



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 10:47 AM UTC

PDB ID : 8OLR / pdb_00008olr
Title : Structure of yeast 20S proteasome in complex with the natural product beta-lactone inhibitor Cystargolide A
Authors : Illigmann, A.; Vielberg, M.-T.; Lakemeyer, M.; Wolf, F.; Staudt, N.; Dema, T.; Stange, P.; Malik, I.; Grond, S.; Sieber, S.A.; Groll, M.; Kaysser, L.; Broetz-Oesterhelt, H.
Deposited on : 2023-03-30
Resolution : 2.80 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

The following versions of software and data (see [references](#) ①) 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

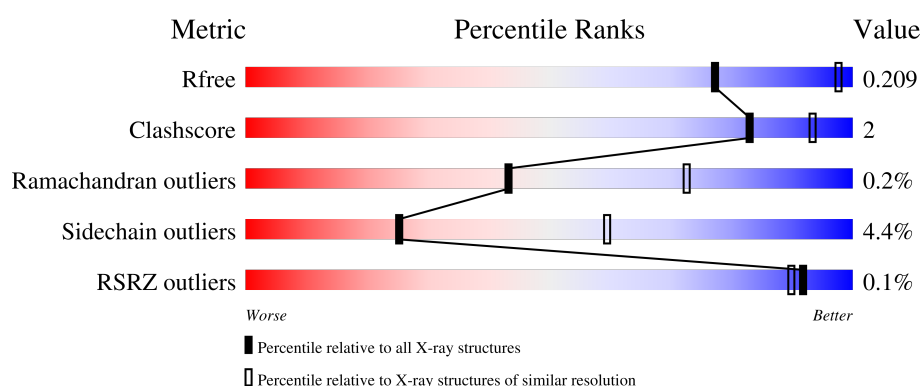
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 Å.

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



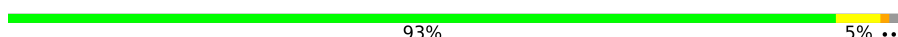
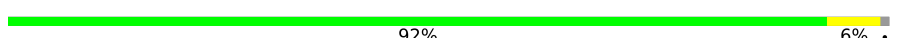
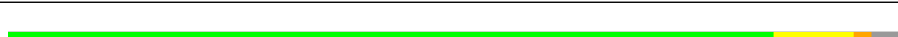
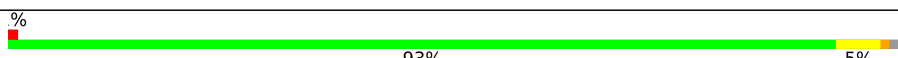
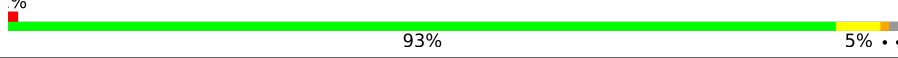
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

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

Mol	Chain	Length	Quality of chain
1	A	250	97% .
1	O	250	96% .
2	B	258	86% 9% 5%
2	P	258	87% 7% 5%
3	C	254	87% 6% . 6%

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

2 Entry composition

There are 18 unique types of molecules in this entry. The entry contains 49760 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Proteasome subunit alpha type-2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	250	Total	C	N	O	S	0	0	0
			1915	1219	315	377	4			
1	O	250	Total	C	N	O	S	0	0	0
			1915	1219	315	377	4			

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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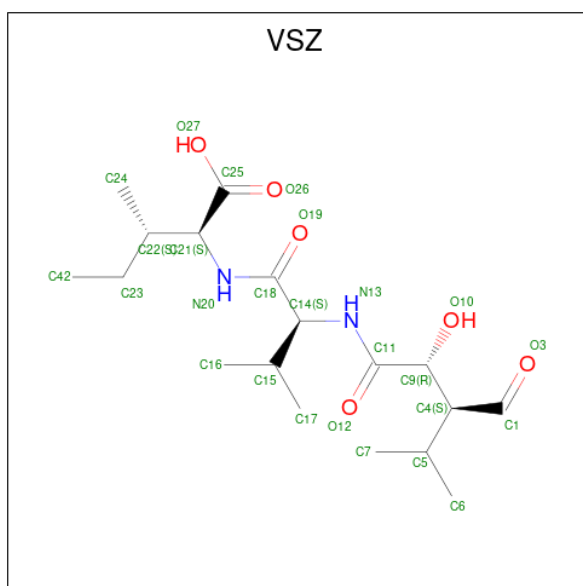
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
15	K	1	Total	Mg	0	0
			1	1		
15	N	1	Total	Mg	0	0
			1	1		
15	W	1	Total	Mg	0	0
			1	1		
15	Y	1	Total	Mg	0	0
			1	1		
15	Z	1	Total	Mg	0	0
			1	1		

- Molecule 16 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

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

- Molecule 17 is Cystargolide A (bound) (CCD ID: VSZ) (formula: C₁₈H₃₂N₂O₆) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
17	H	1	Total	C	N	O	0	0
			26	18	2	6		
17	K	1	Total	C	N	O	0	0
			26	18	2	6		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
17	N	1	Total	C	N	O	0	0
			26	18	2	6		
17	V	1	Total	C	N	O	0	0
			26	18	2	6		
17	Y	1	Total	C	N	O	0	0
			26	18	2	6		
17	b	1	Total	C	N	O	0	0
			26	18	2	6		

- Molecule 18 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
18	A	3	Total	O	0	0
			3	3		
18	B	10	Total	O	0	0
			10	10		
18	C	7	Total	O	0	0
			7	7		
18	D	3	Total	O	0	0
			3	3		
18	E	3	Total	O	0	0
			3	3		
18	F	5	Total	O	0	0
			5	5		
18	G	3	Total	O	0	0
			3	3		
18	H	16	Total	O	0	0
			16	16		
18	I	7	Total	O	0	0
			7	7		
18	J	10	Total	O	0	0
			10	10		
18	K	13	Total	O	0	0
			13	13		
18	L	18	Total	O	0	0
			18	18		
18	M	14	Total	O	0	0
			14	14		
18	N	9	Total	O	0	0
			9	9		
18	O	1	Total	O	0	0
			1	1		

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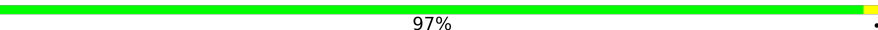
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
18	P	7	Total O 7 7	0	0
18	Q	6	Total O 6 6	0	0
18	R	5	Total O 5 5	0	0
18	S	3	Total O 3 3	0	0
18	T	6	Total O 6 6	0	0
18	U	10	Total O 10 10	0	0
18	V	10	Total O 10 10	0	0
18	W	4	Total O 4 4	0	0
18	X	8	Total O 8 8	0	0
18	Y	14	Total O 14 14	0	0
18	Z	9	Total O 9 9	0	0
18	a	17	Total O 17 17	0	0
18	b	8	Total O 8 8	0	0

3 Residue-property plots [i](#)

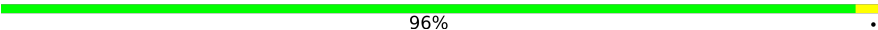
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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:  97%



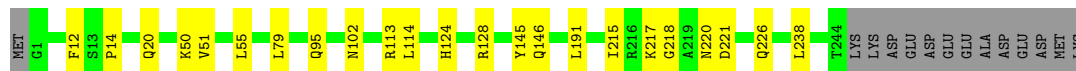
- Molecule 1: Proteasome subunit alpha type-2

Chain O:  96%



- Molecule 2: Proteasome subunit alpha type-3

Chain B:  86% 9% 5%



- Molecule 2: Proteasome subunit alpha type-3

Chain P:  87% 7% 5%



- Molecule 3: Proteasome subunit alpha type-4

Chain C:  87% 6% 6%

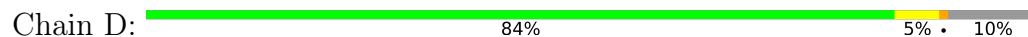


- Molecule 3: Proteasome subunit alpha type-4

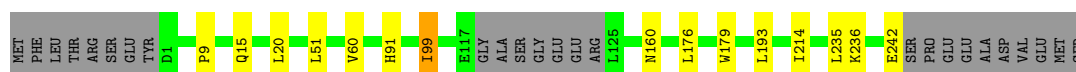
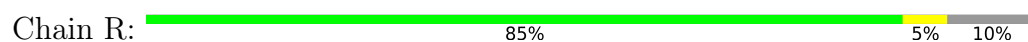
Chain Q:  87% 6% 6%



• Molecule 4: Proteasome subunit alpha type-5



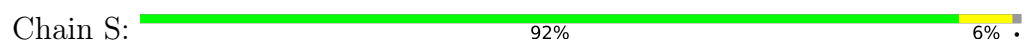
• Molecule 4: Proteasome subunit alpha type-5



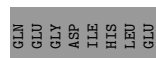
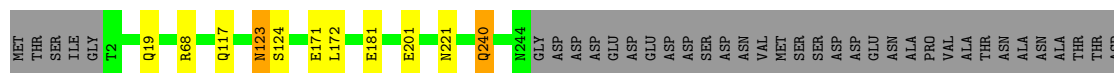
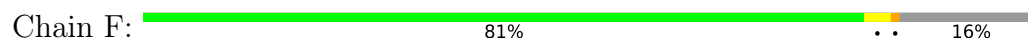
• Molecule 5: Proteasome subunit alpha type-6



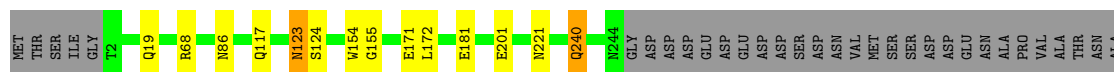
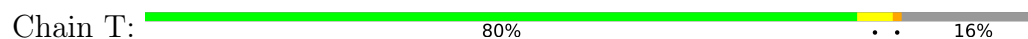
• Molecule 5: Proteasome subunit alpha type-6



• Molecule 6: Probable proteasome subunit alpha type-7



• Molecule 6: Probable proteasome subunit alpha type-7



ASN
ALA
THR
THR
ASP
GLN
GLU
GLY
ASP
ILE
HIS
LEU
GLU

• Molecule 7: Proteasome subunit alpha type-1

Chain G:  90% 6% .

MET SER GLY ALA ALA ALA ALA ALA SER ASP ILE HIS LEU GLU
G2 F23 T26 V73 I78 P79 N83 M14 L115 R122 M125 T133 Q167 T171 R235 L236 Q242 ASP

• Molecule 7: Proteasome subunit alpha type-1

Chain U:  87% 8% . .

MET SER GLY ALA ALA ALA ALA ALA SER ASP ILE HIS LEU GLU
G2 P12 E13 F23 T26 T59 V60 V73 I78 P79 N83 D106 L115 R122 M125 T133 Y146 Q167 T171 V216 R235 L236 Q242 ASP

• Molecule 8: Proteasome subunit beta type-2

Chain H:  86% 9% . .

T1 V4 K7 I14 N30 L34 S38 P39 K40 V55 L68 L98 A101 D104 P105 S112 I113 H114 S118 Y124 L125 S126 L127 E139 Q144 M165 V195 R196 I223 E226 GLN VAL ASP ILE THR ALA

• Molecule 8: Proteasome subunit beta type-2

Chain V:  86% 9% . .

T1 T2 I3 V4 K7 I14 N30 L34 S38 P39 K40 E53 A54 V55 L68 L80 L98 I99 V100 A101 S112 I113 S118 T119 L125 S126 L127 E139 M165 S169 V195 R196 I223 E226 GLN VAL ASP ILE THR ALA

• Molecule 9: Proteasome subunit beta type-3

Chain I:  93% 6%

MET S1 G9 I10 S36 N37 K38 K41 N71 F123 C128 A141 E150 L171 D177 G183 D204

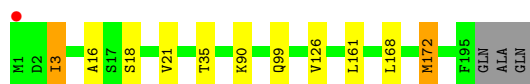
• Molecule 9: Proteasome subunit beta type-3

Chain W:  92% 7%

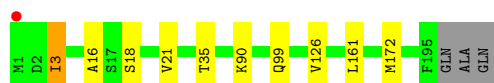
MET S1 G9 I10 S36 N37 K38 K41 N71 R97 F123 C128 A141 E150 L171 R176 D177 G183 D204

• Molecule 10: Proteasome subunit beta type-4

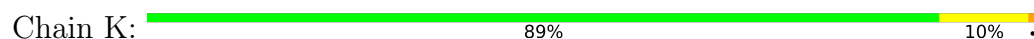
Chain J:  93% 5% . .



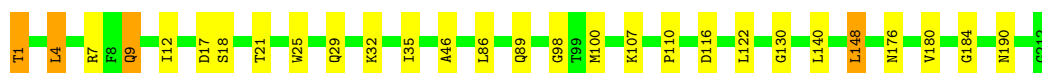
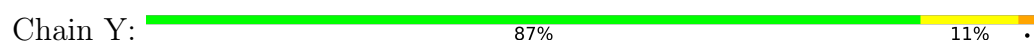
- Molecule 10: Proteasome subunit beta type-4



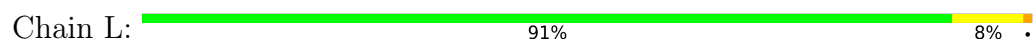
- Molecule 11: Proteasome subunit beta type-5



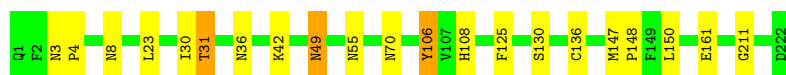
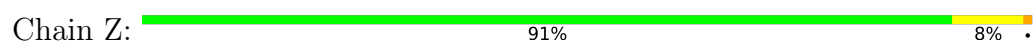
- Molecule 11: Proteasome subunit beta type-5



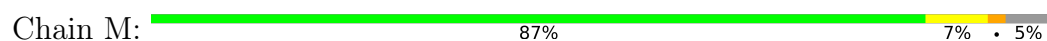
- Molecule 12: Proteasome subunit beta type-6



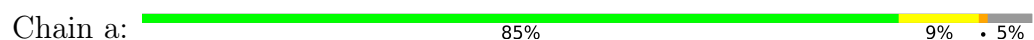
- Molecule 12: Proteasome subunit beta type-6



- Molecule 13: Proteasome subunit beta type-7

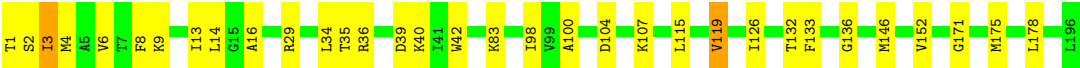
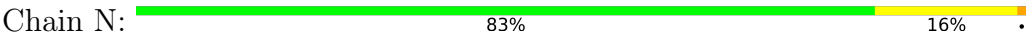


- Molecule 13: Proteasome subunit beta type-7

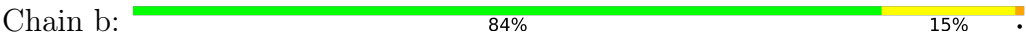




● Molecule 14: Proteasome subunit beta type-1



● Molecule 14: Proteasome subunit beta type-1



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	136.96Å 302.05Å 146.01Å 90.00° 113.09° 90.00°	Depositor
Resolution (Å)	15.00 – 2.80 15.00 – 2.80	Depositor EDS
% Data completeness (in resolution range)	97.2 (15.00-2.80) 97.2 (15.00-2.80)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.16 (at 2.81Å)	Xtriage
Refinement program	REFMAC 5.8.0238	Depositor
R, R_{free}	0.182 , 0.208 0.166 , 0.209	Depositor DCC
R_{free} test set	12970 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	69.5	Xtriage
Anisotropy	0.526	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 68.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	49760	wwPDB-VP
Average B, all atoms (Å ²)	90.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.35% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	1.05	1/1952 (0.1%)	1.37	0/2642
1	O	1.05	0/1952	1.39	0/2642
2	B	1.06	0/1934	1.41	0/2618
2	P	1.06	0/1934	1.40	0/2618
3	C	1.05	0/1910	1.42	0/2586
3	Q	1.05	0/1910	1.43	0/2586
4	D	1.05	0/1837	1.42	2/2475 (0.1%)
4	R	1.05	0/1837	1.43	0/2475
5	E	1.04	0/1800	1.40	0/2433
5	S	1.05	0/1800	1.41	0/2433
6	F	1.04	0/1932	1.42	0/2609
6	T	1.04	0/1932	1.41	0/2609
7	G	1.03	0/1945	1.38	0/2634
7	U	1.04	0/1945	1.39	2/2634 (0.1%)
8	H	1.04	0/1750	1.37	0/2373
8	V	1.04	0/1750	1.37	0/2373
9	I	1.02	0/1611	1.36	1/2174 (0.0%)
9	W	1.04	0/1611	1.37	1/2174 (0.0%)
10	J	1.02	0/1589	1.35	0/2142
10	X	1.02	0/1589	1.33	0/2142
11	K	1.00	0/1681	1.37	0/2274
11	Y	1.00	0/1681	1.37	1/2274 (0.0%)
12	L	1.02	0/1795	1.35	0/2420
12	Z	1.02	0/1795	1.35	0/2420
13	M	1.02	0/1855	1.35	0/2514
13	a	1.02	0/1855	1.35	3/2514 (0.1%)
14	N	1.01	0/1541	1.37	0/2087
14	b	1.02	0/1541	1.38	0/2087
All	All	1.03	1/50264 (0.0%)	1.38	10/67962 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	68	THR	N-CA	5.03	1.49	1.46

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	a	233	ILE	CA-CB-CG1	6.64	121.70	110.40
11	Y	184	GLY	CA-C-O	-5.59	118.29	122.37
9	W	183	GLY	CA-C-O	-5.33	118.61	122.45
9	I	183	GLY	CA-C-O	-5.33	118.62	122.45
13	a	188	ASP	CA-CB-CG	5.26	117.86	112.60
7	U	216	VAL	CA-C-N	5.25	126.17	122.33
7	U	216	VAL	C-N-CA	5.25	126.17	122.33
13	a	233	ILE	CB-CG1-CD1	5.20	124.72	113.80
4	D	30	ILE	CA-C-N	5.14	125.14	121.65
4	D	30	ILE	C-N-CA	5.14	125.14	121.65

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	2	0
1	O	1915	0	1929	7	0
2	B	1904	0	1904	11	0
2	P	1904	0	1904	10	0
3	C	1881	0	1895	10	0
3	Q	1881	0	1895	11	0
4	D	1813	0	1797	8	0
4	R	1813	0	1797	5	0
5	E	1773	0	1775	8	0
5	S	1773	0	1775	11	0
6	F	1892	0	1883	4	0
6	T	1892	0	1883	7	0
7	G	1907	0	1901	6	0
7	U	1907	0	1901	10	0
8	H	1719	0	1718	13	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	V	1719	0	1718	11	0
9	I	1581	0	1574	10	0
9	W	1581	0	1574	11	0
10	J	1561	0	1569	5	0
10	X	1561	0	1569	4	0
11	K	1644	0	1594	12	0
11	Y	1644	0	1594	15	0
12	L	1757	0	1711	11	0
12	Z	1757	0	1711	13	0
13	M	1824	0	1832	15	0
13	a	1824	0	1832	15	0
14	N	1512	0	1480	21	0
14	b	1512	0	1480	21	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	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	26	0	0	1	0
17	K	26	0	0	3	0
17	N	26	0	0	1	0
17	V	26	0	0	1	0
17	Y	26	0	0	3	0
17	b	26	0	0	4	0
18	A	3	0	0	0	0
18	B	10	0	0	0	0
18	C	7	0	0	0	0
18	D	3	0	0	0	0
18	E	3	0	0	0	0
18	F	5	0	0	0	0
18	G	3	0	0	0	0
18	H	16	0	0	1	0
18	I	7	0	0	0	0
18	J	10	0	0	0	0
18	K	13	0	0	0	0
18	L	18	0	0	0	0
18	M	14	0	0	1	0
18	N	9	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
18	O	1	0	0	0	0
18	P	7	0	0	0	0
18	Q	6	0	0	1	0
18	R	5	0	0	0	0
18	S	3	0	0	0	0
18	T	6	0	0	0	0
18	U	10	0	0	0	0
18	V	10	0	0	0	0
18	W	4	0	0	1	0
18	X	8	0	0	0	0
18	Y	14	0	0	1	0
18	Z	9	0	0	0	0
18	a	17	0	0	2	0
18	b	8	0	0	0	0
All	All	49760	0	49124	236	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 2.

All (236) 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)
3:C:160:GLN:HE21	3:C:160:GLN:HA	1.35	0.91
3:Q:160:GLN:HA	3:Q:160:GLN:HE21	1.38	0.86
1:O:12:PHE:H	2:P:20:GLN:HE22	1.29	0.80
7:G:23:PHE:O	7:G:26:THR:HB	1.83	0.78
7:U:23:PHE:O	7:U:26:THR:HB	1.86	0.76
13:M:2:GLN:NE2	18:M:301:HOH:O	2.21	0.72
13:a:2:GLN:NE2	18:a:301:HOH:O	2.24	0.71
14:N:35:THR:HG21	13:a:228:TYR:HE2	1.55	0.71
12:Z:31:THR:HG23	12:Z:36:ASN:HD21	1.56	0.70
1:A:12:PHE:H	2:B:20:GLN:HE22	1.39	0.69
8:V:3:ILE:HG13	8:V:99:ILE:HD12	1.76	0.67
8:H:14:ILE:HD12	8:H:101:ALA:HB3	1.77	0.67
13:M:233:ILE:HD13	13:M:233:ILE:H	1.60	0.66
12:L:31:THR:HG23	12:L:36:ASN:HD21	1.61	0.65
14:b:115:LEU:HD11	17:b:201:VSZ:C23	2.28	0.64
8:V:14:ILE:HD12	8:V:101:ALA:HB3	1.79	0.63
14:N:152:VAL:HA	14:N:175:MET:HE1	1.81	0.62
13:M:228:TYR:HE2	14:b:35:THR:HG21	1.65	0.62
12:L:108:HIS:HD2	12:L:125:PHE:O	1.83	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:b:152:VAL:HA	14:b:175:MET:HE1	1.81	0.61
5:E:12:PHE:H	6:F:19:GLN:HE22	1.47	0.61
11:Y:89:GLN:HG2	18:Y:403:HOH:O	2.00	0.60
2:B:12:PHE:H	3:C:17:GLN:HE22	1.50	0.60
14:N:3:ILE:HG22	14:N:16:ALA:CB	2.32	0.59
11:K:176:ASN:ND2	11:K:190:ASN:HD22	2.00	0.59
8:V:139:GLU:OE2	14:b:29:ARG:NH2	2.35	0.59
8:V:80:LEU:HD13	8:V:119:THR:HG21	1.84	0.58
14:N:3:ILE:HG22	14:N:16:ALA:HB2	1.85	0.58
6:F:123:ASN:HD22	6:F:124:SER:N	2.01	0.57
5:S:12:PHE:H	6:T:19:GLN:HE22	1.50	0.57
14:b:46:SER:HA	17:b:201:VSZ:O3	2.05	0.57
11:Y:1:THR:HG21	17:Y:302:VSZ:O3	2.05	0.56
11:Y:176:ASN:ND2	11:Y:190:ASN:HD22	2.04	0.56
12:Z:3:ASN:HD22	12:Z:4:PRO:HD2	1.70	0.56
6:T:123:ASN:HD22	6:T:124:SER:N	2.02	0.56
8:H:196:ARG:NH2	9:I:150:GLU:O	2.39	0.56
8:H:14:ILE:HD12	8:H:101:ALA:CB	2.36	0.55
12:L:3:ASN:HD22	12:L:4:PRO:HD2	1.71	0.55
17:K:302:VSZ:C18	17:K:302:VSZ:C24	2.85	0.54
12:Z:31:THR:CG2	12:Z:36:ASN:HD21	2.20	0.54
8:H:139:GLU:OE2	14:N:29:ARG:NH2	2.40	0.54
5:S:92:ASN:HD21	12:Z:70:ASN:HD21	1.56	0.54
8:H:1:THR:OG1	17:H:301:VSZ:O10	2.24	0.54
1:O:23:TYR:CD1	7:U:12:PRO:HA	2.42	0.54
6:F:123:ASN:HD22	6:F:123:ASN:C	2.15	0.54
17:Y:302:VSZ:C18	17:Y:302:VSZ:C24	2.85	0.54
13:M:156:ARG:HH11	8:V:165:ASN:HD22	1.55	0.54
8:V:14:ILE:HD12	8:V:101:ALA:CB	2.38	0.54
11:K:4:LEU:HD22	11:K:4:LEU:C	2.33	0.54
12:Z:108:HIS:HD2	12:Z:125:PHE:O	1.90	0.54
14:N:35:THR:HG21	13:a:228:TYR:CE2	2.41	0.53
6:T:123:ASN:HD22	6:T:123:ASN:C	2.16	0.53
14:N:3:ILE:HD12	14:N:98:ILE:HD12	1.90	0.53
4:D:176:LEU:HD22	5:E:55:LEU:CD2	2.39	0.53
9:W:10:ILE:HG21	9:W:141:ALA:HB3	1.91	0.53
10:J:16:ALA:HB2	10:J:161:LEU:HD21	1.91	0.52
17:N:202:VSZ:N13	17:N:202:VSZ:C1	2.73	0.52
9:I:10:ILE:HG21	9:I:141:ALA:HB3	1.91	0.52
12:L:42:LYS:HD2	12:L:55:ASN:HD22	1.73	0.52
8:H:139:GLU:OE1	13:a:187:ARG:NH1	2.37	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:36:SER:HB2	10:J:126:VAL:HG11	1.92	0.51
3:Q:52:LEU:N	18:Q:301:HOH:O	2.35	0.51
8:V:1:THR:OG1	17:V:301:VSZ:O10	2.27	0.51
13:M:187:ARG:NH1	8:V:139:GLU:OE1	2.40	0.51
11:Y:4:LEU:C	11:Y:4:LEU:HD22	2.35	0.51
17:K:302:VSZ:C17	17:K:302:VSZ:N20	2.73	0.51
11:Y:18:SER:OG	11:Y:29:GLN:O	2.26	0.51
8:H:165:ASN:HD22	13:a:156:ARG:HH11	1.59	0.50
3:C:9:PHE:H	4:D:15:GLN:HE22	1.58	0.50
14:N:13:ILE:HG21	14:N:175:MET:HE2	1.92	0.50
1:O:122:THR:HG22	2:P:128:ARG:HH21	1.77	0.50
10:X:21:VAL:HG11	11:Y:122:LEU:HD11	1.93	0.50
13:M:227:GLY:HA3	13:M:231:GLN:HB2	1.94	0.50
9:W:9:GLY:HA3	9:W:41:LYS:HE2	1.94	0.50
5:E:92:ASN:HD21	12:L:70:ASN:HD21	1.60	0.50
11:K:176:ASN:HD21	11:K:190:ASN:HD22	1.59	0.50
2:B:95:GLN:HE22	9:I:71:ASN:HD22	1.60	0.49
10:J:21:VAL:HG11	11:K:122:LEU:HD11	1.93	0.49
9:I:9:GLY:HA3	9:I:41:LYS:HE2	1.94	0.49
12:Z:42:LYS:HD2	12:Z:55:ASN:HD22	1.76	0.49
10:X:16:ALA:HB2	10:X:161:LEU:HD21	1.93	0.49
11:Y:176:ASN:HD21	11:Y:190:ASN:HD22	1.61	0.49
10:J:3:ILE:HG23	10:J:18:SER:HB3	1.94	0.49
9:I:37:ASN:C	9:I:37:ASN:HD22	2.21	0.49
12:L:49:ASN:HD21	12:L:211:GLY:HA2	1.78	0.49
1:O:7:PHE:HB3	3:Q:2:TYR:CE1	2.48	0.49
6:T:155:GLY:HA3	7:U:59:THR:HG21	1.95	0.49
14:b:13:ILE:HG21	14:b:175:MET:HE2	1.95	0.49
12:L:31:THR:CG2	12:L:36:ASN:HD21	2.26	0.48
9:W:141:ALA:HB2	9:W:177:ASP:HB2	1.95	0.48
8:V:196:ARG:NH2	9:W:150:GLU:O	2.45	0.48
10:X:3:ILE:HG23	10:X:18:SER:HB3	1.95	0.48
2:B:146:GLN:HG2	3:C:57:ILE:HG21	1.94	0.48
9:I:141:ALA:HB2	9:I:177:ASP:HB2	1.95	0.48
5:S:71:LEU:HD22	5:S:71:LEU:C	2.39	0.48
3:Q:35:LYS:HG2	3:Q:158:SER:O	2.14	0.48
4:R:91:HIS:CD2	4:R:99:ILE:HG22	2.49	0.47
11:Y:46:ALA:HB3	11:Y:98:GLY:O	2.13	0.47
12:L:108:HIS:CD2	12:L:125:PHE:O	2.66	0.47
3:C:35:LYS:HG2	3:C:158:SER:O	2.14	0.47
13:M:233:ILE:HD13	13:M:233:ILE:N	2.26	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:W:37:ASN:C	9:W:37:ASN:HD22	2.23	0.47
17:Y:302:VSZ:N20	17:Y:302:VSZ:C17	2.77	0.47
4:D:91:HIS:CD2	4:D:99:ILE:HG22	2.50	0.47
3:Q:160:GLN:HE21	3:Q:160:GLN:CA	2.15	0.47
5:E:71:LEU:C	5:E:71:LEU:HD22	2.40	0.46
7:G:167:GLN:HE21	7:G:171:THR:HG23	1.80	0.46
8:H:114:HIS:HB3	18:H:411:HOH:O	2.14	0.46
13:M:97:ALA:HA	13:M:130:VAL:HG21	1.97	0.46
9:I:37:ASN:HD22	9:I:38:LYS:HG3	1.80	0.46
9:W:36:SER:HB2	10:X:126:VAL:HG11	1.96	0.46
14:N:13:ILE:HG21	14:N:175:MET:CE	2.46	0.46
14:N:133:PHE:HA	14:b:132:THR:O	2.15	0.46
12:Z:8:ASN:HA	12:Z:30:ILE:O	2.15	0.46
11:K:4:LEU:HD22	11:K:4:LEU:O	2.16	0.46
12:L:8:ASN:HA	12:L:30:ILE:O	2.16	0.46
14:N:14:LEU:HD11	14:N:100:ALA:HB3	1.97	0.46
14:b:1:THR:OG1	17:b:201:VSZ:O10	2.34	0.46
11:K:1:THR:HG21	17:K:302:VSZ:O3	2.15	0.46
14:b:14:LEU:N	14:b:14:LEU:HD12	2.30	0.46
11:K:46:ALA:HB3	11:K:98:GLY:O	2.16	0.45
2:P:50:LYS:HD3	2:P:50:LYS:HA	1.84	0.45
14:N:136:GLY:HA2	14:b:161:GLN:HE21	1.80	0.45
13:a:97:ALA:HA	13:a:130:VAL:HG21	1.98	0.45
14:N:171:GLY:HA2	13:a:219:TRP:CH2	2.51	0.45
7:U:78:ILE:N	7:U:79:PRO:CD	2.79	0.45
12:L:106:TYR:HD2	12:L:106:TYR:HA	1.64	0.45
14:N:14:LEU:HD12	14:N:14:LEU:N	2.31	0.45
11:Y:4:LEU:HD22	11:Y:4:LEU:O	2.17	0.45
1:O:122:THR:CG2	2:P:128:ARG:HH21	2.30	0.45
13:a:35:ARG:HG3	13:a:36:PHE:CZ	2.52	0.45
13:a:233:ILE:HG22	13:a:233:ILE:OXT	2.16	0.45
14:b:14:LEU:HD11	14:b:100:ALA:HB3	1.99	0.45
9:W:97:ARG:HD2	18:W:401:HOH:O	2.17	0.44
13:M:35:ARG:HG3	13:M:36:PHE:CZ	2.52	0.44
6:F:240:GLN:HE21	6:F:240:GLN:HA	1.82	0.44
9:I:123:PHE:HA	9:I:128:CYS:O	2.17	0.44
11:K:7:ARG:NH1	11:K:110:PRO:O	2.44	0.44
7:U:167:GLN:HE21	7:U:171:THR:HG23	1.82	0.44
6:T:240:GLN:HE21	6:T:240:GLN:HA	1.82	0.44
3:C:201:VAL:O	3:C:202:GLN:CB	2.65	0.44
8:V:98:LEU:HB2	8:V:113:ILE:CG2	2.47	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:65:CYS:SG	5:E:71:LEU:CD1	3.06	0.44
13:M:96:LEU:O	13:M:100:MET:HG2	2.18	0.44
2:P:124:HIS:HB3	3:Q:124:VAL:HG12	1.98	0.44
5:S:65:CYS:SG	5:S:71:LEU:CD1	3.06	0.44
14:b:13:ILE:HG21	14:b:175:MET:CE	2.47	0.44
3:Q:201:VAL:O	3:Q:202:GLN:CB	2.66	0.44
12:Z:36:ASN:HB3	13:a:137:TYR:CD1	2.52	0.44
2:B:95:GLN:NE2	9:I:71:ASN:HD22	2.15	0.43
1:O:14:PRO:HA	2:P:23:TYR:CD1	2.53	0.43
14:b:83:LYS:HG3	14:b:119:VAL:CG2	2.48	0.43
7:G:78:ILE:N	7:G:79:PRO:CD	2.81	0.43
12:Z:36:ASN:HB3	13:a:137:TYR:CE1	2.53	0.43
12:Z:106:TYR:HD2	12:Z:106:TYR:HA	1.65	0.43
2:B:145:TYR:OH	2:B:217:LYS:HB2	2.18	0.43
5:E:77:ALA:N	5:E:78:PRO:CD	2.82	0.43
8:H:98:LEU:HB2	8:H:113:ILE:CG2	2.48	0.43
3:Q:160:GLN:HA	3:Q:160:GLN:NE2	2.20	0.43
5:S:77:ALA:N	5:S:78:PRO:CD	2.81	0.43
14:N:83:LYS:HG3	14:N:119:VAL:CG2	2.49	0.43
4:D:160:ASN:HB3	4:D:179:TRP:CE2	2.54	0.43
5:S:71:LEU:C	5:S:71:LEU:CD2	2.92	0.43
3:C:51:LYS:O	3:C:52:LEU:HB2	2.18	0.42
13:a:171:GLN:HG3	18:a:312:HOH:O	2.19	0.42
14:N:4:MET:HB3	14:N:126:ILE:HG22	2.01	0.42
7:U:78:ILE:HG22	7:U:79:PRO:HD3	2.01	0.42
2:B:14:PRO:HA	3:C:20:TYR:CD1	2.54	0.42
13:M:225:ILE:HD13	14:b:30:VAL:HG21	2.00	0.42
13:a:227:GLY:CA	13:a:231:GLN:HE21	2.33	0.42
8:H:104:ASP:HB2	8:H:105:PRO:HD2	2.01	0.42
3:Q:9:PHE:H	4:R:15:GLN:HE22	1.67	0.42
4:R:160:ASN:HB3	4:R:179:TRP:CE2	2.54	0.42
9:W:37:ASN:HD22	9:W:38:LYS:HG3	1.85	0.42
11:K:12:ILE:HB	11:K:180:VAL:HB	2.02	0.42
7:U:115:LEU:HD12	7:U:115:LEU:HA	1.87	0.42
8:V:112:SER:HB3	8:V:125:LEU:HD13	2.02	0.42
1:A:122:THR:HG22	2:B:128:ARG:HH21	1.84	0.42
5:S:71:LEU:HD22	5:S:71:LEU:O	2.20	0.42
8:H:112:SER:HB3	8:H:125:LEU:HD13	2.01	0.42
2:P:12:PHE:H	3:Q:17:GLN:HE22	1.68	0.42
4:R:9:PRO:HA	5:S:23:TYR:CD1	2.55	0.42
11:Y:1:THR:O	11:Y:130:GLY:HA3	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:124:TYR:OH	14:N:29:ARG:NH2	2.53	0.42
11:Y:7:ARG:NH1	11:Y:110:PRO:O	2.42	0.42
7:G:73:VAL:HG12	7:G:133:THR:HB	2.00	0.41
5:E:71:LEU:C	5:E:71:LEU:CD2	2.93	0.41
14:b:4:MET:HB3	14:b:126:ILE:HG22	2.01	0.41
1:O:6:SER:OG	3:Q:2:TYR:HA	2.20	0.41
5:S:87:LEU:HD21	5:S:107:ALA:HB1	2.02	0.41
4:D:193:LEU:HD12	4:D:193:LEU:HA	1.94	0.41
11:K:86:LEU:C	11:K:86:LEU:HD13	2.44	0.41
11:K:100:MET:HE2	11:K:100:MET:HB2	1.94	0.41
9:W:123:PHE:HA	9:W:128:CYS:O	2.20	0.41
12:Z:49:ASN:HD21	12:Z:211:GLY:HA2	1.85	0.41
17:b:201:VSZ:N13	17:b:201:VSZ:C1	2.83	0.41
2:P:95:GLN:HE22	9:W:71:ASN:HD22	1.67	0.41
14:b:1:THR:O	14:b:128:GLY:HA3	2.20	0.41
4:D:91:HIS:HB3	4:D:99:ILE:CG2	2.51	0.41
14:N:132:THR:O	14:b:133:PHE:HA	2.20	0.41
6:T:86:ASN:HD22	6:T:86:ASN:HA	1.71	0.41
7:U:73:VAL:HG12	7:U:133:THR:HB	2.02	0.41
11:Y:100:MET:HE2	11:Y:100:MET:HB2	1.94	0.41
13:a:96:LEU:O	13:a:100:MET:HG2	2.20	0.41
5:E:87:LEU:HD21	5:E:107:ALA:HB1	2.03	0.41
12:L:147:MET:HE3	9:W:176:ARG:NH2	2.35	0.41
14:N:14:LEU:HB3	14:N:34:LEU:HD22	2.03	0.41
2:P:114:LEU:HD23	2:P:114:LEU:HA	1.97	0.41
5:S:98:PHE:O	13:a:91:TYR:HA	2.21	0.41
11:Y:86:LEU:HD13	11:Y:86:LEU:C	2.46	0.41
2:B:114:LEU:HD23	2:B:114:LEU:HA	1.96	0.41
3:C:11:PRO:HA	4:D:18:TYR:CD1	2.56	0.41
4:D:88:ALA:HA	4:D:99:ILE:HG21	2.02	0.41
7:G:78:ILE:HG22	7:G:79:PRO:HD3	2.02	0.41
7:G:114:ASN:HD22	7:G:114:ASN:HA	1.67	0.41
8:H:68:LEU:HD12	8:H:68:LEU:HA	1.87	0.41
13:M:228:TYR:CE2	14:b:35:THR:HG21	2.51	0.41
13:M:231:GLN:HE21	13:M:231:GLN:HB3	1.62	0.41
7:U:106:ASP:HB3	7:U:146:TYR:CZ	2.56	0.41
14:b:14:LEU:HB3	14:b:34:LEU:HD22	2.03	0.41
11:Y:12:ILE:HB	11:Y:180:VAL:HB	2.02	0.41
2:B:124:HIS:HB3	3:C:124:VAL:HG12	2.03	0.40
2:B:215:ILE:HG12	2:B:226:GLN:HG2	2.03	0.40
13:M:35:ARG:HG3	13:M:36:PHE:CE2	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:231:GLN:OE1	14:b:36:ARG:N	2.30	0.40
11:Y:9:GLN:NE2	11:Y:148:LEU:O	2.55	0.40
14:b:32:ASP:OD2	14:b:185:ARG:NH2	2.54	0.40
4:R:91:HIS:HB3	4:R:99:ILE:CG2	2.51	0.40
12:Z:147:MET:N	12:Z:148:PRO:CD	2.84	0.40
14:N:8:PHE:HB2	14:N:146:MET:O	2.22	0.40
2:P:145:TYR:OH	2:P:217:LYS:HB2	2.21	0.40
10:J:168:LEU:O	10:J:172:MET:HB2	2.22	0.40
11:K:4:LEU:C	11:K:4:LEU:CD2	2.93	0.40
14:N:36:ARG:HG3	14:N:42:TRP:CE2	2.57	0.40
5:S:92:ASN:ND2	12:Z:70:ASN:HD21	2.19	0.40
6:T:154:TRP:CZ3	7:U:60:VAL:HA	2.57	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	248/250 (99%)	240 (97%)	7 (3%)	1 (0%)	30	60
1	O	248/250 (99%)	238 (96%)	9 (4%)	1 (0%)	30	60
2	B	242/258 (94%)	233 (96%)	5 (2%)	4 (2%)	7	25
2	P	242/258 (94%)	233 (96%)	5 (2%)	4 (2%)	7	25
3	C	238/254 (94%)	233 (98%)	3 (1%)	2 (1%)	16	44
3	Q	238/254 (94%)	233 (98%)	3 (1%)	2 (1%)	16	44
4	D	231/260 (89%)	226 (98%)	5 (2%)	0	100	100
4	R	231/260 (89%)	227 (98%)	4 (2%)	0	100	100
5	E	229/234 (98%)	222 (97%)	7 (3%)	0	100	100
5	S	229/234 (98%)	222 (97%)	7 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
6	F	241/288 (84%)	238 (99%)	3 (1%)	0	100	100
6	T	241/288 (84%)	238 (99%)	3 (1%)	0	100	100
7	G	239/252 (95%)	237 (99%)	2 (1%)	0	100	100
7	U	239/252 (95%)	237 (99%)	2 (1%)	0	100	100
8	H	224/232 (97%)	220 (98%)	4 (2%)	0	100	100
8	V	224/232 (97%)	220 (98%)	4 (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%)	187 (97%)	6 (3%)	0	100	100
11	K	210/212 (99%)	206 (98%)	4 (2%)	0	100	100
11	Y	210/212 (99%)	206 (98%)	4 (2%)	0	100	100
12	L	220/222 (99%)	216 (98%)	4 (2%)	0	100	100
12	Z	220/222 (99%)	215 (98%)	5 (2%)	0	100	100
13	M	231/246 (94%)	223 (96%)	8 (4%)	0	100	100
13	a	231/246 (94%)	223 (96%)	8 (4%)	0	100	100
14	N	194/196 (99%)	190 (98%)	4 (2%)	0	100	100
14	b	194/196 (99%)	191 (98%)	3 (2%)	0	100	100
All	All	6284/6614 (95%)	6129 (98%)	141 (2%)	14 (0%)	43	72

All (14) Ramachandran outliers are listed below:

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

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Mol	Chain	Res	Type
3	Q	205	ALA

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	209/209 (100%)	204 (98%)	5 (2%)	43	77
1	O	209/209 (100%)	204 (98%)	5 (2%)	43	77
2	B	203/216 (94%)	196 (97%)	7 (3%)	32	68
2	P	203/216 (94%)	196 (97%)	7 (3%)	32	68
3	C	212/226 (94%)	203 (96%)	9 (4%)	26	61
3	Q	212/226 (94%)	203 (96%)	9 (4%)	26	61
4	D	194/215 (90%)	184 (95%)	10 (5%)	21	53
4	R	194/215 (90%)	184 (95%)	10 (5%)	21	53
5	E	190/193 (98%)	184 (97%)	6 (3%)	34	70
5	S	190/193 (98%)	184 (97%)	6 (3%)	34	70
6	F	201/239 (84%)	192 (96%)	9 (4%)	24	58
6	T	201/239 (84%)	192 (96%)	9 (4%)	24	58
7	G	206/210 (98%)	199 (97%)	7 (3%)	32	68
7	U	206/210 (98%)	198 (96%)	8 (4%)	28	64
8	H	185/190 (97%)	169 (91%)	16 (9%)	10	31
8	V	185/190 (97%)	167 (90%)	18 (10%)	8	25
9	I	172/173 (99%)	170 (99%)	2 (1%)	63	87
9	W	172/173 (99%)	170 (99%)	2 (1%)	63	87
10	J	173/175 (99%)	168 (97%)	5 (3%)	37	73
10	X	173/175 (99%)	168 (97%)	5 (3%)	37	73
11	K	169/169 (100%)	157 (93%)	12 (7%)	13	39
11	Y	169/169 (100%)	157 (93%)	12 (7%)	13	39
12	L	185/185 (100%)	177 (96%)	8 (4%)	26	60

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
12	Z	185/185 (100%)	177 (96%)	8 (4%)	26	60
13	M	199/208 (96%)	189 (95%)	10 (5%)	22	54
13	a	199/208 (96%)	190 (96%)	9 (4%)	24	58
14	N	162/162 (100%)	150 (93%)	12 (7%)	13	37
14	b	162/162 (100%)	152 (94%)	10 (6%)	16	45
All	All	5320/5540 (96%)	5084 (96%)	236 (4%)	25	59

All (236) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	59	GLU
1	A	122	THR
1	A	157	PHE
1	A	250	LEU
2	B	50	LYS
2	B	55	LEU
2	B	79	LEU
2	B	102	ASN
2	B	113	ARG
2	B	191	LEU
2	B	238	LEU
3	C	4	ARG
3	C	38	ASN
3	C	51	LYS
3	C	52	LEU
3	C	77	ASN
3	C	160	GLN
3	C	169	VAL
3	C	180	LYS
3	C	240	GLU
4	D	20	LEU
4	D	51	LEU
4	D	60	VAL
4	D	99	ILE
4	D	176	LEU
4	D	193	LEU
4	D	214	ILE
4	D	235	LEU
4	D	236	LYS

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Mol	Chain	Res	Type
4	D	242	GLU
5	E	9	THR
5	E	29	LYS
5	E	55	LEU
5	E	71	LEU
5	E	188	LEU
5	E	231	LYS
6	F	68	ARG
6	F	117	GLN
6	F	123	ASN
6	F	171	GLU
6	F	172	LEU
6	F	181	GLU
6	F	201	GLU
6	F	221	ASN
6	F	240	GLN
7	G	26	THR
7	G	83	ASN
7	G	115	LEU
7	G	122	ARG
7	G	125	MET
7	G	235	ARG
7	G	236	LEU
8	H	1	THR
8	H	4	VAL
8	H	7	LYS
8	H	14	ILE
8	H	30	ASN
8	H	34	LEU
8	H	38	SER
8	H	40	LYS
8	H	55	VAL
8	H	68	LEU
8	H	113	ILE
8	H	118	SER
8	H	127	LEU
8	H	144	GLN
8	H	195	VAL
8	H	196	ARG
9	I	37	ASN
9	I	171	LEU
10	J	3	ILE

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Mol	Chain	Res	Type
10	J	35	THR
10	J	90	LYS
10	J	99	GLN
10	J	172	MET
11	K	1	THR
11	K	4	LEU
11	K	9	GLN
11	K	17	ASP
11	K	21	THR
11	K	25	TRP
11	K	32	LYS
11	K	35	ILE
11	K	107	LYS
11	K	116	ASP
11	K	140	LEU
11	K	148	LEU
12	L	23	LEU
12	L	31	THR
12	L	49	ASN
12	L	106	TYR
12	L	130	SER
12	L	136	CYS
12	L	150	LEU
12	L	161	GLU
13	M	2	GLN
13	M	10	SER
13	M	48	ASN
13	M	70	LEU
13	M	104	ARG
13	M	161	ARG
13	M	187	ARG
13	M	231	GLN
13	M	232	LYS
13	M	233	ILE
14	N	1	THR
14	N	2	SER
14	N	3	ILE
14	N	6	VAL
14	N	9	LYS
14	N	39	ASP
14	N	40	LYS
14	N	104	ASP

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Mol	Chain	Res	Type
14	N	107	LYS
14	N	115	LEU
14	N	119	VAL
14	N	178	LEU
1	O	1	MET
1	O	59	GLU
1	O	122	THR
1	O	157	PHE
1	O	250	LEU
2	P	50	LYS
2	P	55	LEU
2	P	79	LEU
2	P	102	ASN
2	P	113	ARG
2	P	191	LEU
2	P	238	LEU
3	Q	4	ARG
3	Q	38	ASN
3	Q	51	LYS
3	Q	52	LEU
3	Q	77	ASN
3	Q	160	GLN
3	Q	169	VAL
3	Q	180	LYS
3	Q	240	GLU
4	R	20	LEU
4	R	51	LEU
4	R	60	VAL
4	R	99	ILE
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	55	LEU
5	S	71	LEU
5	S	188	LEU
5	S	231	LYS
6	T	68	ARG

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Mol	Chain	Res	Type
6	T	117	GLN
6	T	123	ASN
6	T	171	GLU
6	T	172	LEU
6	T	181	GLU
6	T	201	GLU
6	T	221	ASN
6	T	240	GLN
7	U	13	GLU
7	U	26	THR
7	U	83	ASN
7	U	115	LEU
7	U	122	ARG
7	U	125	MET
7	U	235	ARG
7	U	236	LEU
8	V	1	THR
8	V	4	VAL
8	V	7	LYS
8	V	14	ILE
8	V	30	ASN
8	V	34	LEU
8	V	38	SER
8	V	40	LYS
8	V	53	GLU
8	V	55	VAL
8	V	68	LEU
8	V	80	LEU
8	V	113	ILE
8	V	118	SER
8	V	127	LEU
8	V	169	SER
8	V	195	VAL
8	V	196	ARG
9	W	37	ASN
9	W	171	LEU
10	X	3	ILE
10	X	35	THR
10	X	90	LYS
10	X	99	GLN
10	X	172	MET
11	Y	1	THR

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Mol	Chain	Res	Type
11	Y	4	LEU
11	Y	9	GLN
11	Y	17	ASP
11	Y	21	THR
11	Y	25	TRP
11	Y	32	LYS
11	Y	35	ILE
11	Y	107	LYS
11	Y	116	ASP
11	Y	140	LEU
11	Y	148	LEU
12	Z	23	LEU
12	Z	31	THR
12	Z	49	ASN
12	Z	106	TYR
12	Z	130	SER
12	Z	136	CYS
12	Z	150	LEU
12	Z	161	GLU
13	a	2	GLN
13	a	10	SER
13	a	48	ASN
13	a	70	LEU
13	a	104	ARG
13	a	161	ARG
13	a	187	ARG
13	a	232	LYS
13	a	233	ILE
14	b	1	THR
14	b	2	SER
14	b	6	VAL
14	b	9	LYS
14	b	39	ASP
14	b	40	LYS
14	b	104	ASP
14	b	107	LYS
14	b	119	VAL
14	b	178	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (169) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	149	GLN
2	B	20	GLN
2	B	95	GLN
2	B	119	GLN
2	B	123	GLN
2	B	155	ASN
2	B	176	GLN
3	C	17	GLN
3	C	38	ASN
3	C	77	ASN
3	C	116	GLN
3	C	120	GLN
3	C	147	GLN
3	C	160	GLN
4	D	15	GLN
4	D	91	HIS
4	D	100	ASN
4	D	146	GLN
4	D	160	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	147	GLN
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	203	ASN
6	F	240	GLN
7	G	83	ASN
7	G	114	ASN
7	G	117	GLN
7	G	121	GLN
7	G	166	GLN
7	G	167	GLN
7	G	175	ASN
8	H	22	GLN

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Mol	Chain	Res	Type
8	H	30	ASN
8	H	66	HIS
8	H	165	ASN
8	H	189	ASN
8	H	194	ASN
9	I	37	ASN
9	I	63	ASN
9	I	168	GLN
9	I	172	ASN
10	J	10	GLN
10	J	55	GLN
10	J	63	ASN
10	J	86	GLN
10	J	191	GLN
11	K	9	GLN
11	K	85	ASN
11	K	133	GLN
11	K	143	ASN
11	K	176	ASN
11	K	208	ASN
12	L	3	ASN
12	L	36	ASN
12	L	49	ASN
12	L	55	ASN
12	L	70	ASN
12	L	80	ASN
12	L	94	GLN
12	L	152	ASN
12	L	153	GLN
12	L	158	ASN
12	L	165	ASN
12	L	197	GLN
13	M	18	ASN
13	M	26	ASN
13	M	48	ASN
13	M	102	GLN
13	M	108	ASN
13	M	149	HIS
13	M	179	ASN
13	M	194	ASN
13	M	213	GLN
14	N	141	ASN

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Mol	Chain	Res	Type
14	N	161	GLN
1	O	149	GLN
2	P	20	GLN
2	P	95	GLN
2	P	119	GLN
2	P	123	GLN
2	P	176	GLN
3	Q	17	GLN
3	Q	38	ASN
3	Q	77	ASN
3	Q	116	GLN
3	Q	120	GLN
3	Q	147	GLN
3	Q	160	GLN
3	Q	233	GLN
4	R	15	GLN
4	R	91	HIS
4	R	100	ASN
4	R	146	GLN
4	R	160	ASN
4	R	225	ASN
5	S	68	HIS
5	S	99	ASN
5	S	116	GLN
5	S	118	ASN
5	S	120	GLN
5	S	151	ASN
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	203	ASN
6	T	240	GLN
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

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Mol	Chain	Res	Type
8	V	22	GLN
8	V	30	ASN
8	V	165	ASN
8	V	189	ASN
9	W	37	ASN
9	W	44	HIS
9	W	63	ASN
9	W	168	GLN
9	W	203	GLN
10	X	55	GLN
10	X	63	ASN
10	X	86	GLN
10	X	191	GLN
11	Y	9	GLN
11	Y	85	ASN
11	Y	133	GLN
11	Y	143	ASN
11	Y	176	ASN
11	Y	208	ASN
12	Z	1	GLN
12	Z	3	ASN
12	Z	8	ASN
12	Z	29	ASN
12	Z	36	ASN
12	Z	49	ASN
12	Z	55	ASN
12	Z	70	ASN
12	Z	80	ASN
12	Z	87	ASN
12	Z	94	GLN
12	Z	153	GLN
12	Z	197	GLN
13	a	18	ASN
13	a	48	ASN
13	a	102	GLN
13	a	108	ASN
13	a	149	HIS
13	a	179	ASN
13	a	194	ASN
13	a	213	GLN
14	b	141	ASN
14	b	161	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 15 ligands modelled in this entry, 9 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	VSZ	Y	302	11	25,25,25	1.09	2 (8%)	31,34,34	1.29	3 (9%)
17	VSZ	H	301	8	25,25,25	1.31	5 (20%)	31,34,34	1.15	2 (6%)
17	VSZ	b	201	14	25,25,25	1.02	3 (12%)	31,34,34	1.06	2 (6%)
17	VSZ	N	202	14	25,25,25	0.91	1 (4%)	31,34,34	0.96	1 (3%)
17	VSZ	V	301	8	25,25,25	1.24	2 (8%)	31,34,34	1.12	2 (6%)
17	VSZ	K	302	11	25,25,25	1.30	2 (8%)	31,34,34	1.32	4 (12%)

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	VSZ	Y	302	11	-	16/40/40/40	-
17	VSZ	H	301	8	-	5/40/40/40	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
17	VSZ	b	201	14	-	10/40/40/40	-
17	VSZ	N	202	14	-	9/40/40/40	-
17	VSZ	V	301	8	-	7/40/40/40	-
17	VSZ	K	302	11	-	12/40/40/40	-

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	K	302	VSZ	C4-C9	-3.68	1.51	1.54
17	H	301	VSZ	C4-C9	-3.37	1.51	1.54
17	V	301	VSZ	C4-C9	-3.30	1.51	1.54
17	K	302	VSZ	C4-C5	-3.25	1.50	1.55
17	Y	302	VSZ	C4-C9	-2.82	1.51	1.54
17	V	301	VSZ	C4-C5	-2.81	1.51	1.55
17	b	201	VSZ	C4-C9	-2.77	1.51	1.54
17	H	301	VSZ	C4-C5	-2.40	1.51	1.55
17	H	301	VSZ	C21-C25	-2.27	1.48	1.52
17	b	201	VSZ	O27-C25	-2.18	1.23	1.30
17	H	301	VSZ	C18-N20	-2.10	1.29	1.34
17	Y	302	VSZ	O27-C25	-2.08	1.24	1.30
17	b	201	VSZ	C21-C25	-2.05	1.49	1.52
17	H	301	VSZ	O27-C25	-2.01	1.24	1.30
17	N	202	VSZ	O27-C25	-2.00	1.24	1.30

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	Y	302	VSZ	O10-C9-C11	-3.62	103.05	110.63
17	K	302	VSZ	C15-C14-C18	-2.91	104.28	111.38
17	K	302	VSZ	O10-C9-C11	-2.85	104.68	110.63
17	b	201	VSZ	O3-C1-C4	-2.84	118.49	125.27
17	K	302	VSZ	C9-C4-C1	-2.82	104.80	110.65
17	Y	302	VSZ	C9-C4-C1	-2.66	105.13	110.65
17	N	202	VSZ	O3-C1-C4	-2.66	118.93	125.27
17	H	301	VSZ	C7-C5-C4	-2.50	107.24	111.76
17	K	302	VSZ	C7-C5-C4	-2.19	107.80	111.76
17	b	201	VSZ	C22-C21-C25	-2.15	105.81	111.64
17	H	301	VSZ	C22-C21-N20	-2.11	107.02	111.35
17	V	301	VSZ	O3-C1-C4	-2.07	120.32	125.27
17	V	301	VSZ	C7-C5-C4	-2.06	108.04	111.76
17	Y	302	VSZ	C15-C14-C18	-2.00	106.49	111.38

There are no chirality outliers.

All (59) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
17	K	302	VSZ	O12-C11-C9-O10
17	K	302	VSZ	C9-C4-C5-C6
17	N	202	VSZ	O12-C11-C9-O10
17	N	202	VSZ	N13-C11-C9-O10
17	N	202	VSZ	N20-C21-C22-C24
17	N	202	VSZ	C25-C21-C22-C23
17	N	202	VSZ	C25-C21-C22-C24
17	V	301	VSZ	C25-C21-C22-C23
17	Y	302	VSZ	O12-C11-C9-O10
17	Y	302	VSZ	N13-C11-C9-O10
17	Y	302	VSZ	C9-C4-C5-C6
17	Y	302	VSZ	C1-C4-C5-C6
17	Y	302	VSZ	C1-C4-C5-C7
17	b	201	VSZ	O12-C11-C9-O10
17	b	201	VSZ	C9-C4-C5-C6
17	b	201	VSZ	C1-C4-C5-C6
17	b	201	VSZ	C21-C22-C23-C42
17	H	301	VSZ	C24-C22-C23-C42
17	N	202	VSZ	N20-C21-C22-C23
17	V	301	VSZ	N20-C21-C22-C24
17	b	201	VSZ	C24-C22-C23-C42
17	K	302	VSZ	C25-C21-C22-C23
17	Y	302	VSZ	C25-C21-C22-C23
17	Y	302	VSZ	N20-C21-C22-C24
17	K	302	VSZ	N13-C11-C9-O10
17	b	201	VSZ	N13-C11-C9-O10
17	H	301	VSZ	C21-C22-C23-C42
17	K	302	VSZ	N20-C21-C22-C24
17	H	301	VSZ	N20-C21-C25-O27
17	K	302	VSZ	C22-C21-C25-O26
17	K	302	VSZ	C22-C21-C25-O27
17	Y	302	VSZ	C22-C21-C25-O26
17	Y	302	VSZ	C22-C21-C25-O27
17	V	301	VSZ	C24-C22-C23-C42
17	K	302	VSZ	C1-C4-C5-C6
17	N	202	VSZ	C9-C4-C5-C6
17	K	302	VSZ	C5-C4-C9-C11
17	Y	302	VSZ	C5-C4-C9-C11
17	V	301	VSZ	C25-C21-C22-C24
17	b	201	VSZ	C22-C21-C25-O26

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Mol	Chain	Res	Type	Atoms
17	b	201	VSZ	C22-C21-C25-O27
17	V	301	VSZ	N20-C21-C22-C23
17	Y	302	VSZ	C24-C22-C23-C42
17	Y	302	VSZ	N20-C21-C22-C23
17	K	302	VSZ	O12-C11-C9-C4
17	N	202	VSZ	O12-C11-C9-C4
17	Y	302	VSZ	O12-C11-C9-C4
17	V	301	VSZ	C21-C22-C23-C42
17	N	202	VSZ	N13-C11-C9-C4
17	Y	302	VSZ	N13-C11-C9-C4
17	Y	302	VSZ	C25-C21-C22-C24
17	K	302	VSZ	C24-C22-C23-C42
17	Y	302	VSZ	C9-C4-C5-C7
17	b	201	VSZ	N13-C11-C9-C4
17	H	301	VSZ	N20-C21-C25-O26
17	V	301	VSZ	N20-C21-C25-O27
17	K	302	VSZ	N20-C21-C22-C23
17	b	201	VSZ	O12-C11-C9-C4
17	H	301	VSZ	N20-C21-C22-C24

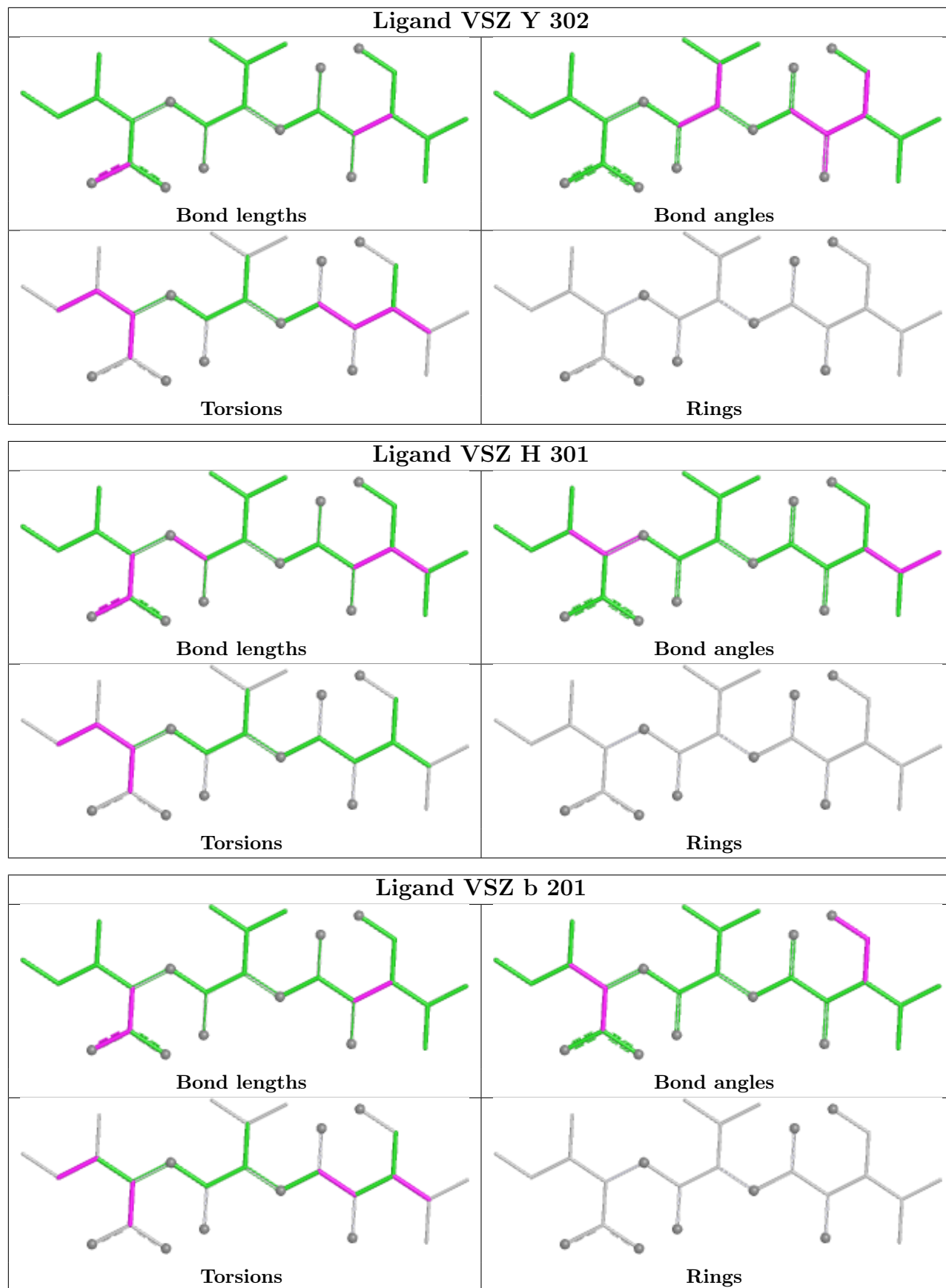
There are no ring outliers.

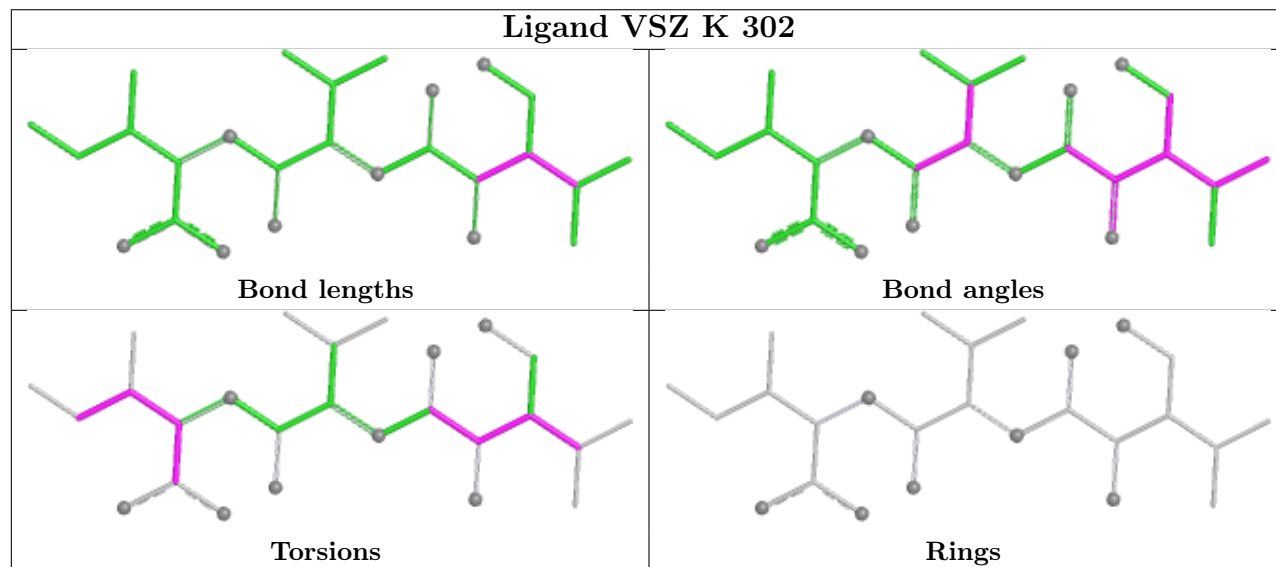
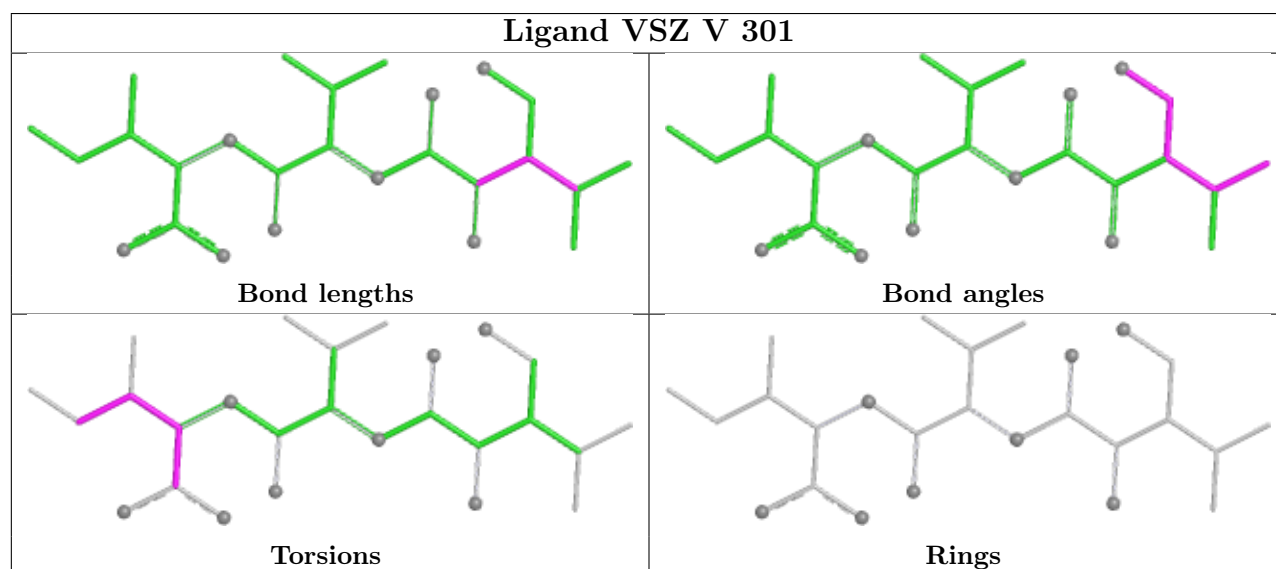
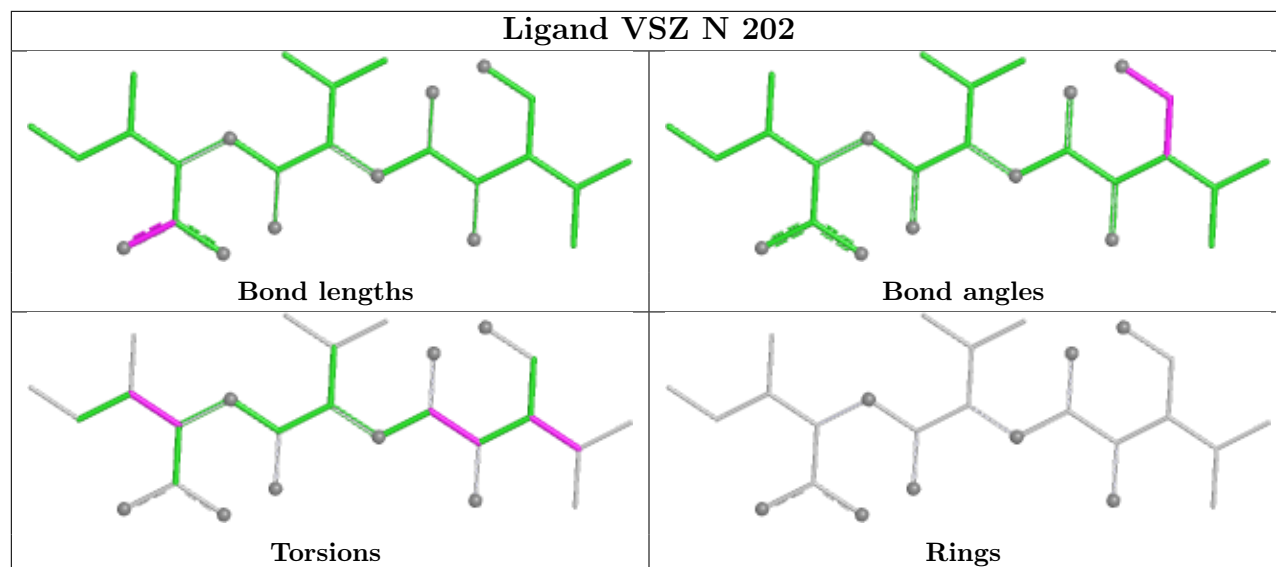
6 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
17	Y	302	VSZ	3	0
17	H	301	VSZ	1	0
17	b	201	VSZ	4	0
17	N	202	VSZ	1	0
17	V	301	VSZ	1	0
17	K	302	VSZ	3	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.





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%)	-0.83	0 100 100	66, 82, 119, 164	0
1	O	250/250 (100%)	-0.77	0 100 100	72, 93, 134, 169	0
2	B	244/258 (94%)	-0.66	0 100 100	66, 94, 149, 208	0
2	P	244/258 (94%)	-0.68	0 100 100	69, 93, 143, 201	0
3	C	240/254 (94%)	-0.62	0 100 100	66, 98, 156, 175	0
3	Q	240/254 (94%)	-0.63	2 (0%) 82 75	76, 110, 177, 197	0
4	D	235/260 (90%)	-0.79	0 100 100	68, 95, 125, 155	0
4	R	235/260 (90%)	-0.66	0 100 100	73, 106, 138, 162	0
5	E	231/234 (98%)	-0.75	0 100 100	72, 97, 130, 160	0
5	S	231/234 (98%)	-0.70	0 100 100	72, 107, 147, 165	0
6	F	243/288 (84%)	-0.81	0 100 100	67, 92, 139, 157	0
6	T	243/288 (84%)	-0.69	0 100 100	70, 102, 149, 178	0
7	G	241/252 (95%)	-0.84	0 100 100	63, 82, 115, 152	0
7	U	241/252 (95%)	-0.76	0 100 100	66, 89, 122, 155	0
8	H	226/232 (97%)	-0.83	1 (0%) 88 84	57, 74, 108, 172	0
8	V	226/232 (97%)	-0.83	1 (0%) 88 84	61, 78, 111, 202	0
9	I	204/205 (99%)	-0.96	0 100 100	54, 71, 96, 122	0
9	W	204/205 (99%)	-0.98	0 100 100	56, 72, 102, 128	0
10	J	195/198 (98%)	-0.90	1 (0%) 87 82	57, 75, 102, 144	0
10	X	195/198 (98%)	-0.90	1 (0%) 87 82	60, 76, 100, 164	0
11	K	212/212 (100%)	-0.94	0 100 100	54, 72, 95, 111	0
11	Y	212/212 (100%)	-0.91	0 100 100	59, 74, 99, 120	0
12	L	222/222 (100%)	-0.90	0 100 100	57, 75, 107, 135	0
12	Z	222/222 (100%)	-0.88	0 100 100	57, 77, 109, 130	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	M	233/246 (94%)	-0.88	0 100 100	57, 78, 105, 128	0
13	a	233/246 (94%)	-0.94	1 (0%) 88 84	56, 76, 100, 116	0
14	N	196/196 (100%)	-0.92	0 100 100	58, 72, 103, 129	0
14	b	196/196 (100%)	-0.92	0 100 100	61, 74, 104, 132	0
All	All	6344/6614 (95%)	-0.81	7 (0%) 92 90	54, 84, 135, 208	0

All (7) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	Q	50	LEU	3.6
10	J	1	MET	3.0
8	V	223	ILE	3.0
10	X	1	MET	2.9
8	H	223	ILE	2.8
3	Q	205	ALA	2.2
13	a	1	THR	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
17	VSZ	N	202	26/26	0.91	0.11	59,80,95,107	0
17	VSZ	Y	302	26/26	0.91	0.09	65,93,105,125	0
17	VSZ	b	201	26/26	0.91	0.12	66,84,98,110	0
17	VSZ	K	302	26/26	0.94	0.09	56,93,114,129	0
17	VSZ	V	301	26/26	0.94	0.09	64,74,95,106	0

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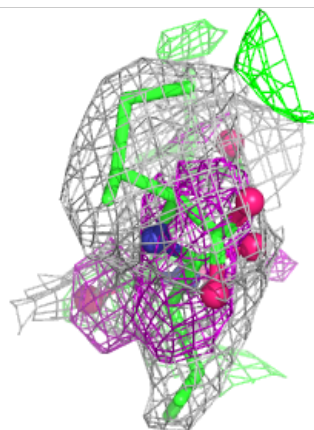
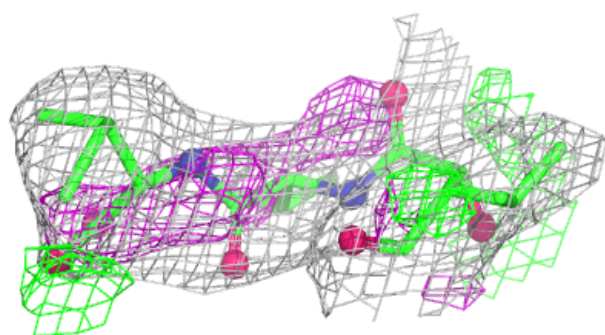
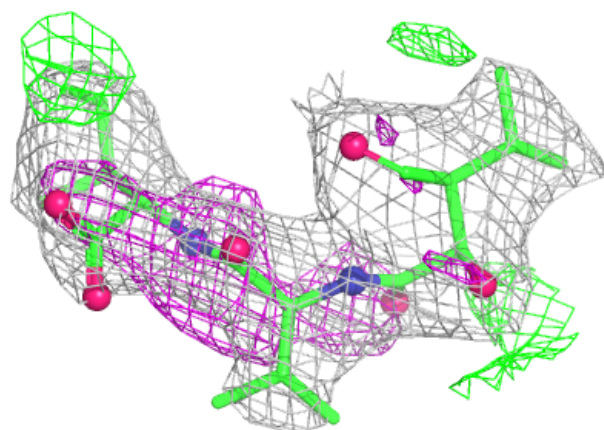
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
17	VSZ	H	301	26/26	0.95	0.09	67,75,95,102	0
15	MG	G	301	1/1	0.97	0.10	74,74,74,74	0
15	MG	Z	301	1/1	0.97	0.07	80,80,80,80	0
16	CL	G	302	1/1	0.98	0.11	69,69,69,69	0
16	CL	U	301	1/1	0.98	0.10	79,79,79,79	0
15	MG	W	301	1/1	0.98	0.06	81,81,81,81	0
15	MG	N	201	1/1	0.98	0.04	65,65,65,65	0
15	MG	Y	301	1/1	0.99	0.03	86,86,86,86	0
15	MG	I	301	1/1	0.99	0.05	77,77,77,77	0
15	MG	K	301	1/1	1.00	0.07	80,80,80,80	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.

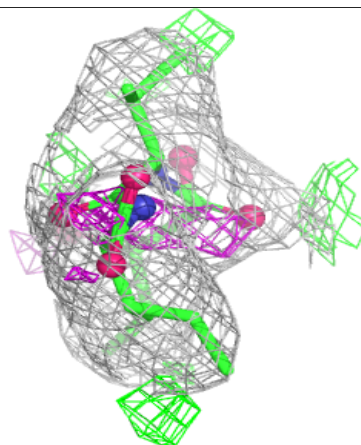
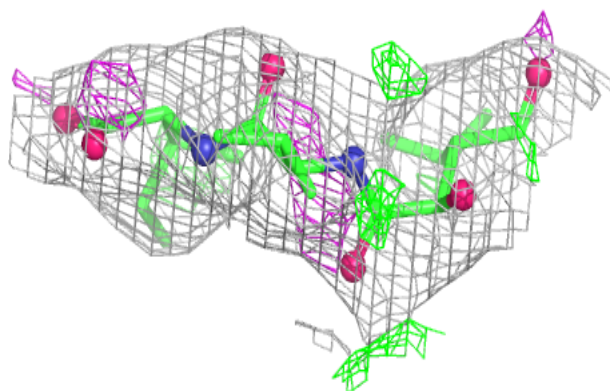
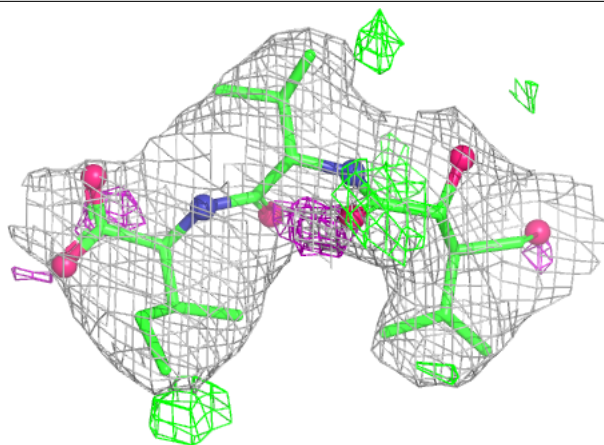
Electron density around VSZ N 202:

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



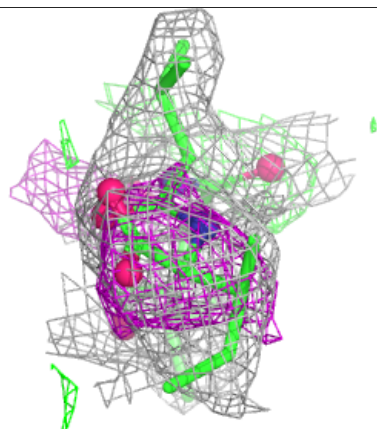
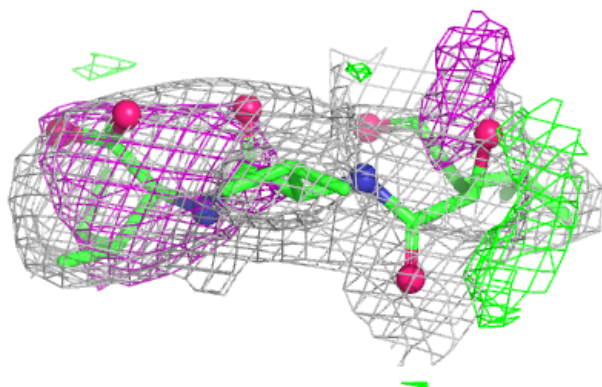
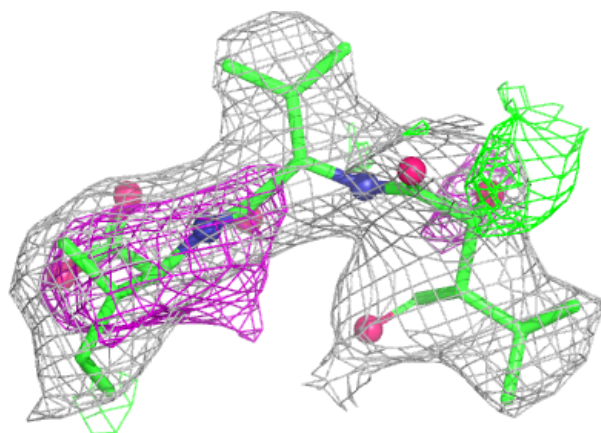
Electron density around VSZ Y 302:

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

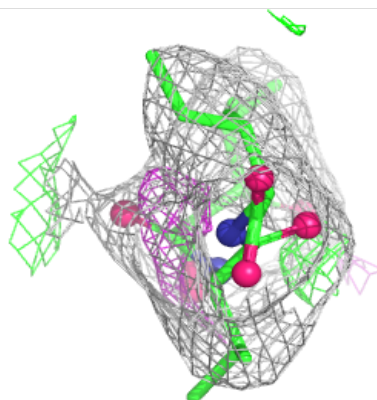
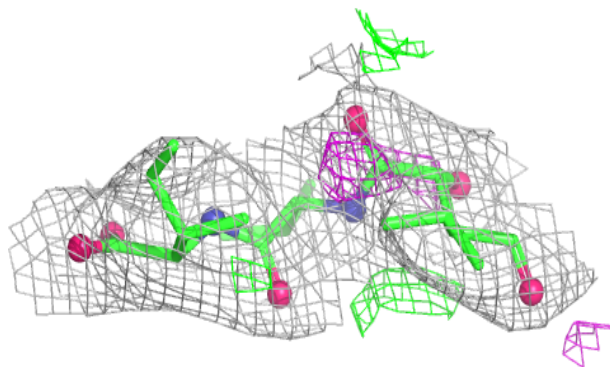
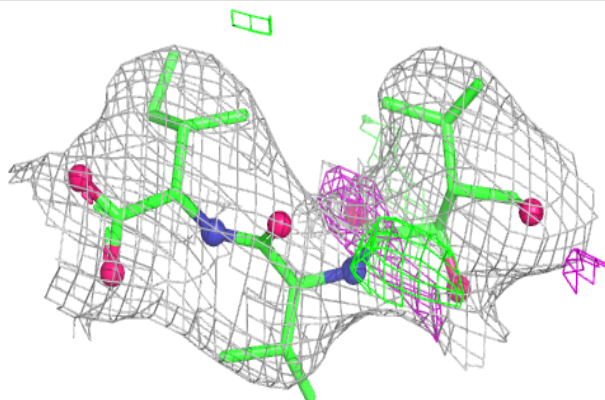


Electron density around VSZ b 201:

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

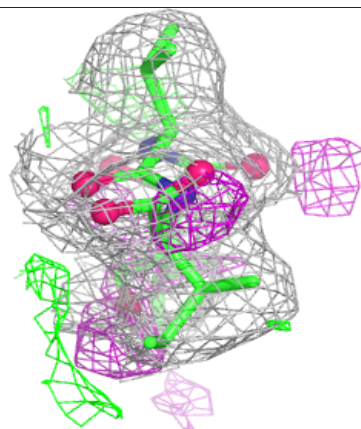
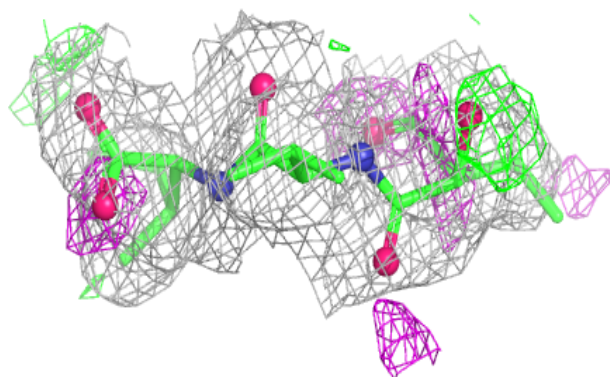
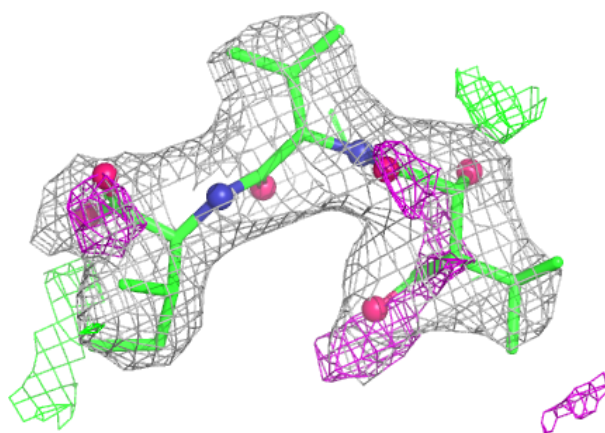
**Electron density around VSZ K 302:**

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

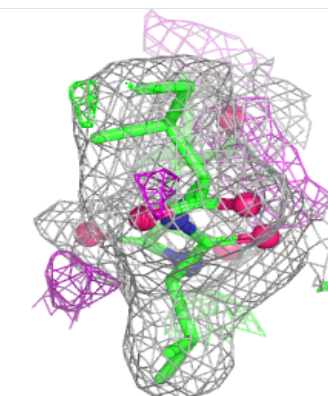
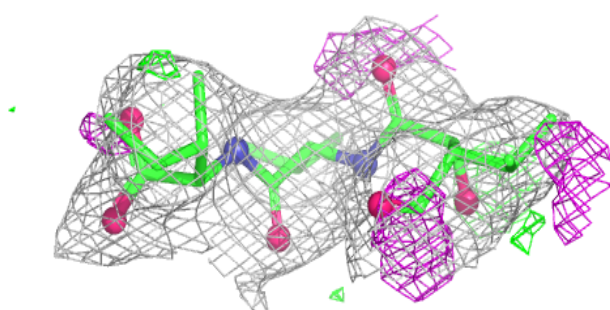
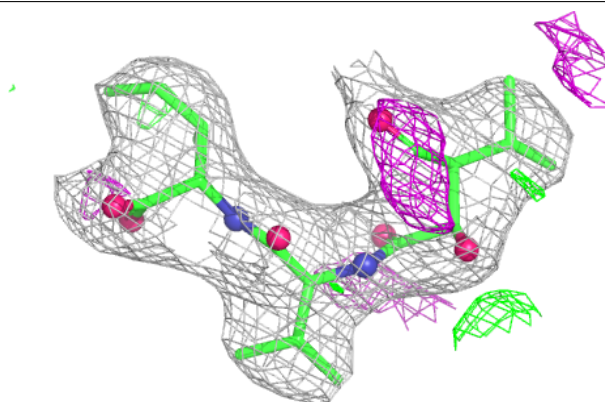


Electron density around VSZ V 301:

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

**Electron density around VSZ 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.