4	ASN	N-CA-C	5.11	116.85	111.28
6	T	174	THR	N-CA-CB	5.04	117.98	110.22
6	T	63	ASN	CB-CA-C	-5.03	104.75	111.89

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
7	U	47	6V1	C1

All (21) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	C	237	GLU	Peptide
4	D	127	ASP	Peptide
4	D	175[A]	GLU	Peptide
4	D	175[B]	GLU	Peptide
4	D	223	GLY	Peptide
5	E	235	GLY	Peptide
9	I	78	GLY	Peptide
10	J	1[A]	MET	Peptide
10	J	1[B]	MET	Peptide
2	P	244	GLU	Peptide
2	P	245	ALA	Peptide
2	P	54	LYS	Peptide
3	Q	47	LYS	Peptide
3	Q	49	SER	Peptide
4	R	130	PRO	Peptide

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Mol	Chain	Res	Type	Group
4	R	223	GLY	Peptide
6	T	5	THR	Peptide
9	W	78	GLY	Peptide
10	X	1	MET	Peptide
11	Y	199	TYR	Peptide
13	a	215	ILE	Peptide

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1788	0	1761	11	0
1	O	1741	0	1683	6	0
2	B	1926	0	1924	8	0
2	P	1909	0	1874	14	0
3	C	1798	0	1718	14	0
3	Q	1820	0	1749	15	0
4	D	1762	0	1709	7	0
4	R	1753	0	1726	6	0
5	E	1822	0	1779	9	0
5	S	1875	0	1818	19	0
6	F	1888	0	1882	10	0
6	T	1856	0	1816	11	0
7	G	1912	0	1882	3	0
7	U	1815	0	1748	8	0
8	H	1664	0	1680	12	0
8	V	1622	0	1594	7	0
9	I	1613	0	1646	9	0
9	W	1599	0	1621	8	0
10	J	1590	0	1581	18	0
10	X	1574	0	1561	13	0
11	K	1550	0	1506	11	0
11	Y	1580	0	1557	19	0
12	L	1636	0	1625	5	0
12	Z	1642	0	1635	4	0
13	M	1692	0	1670	5	0
13	a	1688	0	1658	11	0
14	N	1519	0	1495	9	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
14	b	1524	0	1495	6	0
15	A	4	0	0	0	0
15	B	2	0	0	1	0
15	C	2	0	0	0	0
15	D	2	0	0	0	0
15	E	3	0	0	0	0
15	F	1	0	0	0	0
15	G	2	0	0	0	0
15	H	1	0	0	0	0
15	I	1	0	0	0	0
15	K	3	0	0	0	0
15	M	4	0	0	1	0
15	N	2	0	0	0	0
15	O	4	0	0	0	0
15	P	1	0	0	0	0
15	Q	2	0	0	0	0
15	R	2	0	0	0	0
15	S	3	0	0	0	0
15	U	1	0	0	0	0
15	V	1	0	0	0	0
15	W	1	0	0	0	0
15	Y	4	0	0	0	0
15	a	3	0	0	1	0
15	b	2	0	0	1	0
16	G	1	0	0	0	0
16	L	1	0	0	0	0
16	N	1	0	0	0	0
16	U	1	0	0	0	0
16	Z	1	0	0	0	0
16	b	1	0	0	0	0
17	H	2	0	0	0	0
17	I	2	0	0	0	0
17	J	1	0	0	0	0
17	K	1	0	0	0	0
17	L	1	0	0	0	0
17	V	1	0	0	0	0
17	W	1	0	0	0	0
17	X	1	0	0	0	0
18	H	32	0	44	0	0
18	I	32	0	44	0	0
18	L	16	0	22	0	0
18	M	16	0	22	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
18	W	16	0	22	0	0
18	Z	16	0	22	0	0
18	b	16	0	22	0	0
19	H	28	0	25	1	0
19	K	28	0	25	0	0
19	N	28	0	25	1	0
19	V	28	0	25	0	0
19	Y	28	0	25	0	0
19	b	28	0	25	1	0
20	A	115	0	0	2	0
20	B	131	0	0	2	0
20	C	75	0	0	0	0
20	D	95	0	0	1	0
20	E	147	0	0	2	0
20	F	186	0	0	3	0
20	G	196	0	0	0	0
20	H	159	0	0	7	0
20	I	157	0	0	1	0
20	J	138	0	0	4	0
20	K	105	0	0	0	0
20	L	125	0	0	1	0
20	M	147	0	0	0	0
20	N	162	0	0	0	0
20	O	95	0	0	1	0
20	P	125	0	0	0	0
20	Q	75	0	0	2	0
20	R	132	0	0	0	0
20	S	130	0	0	3	0
20	T	100	0	0	1	0
20	U	107	0	0	1	0
20	V	120	0	0	1	0
20	W	118	0	0	2	0
20	X	125	0	0	0	0
20	Y	142	0	0	0	0
20	Z	169	0	0	1	0
20	a	174	0	0	3	0
20	b	124	0	0	0	0
All	All	52211	0	47741	257	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 (257) 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)
6:F:169[A]:ARG:NH1	20:F:401:HOH:O	2.02	0.92
2:P:25[B]:MET:HE3	2:P:25[B]:MET:HA	1.51	0.92
12:L:144:MET:HE1	12:L:185:ARG:HB2	1.53	0.88
10:X:1:MET:HE1	10:X:134:TYR:H	1.45	0.81
2:P:155:ASN:OD1	3:Q:77:THR:OG1	2.01	0.79
10:J:1[A]:MET:HE1	10:J:134:TYR:H	1.48	0.78
11:Y:35:ILE:HD11	11:Y:45:MET:SD	2.24	0.77
5:S:47:VAL:HG12	5:S:195:LEU:HD22	1.67	0.77
5:E:47:VAL:HG12	5:E:195:LEU:HD22	1.68	0.75
1:A:108:GLN:HE21	1:A:112:ARG:HH12	1.33	0.74
11:K:35:ILE:HD11	11:K:45:MET:SD	2.26	0.74
11:K:141:ARG:NH1	10:X:166:GLU:OE2	2.22	0.73
7:U:108:GLU:OE1	20:U:401:HOH:O	2.06	0.72
10:X:1:MET:HE1	10:X:134:TYR:N	2.05	0.70
10:J:1[A]:MET:HE1	10:J:134:TYR:N	2.06	0.69
8:V:54:MET:HE1	20:W:440:HOH:O	1.93	0.69
1:O:10:THR:HG23	20:O:402:HOH:O	1.93	0.67
5:S:152[B]:ASN:ND2	20:S:402:HOH:O	2.27	0.67
10:J:99[A]:HIS:CD2	20:J:411:HOH:O	2.48	0.67
7:U:118:ILE:HG13	7:U:138:MET:HE1	1.75	0.66
14:b:35:THR:CG2	14:b:45:ARG:HE	2.09	0.66
5:S:18[A]:ARG:HD2	5:S:23:GLU:OE2	1.95	0.66
14:N:35:THR:CG2	14:N:45:ARG:HE	2.09	0.65
9:I:13[A]:MET:HE2	9:I:166:ILE:HB	1.79	0.65
2:P:48:GLU:HB2	2:P:201:MET:HE2	1.78	0.65
13:a:86:ARG:NH1	13:a:133:GLU:OE1	2.30	0.65
2:B:10:THR:OG1	20:B:401:HOH:O	2.14	0.64
8:V:195:LYS:CB	20:V:503:HOH:O	2.44	0.64
2:P:12:PHE:H	3:Q:18:GLN:HE22	1.45	0.64
11:Y:199:TYR:HA	11:Y:200:SER:HB2	1.81	0.63
5:S:65[A]:HIS:CE1	20:S:407:HOH:O	2.52	0.62
3:C:5:ARG:NH1	4:D:125:GLU:OE2	2.32	0.62
12:L:144:MET:CE	12:L:185:ARG:HB2	2.29	0.62
3:C:47:LYS:CB	3:C:48:LYS:HA	2.30	0.61
9:W:13:MET:HE2	9:W:166:ILE:HB	1.82	0.61
3:Q:85:ASN:OD1	10:X:70:ARG:CZ	2.48	0.61
9:I:64:GLN:OE1	10:J:86:ARG:NH2	2.34	0.61
5:S:233:LEU:HB2	5:S:234:GLU:OE2	2.00	0.61
7:U:199:ILE:HD11	7:U:239:LEU:HD23	1.82	0.61
5:E:58:ALA:O	5:E:59:HIS:CB	2.48	0.60
13:a:174:ARG:NH2	20:a:401:HOH:O	2.34	0.60
10:J:101:ASN:HD22	10:J:119:ASP:HA	1.66	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:166:GLU:OE2	11:Y:141[A]:ARG:NH1	2.34	0.60
7:U:195:VAL:O	7:U:199:ILE:HG23	2.01	0.60
4:D:96:THR:OG1	20:D:401:HOH:O	2.16	0.59
6:T:24:GLU:HA	6:T:27:MET:HE3	1.83	0.59
3:C:85[B]:ASN:OD1	10:J:70:ARG:CZ	2.50	0.59
13:M:5:MET:HE2	14:N:116:MET:CB	2.32	0.59
2:B:155:ASN:OD1	3:C:77:THR:OG1	2.18	0.59
6:F:105:ASN:ND2	20:F:403:HOH:O	2.35	0.58
5:S:50:LYS:HB3	5:S:59:HIS:HB3	1.84	0.58
9:I:35:THR:HG21	20:I:415:HOH:O	2.03	0.58
10:X:88:LEU:HB3	10:X:122:ALA:HB2	1.84	0.57
3:C:47:LYS:CB	3:C:48:LYS:CA	2.82	0.57
11:K:99:THR:HG22	11:K:114:VAL:O	2.05	0.57
11:Y:99:THR:HG22	11:Y:114:VAL:O	2.04	0.57
4:R:129:ASP:CB	4:R:130:PRO:HD3	2.34	0.57
5:E:49:LEU:O	5:E:62:LYS:HD2	2.05	0.57
3:C:85[B]:ASN:OD1	10:J:70:ARG:NH2	2.38	0.57
2:B:44:LEU:HD22	2:B:190:LEU:HD13	1.87	0.56
10:J:88:LEU:HB3	10:J:122:ALA:HB2	1.87	0.56
5:S:49:LEU:O	5:S:62:LYS:HD2	2.05	0.56
5:E:101[A]:ARG:NH1	20:E:401:HOH:O	2.39	0.56
14:b:14:LEU:HD23	14:b:44:CYS:SG	2.46	0.56
2:P:25[B]:MET:HA	2:P:25[B]:MET:CE	2.32	0.56
6:T:191:LYS:NZ	20:T:302:HOH:O	2.38	0.55
7:U:58:ASP:O	7:U:59:LYS:CB	2.55	0.55
2:P:44:LEU:HD22	2:P:190:LEU:HD13	1.89	0.55
14:N:14:LEU:HD23	14:N:44:CYS:SG	2.47	0.55
3:Q:41:VAL:HG11	3:Q:134:VAL:HB	1.88	0.54
3:C:35:VAL:HG13	3:C:191:VAL:CG2	2.36	0.54
15:B:301:CL:CL	15:B:302:CL:CL	2.99	0.54
6:T:205:LYS:O	6:T:206:ASP:CG	2.51	0.54
5:S:18[B]:ARG:HG2	5:S:23:GLU:OE2	2.08	0.54
5:S:234:GLU:OE2	5:S:234:GLU:N	2.41	0.54
13:M:5:MET:HE2	14:N:116:MET:HB2	1.88	0.54
14:N:49:ALA:HB3	19:N:304:BO2:H3	1.89	0.54
2:P:194:ILE:CD1	2:P:236:LEU:HB3	2.39	0.53
4:R:129:ASP:CB	4:R:130:PRO:CD	2.87	0.53
5:S:101:ARG:NH1	20:S:406:HOH:O	2.41	0.53
13:a:5:MET:HE2	14:b:116:MET:HB2	1.90	0.53
13:a:5:MET:HE2	14:b:116:MET:CB	2.39	0.53
1:A:51:GLN:HE22	1:A:58[B]:GLU:HB3	1.75	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:13[A]:MET:HE3	9:I:162:LEU:HD12	1.91	0.52
20:Q:406:HOH:O	4:R:128:ALA:HB1	2.09	0.52
10:J:185:LYS:NZ	20:J:401:HOH:O	2.36	0.52
9:W:13:MET:HE1	9:W:166:ILE:N	2.25	0.52
11:Y:40:TYR:HB3	11:Y:73:ARG:NH1	2.25	0.51
1:A:73:LEU:HD22	1:A:135:ILE:HG12	1.92	0.51
15:M:302:CL:CL	15:M:303:CL:CL	3.03	0.51
9:W:13:MET:HE3	9:W:162:LEU:HD12	1.93	0.51
2:P:190:LEU:HG	2:P:236:LEU:HD21	1.93	0.51
3:C:50:VAL:O	3:C:51:ALA:HB3	2.11	0.51
4:R:78:MET:HG3	4:R:82:ILE:HD12	1.91	0.51
3:C:40:ILE:HD11	3:C:210:VAL:HG13	1.93	0.51
9:I:13[A]:MET:HE1	9:I:166:ILE:N	2.27	0.50
3:Q:50:VAL:O	3:Q:51:ALA:HB3	2.12	0.50
9:W:64:GLN:OE1	10:X:86:ARG:NH2	2.43	0.50
13:M:5:MET:HE2	14:N:116:MET:HB3	1.94	0.49
7:U:43:ARG:HB3	7:U:151:VAL:HG13	1.94	0.49
12:L:148:LEU:HD23	12:L:178:VAL:CG1	2.42	0.49
10:J:177:THR:HG22	10:J:195:SER:CB	2.43	0.49
19:H:306:BO2:H16	20:H:407:HOH:O	2.13	0.49
1:O:110:VAL:HG22	1:O:135:ILE:HD12	1.94	0.49
3:Q:85:ASN:OD1	10:X:70:ARG:NH2	2.46	0.49
4:D:78:MET:HG3	4:D:82:ILE:HD12	1.95	0.49
14:b:49:ALA:HB3	19:b:305:BO2:H3	1.93	0.49
6:F:34:SER:OG	6:F:65:ARG:NH1	2.45	0.48
1:A:110:VAL:HG22	1:A:135:ILE:HD12	1.96	0.48
20:H:454:HOH:O	13:a:216:SER:HB3	2.12	0.48
1:O:73:LEU:HD22	1:O:135:ILE:HG12	1.93	0.48
11:K:40:TYR:HB3	11:K:73:ARG:NH1	2.29	0.48
6:T:173:LYS:HB3	6:T:173:LYS:HE2	1.61	0.48
6:T:202:ASP:OD1	6:T:204:VAL:HG12	2.14	0.48
8:H:201:ARG:NH1	20:H:405:HOH:O	2.45	0.48
6:T:74:GLY:HA3	6:T:224:HIS:CD2	2.48	0.48
5:E:68:ASN:ND2	5:E:220:GLU:OE1	2.48	0.47
7:G:11:ARG:HG2	7:G:11:ARG:HH11	1.80	0.47
3:Q:204:LYS:HA	3:Q:205:ASN:O	2.14	0.47
9:I:158:ASP:OD1	9:I:161:HIS:HD2	1.97	0.47
8:H:203:ARG:NH2	9:I:154:GLU:OE1	2.45	0.47
6:T:87:LEU:HD13	6:T:131:PHE:CE1	2.48	0.47
11:Y:40:TYR:CZ	11:Y:73:ARG:HB3	2.49	0.47
6:F:53:VAL:HG12	6:F:208:ALA:HB3	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:W:35:THR:HG21	20:W:428:HOH:O	2.14	0.47
15:a:302:CL:CL	15:b:301:CL:CL	3.06	0.47
6:F:169[A]:ARG:NH1	20:F:408:HOH:O	2.47	0.47
10:X:1:MET:HE2	10:X:1:MET:HB3	1.84	0.47
13:a:92:LEU:HD12	13:a:112:ILE:HD11	1.96	0.47
11:Y:40:TYR:CD2	11:Y:73:ARG:CZ	2.98	0.47
8:H:132:LEU:HD22	14:N:25:TYR:CE2	2.50	0.47
12:Z:148:LEU:HD23	12:Z:178:VAL:CG1	2.45	0.47
10:J:182:ILE:CD1	10:J:191:LEU:HD11	2.45	0.47
1:A:63:LYS:NZ	20:A:405:HOH:O	2.48	0.46
3:Q:63:YCM:HD2	3:Q:84:ILE:HD13	1.96	0.46
1:A:108:GLN:NE2	1:A:112:ARG:HH12	2.08	0.46
8:H:77:VAL:HG12	20:H:542:HOH:O	2.16	0.46
11:K:40:TYR:CZ	11:K:73:ARG:HB3	2.51	0.46
3:Q:106:TYR:CD1	3:Q:106:TYR:C	2.94	0.46
3:Q:199:VAL:O	3:Q:201:SER:N	2.48	0.46
9:W:25[A]:ARG:HG2	9:W:25[A]:ARG:HH11	1.81	0.46
1:A:158:LYS:NZ	20:A:404:HOH:O	2.48	0.46
4:D:164:GLN:OE1	5:E:58:ALA:HB2	2.15	0.46
4:R:96:THR:HG22	4:R:112:VAL:HG22	1.97	0.46
13:a:44:ARG:HD2	20:a:535:HOH:O	2.16	0.45
1:O:10:THR:HB	1:O:20:GLN:HB2	1.98	0.45
3:C:106:TYR:CD1	3:C:106:TYR:C	2.94	0.45
2:P:151:ASP:HB2	2:P:152:PRO:CD	2.47	0.45
7:U:72:ILE:HG21	7:U:114:LEU:HD21	1.98	0.45
13:a:96:MET:HE3	13:a:127:MET:HA	1.98	0.45
2:P:197:LEU:HD22	2:P:201:MET:HE3	1.97	0.45
1:A:206:ASN:C	1:A:206:ASN:HD22	2.25	0.45
11:K:40:TYR:CD2	11:K:73:ARG:CZ	3.00	0.45
10:X:182:ILE:CD1	10:X:191:LEU:HD11	2.47	0.45
3:C:40:ILE:HD11	3:C:210:VAL:CG1	2.46	0.45
8:V:132:LEU:HD22	14:b:25:TYR:CZ	2.52	0.45
11:Y:199:TYR:HA	11:Y:200:SER:CB	2.46	0.45
8:V:213:THR:HB	9:W:198:THR:OG1	2.16	0.45
10:X:46[B]:CYS:SG	10:X:102:LEU:HD22	2.57	0.45
8:H:77:VAL:HG13	20:H:414:HOH:O	2.16	0.44
5:S:237:GLU:O	5:S:238:GLU:CB	2.64	0.44
6:T:34:SER:OG	6:T:65:ARG:NH1	2.47	0.44
11:Y:158:ARG:HE	11:Y:162:GLN:HE21	1.63	0.44
5:E:189:LYS:HG3	5:E:236:LEU:HD23	1.99	0.44
9:I:25[A]:ARG:HG2	9:I:25[A]:ARG:HH11	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:27[A]:GLN:NE2	20:J:404:HOH:O	2.47	0.44
9:W:141:CYS:HB3	9:W:177:ASP:HB2	2.00	0.44
3:C:47:LYS:HA	3:C:205:ASN:HB3	2.00	0.44
8:H:77:VAL:HB	20:H:542:HOH:O	2.17	0.44
12:Z:66:LYS:NZ	20:Z:1406:HOH:O	2.51	0.44
1:A:17:LYS:HE2	1:A:22:GLU:OE2	2.18	0.44
7:G:72:ILE:HG21	7:G:114:LEU:HD21	2.00	0.44
3:Q:63:YCM:HD2	3:Q:84:ILE:CD1	2.48	0.44
8:V:202:TYR:O	8:V:204:CYS:N	2.51	0.44
2:B:33:THR:HB	2:B:166:ASN:O	2.17	0.44
6:F:74:GLY:HA3	6:F:224:HIS:CD2	2.53	0.44
10:J:118:MET:HE2	10:J:124:LEU:HD13	1.99	0.44
5:S:233:LEU:CB	5:S:234:GLU:OE2	2.66	0.43
11:Y:36:GLU:HG2	11:Y:184:TRP:CZ2	2.53	0.43
12:Z:184:GLU:OE2	12:Z:211:ARG:HD2	2.19	0.43
13:a:47:ASN:ND2	20:a:405:HOH:O	2.51	0.43
2:B:48:GLU:HG3	2:B:201:MET:HE3	2.00	0.43
8:H:77:VAL:CG1	20:H:542:HOH:O	2.66	0.43
1:O:206:ASN:C	1:O:206:ASN:HD22	2.27	0.43
5:S:233:LEU:C	5:S:235:GLY:HA3	2.44	0.43
11:Y:52:CYS:SG	11:Y:97[A]:MET:HG3	2.58	0.43
1:A:58[B]:GLU:CD	1:A:58[B]:GLU:H	2.25	0.43
3:C:35:VAL:HG13	3:C:191:VAL:HG22	2.00	0.43
4:D:195:ILE:O	4:D:199:LEU:HD22	2.19	0.43
12:Z:172:MET:HE1	12:Z:197:ILE:HD11	1.99	0.43
9:I:141:CYS:HB3	9:I:177:ASP:HB2	2.00	0.43
6:T:60:GLU:HA	6:T:210:GLU:OE1	2.18	0.43
8:H:201:ARG:HD2	8:H:203:ARG:HB2	2.01	0.43
13:M:96:MET:HE3	13:M:127:MET:HA	2.00	0.43
2:P:246:LYS:HE3	2:P:246:LYS:N	2.34	0.43
2:P:33:THR:HB	2:P:166:ASN:O	2.18	0.42
10:X:38:MET:HE1	10:X:61:GLN:HB2	2.00	0.42
4:D:96:THR:HG22	4:D:112:VAL:HG22	2.02	0.42
3:Q:204:LYS:HA	3:Q:205:ASN:C	2.45	0.42
8:V:178:ILE:HG12	8:V:183:LEU:HD12	2.01	0.42
11:Y:40:TYR:OH	11:Y:73:ARG:HA	2.19	0.42
5:S:233:LEU:C	5:S:234:GLU:OE2	2.62	0.42
10:J:68:LYS:CE	10:J:69:MET:HE2	2.49	0.42
2:B:92[B]:LEU:HD23	20:B:424:HOH:O	2.18	0.42
2:B:151:ASP:HB2	2:B:152:PRO:CD	2.49	0.42
6:F:30:VAL:HG22	6:F:133[A]:CYS:HA	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:226:LYS:HE2	7:G:226:LYS:HB2	1.96	0.42
11:K:83:LEU:HD21	11:K:99:THR:HG21	2.02	0.42
13:M:27:LEU:HD22	13:M:184:TYR:HB2	2.01	0.42
6:F:152:ASP:OD1	6:F:156:VAL:HG12	2.20	0.42
10:X:118:MET:HE2	10:X:124:LEU:HD13	2.01	0.42
2:P:8:ARG:NH2	3:Q:5:ARG:HD2	2.35	0.42
2:P:63:GLU:N	2:P:212:GLU:OE2	2.44	0.42
11:Y:5:ALA:HA	11:Y:13:ILE:O	2.20	0.42
6:F:60:GLU:HA	6:F:210:GLU:OE1	2.20	0.42
10:X:68:LYS:CE	10:X:69:MET:HE2	2.50	0.42
11:K:52:CYS:SG	11:K:97[A]:MET:HG3	2.60	0.42
12:L:43[B]:CYS:SG	20:L:402:HOH:O	2.62	0.42
14:N:35:THR:CG2	14:N:45:ARG:NE	2.81	0.42
8:V:127[B]:MET:HB3	8:V:127[B]:MET:HE2	1.77	0.42
13:a:27:LEU:HD22	13:a:184:TYR:HB2	2.02	0.42
2:B:51:ASN:HB2	2:B:63:GLU:OE1	2.19	0.42
10:J:1[A]:MET:CE	20:J:483:HOH:O	2.67	0.41
3:C:203:GLY:CA	3:C:204:LYS:CB	2.99	0.41
5:E:4:ASN:ND2	20:E:405:HOH:O	2.52	0.41
8:H:132:LEU:HD22	14:N:25:TYR:CZ	2.55	0.41
11:K:96:SER:C	11:K:97[B]:MET:HG3	2.46	0.41
12:L:123:SER:CB	12:L:136:LYS:HG2	2.50	0.41
3:Q:148:ASP:HB2	3:Q:149:PRO:CD	2.50	0.41
11:Y:68:LEU:O	11:Y:71:LYS:HE3	2.20	0.41
11:Y:186[A]:ARG:HE	11:Y:186[A]:ARG:HB2	1.76	0.41
5:E:7:ASP:C	5:E:7:ASP:OD1	2.64	0.41
8:H:178:ILE:HG12	8:H:183:LEU:HD12	2.02	0.41
6:T:30:VAL:HG22	6:T:133[A]:CYS:HA	2.02	0.41
10:J:177:THR:HG22	10:J:195:SER:HB2	2.02	0.41
5:S:50:LYS:CB	5:S:59:HIS:HB3	2.48	0.41
5:S:68:ASN:ND2	5:S:220:GLU:OE1	2.52	0.41
6:T:72:HIS:O	6:T:139:SER:HB2	2.21	0.41
6:F:227:VAL:O	6:F:232[B]:ARG:NH1	2.45	0.41
11:Y:38:ASN:HB2	11:Y:39:PRO:CD	2.50	0.41
13:a:174:ARG:NH1	13:a:206:GLU:O	2.48	0.41
10:J:86:ARG:HD3	10:J:90:ASP:OD1	2.21	0.40
1:O:55:LEU:HD12	7:U:176:THR:HG23	2.03	0.40
20:Q:465:HOH:O	4:R:60:GLU:HG3	2.21	0.40
11:Y:68:LEU:O	11:Y:71:LYS:CE	2.68	0.40
11:K:35:ILE:CD1	11:K:45:MET:SD	3.05	0.40
11:K:36:GLU:HG2	11:K:184:TRP:CZ2	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Q:221:ASN:ND2	3:Q:224:GLU:HB2	2.36	0.40
5:S:176:MET:HA	5:S:179:PHE:CD2	2.56	0.40
11:Y:141[B]:ARG:HD2	11:Y:141[B]:ARG:HA	1.88	0.40
4:D:146:VAL:HG11	4:D:222:PRO:HA	2.04	0.40
8:H:139:GLU:HA	8:H:139:GLU:OE2	2.21	0.40
11:Y:83:LEU:HD21	11:Y:99:THR:HG21	2.03	0.40
1:A:36:GLY:O	1:A:159:ALA:HA	2.21	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	231/234 (99%)	222 (96%)	4 (2%)	5 (2%)	5	2
1	O	228/234 (97%)	218 (96%)	4 (2%)	6 (3%)	4	1
2	B	248/261 (95%)	239 (96%)	7 (3%)	2 (1%)	16	12
2	P	248/261 (95%)	232 (94%)	13 (5%)	3 (1%)	10	7
3	C	236/248 (95%)	224 (95%)	6 (2%)	6 (2%)	4	1
3	Q	236/248 (95%)	218 (92%)	8 (3%)	10 (4%)	2	0
4	D	232/241 (96%)	224 (97%)	4 (2%)	4 (2%)	7	3
4	R	232/241 (96%)	222 (96%)	7 (3%)	3 (1%)	9	6
5	E	232/263 (88%)	226 (97%)	5 (2%)	1 (0%)	30	28
5	S	238/263 (90%)	230 (97%)	6 (2%)	2 (1%)	16	12
6	F	241/255 (94%)	240 (100%)	1 (0%)	0	100	100
6	T	239/255 (94%)	233 (98%)	2 (1%)	4 (2%)	7	3
7	G	241/246 (98%)	235 (98%)	5 (2%)	1 (0%)	30	28
7	U	232/246 (94%)	228 (98%)	4 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
8	H	220/234 (94%)	217 (99%)	3 (1%)	0	100	100
8	V	220/234 (94%)	217 (99%)	2 (1%)	1 (0%)	24	22
9	I	205/205 (100%)	200 (98%)	5 (2%)	0	100	100
9	W	204/205 (100%)	199 (98%)	5 (2%)	0	100	100
10	J	195/201 (97%)	192 (98%)	3 (2%)	0	100	100
10	X	195/201 (97%)	193 (99%)	2 (1%)	0	100	100
11	K	199/204 (98%)	196 (98%)	3 (2%)	0	100	100
11	Y	202/204 (99%)	198 (98%)	3 (2%)	1 (0%)	24	22
12	L	213/213 (100%)	211 (99%)	2 (1%)	0	100	100
12	Z	212/213 (100%)	210 (99%)	2 (1%)	0	100	100
13	M	215/219 (98%)	208 (97%)	7 (3%)	0	100	100
13	a	216/219 (99%)	209 (97%)	7 (3%)	0	100	100
14	N	201/205 (98%)	199 (99%)	2 (1%)	0	100	100
14	b	202/205 (98%)	200 (99%)	2 (1%)	0	100	100
All	All	6213/6458 (96%)	6040 (97%)	124 (2%)	49 (1%)	16	12

All (49) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	50	LYS
1	A	52	LYS
1	A	53	SER
4	D	176	GLY
5	E	59	HIS
1	O	52	LYS
1	O	53	SER
2	P	204	SER
3	Q	47	LYS
3	Q	201	SER
3	Q	206	ILE
3	Q	221	ASN
4	R	130	PRO
5	S	238	GLU
6	T	208	ALA
11	Y	200	SER
3	C	200	GLN
1	O	50	LYS

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Mol	Chain	Res	Type
1	O	231	ALA
2	P	52	ILE
2	P	54	LYS
3	Q	200	GLN
6	T	7	TYR
6	T	206	ASP
8	V	203	ARG
1	A	176	ARG
3	C	50	VAL
3	C	204	LYS
4	D	175[A]	GLU
4	D	175[B]	GLU
1	O	176	ARG
4	R	128	ALA
3	C	216	SER
4	D	126	GLU
3	Q	48	LYS
3	Q	50	VAL
5	S	3	ARG
6	T	6	GLY
1	A	201	GLN
3	C	51	ALA
7	G	209	ASP
1	O	201	GLN
3	Q	216	SER
4	R	129	ASP
2	B	204	SER
3	Q	51	ALA
3	C	203	GLY
2	B	203	VAL
3	Q	203	GLY

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	185/191 (97%)	172 (93%)	13 (7%)	14	11
1	O	176/191 (92%)	167 (95%)	9 (5%)	21	21
2	B	200/221 (90%)	193 (96%)	7 (4%)	32	35
2	P	197/221 (89%)	186 (94%)	11 (6%)	19	18
3	C	179/210 (85%)	169 (94%)	10 (6%)	19	18
3	Q	184/210 (88%)	172 (94%)	12 (6%)	15	13
4	D	189/203 (93%)	183 (97%)	6 (3%)	34	38
4	R	187/203 (92%)	185 (99%)	2 (1%)	65	74
5	E	192/223 (86%)	185 (96%)	7 (4%)	31	34
5	S	197/223 (88%)	191 (97%)	6 (3%)	36	41
6	F	199/212 (94%)	187 (94%)	12 (6%)	17	15
6	T	192/212 (91%)	182 (95%)	10 (5%)	21	20
7	G	202/207 (98%)	194 (96%)	8 (4%)	28	29
7	U	186/207 (90%)	178 (96%)	8 (4%)	26	27
8	H	181/195 (93%)	172 (95%)	9 (5%)	22	22
8	V	172/195 (88%)	163 (95%)	9 (5%)	21	20
9	I	176/174 (101%)	174 (99%)	2 (1%)	65	74
9	W	173/174 (99%)	170 (98%)	3 (2%)	53	62
10	J	166/170 (98%)	159 (96%)	7 (4%)	26	28
10	X	164/170 (96%)	158 (96%)	6 (4%)	30	33
11	K	155/159 (98%)	147 (95%)	8 (5%)	21	20
11	Y	159/159 (100%)	155 (98%)	4 (2%)	42	48
12	L	175/178 (98%)	167 (95%)	8 (5%)	24	25
12	Z	175/178 (98%)	169 (97%)	6 (3%)	32	35
13	M	180/181 (99%)	178 (99%)	2 (1%)	65	74
13	a	178/181 (98%)	174 (98%)	4 (2%)	45	53
14	N	158/159 (99%)	155 (98%)	3 (2%)	50	58
14	b	158/159 (99%)	154 (98%)	4 (2%)	42	48
All	All	5035/5366 (94%)	4839 (96%)	196 (4%)	29	31

All (196) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	17	LYS
1	A	50	LYS
1	A	53	SER
1	A	61	VAL
1	A	69	LYS
1	A	73	LEU
1	A	131	VAL
1	A	174	GLU
1	A	189	THR
1	A	206	ASN
1	A	223	THR
1	A	226	LYS
1	A	227	ASP
2	B	33	THR
2	B	43	VAL
2	B	59	VAL
2	B	190	LEU
2	B	229	LYS
2	B	238	LYS
2	B	249	ARG
3	C	35	VAL
3	C	45	VAL
3	C	105	GLU
3	C	113	SER
3	C	148	ASP
3	C	179	GLU
3	C	183	THR
3	C	205	ASN
3	C	208	LEU
3	C	225	ILE
4	D	46	VAL
4	D	65	GLU
4	D	95	GLU
4	D	126	GLU
4	D	199	LEU
4	D	207	GLU
5	E	29	VAL
5	E	61	LYS
5	E	101[A]	ARG
5	E	101[B]	ARG
5	E	180	MET
5	E	181	GLU
5	E	189	LYS

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Mol	Chain	Res	Type
6	F	17	ASP
6	F	28	LYS
6	F	53	VAL
6	F	81	LEU
6	F	86	SER
6	F	87	LEU
6	F	174	THR
6	F	187	ARG
6	F	190	VAL
6	F	240	LYS
6	F	243	LEU
6	F	244	LYS
7	G	42	VAL
7	G	78	CYS
7	G	88	ARG
7	G	150	GLN
7	G	183	VAL
7	G	190	THR
7	G	206	LEU
7	G	226	LYS
8	H	6	VAL
8	H	12	ILE
8	H	65	LEU
8	H	68	LEU
8	H	132	LEU
8	H	183	LEU
8	H	199	LEU
8	H	215	LYS
8	H	220	GLU
9	I	35	THR
9	I	69	ARG
10	J	1[A]	MET
10	J	1[B]	MET
10	J	62	LYS
10	J	88	LEU
10	J	95	ARG
10	J	102	LEU
10	J	155	ARG
11	K	12	VAL
11	K	41	LEU
11	K	42	LEU
11	K	138	VAL

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Mol	Chain	Res	Type
11	K	147	LEU
11	K	158	ARG
11	K	174	VAL
11	K	187	VAL
12	L	3[A]	SER
12	L	3[B]	SER
12	L	81	LYS
12	L	161	VAL
12	L	169	ASP
12	L	172	MET
12	L	174	LEU
12	L	207	THR
13	M	154	LEU
13	M	206	GLU
14	N	22	THR
14	N	35	THR
14	N	196	LYS
1	O	10	THR
1	O	53	SER
1	O	73	LEU
1	O	131	VAL
1	O	181	LEU
1	O	189	THR
1	O	206	ASN
1	O	223	THR
1	O	226	LYS
2	P	7[A]	SER
2	P	7[B]	SER
2	P	33	THR
2	P	43	VAL
2	P	59	VAL
2	P	124	PHE
2	P	190	LEU
2	P	204	SER
2	P	235	GLN
2	P	246	LYS
2	P	249	ARG
3	Q	45	VAL
3	Q	56	GLU
3	Q	98	VAL
3	Q	105	GLU
3	Q	148	ASP

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Mol	Chain	Res	Type
3	Q	170	GLU
3	Q	183	THR
3	Q	197	GLU
3	Q	206	ILE
3	Q	208	LEU
3	Q	225	ILE
3	Q	227	LYS
4	R	32	LYS
4	R	46	VAL
5	S	3	ARG
5	S	29	VAL
5	S	45	VAL
5	S	101	ARG
5	S	180	MET
5	S	202	GLU
6	T	17	ASP
6	T	53	VAL
6	T	81	LEU
6	T	86	SER
6	T	87	LEU
6	T	174	THR
6	T	190	VAL
6	T	240	LYS
6	T	241	GLU
6	T	243	LEU
7	U	42	VAL
7	U	78	CYS
7	U	150	GLN
7	U	151	VAL
7	U	182	LYS
7	U	199	ILE
7	U	206	LEU
7	U	223	GLU
8	V	6	VAL
8	V	12	ILE
8	V	65	LEU
8	V	68	LEU
8	V	104[A]	ASP
8	V	104[B]	ASP
8	V	132	LEU
8	V	183	LEU
8	V	213	THR

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Mol	Chain	Res	Type
9	W	35	THR
9	W	69	ARG
9	W	193	LYS
10	X	1	MET
10	X	62	LYS
10	X	88	LEU
10	X	95	ARG
10	X	102	LEU
10	X	158	GLU
11	Y	12	VAL
11	Y	41	LEU
11	Y	138	VAL
11	Y	147	LEU
12	Z	73	LYS
12	Z	169	ASP
12	Z	172	MET
12	Z	174	LEU
12	Z	207	THR
12	Z	208	VAL
13	a	71	VAL
13	a	154	LEU
13	a	198	GLU
13	a	216	SER
14	b	22	THR
14	b	35	THR
14	b	145	GLU
14	b	196	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (66) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	51	GLN
1	A	62	HIS
1	A	94	GLN
1	A	108	GLN
1	A	206	ASN
2	B	40	ASN
2	B	102	GLN
2	B	142	HIS
2	B	146	GLN
3	C	175	ASN
5	E	8	ASN

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Mol	Chain	Res	Type
5	E	16	GLN
5	E	65	HIS
6	F	143	ASN
7	G	33	ASN
7	G	68	HIS
7	G	100	ASN
8	H	57	GLN
8	H	80	ASN
8	H	153	ASN
8	H	172	ASN
9	I	161	HIS
9	I	168	GLN
9	I	172	ASN
10	J	61	GLN
10	J	63	ASN
10	J	65	GLN
10	J	101	ASN
11	K	119	ASN
11	K	162	GLN
13	M	162	GLN
13	M	188	GLN
14	N	106	GLN
1	O	62	HIS
1	O	94	GLN
1	O	118	GLN
1	O	206	ASN
2	P	40	ASN
2	P	102	GLN
2	P	235	GLN
3	Q	18	GLN
3	Q	175	ASN
4	R	97	GLN
4	R	186	HIS
5	S	60	GLN
5	S	86	ASN
6	T	63	ASN
6	T	68	ASN
6	T	143	ASN
7	U	68	HIS
8	V	57	GLN
8	V	80	ASN
8	V	172	ASN

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Mol	Chain	Res	Type
9	W	168	GLN
10	X	24	ASN
10	X	61	GLN
10	X	63	ASN
10	X	65	GLN
10	X	174	ASN
11	Y	119	ASN
11	Y	162	GLN
12	Z	79	ASN
13	a	47	ASN
13	a	65	GLN
13	a	162	GLN
13	a	188	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

12 non-standard protein/DNA/RNA residues are modelled in this entry.

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	$\# Z > 2$
5	6V1	S	148	5	13,15,16	2.17	4 (30%)	10,20,22	3.23	6 (60%)
7	6V1	G	161	7	13,15,16	1.60	2 (15%)	10,20,22	2.15	5 (50%)
3	YCM	C	63	3	7,9,10	0.87	0	5,10,12	1.04	0
3	YCM	Q	63	3	7,9,10	1.30	1 (14%)	5,10,12	3.08	4 (80%)
7	YCM	G	137	7	7,9,10	1.71	1 (14%)	5,10,12	2.04	2 (40%)
7	6V1	G	47	7	13,15,16	2.23	3 (23%)	10,20,22	1.69	2 (20%)
7	6V1	U	47	7	13,15,16	2.04	4 (30%)	10,20,22	2.49	4 (40%)
7	6V1	U	161	7	13,15,16	1.56	2 (15%)	10,20,22	2.31	4 (40%)
10	6V1	X	91	10	13,15,16	1.70	2 (15%)	10,20,22	4.47	6 (60%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	6V1	E	148	5	13,15,16	2.06	3 (23%)	10,20,22	2.95	5 (50%)
10	6V1	J	91	10	13,15,16	2.21	3 (23%)	10,20,22	3.91	6 (60%)
7	YCM	U	137	7	7,9,10	1.12	1 (14%)	5,10,12	1.20	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	6V1	S	148	5	-	0/6/25/27	0/1/1/1
7	6V1	G	161	7	-	1/6/25/27	0/1/1/1
3	YCM	C	63	3	-	0/6/8/10	-
3	YCM	Q	63	3	-	4/6/8/10	-
7	YCM	G	137	7	-	2/6/8/10	-
7	6V1	G	47	7	-	1/6/25/27	0/1/1/1
7	6V1	U	47	7	1/1/5/6	0/6/25/27	0/1/1/1
7	6V1	U	161	7	-	1/6/25/27	0/1/1/1
10	6V1	X	91	10	-	2/6/25/27	0/1/1/1
5	6V1	E	148	5	-	2/6/25/27	0/1/1/1
10	6V1	J	91	10	-	2/6/25/27	0/1/1/1
7	YCM	U	137	7	-	2/6/8/10	-

All (26) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	J	91	6V1	C1-SG	-6.57	1.76	1.83
7	G	47	6V1	CB-SG	-6.44	1.75	1.82
5	S	148	6V1	CB-SG	-6.05	1.76	1.82
5	E	148	6V1	CB-SG	-5.48	1.76	1.82
7	U	47	6V1	CB-SG	-5.00	1.77	1.82
10	X	91	6V1	C1-SG	-4.67	1.78	1.83
7	G	47	6V1	C4-N3	-3.40	1.33	1.38
7	G	161	6V1	C2-N3	-3.35	1.34	1.38
7	U	47	6V1	C1-SG	-3.29	1.79	1.83
5	E	148	6V1	C2-N3	-3.28	1.34	1.38
7	G	137	YCM	CB-SG	-3.26	1.68	1.81
5	S	148	6V1	C2-N3	-3.23	1.34	1.38
7	U	161	6V1	CB-SG	-3.21	1.78	1.82
7	G	161	6V1	CB-SG	-3.12	1.79	1.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	U	47	6V1	C2-N3	-2.85	1.34	1.38
7	G	47	6V1	C2-N3	-2.75	1.35	1.38
3	Q	63	YCM	CD-SG	-2.70	1.74	1.81
10	J	91	6V1	C4-N3	-2.68	1.34	1.38
5	S	148	6V1	C4-N3	-2.64	1.34	1.38
7	U	47	6V1	C4-N3	-2.59	1.34	1.38
10	X	91	6V1	C4-N3	-2.42	1.35	1.38
5	E	148	6V1	C1-SG	-2.39	1.80	1.83
7	U	137	YCM	CB-SG	-2.27	1.72	1.81
10	J	91	6V1	CB-SG	-2.25	1.79	1.82
7	U	161	6V1	C2-N3	-2.24	1.35	1.38
5	S	148	6V1	C5-C4	2.21	1.54	1.50

All (44) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	X	91	6V1	C5-C4-N3	8.12	113.18	108.07
10	J	91	6V1	C5-C4-N3	7.42	112.74	108.07
10	X	91	6V1	C2-N3-C4	-6.82	109.08	113.07
5	E	148	6V1	C5-C4-N3	6.78	112.34	108.07
5	S	148	6V1	C2-N3-C4	-6.11	109.49	113.07
10	X	91	6V1	O7-C2-N3	5.86	131.24	124.14
10	J	91	6V1	O7-C2-N3	5.73	131.09	124.14
5	S	148	6V1	C5-C4-N3	5.65	111.63	108.07
10	J	91	6V1	C2-N3-C4	-5.22	110.01	113.07
10	X	91	6V1	C6-N3-C2	5.04	129.27	123.37
7	U	47	6V1	C2-N3-C4	-4.94	110.18	113.07
3	Q	63	YCM	CE-CD-SG	-4.66	99.08	113.81
10	J	91	6V1	C6-N3-C2	4.50	128.64	123.37
7	U	47	6V1	C5-C4-N3	4.40	110.84	108.07
7	U	161	6V1	O8-C4-N3	4.21	128.46	123.94
5	E	148	6V1	C2-N3-C4	-4.03	110.71	113.07
5	S	148	6V1	C6-N3-C4	4.02	127.27	122.52
10	X	91	6V1	O8-C4-C5	-3.88	121.60	127.28
7	G	137	YCM	CE-CD-SG	3.60	125.19	113.81
7	U	161	6V1	O8-C4-C5	-3.44	122.24	127.28
7	U	161	6V1	C2-N3-C4	-3.42	111.07	113.07
3	Q	63	YCM	CA-CB-SG	-3.39	101.00	113.51
7	G	47	6V1	C2-N3-C4	-3.33	111.12	113.07
7	G	47	6V1	C5-C4-N3	3.17	110.06	108.07
7	G	161	6V1	C6-N3-C2	3.12	127.03	123.37
10	X	91	6V1	O7-C2-C1	-3.09	117.79	124.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	G	161	6V1	O8-C4-N3	3.07	127.23	123.94
10	J	91	6V1	O8-C4-C5	-3.07	122.79	127.28
3	Q	63	YCM	CB-SG-CD	3.03	131.27	104.24
5	E	148	6V1	C6-N3-C2	2.90	126.77	123.37
5	S	148	6V1	CB-CA-C	-2.81	103.17	110.80
7	U	161	6V1	C6-N3-C4	2.74	125.76	122.52
5	E	148	6V1	O8-C4-C5	-2.61	123.46	127.28
7	G	161	6V1	O8-C4-C5	-2.57	123.53	127.28
7	U	47	6V1	O8-C4-C5	-2.56	123.53	127.28
7	G	161	6V1	C3-C6-N3	-2.50	103.08	111.66
10	J	91	6V1	O7-C2-C1	-2.40	119.29	124.52
5	E	148	6V1	CB-CA-C	-2.35	104.42	110.80
7	G	161	6V1	O7-C2-N3	2.33	126.97	124.14
7	U	47	6V1	C6-N3-C2	2.24	126.00	123.37
5	S	148	6V1	O8-C4-C5	-2.12	124.18	127.28
5	S	148	6V1	O7-C2-N3	-2.09	121.61	124.14
3	Q	63	YCM	CB-CA-C	-2.07	105.18	110.80
7	G	137	YCM	CA-CB-SG	-2.00	106.14	113.51

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
7	U	47	6V1	C1

All (17) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	G	137	YCM	SG-CD-CE-NZ2
10	J	91	6V1	C3-C6-N3-C2
10	J	91	6V1	C3-C6-N3-C4
3	Q	63	YCM	CE-CD-SG-CB
3	Q	63	YCM	SG-CD-CE-OZ1
3	Q	63	YCM	SG-CD-CE-NZ2
10	X	91	6V1	C3-C6-N3-C2
10	X	91	6V1	C3-C6-N3-C4
5	E	148	6V1	C3-C6-N3-C2
5	E	148	6V1	C3-C6-N3-C4
7	G	137	YCM	CE-CD-SG-CB
7	U	137	YCM	CE-CD-SG-CB
7	G	47	6V1	C5-C1-SG-CB
7	G	161	6V1	N-CA-CB-SG
7	U	161	6V1	N-CA-CB-SG

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Mol	Chain	Res	Type	Atoms
3	Q	63	YCM	CA-CB-SG-CD
7	U	137	YCM	SG-CD-CE-NZ2

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	Q	63	YCM	2	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 82 ligands modelled in this entry, 67 are monoatomic - leaving 15 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	$\# Z > 2$
18	1PE	L	301	-	15,15,15	0.56	0	14,14,14	0.67	0
18	1PE	W	303	-	15,15,15	0.58	0	14,14,14	0.38	0
19	BO2	V	303	8	25,29,29	0.80	0	33,38,38	1.50	2 (6%)
19	BO2	K	305	11	25,29,29	0.70	0	33,38,38	1.26	4 (12%)
19	BO2	N	304	14	25,29,29	0.96	0	33,38,38	1.78	9 (27%)
18	1PE	Z	301	-	15,15,15	0.58	0	14,14,14	0.45	0
18	1PE	H	304	-	15,15,15	0.51	0	14,14,14	0.52	0
18	1PE	b	303	-	15,15,15	0.61	0	14,14,14	0.65	0
18	1PE	H	305	-	15,15,15	0.56	0	14,14,14	0.38	0
19	BO2	H	306	8	25,29,29	1.11	1 (4%)	33,38,38	1.22	1 (3%)
18	1PE	I	304	-	15,15,15	0.52	0	14,14,14	0.44	0
18	1PE	I	303	-	15,15,15	0.55	0	14,14,14	0.85	1 (7%)
19	BO2	b	305	14	25,29,29	0.93	1 (4%)	33,38,38	1.35	5 (15%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
19	BO2	Y	305	11	25,29,29	0.73	1 (4%)	33,38,38	1.15	1 (3%)
18	1PE	M	305	-	15,15,15	0.53	0	14,14,14	0.32	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
18	1PE	L	301	-	-	6/13/13/13	-
18	1PE	W	303	-	-	9/13/13/13	-
19	BO2	V	303	8	-	5/23/28/28	0/2/2/2
19	BO2	K	305	11	-	3/23/28/28	0/2/2/2
19	BO2	N	304	14	-	0/23/28/28	0/2/2/2
18	1PE	Z	301	-	-	6/13/13/13	-
18	1PE	H	304	-	-	7/13/13/13	-
18	1PE	b	303	-	-	5/13/13/13	-
18	1PE	H	305	-	-	4/13/13/13	-
19	BO2	H	306	8	-	5/23/28/28	0/2/2/2
18	1PE	I	304	-	-	10/13/13/13	-
18	1PE	I	303	-	-	6/13/13/13	-
19	BO2	b	305	14	-	0/23/28/28	0/2/2/2
19	BO2	Y	305	11	-	3/23/28/28	0/2/2/2
18	1PE	M	305	-	-	6/13/13/13	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	H	306	BO2	C11-C10	-2.28	1.48	1.54
19	Y	305	BO2	C16-C17	2.17	1.42	1.38
19	b	305	BO2	C15-C14	2.04	1.42	1.38

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	V	303	BO2	C7-C2-N1	5.02	123.29	117.42
19	N	304	BO2	C6-N1-C2	4.66	122.94	116.93
19	H	306	BO2	C7-C2-N1	4.26	122.39	117.42
19	N	304	BO2	C3-C2-N1	-3.55	117.42	121.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	K	305	BO2	C7-C2-N1	3.38	121.37	117.42
19	N	304	BO2	C5-N4-C3	3.18	122.43	116.85
19	b	305	BO2	C6-C5-N4	-3.03	118.19	121.96
19	K	305	BO2	C2-C3-N4	-3.02	118.01	121.97
19	N	304	BO2	C2-C7-N9	2.88	120.73	115.19
19	N	304	BO2	C6-C5-N4	-2.88	118.38	121.96
19	b	305	BO2	C5-N4-C3	2.58	121.37	116.85
19	K	305	BO2	C5-N4-C3	2.55	121.31	116.85
19	N	304	BO2	O8-C7-C2	-2.53	115.50	121.08
19	N	304	BO2	C7-C2-N1	2.48	120.31	117.42
19	V	303	BO2	C15-C16-C17	-2.47	117.19	120.24
19	b	305	BO2	C7-C2-N1	2.46	120.30	117.42
19	b	305	BO2	C3-C2-N1	-2.41	118.76	121.60
19	Y	305	BO2	C7-C2-N1	2.36	120.18	117.42
19	K	305	BO2	C3-C2-C7	-2.35	116.71	119.71
19	b	305	BO2	B26-C21-C22	-2.26	108.04	112.31
19	N	304	BO2	B26-C21-C22	-2.08	108.39	112.31
18	I	303	1PE	C25-OH5-C14	2.06	122.27	113.26
19	N	304	BO2	C5-C6-N1	-2.06	119.29	122.19

There are no chirality outliers.

All (75) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
19	H	306	BO2	N1-C2-C7-N9
19	H	306	BO2	C3-C2-C7-O8
19	H	306	BO2	C3-C2-C7-N9
19	V	303	BO2	C3-C2-C7-O8
19	V	303	BO2	C3-C2-C7-N9
19	H	306	BO2	N1-C2-C7-O8
19	V	303	BO2	N1-C2-C7-O8
19	V	303	BO2	N1-C2-C7-N9
18	b	303	1PE	C24-C14-OH5-C25
18	W	303	1PE	OH6-C15-C25-OH5
18	Z	301	1PE	OH6-C15-C25-OH5
18	L	301	1PE	C16-C26-OH6-C15
18	M	305	1PE	OH5-C14-C24-OH4
18	b	303	1PE	OH4-C13-C23-OH3
18	H	305	1PE	OH4-C13-C23-OH3
18	I	303	1PE	OH6-C15-C25-OH5
18	L	301	1PE	OH5-C14-C24-OH4
18	L	301	1PE	OH6-C15-C25-OH5

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Mol	Chain	Res	Type	Atoms
18	W	303	1PE	OH2-C12-C22-OH3
18	H	305	1PE	OH5-C14-C24-OH4
18	H	304	1PE	OH4-C13-C23-OH3
19	K	305	BO2	C3-C2-C7-N9
19	Y	305	BO2	C3-C2-C7-N9
18	I	304	1PE	OH4-C13-C23-OH3
18	H	304	1PE	OH2-C12-C22-OH3
18	I	303	1PE	C15-C25-OH5-C14
18	M	305	1PE	OH6-C15-C25-OH5
18	W	303	1PE	OH7-C16-C26-OH6
18	Z	301	1PE	OH4-C13-C23-OH3
18	H	304	1PE	OH7-C16-C26-OH6
18	I	304	1PE	C24-C14-OH5-C25
18	Z	301	1PE	C16-C26-OH6-C15
18	L	301	1PE	OH2-C12-C22-OH3
18	H	305	1PE	OH2-C12-C22-OH3
18	I	303	1PE	OH2-C12-C22-OH3
18	L	301	1PE	C25-C15-OH6-C26
19	V	303	BO2	C21-C22-C23-C24
18	W	303	1PE	C12-C22-OH3-C23
18	W	303	1PE	C24-C14-OH5-C25
18	L	301	1PE	C13-C23-OH3-C22
18	W	303	1PE	C23-C13-OH4-C24
18	b	303	1PE	OH2-C12-C22-OH3
18	I	304	1PE	C16-C26-OH6-C15
18	I	304	1PE	C23-C13-OH4-C24
18	I	303	1PE	C24-C14-OH5-C25
18	I	304	1PE	OH6-C15-C25-OH5
18	b	303	1PE	OH7-C16-C26-OH6
18	H	305	1PE	OH7-C16-C26-OH6
18	M	305	1PE	C23-C13-OH4-C24
18	I	304	1PE	OH7-C16-C26-OH6
18	I	303	1PE	C12-C22-OH3-C23
18	Z	301	1PE	C23-C13-OH4-C24
18	I	304	1PE	C13-C23-OH3-C22
18	M	305	1PE	OH4-C13-C23-OH3
18	H	304	1PE	C13-C23-OH3-C22
18	I	303	1PE	OH5-C14-C24-OH4
18	b	303	1PE	OH5-C14-C24-OH4
18	H	304	1PE	C12-C22-OH3-C23
19	H	306	BO2	C21-C22-C23-C24
19	K	305	BO2	C21-C22-C23-C24

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Mol	Chain	Res	Type	Atoms
19	Y	305	BO2	C21-C22-C23-C24
18	Z	301	1PE	C12-C22-OH3-C23
18	W	303	1PE	C13-C23-OH3-C22
18	H	304	1PE	C16-C26-OH6-C15
18	Z	301	1PE	OH2-C12-C22-OH3
19	K	305	BO2	C3-C2-C7-O8
18	W	303	1PE	C14-C24-OH4-C13
18	I	304	1PE	C12-C22-OH3-C23
18	M	305	1PE	C12-C22-OH3-C23
18	H	304	1PE	C25-C15-OH6-C26
18	W	303	1PE	C25-C15-OH6-C26
18	I	304	1PE	C15-C25-OH5-C14
18	M	305	1PE	OH7-C16-C26-OH6
19	Y	305	BO2	C3-C2-C7-O8
18	I	304	1PE	OH5-C14-C24-OH4

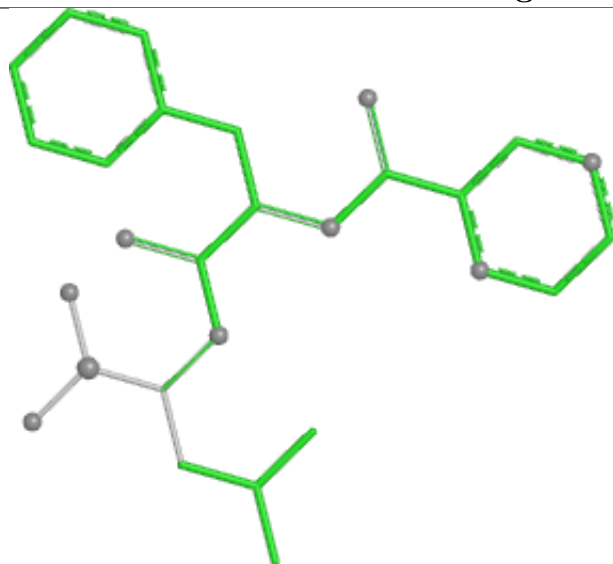
There are no ring outliers.

3 monomers are involved in 3 short contacts:

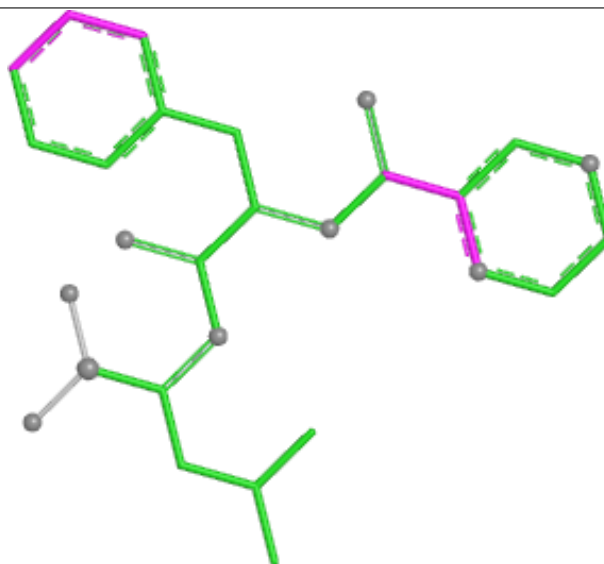
Mol	Chain	Res	Type	Clashes	Symm-Clashes
19	N	304	BO2	1	0
19	H	306	BO2	1	0
19	b	305	BO2	1	0

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

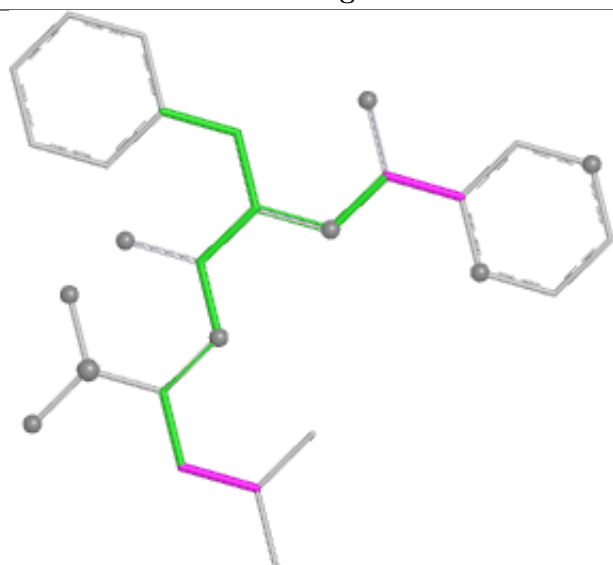
Ligand BO2 V 303



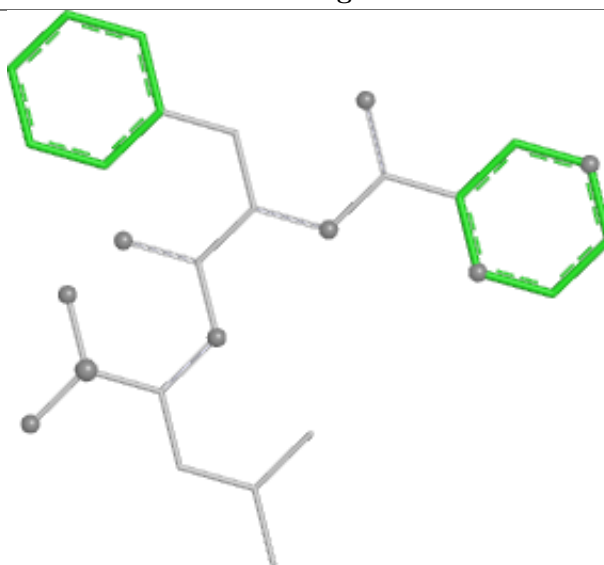
Bond lengths



Bond angles

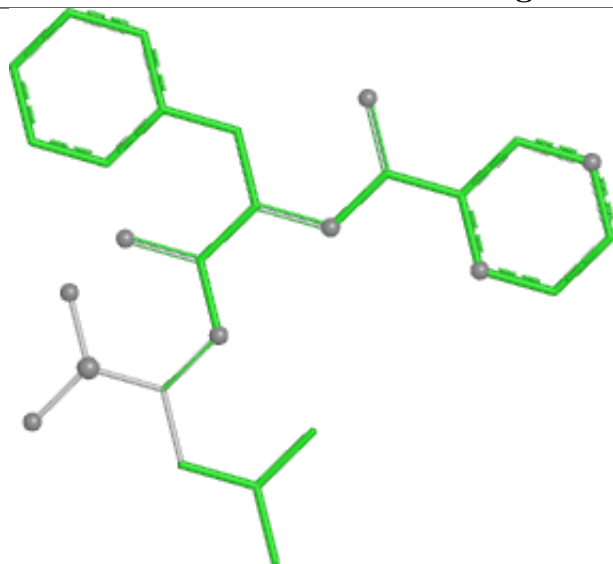


Torsions

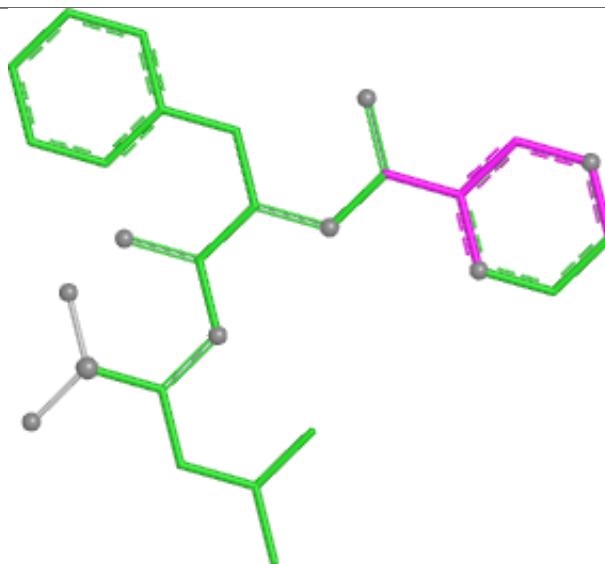


Rings

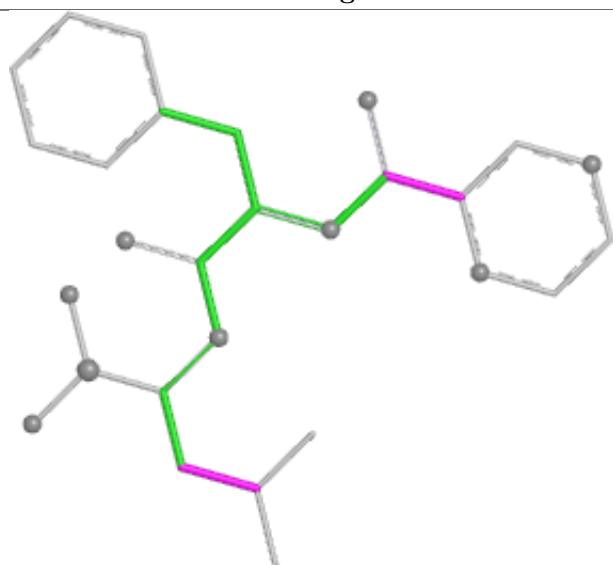
Ligand BO2 K 305



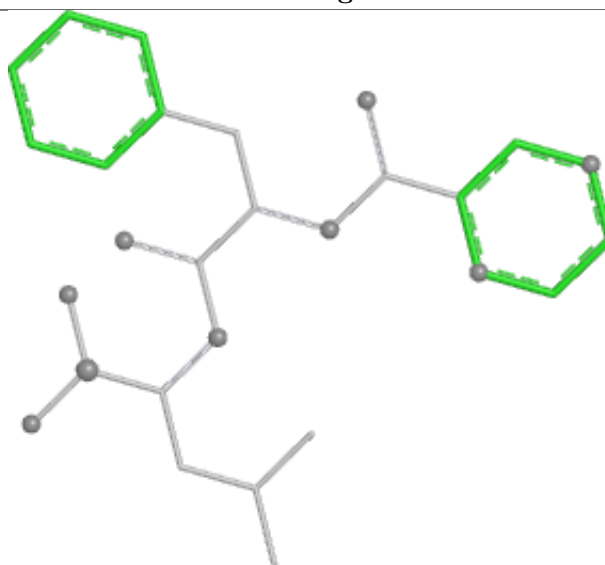
Bond lengths



Bond angles

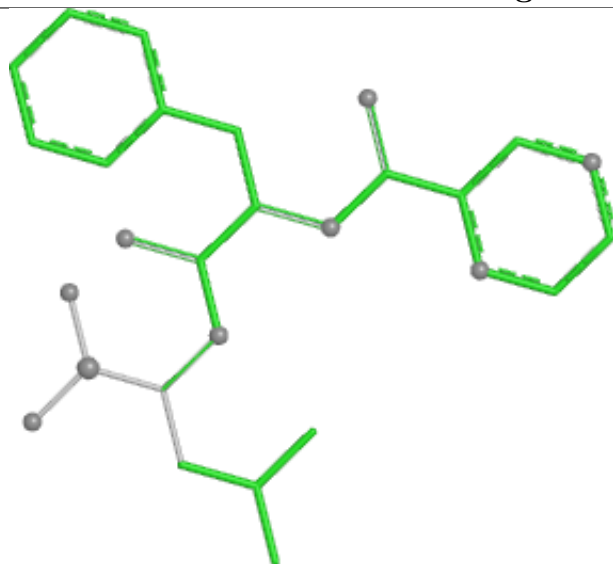


Torsions

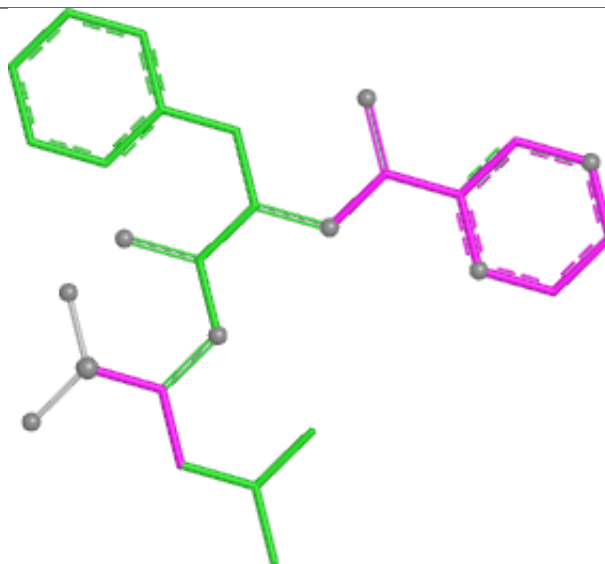


Rings

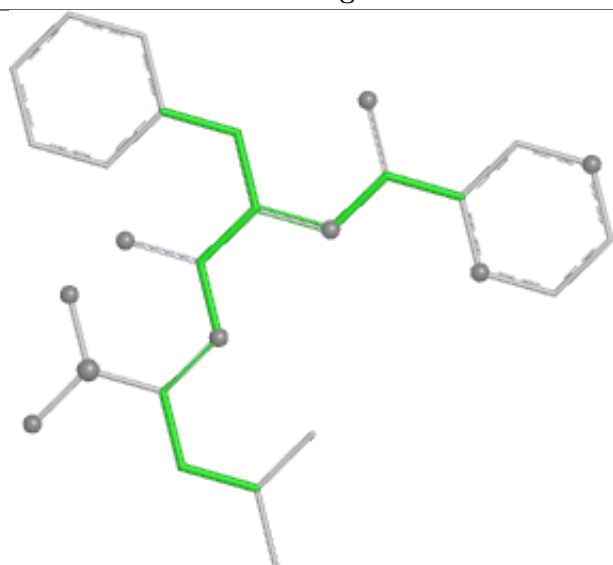
Ligand BO2 N 304



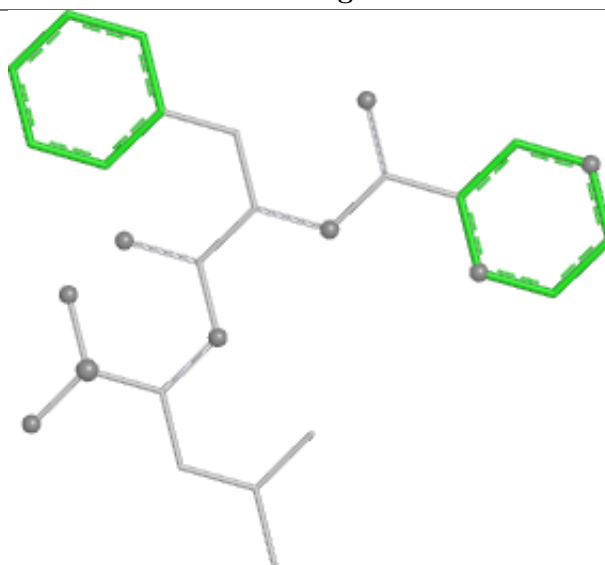
Bond lengths



Bond angles

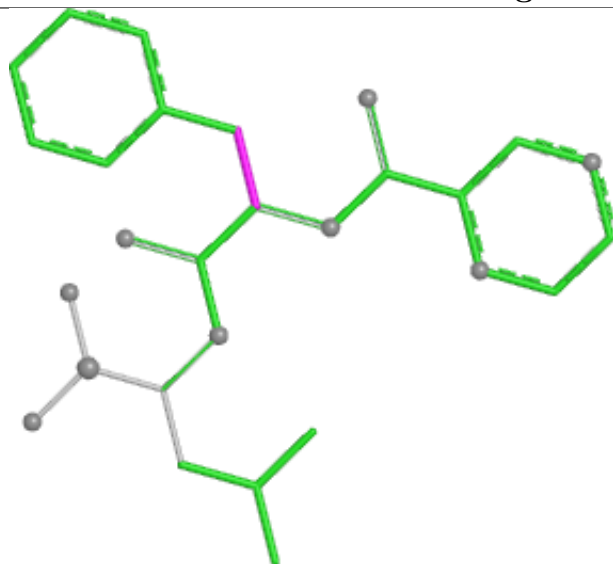


Torsions

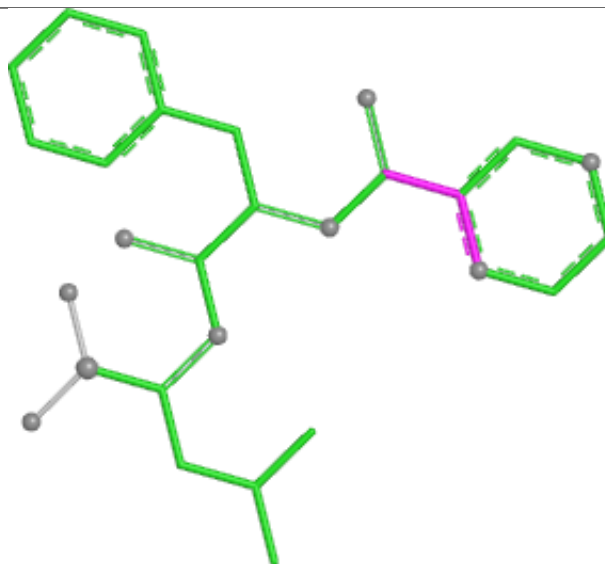


Rings

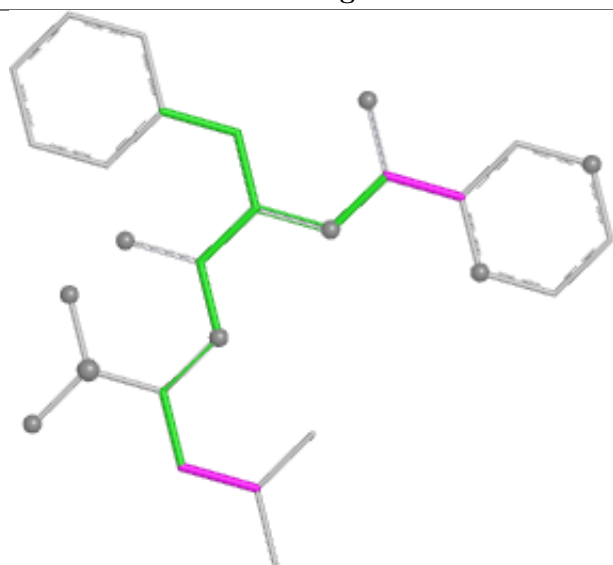
Ligand BO2 H 306



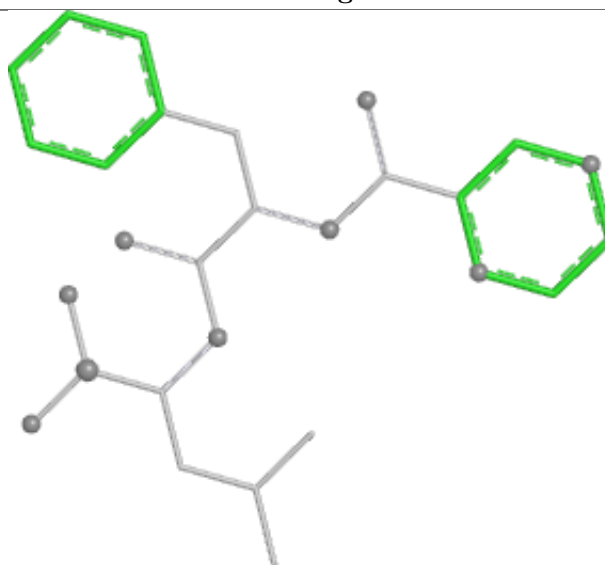
Bond lengths



Bond angles

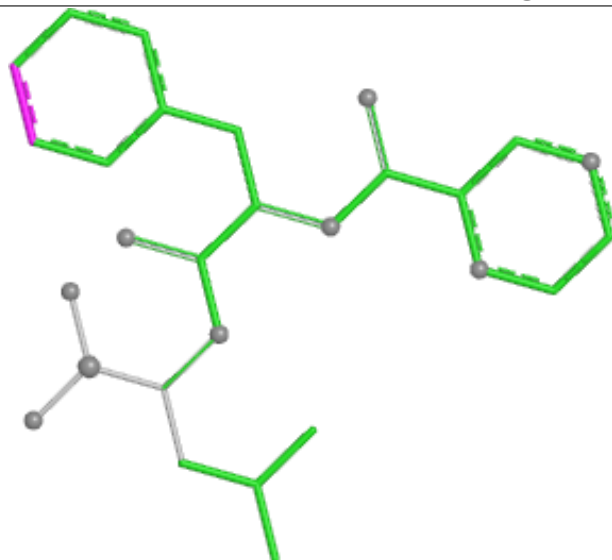


Torsions

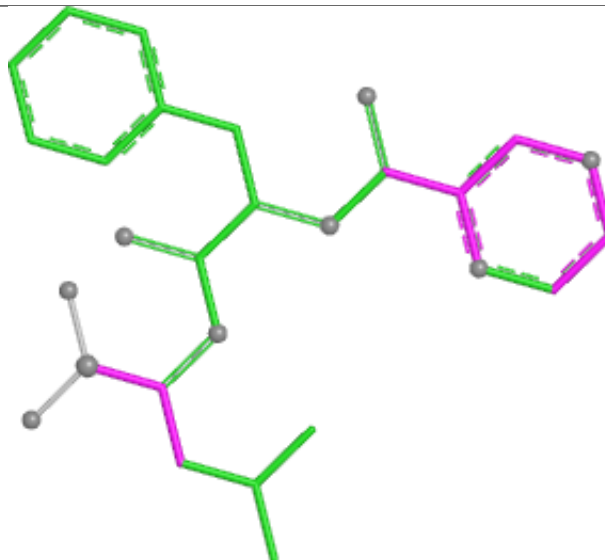


Rings

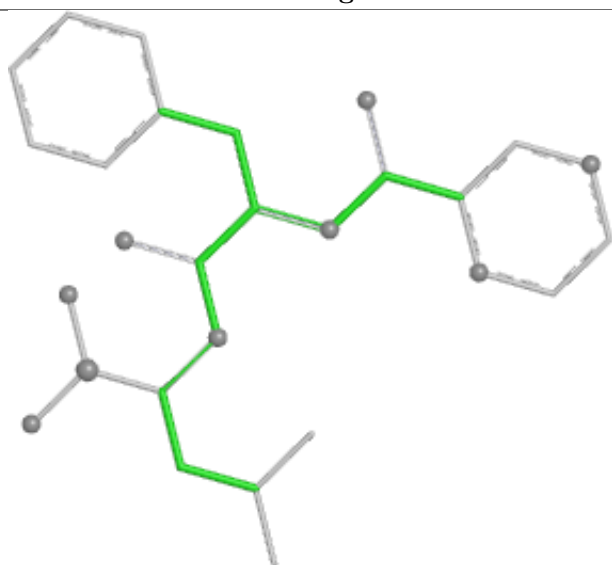
Ligand BO2 b 305



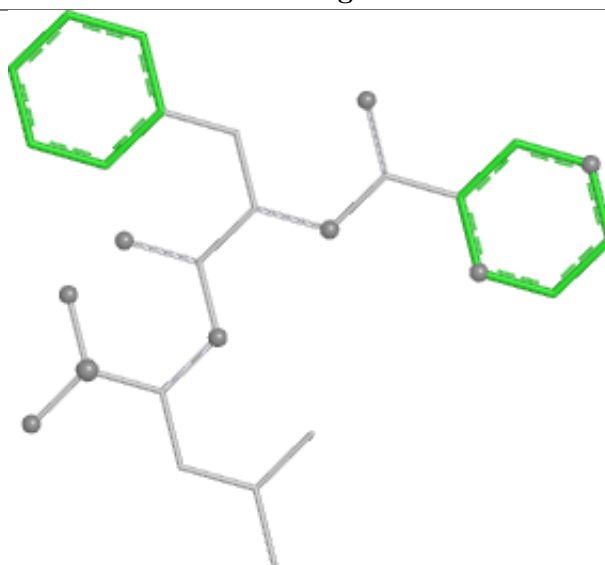
Bond lengths



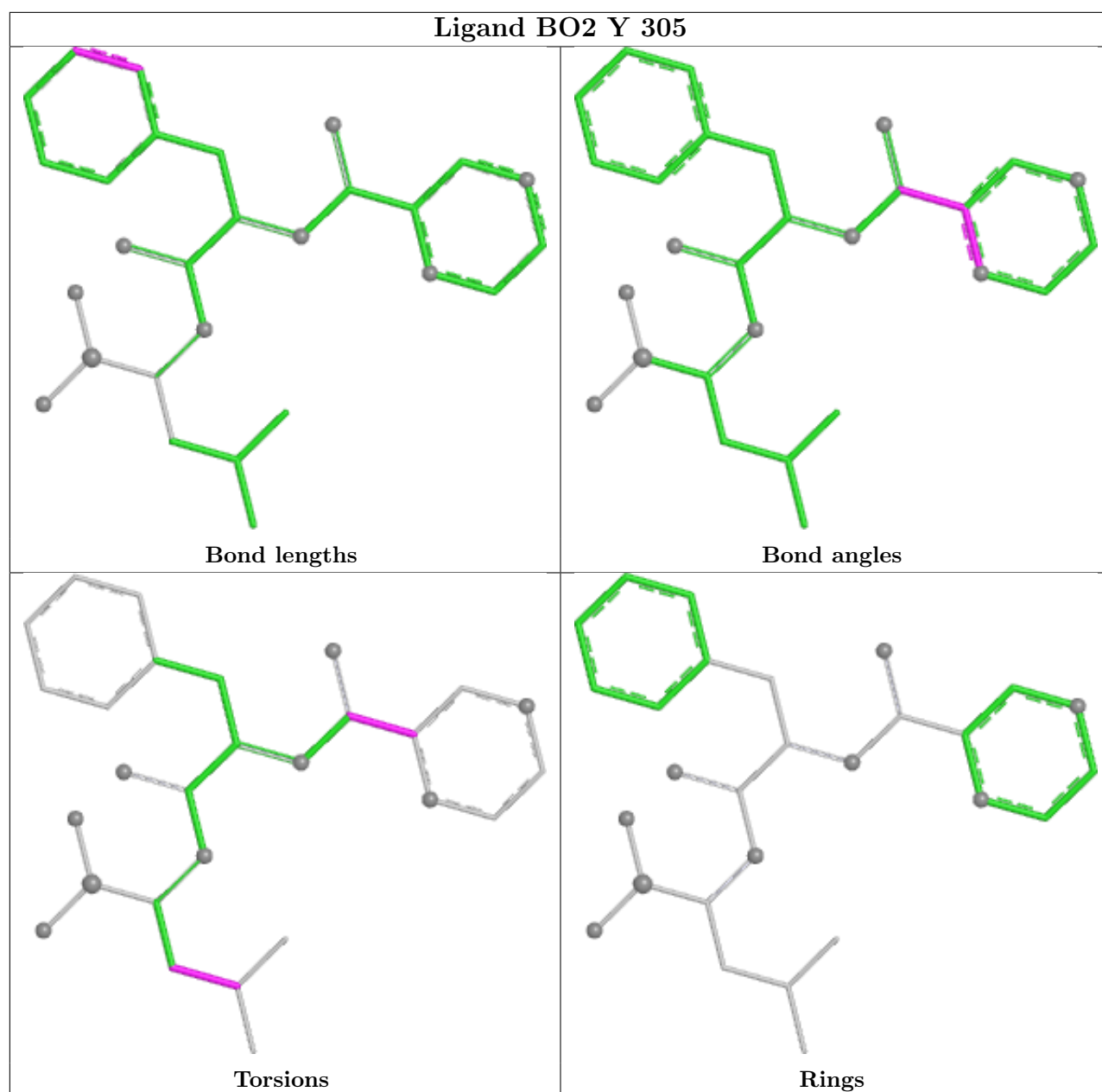
Bond angles



Torsions



Rings



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	230/234 (98%)	-0.08	4 (1%) 69 71	24, 46, 82, 94	3 (1%)
1	O	230/234 (98%)	0.56	15 (6%) 25 26	43, 63, 103, 122	0
2	B	248/261 (95%)	0.11	5 (2%) 65 67	21, 52, 94, 132	2 (0%)
2	P	248/261 (95%)	0.27	7 (2%) 55 57	34, 57, 100, 142	2 (0%)
3	C	236/248 (95%)	0.38	6 (2%) 58 61	27, 62, 101, 125	2 (0%)
3	Q	238/248 (95%)	0.56	17 (7%) 22 23	38, 66, 116, 153	0
4	D	233/241 (96%)	0.31	5 (2%) 63 66	31, 57, 85, 118	1 (0%)
4	R	233/241 (96%)	0.13	8 (3%) 48 50	22, 47, 75, 97	1 (0%)
5	E	233/263 (88%)	-0.02	9 (3%) 43 45	26, 43, 89, 116	1 (0%)
5	S	237/263 (90%)	0.15	9 (3%) 44 46	24, 51, 89, 114	3 (1%)
6	F	239/255 (93%)	-0.33	0 100 100	20, 37, 59, 74	4 (1%)
6	T	240/255 (94%)	0.46	8 (3%) 49 51	32, 60, 90, 114	1 (0%)
7	G	241/246 (97%)	-0.16	2 (0%) 82 84	21, 42, 74, 108	2 (0%)
7	U	235/246 (95%)	0.45	7 (2%) 52 55	33, 68, 100, 131	1 (0%)
8	H	220/234 (94%)	-0.25	3 (1%) 73 75	21, 38, 69, 109	2 (0%)
8	V	220/234 (94%)	0.07	5 (2%) 61 64	25, 49, 79, 105	2 (0%)
9	I	204/205 (99%)	-0.38	0 100 100	21, 38, 58, 76	3 (1%)
9	W	204/205 (99%)	-0.05	0 100 100	26, 47, 70, 77	2 (0%)
10	J	195/201 (97%)	-0.25	1 (0%) 87 88	17, 43, 60, 75	3 (1%)
10	X	195/201 (97%)	-0.17	1 (0%) 87 88	20, 43, 58, 73	2 (1%)
11	K	200/204 (98%)	-0.16	1 (0%) 87 88	24, 44, 69, 81	1 (0%)
11	Y	201/204 (98%)	-0.27	4 (1%) 65 67	21, 39, 63, 80	3 (1%)
12	L	213/213 (100%)	-0.18	0 100 100	25, 45, 68, 82	2 (0%)
12	Z	213/213 (100%)	-0.38	0 100 100	28, 39, 61, 73	1 (0%)

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å ²)	Q<0.9
13	M	216/219 (98%)	-0.32	1 (0%)	87 88	28, 41, 64, 90	1 (0%)
13	a	216/219 (98%)	-0.20	2 (0%)	81 83	27, 42, 64, 83	2 (0%)
14	N	202/205 (98%)	-0.39	2 (0%)	79 81	21, 38, 57, 87	1 (0%)
14	b	203/205 (99%)	-0.15	1 (0%)	87 88	34, 46, 72, 101	1 (0%)
All	All	6223/6458 (96%)	0.00	123 (1%)	65 67	17, 47, 87, 153	49 (0%)

All (123) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
11	K	40	TYR	5.1
11	Y	201	GLY	4.6
5	S	57	ALA	4.4
8	V	204	CYS	4.3
11	Y	40	TYR	4.3
5	E	56	LEU	4.1
5	E	54	SER	4.0
5	E	59	HIS	3.8
5	E	57	ALA	3.7
5	S	2	PHE	3.7
13	a	216	SER	3.5
7	U	186	LYS	3.5
5	S	56	LEU	3.4
2	P	203	VAL	3.4
6	T	208	ALA	3.4
8	H	204	CYS	3.4
2	P	61	PHE	3.3
4	D	241	ILE	3.3
1	A	231	ALA	3.2
3	Q	50	VAL	3.2
4	R	241	ILE	3.2
5	E	58	ALA	3.1
3	Q	53	LEU	3.1
1	O	232	ILE	3.1
1	O	188	HIS	3.1
13	a	215	ILE	3.1
4	R	130	PRO	3.0
2	P	124	PHE	3.0
1	O	231	ALA	2.9
3	Q	48	LYS	2.9
4	R	120[A]	ALA	2.9
4	R	128	ALA	2.9

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Mol	Chain	Res	Type	RSRZ
5	E	51	ARG	2.9
4	R	131	GLY	2.9
6	T	142	VAL	2.8
2	P	51	ASN	2.8
14	N	200	ALA	2.8
3	Q	203	GLY	2.8
6	T	6	GLY	2.8
2	B	202	ASP	2.8
3	Q	225	ILE	2.8
5	S	18[A]	ARG	2.7
1	A	3	ARG	2.7
14	b	199	VAL	2.7
1	O	230	ALA	2.7
6	T	204	VAL	2.7
3	Q	232	ILE	2.7
11	Y	200	SER	2.7
3	C	53	LEU	2.7
4	D	131	GLY	2.7
3	C	138	PHE	2.6
3	Q	202	GLY	2.6
6	T	5	THR	2.6
13	M	215	ILE	2.6
4	R	127	ASP	2.6
2	P	245	ALA	2.6
7	G	187	PHE	2.5
7	U	193	GLN	2.5
1	O	3	ARG	2.5
5	S	54	SER	2.5
7	G	189	TRP	2.5
3	Q	220	LEU	2.5
1	O	56	TYR	2.5
5	E	53	GLN	2.5
2	P	55	LEU	2.5
6	T	54	LEU	2.5
1	O	215	ALA	2.4
6	T	209	PHE	2.4
8	V	220	GLU	2.4
3	Q	196	LEU	2.4
8	V	199	LEU	2.4
4	R	54	ILE	2.4
3	Q	51	ALA	2.4
4	R	129	ASP	2.4

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Mol	Chain	Res	Type	RSRZ
3	Q	98	VAL	2.4
1	O	177	TYR	2.3
14	N	202	LEU	2.3
7	U	185	LYS	2.3
8	V	203	ARG	2.3
1	O	54	ILE	2.3
3	Q	206	ILE	2.3
3	Q	205	ASN	2.3
1	O	225	VAL	2.3
3	Q	59	VAL	2.3
2	B	2	SER	2.3
2	B	61	PHE	2.3
2	B	205	LYS	2.3
5	S	239	ARG	2.2
7	U	245	ARG	2.2
10	X	196	PHE	2.2
4	D	128	ALA	2.2
5	E	52	ALA	2.2
1	A	181	LEU	2.2
8	V	202	TYR	2.2
5	S	51	ARG	2.2
3	Q	47	LYS	2.2
1	O	189	THR	2.2
3	C	97	THR	2.2
3	Q	138	PHE	2.2
4	D	129	ASP	2.2
3	C	49	SER	2.2
10	J	1[A]	MET	2.2
8	H	202	TYR	2.1
1	O	51	GLN	2.1
11	Y	73	ARG	2.1
5	E	201	ALA	2.1
1	O	181	LEU	2.1
1	A	54	ILE	2.1
1	O	194	LEU	2.1
3	Q	49	SER	2.1
7	U	2	SER	2.1
5	S	53	GLN	2.1
8	H	197	THR	2.1
3	C	206	ILE	2.1
2	B	203	VAL	2.1
2	P	204	SER	2.1

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Mol	Chain	Res	Type	RSRZ
1	O	50	LYS	2.0
4	D	86	LYS	2.0
3	C	203	GLY	2.0
5	S	58	ALA	2.0
6	T	239	ALA	2.0
7	U	241	ALA	2.0
7	U	194	THR	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [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
7	6V1	U	47	15/16	0.84	0.16	82,108,112,115	0
7	YCM	G	137	10/11	0.89	0.13	35,43,60,61	0
7	YCM	U	137	10/11	0.89	0.12	57,65,83,84	0
3	YCM	C	63	10/11	0.90	0.11	55,60,68,69	0
7	6V1	U	161	15/16	0.92	0.12	58,72,79,80	0
7	6V1	G	47	15/16	0.93	0.10	42,58,60,61	0
5	6V1	E	148	15/16	0.93	0.11	32,51,59,59	0
5	6V1	S	148	15/16	0.93	0.12	39,63,69,69	0
10	6V1	X	91	15/16	0.94	0.12	38,59,64,70	0
7	6V1	G	161	15/16	0.95	0.11	33,54,60,63	0
10	6V1	J	91	15/16	0.95	0.11	36,55,59,59	0
3	YCM	Q	63	10/11	0.96	0.07	54,57,66,68	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
18	1PE	I	304	16/16	0.82	0.16	62,76,88,88	0
15	CL	Q	301	1/1	0.83	0.16	78,78,78,78	0
18	1PE	M	305	16/16	0.85	0.14	75,80,95,96	0
15	CL	O	304	1/1	0.87	0.18	70,70,70,70	0
15	CL	D	301	1/1	0.88	0.18	73,73,73,73	0
18	1PE	H	305	16/16	0.88	0.14	65,69,89,90	0
18	1PE	W	303	16/16	0.88	0.13	56,63,79,79	0
18	1PE	b	303	16/16	0.89	0.13	52,59,77,78	0
19	BO2	V	303	28/28	0.89	0.12	49,54,66,67	0
18	1PE	Z	301	16/16	0.90	0.14	57,71,80,80	0
15	CL	O	303	1/1	0.90	0.10	87,87,87,87	0
19	BO2	H	306	28/28	0.90	0.11	38,45,67,67	0
15	CL	Q	302	1/1	0.90	0.23	70,70,70,70	0
15	CL	C	302	1/1	0.91	0.16	69,69,69,69	0
18	1PE	I	303	16/16	0.91	0.11	56,60,68,72	0
15	CL	S	301	1/1	0.91	0.24	75,75,75,75	0
18	1PE	L	301	16/16	0.91	0.13	55,70,75,76	0
15	CL	S	302	1/1	0.91	0.15	69,69,69,69	0
15	CL	O	302	1/1	0.92	0.17	60,60,60,60	0
15	CL	Y	304	1/1	0.92	0.21	70,70,70,70	0
15	CL	K	304	1/1	0.92	0.18	71,71,71,71	0
15	CL	R	302	1/1	0.93	0.28	58,58,58,58	0
15	CL	C	301	1/1	0.93	0.12	66,66,66,66	0
15	CL	D	302	1/1	0.93	0.12	65,65,65,65	0
15	CL	V	302	1/1	0.93	0.16	60,60,60,60	0
15	CL	K	303	1/1	0.93	0.17	68,68,68,68	0
15	CL	G	302	1/1	0.94	0.09	62,62,62,62	0
15	CL	a	303	1/1	0.94	0.10	66,66,66,66	0
17	MG	I	301	1/1	0.94	0.11	37,37,37,37	0
18	1PE	H	304	16/16	0.94	0.09	46,51,64,67	0
15	CL	A	302	1/1	0.94	0.09	69,69,69,69	0
15	CL	S	303	1/1	0.94	0.15	61,61,61,61	0
19	BO2	N	304	28/28	0.94	0.08	35,37,44,47	0
15	CL	B	302	1/1	0.94	0.21	62,62,62,62	0
19	BO2	b	305	28/28	0.94	0.09	37,43,53,55	0
15	CL	b	302	1/1	0.95	0.20	64,64,64,64	0
15	CL	K	302	1/1	0.95	0.13	74,74,74,74	0
15	CL	M	301	1/1	0.95	0.31	68,68,68,68	0
15	CL	a	302	1/1	0.95	0.13	49,49,49,49	0
15	CL	M	304	1/1	0.95	0.14	58,58,58,58	0
15	CL	Y	302	1/1	0.96	0.09	68,68,68,68	0
15	CL	Y	303	1/1	0.96	0.10	64,64,64,64	0
15	CL	E	301	1/1	0.96	0.12	65,65,65,65	0

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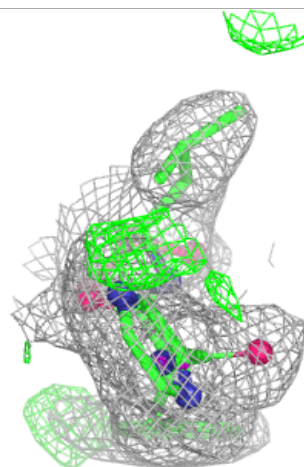
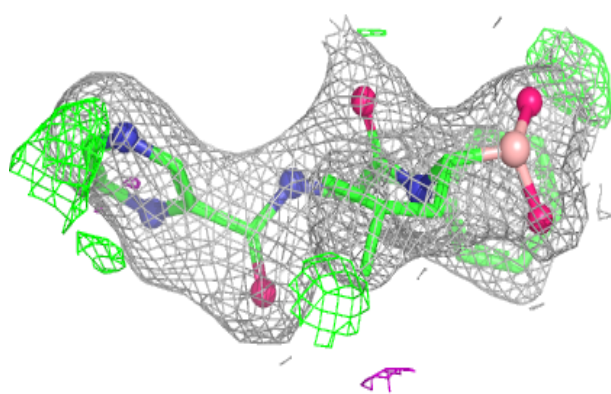
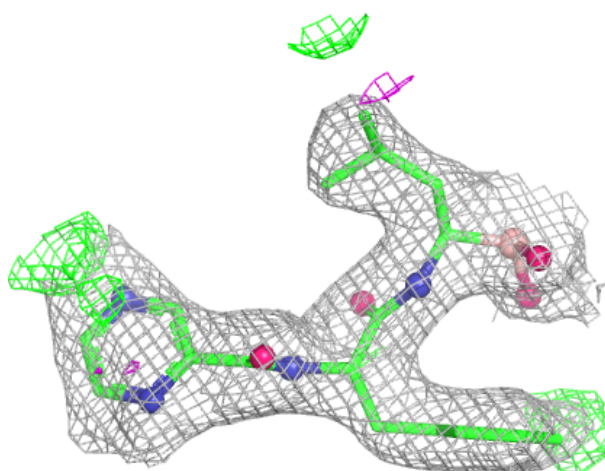
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
15	CL	a	301	1/1	0.96	0.14	67,67,67,67	0
15	CL	M	302	1/1	0.96	0.23	65,65,65,65	0
15	CL	E	303	1/1	0.96	0.14	60,60,60,60	0
15	CL	b	301	1/1	0.96	0.20	68,68,68,68	0
15	CL	A	304	1/1	0.96	0.17	59,59,59,59	0
16	K	L	302	1/1	0.96	0.11	49,49,49,49	0
16	K	b	304	1/1	0.96	0.15	46,46,46,46	0
15	CL	U	301	1/1	0.96	0.15	64,64,64,64	0
15	CL	R	301	1/1	0.96	0.12	61,61,61,61	0
17	MG	K	301	1/1	0.97	0.07	34,34,34,34	0
15	CL	I	302	1/1	0.97	0.07	44,44,44,44	0
15	CL	N	302	1/1	0.97	0.20	59,59,59,59	0
15	CL	E	302	1/1	0.97	0.11	53,53,53,53	0
15	CL	A	301	1/1	0.97	0.10	48,48,48,48	0
15	CL	F	301	1/1	0.97	0.13	56,56,56,56	0
15	CL	P	301	1/1	0.97	0.10	51,51,51,51	0
15	CL	B	301	1/1	0.97	0.09	45,45,45,45	0
15	CL	W	302	1/1	0.97	0.09	52,52,52,52	0
16	K	N	303	1/1	0.97	0.14	45,45,45,45	0
16	K	Z	302	1/1	0.97	0.08	42,42,42,42	0
19	BO2	K	305	28/28	0.97	0.06	32,37,41,42	0
15	CL	Y	301	1/1	0.97	0.15	67,67,67,67	0
15	CL	H	303	1/1	0.97	0.11	47,47,47,47	0
19	BO2	Y	305	28/28	0.97	0.05	29,32,37,38	0
17	MG	I	305	1/1	0.97	0.12	31,31,31,31	0
17	MG	L	303	1/1	0.98	0.13	37,37,37,37	0
17	MG	V	301	1/1	0.98	0.07	57,57,57,57	0
17	MG	W	301	1/1	0.98	0.08	36,36,36,36	0
15	CL	N	301	1/1	0.98	0.05	37,37,37,37	0
15	CL	M	303	1/1	0.98	0.12	47,47,47,47	0
17	MG	H	302	1/1	0.98	0.16	34,34,34,34	0
15	CL	O	301	1/1	0.98	0.08	59,59,59,59	0
15	CL	A	303	1/1	0.98	0.12	52,52,52,52	0
16	K	U	302	1/1	0.98	0.10	46,46,46,46	0
17	MG	X	301	1/1	0.99	0.03	49,49,49,49	0
15	CL	G	301	1/1	0.99	0.19	50,50,50,50	0
17	MG	H	301	1/1	0.99	0.03	53,53,53,53	0
16	K	G	303	1/1	0.99	0.07	37,37,37,37	0
17	MG	J	301	1/1	1.00	0.02	48,48,48,48	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.

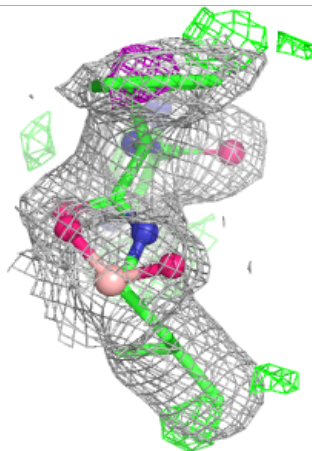
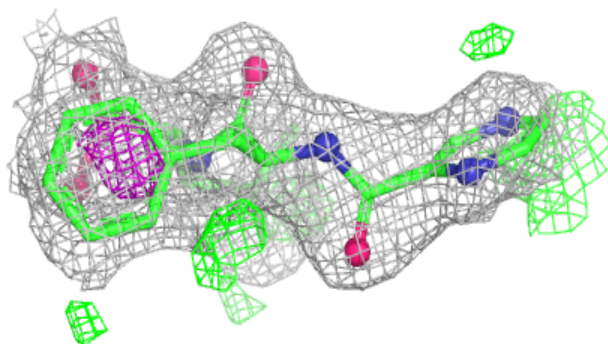
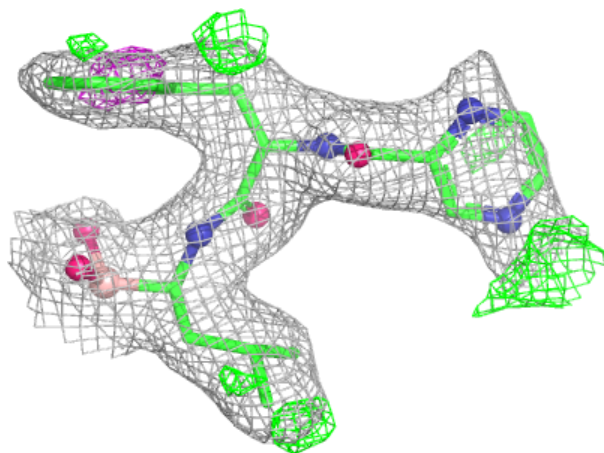
Electron density around BO2 V 303:

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



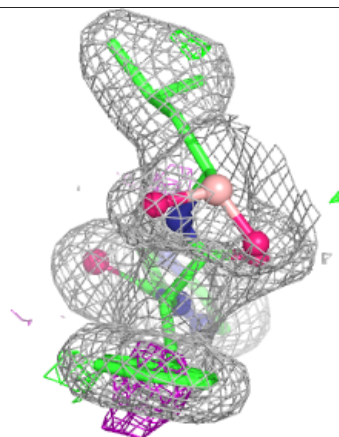
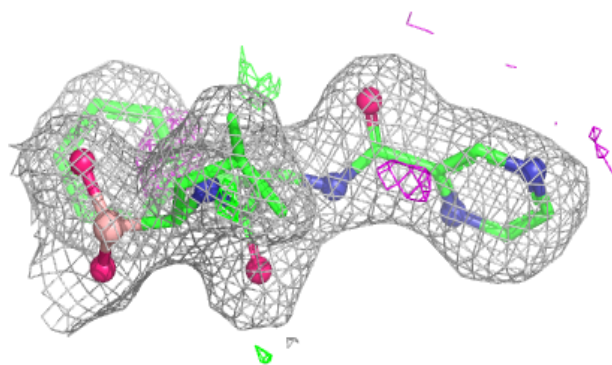
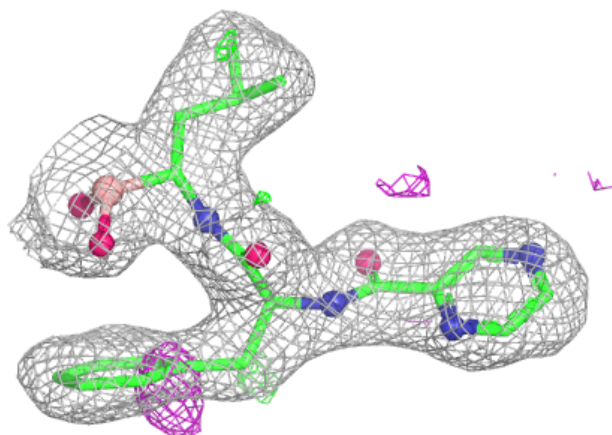
Electron density around BO2 H 306:

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



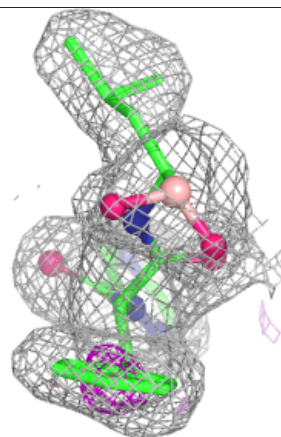
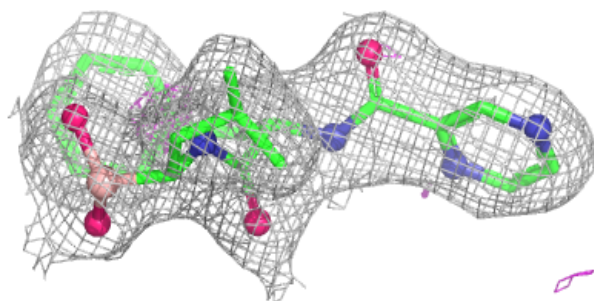
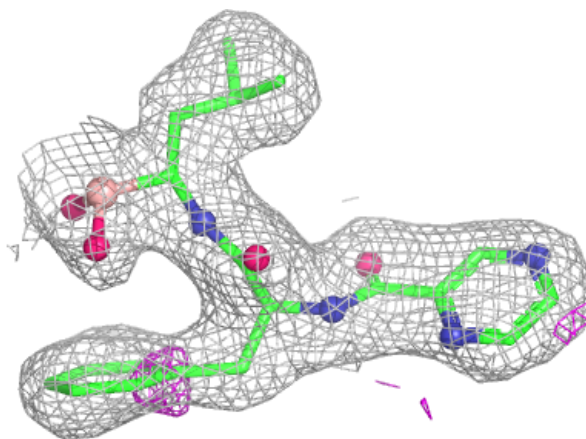
Electron density around BO2 N 304:

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



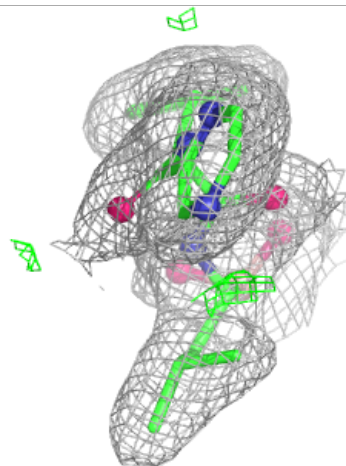
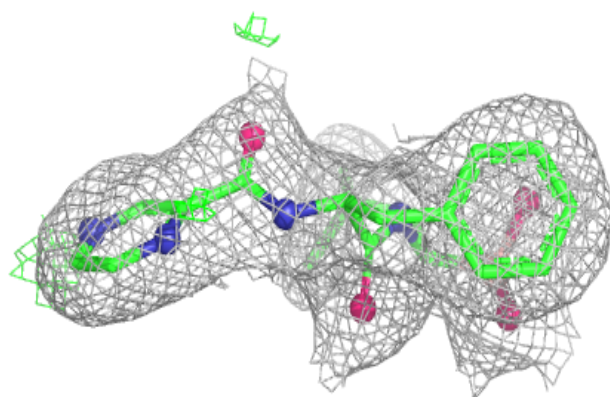
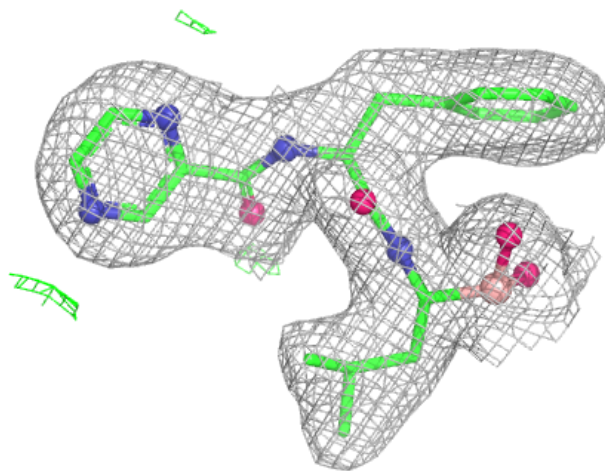
Electron density around BO2 b 305:

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



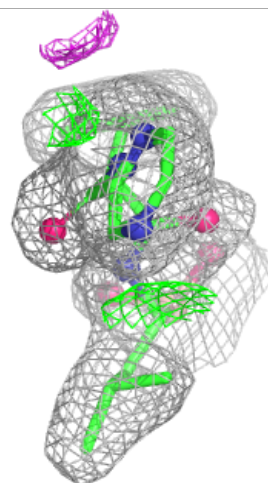
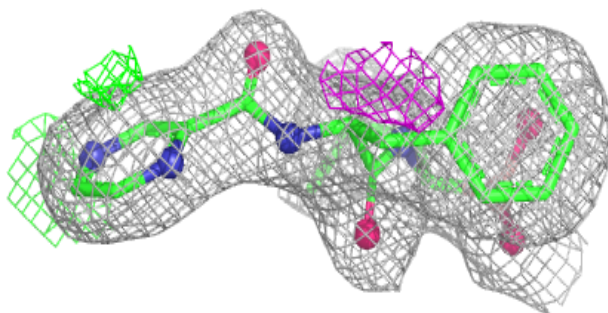
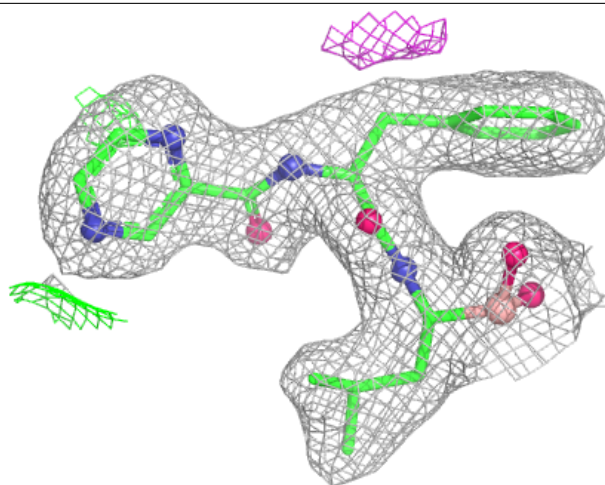
Electron density around BO2 K 305:

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



Electron density around BO2 Y 305:

$2mF_o-DF_c$ (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.