



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 17, 2026 – 08:31 PM UTC

PDB ID : 5HL7 / pdb_00005hl7
Title : The crystal structure of the large ribosomal subunit of *Staphylococcus aureus* in complex with lefamulin
Authors : Eyal, Z.; Matzov, D.; Krupkin, M.; Rozenberg, H.; Zimmerman, E.; Bashan, A.; Yonath, A.
Deposited on : 2016-01-14
Resolution : 3.55 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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

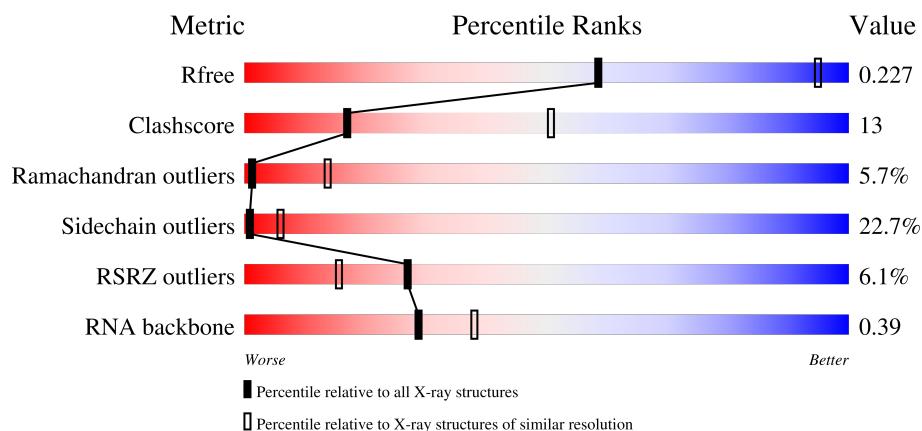
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.55 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	1410 (3.62-3.50)
Clashscore	190562	1480 (3.62-3.50)
Ramachandran outliers	187476	1440 (3.62-3.50)
Sidechain outliers	187428	1441 (3.62-3.50)
RSRZ outliers	180081	1409 (3.62-3.50)
RNA backbone	3983	1006 (4.02-3.06)

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	277	10% 66% 24% 6% ••
2	X	2923	3% 44% 39% 10% 7%
3	Y	114	3% 43% 52% 5%

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Mol	Chain	Length	Quality of chain
4	B	220	
5	C	207	
6	D	179	
7	E	178	
8	G	145	
9	H	122	
10	I	140	
11	J	144	
12	K	122	
13	L	119	
14	M	116	
15	N	118	
16	O	102	
17	P	117	
18	Q	91	
19	R	105	
20	S	217	
21	T	94	
22	U	62	
23	V	69	
24	W	59	
25	Z	58	
26	2	45	
27	3	66	
28	4	37	

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
30	MG	A	303	-	-	-	X
30	MG	A	304	-	-	-	X
30	MG	X	3002	-	-	-	X
30	MG	X	3165	-	-	-	X
30	MG	X	3250	-	-	-	X
30	MG	X	3265	-	-	-	X
30	MG	X	3287	-	-	-	X
30	MG	X	3291	-	-	-	X
30	MG	X	3327	-	-	-	X
30	MG	X	3342	-	-	-	X
30	MG	X	3347	-	-	-	X
30	MG	X	3349	-	-	-	X
30	MG	X	3351	-	-	-	X
30	MG	X	3358	-	-	-	X
30	MG	X	3370	-	-	-	X
30	MG	X	3385	-	-	-	X
30	MG	X	3417	-	-	-	X
30	MG	X	3424	-	-	-	X
30	MG	X	3488	-	-	-	X
30	MG	Y	205	-	-	-	X
35	EPE	N	201	-	-	X	-

2 Entry composition

There are 35 unique types of molecules in this entry. The entry contains 81462 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 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	269	Total	C	N	O	S	0	0	0
			1667	1007	331	324	5			

- Molecule 2 is a RNA chain called 23S ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	X	2705	Total	C	N	O	P	0	0	0
			57983	25884	10620	18774	2705			

- Molecule 3 is a RNA chain called 5S ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	Y	114	Total	C	N	O	P	0	0	0
			2430	1086	436	794	114			

- Molecule 4 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	B	215	Total	C	N	O	S	0	0	0
			1547	967	289	286	5			

- Molecule 5 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	C	199	Total	C	N	O	S	0	0	0
			1324	823	250	249	2			

- Molecule 6 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	D	165	Total	C	N	O	S	0	0	0
			853	512	165	174	2			

- Molecule 7 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	E	157	Total	C	N	O	S	0	0	0
			915	559	172	182	2			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	174	LYS	GLY	conflict	UNP Q2FW21

- Molecule 8 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	G	145	Total	C	N	O	S	0	0	0
			1090	682	202	203	3			

- Molecule 9 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	H	122	Total	C	N	O	S	0	0	0
			884	548	167	165	4			

- Molecule 10 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	I	131	Total	C	N	O	S	0	0	0
			819	498	164	156	1			

- Molecule 11 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	J	138	Total	C	N	O	S	0	0	0
			1001	641	187	170	3			

- Molecule 12 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	K	119	Total	C	N	O	S	0	0	0
			906	556	175	174	1			

- Molecule 13 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
13	L	109	Total	C	N	O	0	0	0
			673	411	134	128			

- Molecule 14 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
14	M	110	Total	C	N	O	0	0	0
			807	510	162	135			

- Molecule 15 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	N	116	Total	C	N	O	S	0	0	0
			922	581	183	154	4			

- Molecule 16 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	O	102	Total	C	N	O	S	0	0	0
			751	477	138	135	1			

- Molecule 17 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	P	112	Total	C	N	O	S	0	0	0
			853	531	161	158	3			

- Molecule 18 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
18	Q	90	Total	C	N	O	S	0	0	0
			583	365	103	112	3			

- Molecule 19 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	R	102	Total	C	N	O	S	0	0	0
			627	382	120	124	1			

- Molecule 20 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	S	167	Total	C	N	O	S	0	0	0
			1087	682	191	212	2			

- Molecule 21 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
21	T	75	Total	C	N	O		0	0	0
			559	349	110	100				

- Molecule 22 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	U	42	Total	C	N	O		0	0	0
			242	149	48	45				

- Molecule 23 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	V	65	Total	C	N	O		0	0	0
			486	299	89	98				

- Molecule 24 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
24	W	57	Total	C	N	O		0	0	0
			437	271	82	84				

- Molecule 25 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
25	Z	43	Total	C	N	O	S	0	0	0
			339	208	70	57	4			

- Molecule 26 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	2	43	Total	C	N	O	S	0	0	0
			350	213	85	51	1			

- Molecule 27 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
27	3	60	Total	C	N	O	S	0	0	0
			405	248	81	74	2			

- Molecule 28 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
28	4	36	Total	C	N	O	S	0	0	0
			181	107	36	36	2			

- Molecule 29 is MANGANESE (II) ION (CCD ID: MN) (formula: Mn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
29	A	1	Total	Mn	0	0
			1	1		
29	X	268	Total	Mn	0	0
			268	268		
29	Y	2	Total	Mn	0	0
			2	2		
29	R	1	Total	Mn	0	0
			1	1		
29	T	1	Total	Mn	0	0
			1	1		
29	Z	1	Total	Mn	0	0
			1	1		

- Molecule 30 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

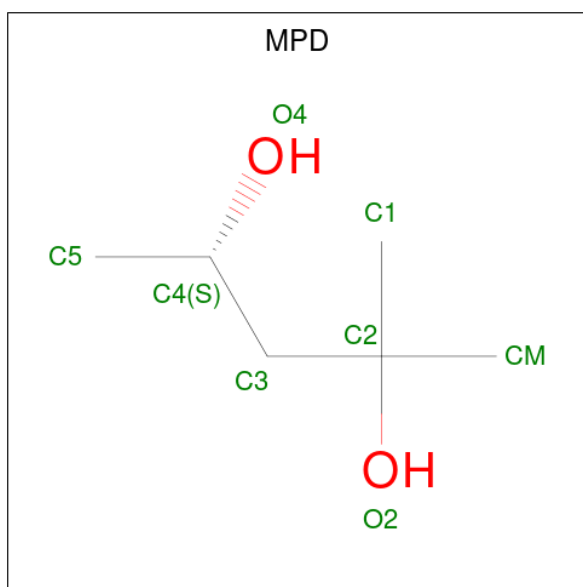
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
30	A	3	Total	Mg	0	0
			3	3		
30	X	218	Total	Mg	0	0
			218	218		
30	Y	10	Total	Mg	0	0
			10	10		
30	C	2	Total	Mg	0	0
			2	2		
30	G	2	Total	Mg	0	0
			2	2		
30	I	1	Total	Mg	0	0
			1	1		
30	J	1	Total	Mg	0	0
			1	1		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
30	M	1	Total Mg 1 1	0	0
30	O	1	Total Mg 1 1	0	0
30	P	1	Total Mg 1 1	0	0

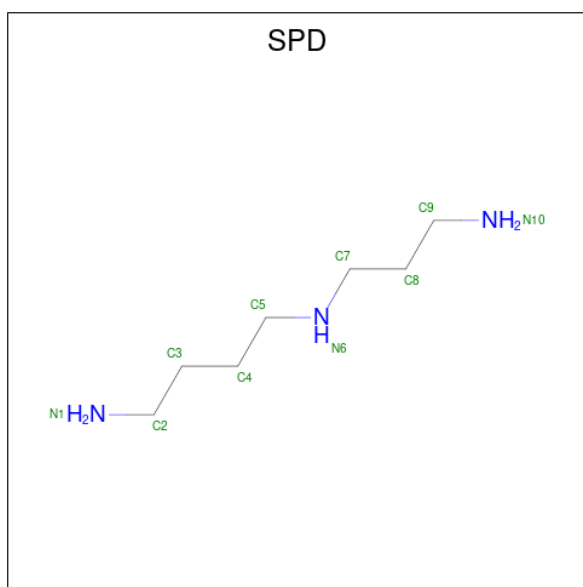
-
- Chemical structure of compound 62B, a complex polycyclic molecule. The structure features a central bicyclic core with several stereocenters labeled with C and S. Key functional groups include a hydroxyl group (OH) at C11(S), a carboxylic acid group (COOH) at C2, and a sulfonamide group (SO₂NH₂) at C23(R). The molecule is highly substituted with various rings and side chains, including a cyclohexane ring fused to a cyclopentane ring, and a cyclohexane ring fused to a cyclohexane ring. Stereochemistry is indicated by wedged and dashed bonds, and specific configurations are noted for several centers (e.g., C11(S), C23(R), C26(R), C28(R)).

- Molecule 32 is (4S)-2-METHYL-2,4-PENTANEDIOL (CCD ID: MPD) (formula: C₆H₁₄O₂).



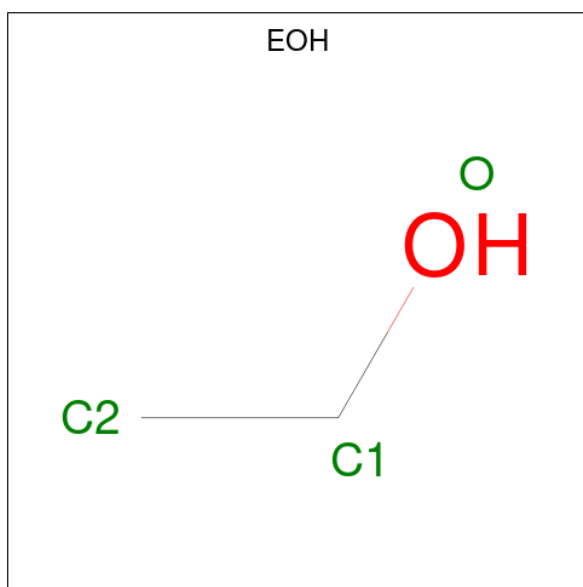
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
32	X	1	Total	C	O	0	0
			8	6	2		
32	X	1	Total	C	O	0	0
			8	6	2		
32	X	1	Total	C	O	0	0
			8	6	2		
32	X	1	Total	C	O	0	0
			8	6	2		
32	X	1	Total	C	O	0	0
			8	6	2		
32	X	1	Total	C	O	0	0
			8	6	2		
32	X	1	Total	C	O	0	0
			8	6	2		
32	J	1	Total	C	O	0	0
			8	6	2		
32	Q	1	Total	C	O	0	0
			8	6	2		
32	Z	1	Total	C	O	0	0
			8	6	2		

- Molecule 33 is SPERMIDINE (CCD ID: SPD) (formula: $C_7H_{19}N_3$).



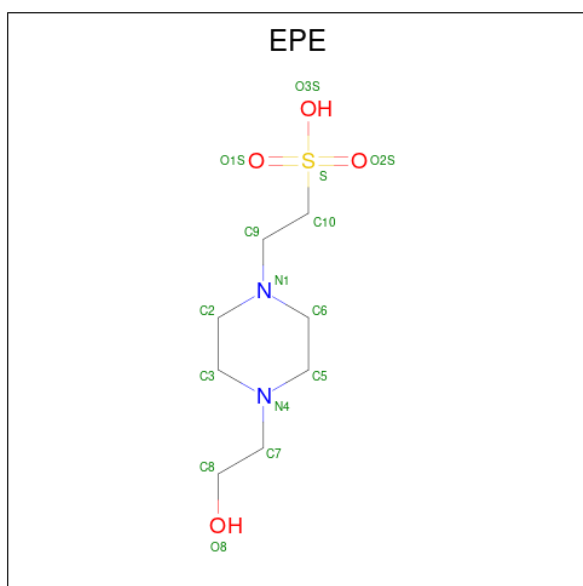
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
33	X	1	Total	C	N	0	0
			10	7	3		
33	X	1	Total	C	N	0	0
			10	7	3		
33	X	1	Total	C	N	0	0
			10	7	3		
33	X	1	Total	C	N	0	0
			10	7	3		
33	X	1	Total	C	N	0	0
			10	7	3		
33	X	1	Total	C	N	0	0
			10	7	3		
33	Y	1	Total	C	N	0	0
			10	7	3		

- Molecule 34 is ETHANOL (CCD ID: EOH) (formula: C₂H₆O).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
34	X	1	Total	C	O	0	0
			3	2	1		
34	X	1	Total	C	O	0	0
			3	2	1		
34	S	1	Total	C	O	0	0
			3	2	1		

- Molecule 35 is 4-(2-HYDROXYETHYL)-1-PIPERAZINE ETHANESULFONIC ACID (CCD ID: EPE) (formula: $C_8H_{18}N_2O_4S$).

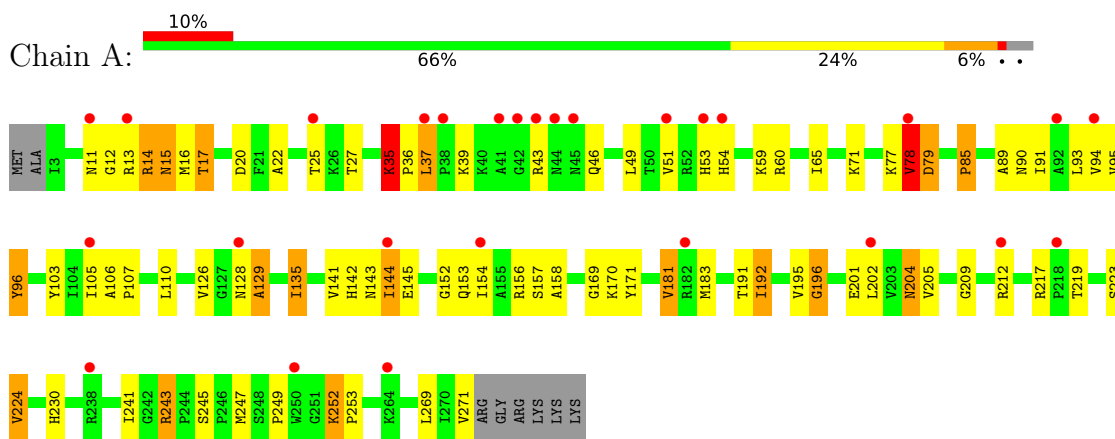


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
35	N	1	Total	C	N	O	S	0	0
			15	8	2	4	1		

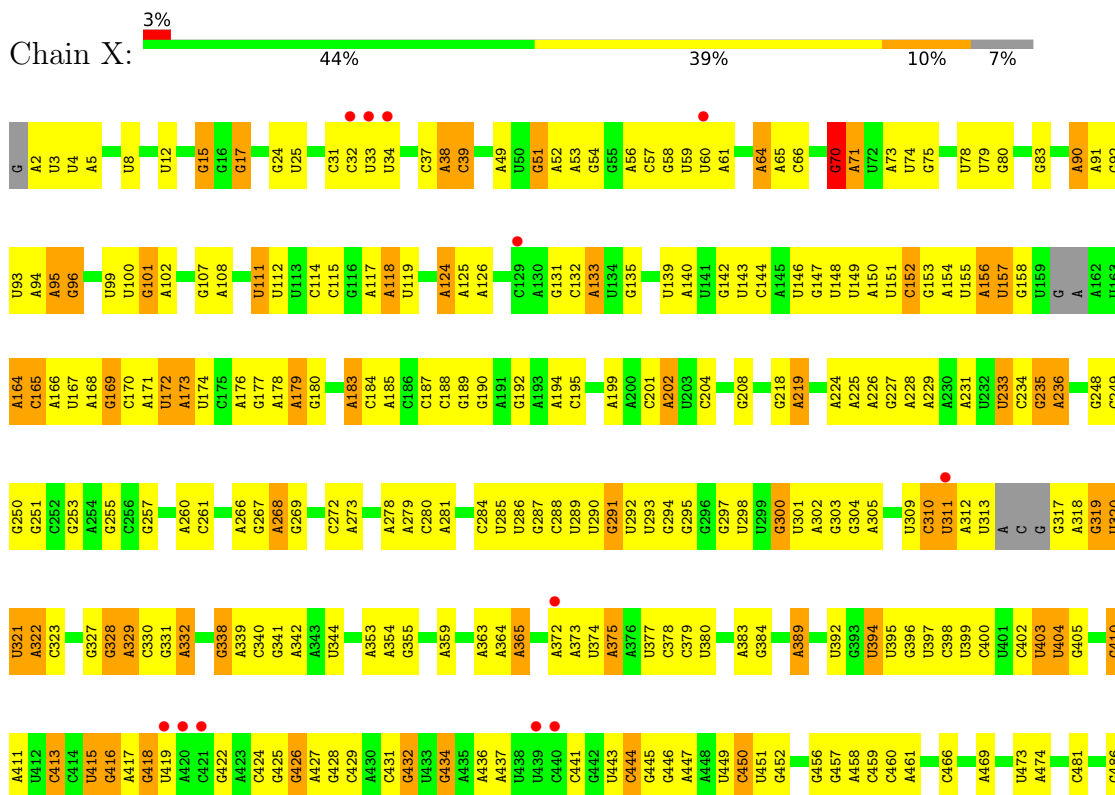
3 Residue-property plots [i](#)

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: 50S ribosomal protein L2

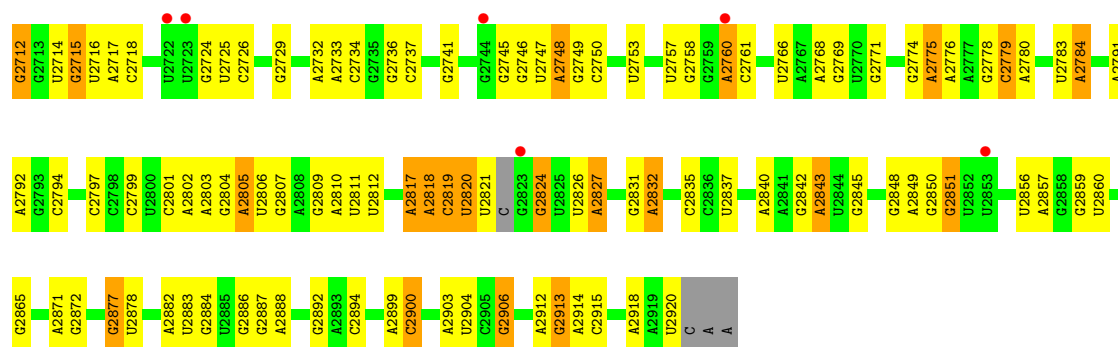


• Molecule 2: 23S ribosomal RNA

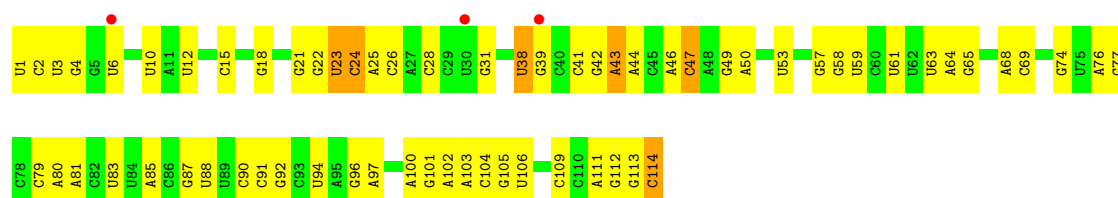




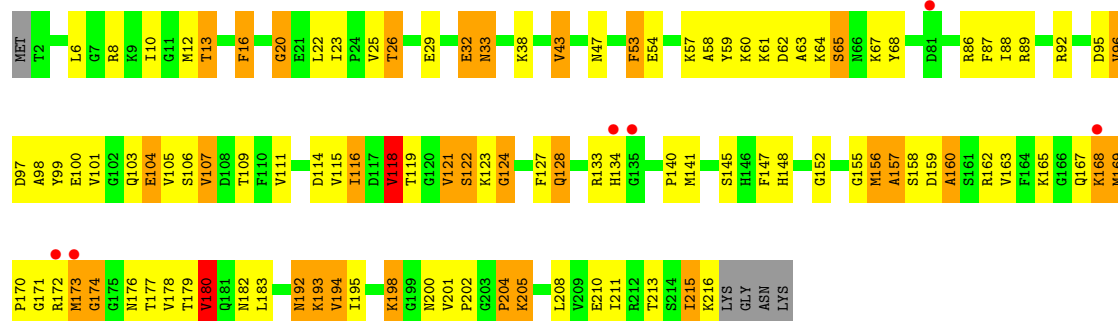




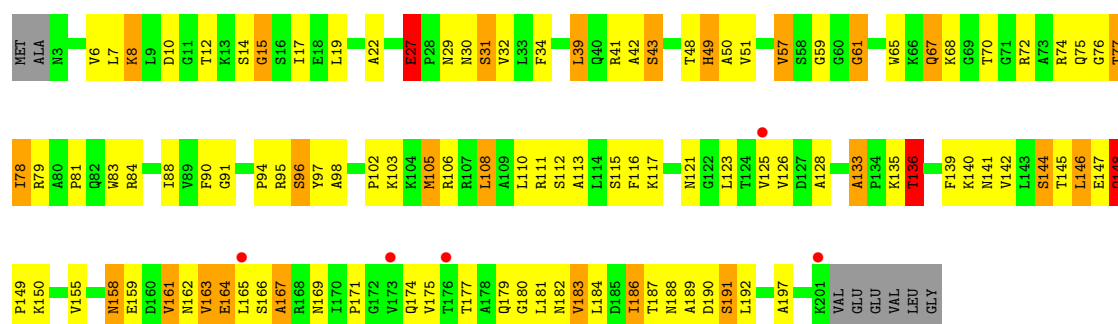
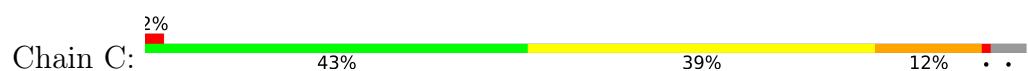
• Molecule 3: 5S ribosomal RNA



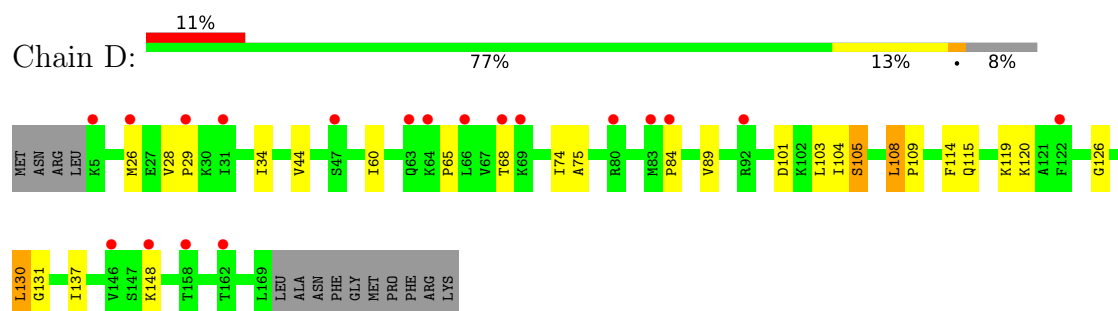
• Molecule 4: 50S ribosomal protein L3



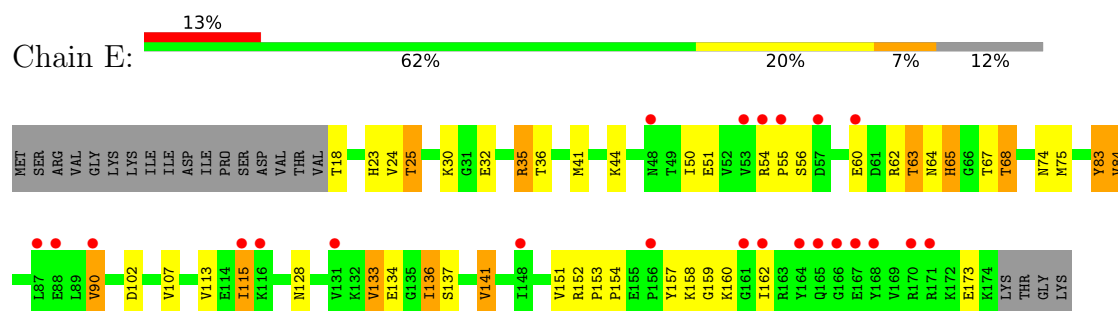
• Molecule 5: 50S ribosomal protein L4



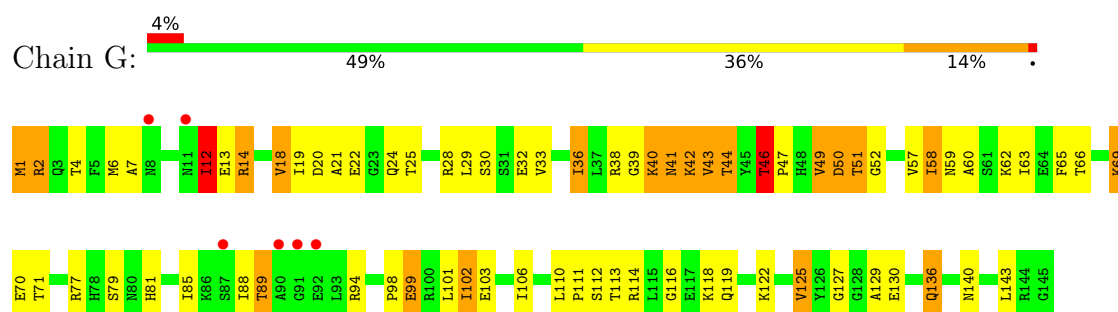
- Molecule 6: 50S ribosomal protein L5



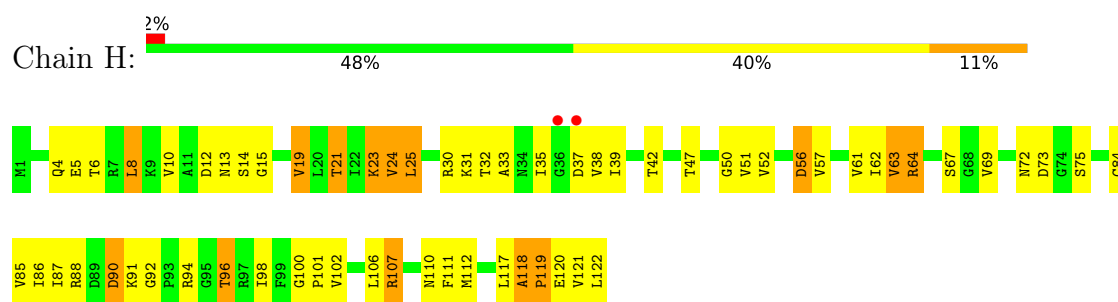
- Molecule 7: 50S ribosomal protein L6



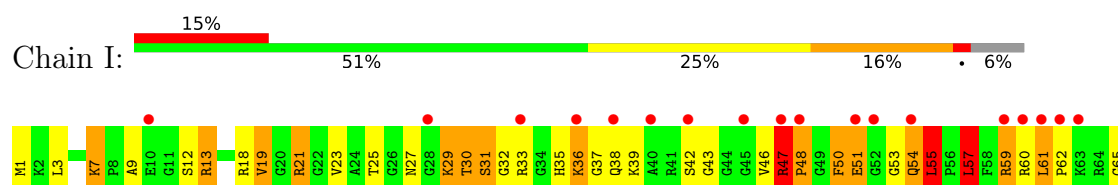
- Molecule 8: 50S ribosomal protein L13

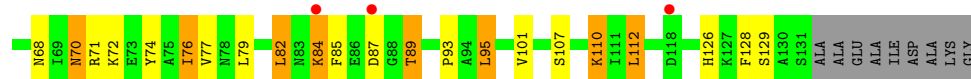


- Molecule 9: 50S ribosomal protein L14

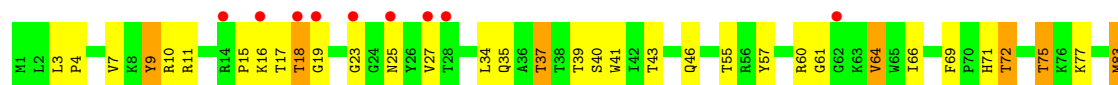


- Molecule 10: 50S ribosomal protein L15

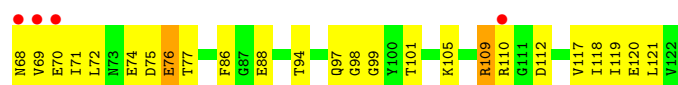




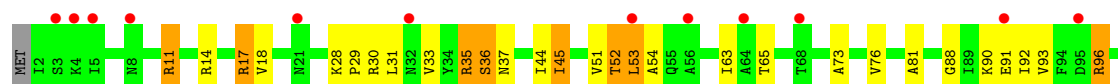
- Molecule 11: 50S ribosomal protein L16



- Molecule 12: 50S ribosomal protein L17



- Molecule 13: 50S ribosomal protein L18

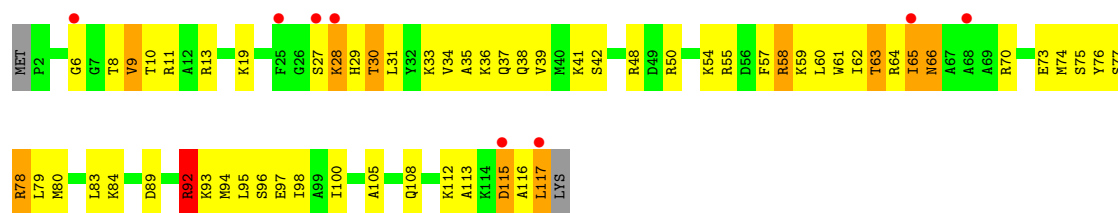


- Molecule 14: 50S ribosomal protein L19

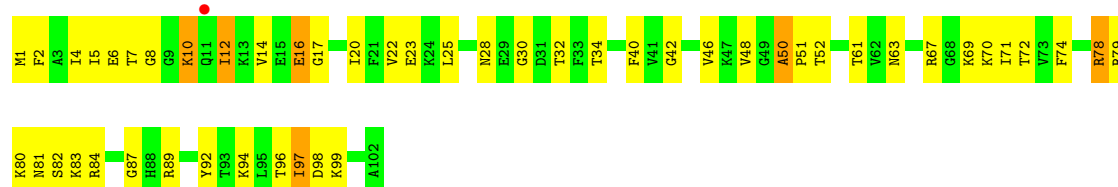


- Molecule 15: 50S ribosomal protein L20

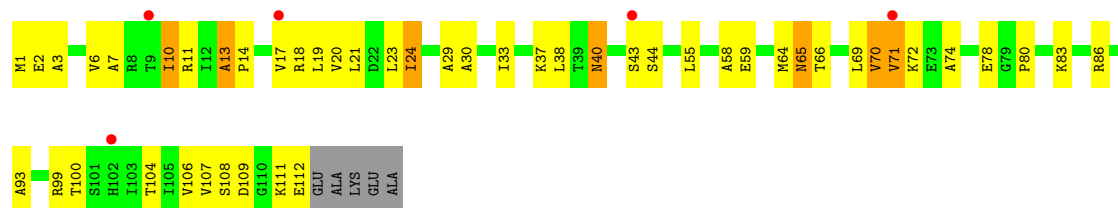




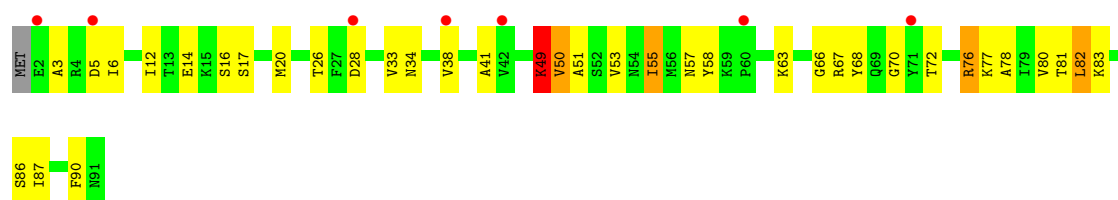
• Molecule 16: 50S ribosomal protein L21



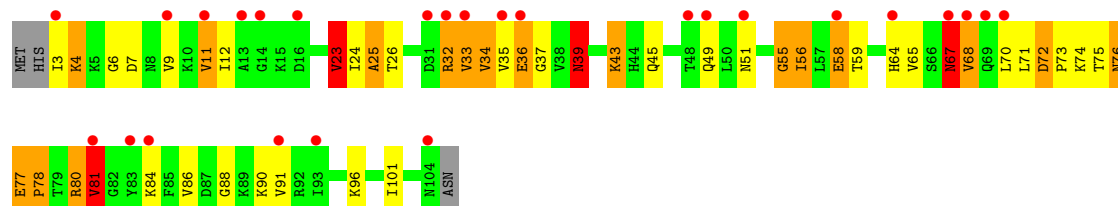
• Molecule 17: 50S ribosomal protein L22



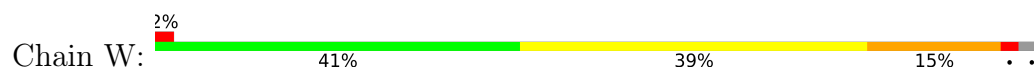
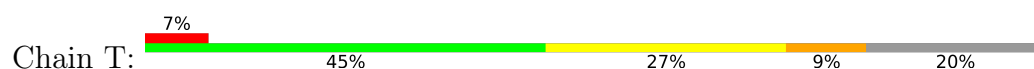
• Molecule 18: 50S ribosomal protein L23



• Molecule 19: 50S ribosomal protein L24

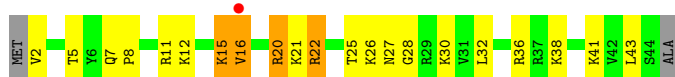


Chain S: %





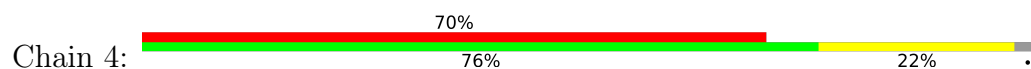
- Molecule 26: 50S ribosomal protein L34



- Molecule 27: 50S ribosomal protein L35



- Molecule 28: 50S ribosomal protein L36



4 Data and refinement statistics

Property	Value	Source
Space group	P 65 2 2	Depositor
Cell constants a, b, c, α , β , γ	282.11Å 282.11Å 875.34Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	49.93 – 3.55 49.93 – 3.55	Depositor EDS
% Data completeness (in resolution range)	95.4 (49.93-3.55) 95.6 (49.93-3.55)	Depositor EDS
R_{merge}	0.21	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.53 (at 3.57Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.187 , 0.227 0.189 , 0.227	Depositor DCC
R_{free} test set	11848 reflections (4.79%)	wwPDB-VP
Wilson B-factor (Å ²)	105.6	Xtriage
Anisotropy	0.307	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.24 , 59.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	81462	wwPDB-VP
Average B, all atoms (Å ²)	110.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.34% 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: MN, EOH, MG, 62B, SPD, MPD, EPE

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	0.39	0/1697	1.00	8/2332 (0.3%)
2	X	0.50	1/64923 (0.0%)	0.70	5/101215 (0.0%)
3	Y	0.46	0/2717	0.65	0/4232
4	B	0.91	2/1570 (0.1%)	1.33	23/2117 (1.1%)
5	C	1.02	3/1343 (0.2%)	1.52	24/1838 (1.3%)
6	D	0.56	0/855	1.04	3/1185 (0.3%)
7	E	0.71	1/925 (0.1%)	1.10	3/1279 (0.2%)
8	G	1.02	3/1112 (0.3%)	1.34	11/1507 (0.7%)
9	H	0.81	0/891	1.17	6/1203 (0.5%)
10	I	1.12	4/827 (0.5%)	1.57	16/1121 (1.4%)
11	J	0.85	1/1023 (0.1%)	1.34	14/1388 (1.0%)
12	K	0.48	0/909	0.91	0/1217
13	L	0.75	0/678	1.18	5/927 (0.5%)
14	M	0.94	1/819 (0.1%)	1.29	5/1107 (0.5%)
15	N	1.05	1/934 (0.1%)	1.33	7/1241 (0.6%)
16	O	1.00	0/761	1.58	9/1022 (0.9%)
17	P	0.59	0/861	1.00	4/1160 (0.3%)
18	Q	0.84	1/589 (0.2%)	1.27	5/808 (0.6%)
19	R	1.13	3/631 (0.5%)	1.32	3/863 (0.3%)
20	S	0.86	2/1099 (0.2%)	1.29	9/1509 (0.6%)
21	T	0.78	0/565	1.15	2/751 (0.3%)
22	U	0.58	0/247	1.03	1/344 (0.3%)
23	V	0.56	0/487	1.03	2/654 (0.3%)
24	W	0.95	1/439 (0.2%)	1.25	1/593 (0.2%)
25	Z	0.96	0/345	1.19	4/460 (0.9%)
26	2	0.85	0/353	1.29	3/463 (0.6%)
27	3	1.06	0/409	1.50	8/550 (1.5%)
28	4	0.80	0/180	1.38	1/249 (0.4%)
All	All	0.60	24/88189 (0.0%)	0.85	182/133335 (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
1	A	0	1
4	B	0	2
5	C	0	2
10	I	0	1
16	O	0	1
17	P	0	1
20	S	0	1
27	3	0	2
All	All	0	11

The worst 5 of 24 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	R	68	VAL	CA-CB	14.12	1.68	1.54
19	R	67	ASN	CA-C	6.44	1.61	1.52
15	N	34	VAL	CA-CB	-6.04	1.47	1.54
8	G	50	ASP	CA-C	-6.04	1.45	1.52
10	I	55	LEU	CA-C	5.92	1.60	1.52

The worst 5 of 182 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	O	50	ALA	CA-C-N	-19.29	100.36	119.85
16	O	50	ALA	C-N-CA	-19.29	100.36	119.85
5	C	184	LEU	N-CA-C	10.59	122.91	111.36
8	G	46	THR	CA-C-N	10.29	130.59	119.28
8	G	46	THR	C-N-CA	10.29	130.59	119.28

There are no chirality outliers.

5 of 11 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	77	LYS	Peptide
4	B	104	GLU	Peptide
4	B	57	LYS	Peptide
5	C	161	VAL	Peptide
5	C	27	GLU	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	1667	0	1292	50	0
2	X	57983	0	29161	924	0
3	Y	2430	0	1229	57	0
4	B	1547	0	1514	68	0
5	C	1324	0	1175	62	0
6	D	853	0	444	7	0
7	E	915	0	648	24	0
8	G	1090	0	1034	51	0
9	H	884	0	902	45	0
10	I	819	0	687	45	0
11	J	1001	0	971	37	0
12	K	906	0	930	37	0
13	L	673	0	538	20	0
14	M	807	0	803	32	0
15	N	922	0	973	63	0
16	O	751	0	743	23	0
17	P	853	0	900	31	0
18	Q	583	0	472	21	0
19	R	627	0	510	24	0
20	S	1087	0	934	26	0
21	T	559	0	569	24	0
22	U	242	0	141	5	0
23	V	486	0	469	11	0
24	W	437	0	467	25	0
25	Z	339	0	350	24	0
26	2	350	0	383	12	0
27	3	405	0	363	20	0
28	4	181	0	76	5	0
29	A	1	0	0	0	0
29	R	1	0	0	0	0
29	T	1	0	0	0	0
29	X	268	0	0	0	0
29	Y	2	0	0	0	0
29	Z	1	0	0	0	0
30	A	3	0	0	0	0
30	C	2	0	0	0	0
30	G	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
30	I	1	0	0	0	0
30	J	1	0	0	0	0
30	M	1	0	0	0	0
30	O	1	0	0	0	0
30	P	1	0	0	0	0
30	X	218	0	0	0	0
30	Y	10	0	0	0	0
31	X	35	0	0	1	0
32	J	8	0	14	1	0
32	Q	8	0	14	0	0
32	X	64	0	112	7	0
32	Z	8	0	14	0	0
33	X	70	0	133	9	0
33	Y	10	0	19	1	0
34	S	3	0	6	0	0
34	X	6	0	12	0	0
35	N	15	0	17	17	0
All	All	81462	0	49019	1593	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 13.

The worst 5 of 1593 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)
19:R:11:VAL:HA	19:R:67:ASN:HB2	1.48	0.96
2:X:956:A:H2'	11:J:11:ARG:HH11	1.30	0.96
2:X:83:G:H21	2:X:102:A:H2	1.15	0.93
4:B:124:GLY:HA2	4:B:174:GLY:HA3	1.53	0.91
3:Y:21:G:H1	3:Y:58:G:H1	1.08	0.91

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	267/277 (96%)	222 (83%)	27 (10%)	18 (7%)	1	11
4	B	213/220 (97%)	187 (88%)	17 (8%)	9 (4%)	2	19
5	C	197/207 (95%)	155 (79%)	31 (16%)	11 (6%)	1	14
6	D	163/179 (91%)	131 (80%)	17 (10%)	15 (9%)	0	6
7	E	155/178 (87%)	120 (77%)	26 (17%)	9 (6%)	1	13
8	G	143/145 (99%)	131 (92%)	8 (6%)	4 (3%)	4	26
9	H	120/122 (98%)	102 (85%)	16 (13%)	2 (2%)	7	35
10	I	129/140 (92%)	91 (70%)	25 (19%)	13 (10%)	0	5
11	J	136/144 (94%)	110 (81%)	15 (11%)	11 (8%)	1	8
12	K	117/122 (96%)	101 (86%)	9 (8%)	7 (6%)	1	13
13	L	107/119 (90%)	86 (80%)	16 (15%)	5 (5%)	2	17
14	M	108/116 (93%)	85 (79%)	18 (17%)	5 (5%)	2	17
15	N	114/118 (97%)	108 (95%)	6 (5%)	0	100	100
16	O	100/102 (98%)	90 (90%)	5 (5%)	5 (5%)	1	16
17	P	110/117 (94%)	101 (92%)	8 (7%)	1 (1%)	14	47
18	Q	88/91 (97%)	74 (84%)	9 (10%)	5 (6%)	1	14
19	R	100/105 (95%)	71 (71%)	17 (17%)	12 (12%)	0	4
20	S	165/217 (76%)	121 (73%)	23 (14%)	21 (13%)	0	3
21	T	73/94 (78%)	63 (86%)	10 (14%)	0	100	100
22	U	40/62 (64%)	32 (80%)	6 (15%)	2 (5%)	1	16
23	V	63/69 (91%)	55 (87%)	5 (8%)	3 (5%)	2	16
24	W	55/59 (93%)	51 (93%)	3 (6%)	1 (2%)	6	34
25	Z	41/58 (71%)	36 (88%)	4 (10%)	1 (2%)	4	29
26	2	41/45 (91%)	39 (95%)	1 (2%)	1 (2%)	4	29
27	3	58/66 (88%)	42 (72%)	9 (16%)	7 (12%)	0	4
28	4	34/37 (92%)	26 (76%)	8 (24%)	0	100	100
All	All	2937/3209 (92%)	2430 (83%)	339 (12%)	168 (6%)	1	14

5 of 168 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	27	THR
1	A	35	LYS
1	A	36	PRO
1	A	51	VAL
1	A	78	VAL

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	112/224 (50%)	96 (86%)	16 (14%)	3	18
4	B	150/177 (85%)	118 (79%)	32 (21%)	1	7
5	C	106/169 (63%)	76 (72%)	30 (28%)	0	3
6	D	15/158 (10%)	12 (80%)	3 (20%)	1	8
7	E	51/156 (33%)	38 (74%)	13 (26%)	0	4
8	G	106/123 (86%)	84 (79%)	22 (21%)	1	7
9	H	91/100 (91%)	71 (78%)	20 (22%)	1	6
10	I	56/108 (52%)	33 (59%)	23 (41%)	0	0
11	J	90/119 (76%)	77 (86%)	13 (14%)	3	18
12	K	91/102 (89%)	74 (81%)	17 (19%)	1	9
13	L	40/95 (42%)	30 (75%)	10 (25%)	0	4
14	M	75/102 (74%)	50 (67%)	25 (33%)	0	2
15	N	91/98 (93%)	70 (77%)	21 (23%)	1	5
16	O	71/86 (83%)	57 (80%)	14 (20%)	1	8
17	P	89/94 (95%)	75 (84%)	14 (16%)	2	15
18	Q	41/82 (50%)	35 (85%)	6 (15%)	3	17
19	R	44/90 (49%)	24 (54%)	20 (46%)	0	0
20	S	88/190 (46%)	70 (80%)	18 (20%)	1	7
21	T	53/75 (71%)	39 (74%)	14 (26%)	0	3
22	U	8/52 (15%)	8 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
23	V	47/62 (76%)	36 (77%)	11 (23%)	1	5
24	W	50/53 (94%)	38 (76%)	12 (24%)	1	5
25	Z	38/51 (74%)	28 (74%)	10 (26%)	0	4
26	2	35/40 (88%)	27 (77%)	8 (23%)	1	6
27	3	33/57 (58%)	26 (79%)	7 (21%)	1	7
28	4	2/35 (6%)	1 (50%)	1 (50%)	0	0
All	All	1673/2698 (62%)	1293 (77%)	380 (23%)	1	6

5 of 380 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
15	N	63	THR
19	R	33	VAL
15	N	84	LYS
17	P	17	VAL
20	S	18	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 21 such sidechains are listed below:

Mol	Chain	Res	Type
17	P	40	ASN
22	U	20	HIS
26	2	7	GLN
22	U	30	ASN
20	S	10	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	X	2685/2923 (91%)	652 (24%)	36 (1%)
3	Y	113/114 (99%)	18 (15%)	0
All	All	2798/3037 (92%)	670 (23%)	36 (1%)

5 of 670 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	X	8	U
2	X	15	G

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Mol	Chain	Res	Type
2	X	17	G
2	X	34	U
2	X	38	A

5 of 36 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
2	X	1885	G
2	X	2611	U
2	X	1901	C
2	X	2378	G
2	X	890	G

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 538 ligands modelled in this entry, 514 are monoatomic - leaving 24 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
32	MPD	X	3004	-	7,7,7	1.04	1 (14%)	9,10,10	0.75	0
32	MPD	X	3009	-	7,7,7	0.55	0	9,10,10	0.35	0
34	EOH	X	3500	-	2,2,2	0.63	0	1,1,1	0.51	0
33	SPD	Y	213	-	9,9,9	0.19	0	8,8,8	0.14	0
35	EPE	N	201	-	15,15,15	1.17	1 (6%)	19,20,20	1.52	3 (15%)
32	MPD	X	3005	-	7,7,7	0.91	0	9,10,10	0.70	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
32	MPD	X	3011	-	7,7,7	1.17	1 (14%)	9,10,10	0.49	0
32	MPD	Q	101	-	7,7,7	0.66	0	9,10,10	0.28	0
32	MPD	X	3007	-	7,7,7	0.35	0	9,10,10	0.43	0
32	MPD	Z	101	-	7,7,7	0.55	0	9,10,10	0.26	0
31	62B	X	3003	-	37,38,38	1.00	2 (5%)	56,60,60	3.22	18 (32%)
33	SPD	X	3492	-	9,9,9	0.40	0	8,8,8	0.42	0
33	SPD	X	3498	-	9,9,9	0.37	0	8,8,8	0.64	0
32	MPD	X	3008	-	7,7,7	1.07	1 (14%)	9,10,10	0.71	0
32	MPD	X	3006	-	7,7,7	0.90	1 (14%)	9,10,10	0.61	0
33	SPD	X	3495	-	9,9,9	0.23	0	8,8,8	0.37	0
33	SPD	X	3497	-	9,9,9	0.11	0	8,8,8	0.34	0
32	MPD	X	3010	-	7,7,7	0.87	0	9,10,10	0.45	0
33	SPD	X	3496	-	9,9,9	0.26	0	8,8,8	0.21	0
34	EOH	S	301	-	2,2,2	0.73	0	1,1,1	0.29	0
32	MPD	J	201	-	7,7,7	1.20	1 (14%)	9,10,10	0.73	0
33	SPD	X	3494	-	9,9,9	0.21	0	8,8,8	0.32	0
34	EOH	X	3499	-	2,2,2	0.63	0	1,1,1	0.49	0
33	SPD	X	3493	-	9,9,9	0.33	0	8,8,8	0.55	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
32	MPD	X	3004	-	-	5/5/5/5	-
32	MPD	X	3009	-	-	4/5/5/5	-
33	SPD	Y	213	-	-	2/7/7/7	-
35	EPE	N	201	-	-	5/9/19/19	0/1/1/1
32	MPD	X	3005	-	-	4/5/5/5	-
32	MPD	X	3011	-	-	3/5/5/5	-
32	MPD	Q	101	-	-	1/5/5/5	-
32	MPD	X	3007	-	-	0/5/5/5	-
32	MPD	Z	101	-	-	0/5/5/5	-
31	62B	X	3003	-	-	2/12/86/86	0/4/4/4
33	SPD	X	3492	-	-	4/7/7/7	-
33	SPD	X	3498	-	-	2/7/7/7	-
32	MPD	X	3008	-	-	3/5/5/5	-
32	MPD	X	3006	-	-	1/5/5/5	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
33	SPD	X	3495	-	-	5/7/7/7	-
33	SPD	X	3497	-	-	4/7/7/7	-
32	MPD	X	3010	-	-	0/5/5/5	-
33	SPD	X	3496	-	-	1/7/7/7	-
32	MPD	J	201	-	-	1/5/5/5	-
33	SPD	X	3494	-	-	3/7/7/7	-
33	SPD	X	3493	-	-	1/7/7/7	-

The worst 5 of 8 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	X	3003	62B	C10-C11	3.90	1.60	1.56
35	N	201	EPE	C10-S	-3.88	1.72	1.77
31	X	3003	62B	C13-C12	-3.45	1.49	1.55
32	J	201	MPD	C3-C2	2.61	1.61	1.54
32	X	3011	MPD	C3-C2	2.44	1.61	1.54

The worst 5 of 21 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	X	3003	62B	C18-C12-C11	10.92	115.64	108.16
31	X	3003	62B	C15-C5-C14	-8.14	100.50	108.81
31	X	3003	62B	C6-C5-C14	7.40	117.16	112.13
31	X	3003	62B	C24-C25-C26	-7.23	103.25	111.53
31	X	3003	62B	C13-C12-C19	-6.14	98.31	110.83

There are no chirality outliers.

5 of 51 torsion outliers are listed below:

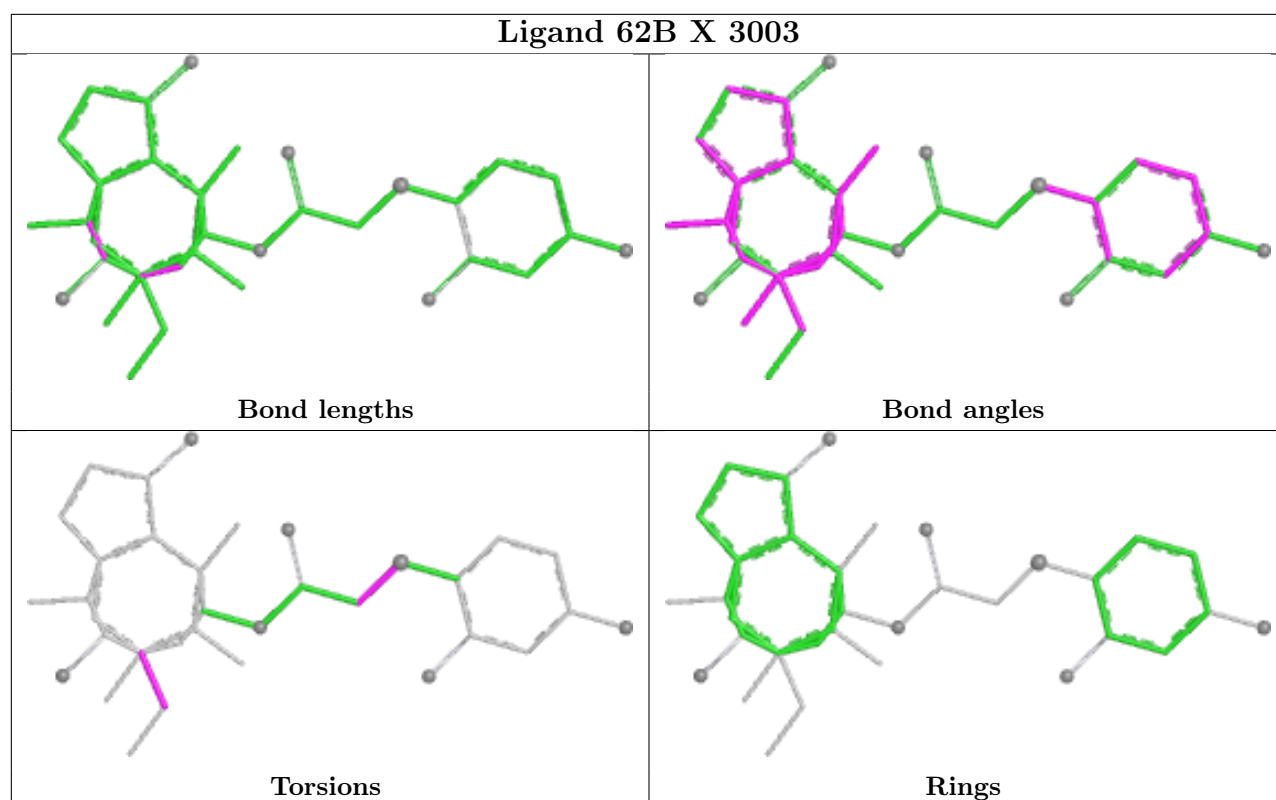
Mol	Chain	Res	Type	Atoms
32	X	3004	MPD	C2-C3-C4-O4
32	X	3004	MPD	C2-C3-C4-C5
35	N	201	EPE	N4-C7-C8-O8
33	X	3495	SPD	N6-C7-C8-C9
33	X	3498	SPD	C8-C7-N6-C5

There are no ring outliers.

14 monomers are involved in 36 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
32	X	3004	MPD	2	0
33	Y	213	SPD	1	0
35	N	201	EPE	17	0
32	X	3005	MPD	1	0
31	X	3003	62B	1	0
33	X	3498	SPD	1	0
32	X	3008	MPD	1	0
32	X	3006	MPD	2	0
33	X	3495	SPD	2	0
33	X	3497	SPD	3	0
32	X	3010	MPD	1	0
32	J	201	MPD	1	0
33	X	3494	SPD	1	0
33	X	3493	SPD	2	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 ⓘ

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	269/277 (97%)	0.72	27 (10%) 12 8	92, 138, 160, 172	0
2	X	2705/2923 (92%)	-0.16	90 (3%) 49 27	53, 101, 188, 280	0
3	Y	114/114 (100%)	-0.21	3 (2%) 57 32	76, 125, 175, 180	0
4	B	215/220 (97%)	0.21	6 (2%) 55 30	62, 81, 99, 116	0
5	C	199/207 (96%)	0.03	5 (2%) 58 33	64, 96, 113, 138	0
6	D	165/179 (92%)	0.68	19 (11%) 9 7	166, 193, 231, 239	0
7	E	157/178 (88%)	0.84	23 (14%) 6 5	133, 172, 206, 212	0
8	G	145/145 (100%)	0.01	6 (4%) 41 22	64, 79, 91, 96	0
9	H	122/122 (100%)	-0.21	2 (1%) 70 42	84, 102, 123, 128	0
10	I	131/140 (93%)	0.84	21 (16%) 5 4	58, 116, 136, 142	0
11	J	138/144 (95%)	0.34	9 (6%) 25 15	77, 103, 135, 152	0
12	K	119/122 (97%)	0.49	10 (8%) 17 11	67, 84, 108, 141	0
13	L	109/119 (91%)	0.45	12 (11%) 10 7	121, 130, 157, 189	0
14	M	110/116 (94%)	0.13	6 (5%) 30 17	85, 99, 132, 156	0
15	N	116/118 (98%)	0.35	8 (6%) 23 14	54, 70, 90, 96	0
16	O	102/102 (100%)	-0.21	1 (0%) 79 54	54, 88, 103, 109	0
17	P	112/117 (95%)	0.32	5 (4%) 38 20	64, 75, 114, 139	0
18	Q	90/91 (98%)	0.63	7 (7%) 19 12	98, 122, 138, 170	0
19	R	102/105 (97%)	1.24	26 (25%) 1 2	98, 121, 189, 206	0
20	S	167/217 (76%)	0.09	2 (1%) 76 49	87, 109, 199, 218	0
21	T	75/94 (79%)	0.34	7 (9%) 14 9	85, 97, 115, 129	0
22	U	42/62 (67%)	1.81	21 (50%) 0 1	160, 172, 203, 213	0
23	V	65/69 (94%)	0.61	6 (9%) 14 9	134, 145, 159, 163	0
24	W	57/59 (96%)	-0.09	1 (1%) 67 40	63, 77, 99, 101	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
25	Z	43/58 (74%)	0.14	0 100 100	54, 76, 131, 136	0
26	2	43/45 (95%)	0.18	1 (2%) 61 34	83, 92, 102, 105	0
27	3	60/66 (90%)	0.85	5 (8%) 17 11	80, 89, 105, 109	0
28	4	36/37 (97%)	3.29	26 (72%) 0 0	159, 164, 174, 178	0
All	All	5808/6246 (92%)	0.15	355 (6%) 27 15	53, 103, 190, 280	0

The worst 5 of 355 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
28	4	36	GLN	10.7
28	4	2	LYS	7.6
18	Q	71	TYR	5.6
4	B	173	MET	5.5
1	A	53	HIS	5.5

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
30	MG	X	3435	1/1	0.06	0.29	153,153,153,153	0
30	MG	X	3228	1/1	0.18	0.24	150,150,150,150	0
33	SPD	X	3492	10/10	0.26	0.36	105,105,105,105	0
30	MG	X	3387	1/1	0.35	0.24	175,175,175,175	0
30	MG	X	3327	1/1	0.37	0.46	126,126,126,126	0
30	MG	X	3445	1/1	0.39	0.39	104,104,104,104	0
30	MG	X	3351	1/1	0.40	0.47	116,116,116,116	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
30	MG	X	3349	1/1	0.41	0.58	127,127,127,127	0
30	MG	X	3433	1/1	0.42	0.30	124,124,124,124	0
30	MG	X	3283	1/1	0.43	0.19	129,129,129,129	0
30	MG	X	3340	1/1	0.46	0.20	84,84,84,84	0
30	MG	X	3450	1/1	0.47	0.32	132,132,132,132	0
30	MG	X	3474	1/1	0.47	0.20	106,106,106,106	0
30	MG	X	3260	1/1	0.47	0.25	123,123,123,123	0
30	MG	Y	210	1/1	0.48	0.35	105,105,105,105	0
30	MG	Y	205	1/1	0.49	0.43	94,94,94,94	0
30	MG	A	304	1/1	0.51	0.53	105,105,105,105	0
30	MG	X	3310	1/1	0.52	0.30	129,129,129,129	0
30	MG	X	3253	1/1	0.54	0.34	112,112,112,112	0
30	MG	X	3337	1/1	0.56	0.37	89,89,89,89	0
30	MG	X	3252	1/1	0.57	0.40	114,114,114,114	0
30	MG	X	3259	1/1	0.57	0.26	122,122,122,122	0
30	MG	X	3385	1/1	0.57	0.45	88,88,88,88	0
29	MN	X	3460	1/1	0.58	0.28	182,182,182,182	0
30	MG	G	201	1/1	0.58	0.27	89,89,89,89	0
30	MG	X	3002	1/1	0.58	0.62	100,100,100,100	0
30	MG	X	3394	1/1	0.59	0.20	98,98,98,98	0
30	MG	X	3293	1/1	0.61	0.31	117,117,117,117	0
30	MG	X	3165	1/1	0.63	0.41	84,84,84,84	0
30	MG	Y	203	1/1	0.63	0.13	96,96,96,96	0
30	MG	X	3339	1/1	0.63	0.26	108,108,108,108	0
32	MPD	X	3010	8/8	0.64	0.20	113,113,113,113	0
30	MG	X	3290	1/1	0.64	0.26	98,98,98,98	0
30	MG	X	3295	1/1	0.65	0.32	100,100,100,100	0
30	MG	X	3244	1/1	0.65	0.34	109,109,109,109	0
30	MG	X	3345	1/1	0.66	0.10	65,65,65,65	0
30	MG	X	3382	1/1	0.66	0.38	126,126,126,126	0
30	MG	X	3417	1/1	0.67	0.50	82,82,82,82	0
30	MG	X	3406	1/1	0.67	0.27	71,71,71,71	0
30	MG	X	3333	1/1	0.68	0.39	97,97,97,97	0
30	MG	X	3272	1/1	0.68	0.22	104,104,104,104	0
32	MPD	Q	101	8/8	0.68	0.14	137,137,137,137	0
30	MG	X	3299	1/1	0.68	0.22	149,149,149,149	0
33	SPD	X	3497	10/10	0.68	0.15	96,96,96,96	0
30	MG	X	3438	1/1	0.69	0.17	84,84,84,84	0
30	MG	X	3341	1/1	0.69	0.15	96,96,96,96	0
30	MG	X	3396	1/1	0.69	0.23	108,108,108,108	0
30	MG	X	3344	1/1	0.69	0.33	91,91,91,91	0
30	MG	X	3386	1/1	0.70	0.25	88,88,88,88	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
30	MG	X	3308	1/1	0.71	0.18	77,77,77,77	0
30	MG	X	3250	1/1	0.71	0.64	89,89,89,89	0
30	MG	X	3488	1/1	0.71	0.42	100,100,100,100	0
29	MN	X	3146	1/1	0.71	0.10	122,122,122,122	0
30	MG	X	3292	1/1	0.71	0.33	89,89,89,89	0
30	MG	Y	206	1/1	0.71	0.32	104,104,104,104	0
30	MG	X	3305	1/1	0.72	0.27	123,123,123,123	0
30	MG	X	3342	1/1	0.72	0.52	80,80,80,80	0
29	MN	X	3324	1/1	0.72	0.10	164,164,164,164	0
30	MG	X	3265	1/1	0.72	0.57	96,96,96,96	0
32	MPD	J	201	8/8	0.72	0.34	125,125,125,125	0
30	MG	X	3490	1/1	0.72	0.18	100,100,100,100	0
30	MG	X	3347	1/1	0.72	0.41	108,108,108,108	0
30	MG	X	3226	1/1	0.72	0.36	102,102,102,102	0
30	MG	X	3269	1/1	0.73	0.15	132,132,132,132	0
30	MG	X	3393	1/1	0.73	0.24	104,104,104,104	0
30	MG	X	3384	1/1	0.73	0.22	102,102,102,102	0
30	MG	X	3309	1/1	0.74	0.29	105,105,105,105	0
29	MN	X	3316	1/1	0.74	0.14	173,173,173,173	0
30	MG	X	3304	1/1	0.74	0.23	117,117,117,117	0
30	MG	X	3391	1/1	0.75	0.34	107,107,107,107	0
30	MG	X	3362	1/1	0.75	0.24	114,114,114,114	0
29	MN	Y	208	1/1	0.75	0.09	164,164,164,164	0
29	MN	X	3210	1/1	0.76	0.13	201,201,201,201	0
30	MG	X	3277	1/1	0.76	0.39	97,97,97,97	0
30	MG	X	3398	1/1	0.76	0.33	99,99,99,99	0
30	MG	X	3358	1/1	0.76	0.47	88,88,88,88	0
30	MG	X	3294	1/1	0.76	0.24	108,108,108,108	0
30	MG	X	3424	1/1	0.76	0.52	89,89,89,89	0
30	MG	X	3363	1/1	0.76	0.23	82,82,82,82	0
30	MG	X	3336	1/1	0.76	0.24	99,99,99,99	0
30	MG	X	3370	1/1	0.77	0.44	113,113,113,113	0
30	MG	X	3291	1/1	0.77	0.41	86,86,86,86	0
30	MG	X	3268	1/1	0.77	0.24	62,62,62,62	0
29	MN	X	3466	1/1	0.77	0.15	155,155,155,155	0
30	MG	X	3334	1/1	0.78	0.25	89,89,89,89	0
30	MG	X	3428	1/1	0.78	0.08	105,105,105,105	0
30	MG	A	303	1/1	0.78	0.93	94,94,94,94	0
30	MG	X	3331	1/1	0.78	0.38	86,86,86,86	0
29	MN	X	3326	1/1	0.78	0.11	145,145,145,145	0
33	SPD	X	3498	10/10	0.78	0.39	93,93,93,93	0
30	MG	X	3303	1/1	0.79	0.18	101,101,101,101	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
30	MG	X	3280	1/1	0.79	0.20	159,159,159,159	0
30	MG	X	3255	1/1	0.79	0.17	94,94,94,94	0
30	MG	X	3400	1/1	0.79	0.19	90,90,90,90	0
30	MG	Y	207	1/1	0.79	0.26	78,78,78,78	0
30	MG	A	302	1/1	0.79	0.22	92,92,92,92	0
30	MG	Y	211	1/1	0.79	0.28	115,115,115,115	0
30	MG	X	3287	1/1	0.80	0.44	102,102,102,102	0
30	MG	X	3412	1/1	0.80	0.28	106,106,106,106	0
30	MG	X	3123	1/1	0.80	0.16	69,69,69,69	0
32	MPD	X	3008	8/8	0.80	0.18	94,94,94,94	0
30	MG	X	3449	1/1	0.80	0.16	86,86,86,86	0
30	MG	X	3205	1/1	0.81	0.11	98,98,98,98	0
30	MG	Y	209	1/1	0.81	0.14	153,153,153,153	0
30	MG	X	3377	1/1	0.81	0.23	121,121,121,121	0
30	MG	X	3335	1/1	0.81	0.23	61,61,61,61	0
29	MN	X	3461	1/1	0.81	0.17	149,149,149,149	0
30	MG	X	3227	1/1	0.81	0.39	95,95,95,95	0
30	MG	X	3482	1/1	0.81	0.24	90,90,90,90	0
30	MG	X	3350	1/1	0.81	0.24	100,100,100,100	0
29	MN	X	3209	1/1	0.81	0.07	150,150,150,150	0
30	MG	X	3288	1/1	0.81	0.28	81,81,81,81	0
29	MN	X	3203	1/1	0.81	0.07	145,145,145,145	0
30	MG	X	3273	1/1	0.81	0.27	124,124,124,124	0
34	EOH	X	3499	3/3	0.81	0.30	80,80,80,80	0
30	MG	X	3229	1/1	0.82	0.35	98,98,98,98	0
32	MPD	X	3009	8/8	0.82	0.33	129,129,129,129	0
30	MG	X	3328	1/1	0.82	0.29	103,103,103,103	0
30	MG	X	3274	1/1	0.82	0.16	99,99,99,99	0
30	MG	X	3352	1/1	0.82	0.86	94,94,94,94	0
29	MN	X	3237	1/1	0.82	0.07	167,167,167,167	0
33	SPD	X	3494	10/10	0.82	0.18	87,87,87,87	0
30	MG	X	3429	1/1	0.82	0.16	102,102,102,102	0
30	MG	X	3361	1/1	0.82	0.18	86,86,86,86	0
29	MN	X	3447	1/1	0.82	0.08	128,128,128,128	0
29	MN	X	3320	1/1	0.83	0.17	107,107,107,107	0
30	MG	X	3356	1/1	0.83	0.12	83,83,83,83	0
29	MN	X	3468	1/1	0.83	0.10	104,104,104,104	0
30	MG	X	3487	1/1	0.83	0.38	109,109,109,109	0
30	MG	X	3419	1/1	0.83	0.18	107,107,107,107	0
30	MG	X	3443	1/1	0.83	0.23	118,118,118,118	0
30	MG	X	3359	1/1	0.83	0.56	91,91,91,91	0
29	MN	X	3231	1/1	0.83	0.17	161,161,161,161	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
34	EOH	X	3500	3/3	0.83	0.64	99,99,99,99	0
30	MG	X	3141	1/1	0.84	0.20	85,85,85,85	0
32	MPD	X	3007	8/8	0.84	0.13	132,132,132,132	0
30	MG	X	3420	1/1	0.84	0.38	75,75,75,75	0
29	MN	X	3471	1/1	0.84	0.25	130,130,130,130	0
30	MG	X	3302	1/1	0.84	0.12	100,100,100,100	0
30	MG	X	3196	1/1	0.84	0.22	89,89,89,89	0
30	MG	X	3354	1/1	0.84	0.14	75,75,75,75	0
30	MG	X	3238	1/1	0.84	0.26	85,85,85,85	0
29	MN	X	3478	1/1	0.84	0.06	132,132,132,132	0
33	SPD	X	3496	10/10	0.84	0.34	102,102,102,102	0
30	MG	X	3408	1/1	0.84	0.30	97,97,97,97	0
30	MG	X	3410	1/1	0.84	0.18	95,95,95,95	0
30	MG	X	3249	1/1	0.84	0.27	109,109,109,109	0
29	MN	X	3479	1/1	0.84	0.14	171,171,171,171	0
34	EOH	S	301	3/3	0.84	0.56	90,90,90,90	0
30	MG	X	3285	1/1	0.85	0.29	75,75,75,75	0
29	MN	X	3120	1/1	0.85	0.19	166,166,166,166	0
29	MN	X	3425	1/1	0.85	0.17	101,101,101,101	0
30	MG	X	3233	1/1	0.85	0.14	68,68,68,68	0
29	MN	X	3446	1/1	0.85	0.14	142,142,142,142	0
29	MN	X	3175	1/1	0.85	0.13	122,122,122,122	0
30	MG	X	3306	1/1	0.85	0.26	95,95,95,95	0
30	MG	I	201	1/1	0.85	0.73	80,80,80,80	0
30	MG	X	3489	1/1	0.85	0.27	62,62,62,62	0
30	MG	X	3087	1/1	0.85	0.24	55,55,55,55	0
29	MN	R	201	1/1	0.85	0.13	123,123,123,123	0
30	MG	X	3348	1/1	0.86	0.28	72,72,72,72	0
30	MG	X	3329	1/1	0.86	0.28	63,63,63,63	0
29	MN	X	3263	1/1	0.86	0.10	166,166,166,166	0
30	MG	X	3444	1/1	0.86	0.14	100,100,100,100	0
32	MPD	Z	101	8/8	0.86	0.19	145,145,145,145	0
30	MG	X	3413	1/1	0.86	0.34	90,90,90,90	0
30	MG	X	3144	1/1	0.86	0.28	71,71,71,71	0
33	SPD	X	3495	10/10	0.86	0.16	83,83,83,83	0
30	MG	X	3366	1/1	0.86	0.28	99,99,99,99	0
29	MN	X	3480	1/1	0.86	0.10	175,175,175,175	0
30	MG	X	3373	1/1	0.86	0.24	97,97,97,97	0
33	SPD	Y	213	10/10	0.86	0.36	101,101,101,101	0
29	MN	X	3235	1/1	0.86	0.10	155,155,155,155	0
29	MN	X	3380	1/1	0.86	0.11	151,151,151,151	0
29	MN	X	3182	1/1	0.86	0.08	133,133,133,133	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
30	MG	X	3130	1/1	0.87	0.27	72,72,72,72	0
30	MG	X	3411	1/1	0.87	0.21	82,82,82,82	0
30	MG	X	3485	1/1	0.87	0.23	102,102,102,102	0
29	MN	X	3202	1/1	0.87	0.18	173,173,173,173	0
30	MG	X	3378	1/1	0.87	0.22	83,83,83,83	0
29	MN	X	3225	1/1	0.87	0.15	157,157,157,157	0
30	MG	X	3213	1/1	0.87	0.35	86,86,86,86	0
30	MG	X	3224	1/1	0.87	0.33	66,66,66,66	0
30	MG	X	3236	1/1	0.87	0.31	88,88,88,88	0
30	MG	X	3372	1/1	0.87	0.18	78,78,78,78	0
30	MG	X	3451	1/1	0.87	0.23	115,115,115,115	0
32	MPD	X	3006	8/8	0.88	0.44	82,82,82,82	0
30	MG	X	3414	1/1	0.88	0.27	89,89,89,89	0
30	MG	X	3300	1/1	0.88	0.30	94,94,94,94	0
30	MG	X	3286	1/1	0.88	0.33	77,77,77,77	0
30	MG	X	3246	1/1	0.88	0.23	72,72,72,72	0
30	MG	X	3365	1/1	0.88	0.14	76,76,76,76	0
29	MN	X	3194	1/1	0.88	0.09	138,138,138,138	0
30	MG	X	3142	1/1	0.88	0.19	72,72,72,72	0
29	MN	X	3437	1/1	0.88	0.07	153,153,153,153	0
30	MG	X	3434	1/1	0.88	0.29	64,64,64,64	0
29	MN	X	3155	1/1	0.88	0.32	110,110,110,110	0
29	MN	X	3094	1/1	0.88	0.09	124,124,124,124	0
30	MG	X	3440	1/1	0.88	0.14	79,79,79,79	0
29	MN	X	3325	1/1	0.88	0.07	187,187,187,187	0
29	MN	X	3114	1/1	0.88	0.10	122,122,122,122	0
30	MG	X	3383	1/1	0.88	0.12	75,75,75,75	0
29	MN	X	3183	1/1	0.88	0.06	125,125,125,125	0
30	MG	X	3343	1/1	0.88	0.23	73,73,73,73	0
30	MG	C	301	1/1	0.89	0.46	64,64,64,64	0
30	MG	X	3371	1/1	0.89	0.25	88,88,88,88	0
29	MN	X	3321	1/1	0.89	0.05	159,159,159,159	0
30	MG	J	202	1/1	0.89	0.15	92,92,92,92	0
32	MPD	X	3005	8/8	0.89	0.20	78,78,78,78	0
29	MN	X	3322	1/1	0.89	0.12	137,137,137,137	0
30	MG	X	3281	1/1	0.89	0.22	113,113,113,113	0
29	MN	X	3186	1/1	0.89	0.12	143,143,143,143	0
30	MG	X	3473	1/1	0.89	0.21	82,82,82,82	0
29	MN	X	3150	1/1	0.89	0.07	110,110,110,110	0
30	MG	X	3415	1/1	0.89	0.43	81,81,81,81	0
29	MN	X	3469	1/1	0.89	0.08	140,140,140,140	0
30	MG	X	3357	1/1	0.89	0.23	95,95,95,95	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
29	MN	X	3197	1/1	0.89	0.12	138,138,138,138	0
29	MN	X	3119	1/1	0.89	0.09	140,140,140,140	0
30	MG	X	3266	1/1	0.89	0.28	90,90,90,90	0
29	MN	X	3404	1/1	0.89	0.11	131,131,131,131	0
29	MN	X	3019	1/1	0.89	0.20	109,109,109,109	0
29	MN	X	3133	1/1	0.89	0.10	133,133,133,133	0
29	MN	X	3317	1/1	0.89	0.07	137,137,137,137	0
30	MG	X	3367	1/1	0.89	0.42	83,83,83,83	0
30	MG	X	3369	1/1	0.89	0.33	70,70,70,70	0
29	MN	X	3044	1/1	0.89	0.13	116,116,116,116	0
35	EPE	N	201	15/15	0.89	0.17	73,73,73,73	0
30	MG	X	3278	1/1	0.90	0.26	82,82,82,82	0
30	MG	X	3381	1/1	0.90	0.42	97,97,97,97	0
29	MN	X	3462	1/1	0.90	0.08	152,152,152,152	0
29	MN	X	3025	1/1	0.90	0.10	128,128,128,128	0
30	MG	X	3282	1/1	0.90	0.08	85,85,85,85	0
29	MN	X	3124	1/1	0.90	0.07	147,147,147,147	0
30	MG	X	3261	1/1	0.90	0.13	91,91,91,91	0
29	MN	X	3312	1/1	0.90	0.07	115,115,115,115	0
30	MG	X	3242	1/1	0.90	0.18	65,65,65,65	0
30	MG	X	3267	1/1	0.90	0.16	72,72,72,72	0
30	MG	X	3289	1/1	0.90	0.16	110,110,110,110	0
30	MG	X	3346	1/1	0.90	0.20	68,68,68,68	0
30	MG	X	3397	1/1	0.90	0.15	78,78,78,78	0
29	MN	X	3101	1/1	0.90	0.23	131,131,131,131	0
29	MN	X	3173	1/1	0.90	0.07	129,129,129,129	0
30	MG	X	3441	1/1	0.90	0.27	96,96,96,96	0
29	MN	X	3458	1/1	0.90	0.12	127,127,127,127	0
30	MG	Y	212	1/1	0.90	0.29	95,95,95,95	0
30	MG	X	3129	1/1	0.90	0.18	79,79,79,79	0
29	MN	X	3379	1/1	0.90	0.07	158,158,158,158	0
29	MN	X	3208	1/1	0.90	0.13	141,141,141,141	0
29	MN	T	101	1/1	0.91	0.13	121,121,121,121	0
30	MG	X	3256	1/1	0.91	0.21	69,69,69,69	0
30	MG	X	3218	1/1	0.91	0.42	75,75,75,75	0
30	MG	X	3221	1/1	0.91	0.20	89,89,89,89	0
29	MN	X	3459	1/1	0.91	0.10	161,161,161,161	0
30	MG	P	201	1/1	0.91	0.16	63,63,63,63	0
29	MN	X	3211	1/1	0.91	0.12	144,144,144,144	0
29	MN	X	3223	1/1	0.91	0.07	119,119,119,119	0
29	MN	X	3058	1/1	0.91	0.13	101,101,101,101	0
29	MN	X	3463	1/1	0.91	0.09	134,134,134,134	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
30	MG	X	3232	1/1	0.91	0.13	74,74,74,74	0
29	MN	X	3153	1/1	0.91	0.10	123,123,123,123	0
29	MN	A	301	1/1	0.91	0.10	138,138,138,138	0
30	MG	X	3483	1/1	0.91	0.21	91,91,91,91	0
29	MN	X	3162	1/1	0.91	0.08	118,118,118,118	0
30	MG	X	3276	1/1	0.91	0.28	67,67,67,67	0
29	MN	X	3199	1/1	0.91	0.12	143,143,143,143	0
29	MN	X	3166	1/1	0.91	0.11	92,92,92,92	0
29	MN	X	3168	1/1	0.91	0.16	115,115,115,115	0
30	MG	X	3247	1/1	0.91	0.28	85,85,85,85	0
29	MN	X	3046	1/1	0.91	0.15	91,91,91,91	0
30	MG	X	3180	1/1	0.91	0.25	78,78,78,78	0
29	MN	X	3147	1/1	0.91	0.07	119,119,119,119	0
30	MG	X	3355	1/1	0.91	0.50	91,91,91,91	0
29	MN	X	3148	1/1	0.91	0.17	144,144,144,144	0
30	MG	X	3388	1/1	0.91	0.23	85,85,85,85	0
29	MN	X	3422	1/1	0.92	0.07	154,154,154,154	0
30	MG	X	3222	1/1	0.92	0.13	80,80,80,80	0
30	MG	X	3307	1/1	0.92	0.14	71,71,71,71	0
29	MN	X	3158	1/1	0.92	0.09	117,117,117,117	0
29	MN	X	3314	1/1	0.92	0.09	147,147,147,147	0
30	MG	X	3476	1/1	0.92	0.17	64,64,64,64	0
30	MG	X	3477	1/1	0.92	0.08	80,80,80,80	0
30	MG	X	3143	1/1	0.92	0.23	59,59,59,59	0
30	MG	X	3423	1/1	0.92	0.20	79,79,79,79	0
29	MN	X	3181	1/1	0.92	0.08	142,142,142,142	0
30	MG	X	3426	1/1	0.92	0.14	104,104,104,104	0
32	MPD	X	3011	8/8	0.92	0.24	75,75,75,75	0
29	MN	X	3159	1/1	0.92	0.10	118,118,118,118	0
30	MG	X	3368	1/1	0.92	0.26	87,87,87,87	0
30	MG	X	3230	1/1	0.92	0.11	80,80,80,80	0
30	MG	X	3491	1/1	0.92	0.17	86,86,86,86	0
33	SPD	X	3493	10/10	0.92	0.23	83,83,83,83	0
30	MG	X	3504	1/1	0.92	0.20	74,74,74,74	0
29	MN	X	3470	1/1	0.92	0.17	148,148,148,148	0
30	MG	Y	204	1/1	0.92	0.19	78,78,78,78	0
30	MG	X	3332	1/1	0.92	0.13	81,81,81,81	0
30	MG	X	3297	1/1	0.92	0.14	81,81,81,81	0
29	MN	X	3360	1/1	0.92	0.06	146,146,146,146	0
29	MN	X	3319	1/1	0.92	0.04	158,158,158,158	0
30	MG	X	3212	1/1	0.92	0.21	78,78,78,78	0
29	MN	X	3154	1/1	0.92	0.11	124,124,124,124	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
29	MN	X	3311	1/1	0.92	0.09	124,124,124,124	0
30	MG	G	202	1/1	0.93	0.22	77,77,77,77	0
29	MN	X	3071	1/1	0.93	0.11	98,98,98,98	0
29	MN	X	3102	1/1	0.93	0.14	124,124,124,124	0
30	MG	X	3475	1/1	0.93	0.28	93,93,93,93	0
30	MG	X	3375	1/1	0.93	0.15	76,76,76,76	0
29	MN	X	3184	1/1	0.93	0.05	128,128,128,128	0
29	MN	X	3157	1/1	0.93	0.10	108,108,108,108	0
29	MN	X	3192	1/1	0.93	0.08	138,138,138,138	0
29	MN	Z	102	1/1	0.93	0.15	112,112,112,112	0
29	MN	X	3135	1/1	0.93	0.07	115,115,115,115	0
29	MN	X	3195	1/1	0.93	0.17	139,139,139,139	0
29	MN	X	3454	1/1	0.93	0.11	126,126,126,126	0
29	MN	X	3139	1/1	0.93	0.18	117,117,117,117	0
29	MN	X	3198	1/1	0.93	0.08	125,125,125,125	0
29	MN	X	3111	1/1	0.93	0.11	130,130,130,130	0
29	MN	X	3163	1/1	0.93	0.06	124,124,124,124	0
29	MN	X	3112	1/1	0.93	0.10	124,124,124,124	0
30	MG	X	3298	1/1	0.93	0.30	95,95,95,95	0
30	MG	X	3364	1/1	0.93	0.21	83,83,83,83	0
29	MN	X	3072	1/1	0.93	0.08	123,123,123,123	0
29	MN	X	3323	1/1	0.93	0.11	141,141,141,141	0
29	MN	X	3149	1/1	0.93	0.07	109,109,109,109	0
29	MN	X	3174	1/1	0.93	0.06	121,121,121,121	0
29	MN	X	3073	1/1	0.93	0.09	95,95,95,95	0
29	MN	X	3176	1/1	0.93	0.12	128,128,128,128	0
29	MN	X	3045	1/1	0.93	0.17	96,96,96,96	0
29	MN	X	3140	1/1	0.94	0.06	105,105,105,105	0
30	MG	X	3207	1/1	0.94	0.15	66,66,66,66	0
29	MN	X	3315	1/1	0.94	0.07	104,104,104,104	0
30	MG	X	3395	1/1	0.94	0.06	79,79,79,79	0
30	MG	X	3254	1/1	0.94	0.12	66,66,66,66	0
30	MG	X	3448	1/1	0.94	0.21	72,72,72,72	0
29	MN	X	3115	1/1	0.94	0.12	116,116,116,116	0
29	MN	X	3439	1/1	0.94	0.33	94,94,94,94	0
30	MG	M	201	1/1	0.94	0.12	68,68,68,68	0
30	MG	X	3258	1/1	0.94	0.07	80,80,80,80	0
32	MPD	X	3004	8/8	0.94	0.29	135,135,135,135	0
29	MN	X	3160	1/1	0.94	0.06	100,100,100,100	0
29	MN	X	3100	1/1	0.94	0.05	96,96,96,96	0
29	MN	X	3185	1/1	0.94	0.05	101,101,101,101	0
29	MN	X	3070	1/1	0.94	0.21	129,129,129,129	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
29	MN	X	3187	1/1	0.94	0.10	137,137,137,137	0
29	MN	X	3191	1/1	0.94	0.06	138,138,138,138	0
29	MN	X	3024	1/1	0.94	0.07	120,120,120,120	0
30	MG	X	3484	1/1	0.94	0.14	77,77,77,77	0
29	MN	X	3131	1/1	0.94	0.08	126,126,126,126	0
30	MG	X	3486	1/1	0.94	0.45	90,90,90,90	0
30	MG	X	3301	1/1	0.94	0.13	72,72,72,72	0
29	MN	X	3001	1/1	0.94	0.27	97,97,97,97	0
29	MN	X	3464	1/1	0.94	0.09	149,149,149,149	0
29	MN	X	3262	1/1	0.94	0.05	143,143,143,143	0
29	MN	X	3134	1/1	0.94	0.18	121,121,121,121	0
30	MG	X	3241	1/1	0.94	0.27	78,78,78,78	0
29	MN	X	3067	1/1	0.94	0.17	104,104,104,104	0
29	MN	X	3402	1/1	0.94	0.06	108,108,108,108	0
30	MG	X	3353	1/1	0.94	0.15	79,79,79,79	0
29	MN	X	3069	1/1	0.94	0.10	103,103,103,103	0
29	MN	X	3472	1/1	0.94	0.17	110,110,110,110	0
29	MN	X	3405	1/1	0.94	0.09	103,103,103,103	0
29	MN	X	3177	1/1	0.95	0.08	125,125,125,125	0
29	MN	X	3178	1/1	0.95	0.05	126,126,126,126	0
29	MN	X	3465	1/1	0.95	0.16	117,117,117,117	0
30	MG	X	3167	1/1	0.95	0.07	62,62,62,62	0
30	MG	X	3430	1/1	0.95	0.10	74,74,74,74	0
30	MG	X	3432	1/1	0.95	0.12	71,71,71,71	0
29	MN	X	3065	1/1	0.95	0.14	97,97,97,97	0
29	MN	X	3078	1/1	0.95	0.10	111,111,111,111	0
30	MG	C	302	1/1	0.95	0.09	78,78,78,78	0
29	MN	X	3151	1/1	0.95	0.11	97,97,97,97	0
29	MN	X	3116	1/1	0.95	0.10	111,111,111,111	0
29	MN	X	3401	1/1	0.95	0.05	104,104,104,104	0
29	MN	X	3080	1/1	0.95	0.14	78,78,78,78	0
29	MN	X	3081	1/1	0.95	0.15	109,109,109,109	0
30	MG	O	201	1/1	0.95	0.19	51,51,51,51	0
29	MN	X	3121	1/1	0.95	0.07	104,104,104,104	0
30	MG	X	3389	1/1	0.95	0.44	94,94,94,94	0
29	MN	X	3418	1/1	0.95	0.05	124,124,124,124	0
29	MN	Y	202	1/1	0.95	0.05	105,105,105,105	0
29	MN	X	3264	1/1	0.95	0.04	117,117,117,117	0
29	MN	X	3084	1/1	0.95	0.13	123,123,123,123	0
29	MN	X	3436	1/1	0.95	0.11	119,119,119,119	0
29	MN	X	3125	1/1	0.95	0.08	123,123,123,123	0
29	MN	X	3090	1/1	0.95	0.09	97,97,97,97	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
30	MG	X	3399	1/1	0.95	0.19	79,79,79,79	0
29	MN	X	3034	1/1	0.95	0.11	77,77,77,77	0
29	MN	X	3097	1/1	0.95	0.10	109,109,109,109	0
30	MG	X	3279	1/1	0.95	0.29	67,67,67,67	0
29	MN	X	3453	1/1	0.95	0.06	126,126,126,126	0
29	MN	X	3068	1/1	0.95	0.21	94,94,94,94	0
30	MG	X	3239	1/1	0.95	0.31	91,91,91,91	0
29	MN	X	3049	1/1	0.95	0.13	93,93,93,93	0
29	MN	X	3037	1/1	0.95	0.05	90,90,90,90	0
29	MN	X	3059	1/1	0.95	0.14	111,111,111,111	0
30	MG	X	3416	1/1	0.95	0.20	90,90,90,90	0
30	MG	X	3138	1/1	0.95	0.14	72,72,72,72	0
29	MN	X	3060	1/1	0.95	0.07	90,90,90,90	0
30	MG	X	3338	1/1	0.95	0.11	82,82,82,82	0
29	MN	X	3113	1/1	0.95	0.12	96,96,96,96	0
29	MN	X	3164	1/1	0.96	0.06	111,111,111,111	0
29	MN	X	3096	1/1	0.96	0.15	100,100,100,100	0
29	MN	X	3051	1/1	0.96	0.05	97,97,97,97	0
29	MN	X	3374	1/1	0.96	0.06	104,104,104,104	0
29	MN	X	3376	1/1	0.96	0.04	119,119,119,119	0
29	MN	X	3206	1/1	0.96	0.14	95,95,95,95	0
30	MG	Y	201	1/1	0.96	0.23	66,66,66,66	0
30	MG	X	3240	1/1	0.96	0.26	78,78,78,78	0
29	MN	X	3171	1/1	0.96	0.06	114,114,114,114	0
29	MN	X	3392	1/1	0.96	0.06	89,89,89,89	0
29	MN	X	3054	1/1	0.96	0.11	97,97,97,97	0
30	MG	X	3296	1/1	0.96	0.12	45,45,45,45	0
29	MN	X	3056	1/1	0.96	0.15	88,88,88,88	0
29	MN	X	3057	1/1	0.96	0.07	68,68,68,68	0
30	MG	X	3248	1/1	0.96	0.17	69,69,69,69	0
29	MN	X	3216	1/1	0.96	0.07	94,94,94,94	0
29	MN	X	3219	1/1	0.96	0.09	85,85,85,85	0
29	MN	X	3421	1/1	0.96	0.13	111,111,111,111	0
29	MN	X	3105	1/1	0.96	0.07	97,97,97,97	0
29	MN	X	3110	1/1	0.96	0.13	117,117,117,117	0
29	MN	X	3043	1/1	0.96	0.10	81,81,81,81	0
29	MN	X	3234	1/1	0.96	0.06	144,144,144,144	0
29	MN	X	3179	1/1	0.96	0.04	106,106,106,106	0
29	MN	X	3076	1/1	0.96	0.07	90,90,90,90	0
29	MN	X	3077	1/1	0.96	0.12	100,100,100,100	0
31	62B	X	3003	35/35	0.96	0.13	65,65,65,65	0
29	MN	X	3452	1/1	0.96	0.04	120,120,120,120	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
29	MN	X	3013	1/1	0.96	0.06	70,70,70,70	0
29	MN	X	3036	1/1	0.96	0.08	86,86,86,86	0
29	MN	X	3457	1/1	0.96	0.11	135,135,135,135	0
30	MG	X	3442	1/1	0.96	0.14	71,71,71,71	0
29	MN	X	3061	1/1	0.96	0.07	92,92,92,92	0
29	MN	X	3117	1/1	0.96	0.06	107,107,107,107	0
30	MG	X	3271	1/1	0.96	0.15	92,92,92,92	0
29	MN	X	3082	1/1	0.96	0.07	112,112,112,112	0
29	MN	X	3188	1/1	0.96	0.12	114,114,114,114	0
29	MN	X	3189	1/1	0.96	0.06	154,154,154,154	0
30	MG	X	3214	1/1	0.96	0.22	86,86,86,86	0
29	MN	X	3027	1/1	0.96	0.13	68,68,68,68	0
29	MN	X	3318	1/1	0.96	0.04	128,128,128,128	0
29	MN	X	3089	1/1	0.96	0.09	113,113,113,113	0
30	MG	X	3390	1/1	0.96	0.15	63,63,63,63	0
29	MN	X	3193	1/1	0.96	0.05	110,110,110,110	0
30	MG	X	3481	1/1	0.96	0.10	82,82,82,82	0
29	MN	X	3122	1/1	0.96	0.09	99,99,99,99	0
29	MN	X	3042	1/1	0.96	0.13	74,74,74,74	0
29	MN	X	3050	1/1	0.96	0.14	98,98,98,98	0
30	MG	X	3284	1/1	0.96	0.09	72,72,72,72	0
29	MN	X	3128	1/1	0.96	0.07	93,93,93,93	0
29	MN	X	3190	1/1	0.97	0.06	124,124,124,124	0
29	MN	X	3092	1/1	0.97	0.09	90,90,90,90	0
29	MN	X	3093	1/1	0.97	0.09	81,81,81,81	0
29	MN	X	3243	1/1	0.97	0.09	114,114,114,114	0
29	MN	X	3467	1/1	0.97	0.17	72,72,72,72	0
29	MN	X	3245	1/1	0.97	0.03	129,129,129,129	0
29	MN	X	3257	1/1	0.97	0.10	93,93,93,93	0
29	MN	X	3170	1/1	0.97	0.07	104,104,104,104	0
29	MN	X	3403	1/1	0.97	0.10	114,114,114,114	0
29	MN	X	3038	1/1	0.97	0.04	106,106,106,106	0
29	MN	X	3095	1/1	0.97	0.04	79,79,79,79	0
29	MN	X	3407	1/1	0.97	0.14	83,83,83,83	0
29	MN	X	3409	1/1	0.97	0.04	87,87,87,87	0
29	MN	X	3052	1/1	0.97	0.11	90,90,90,90	0
30	MG	X	3275	1/1	0.97	0.07	71,71,71,71	0
29	MN	X	3053	1/1	0.97	0.14	58,58,58,58	0
29	MN	X	3313	1/1	0.97	0.13	117,117,117,117	0
29	MN	X	3098	1/1	0.97	0.03	92,92,92,92	0
29	MN	X	3200	1/1	0.97	0.08	123,123,123,123	0
29	MN	X	3099	1/1	0.97	0.08	82,82,82,82	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
29	MN	X	3020	1/1	0.97	0.07	107,107,107,107	0
29	MN	X	3055	1/1	0.97	0.09	86,86,86,86	0
29	MN	X	3088	1/1	0.97	0.07	101,101,101,101	0
29	MN	X	3103	1/1	0.97	0.08	85,85,85,85	0
29	MN	X	3012	1/1	0.97	0.16	79,79,79,79	0
29	MN	X	3108	1/1	0.97	0.08	89,89,89,89	0
29	MN	X	3455	1/1	0.97	0.05	116,116,116,116	0
30	MG	X	3137	1/1	0.97	0.28	63,63,63,63	0
29	MN	X	3456	1/1	0.97	0.07	113,113,113,113	0
29	MN	X	3132	1/1	0.97	0.04	104,104,104,104	0
29	MN	X	3161	1/1	0.97	0.06	93,93,93,93	0
29	MN	X	3109	1/1	0.97	0.09	92,92,92,92	0
29	MN	X	3033	1/1	0.97	0.14	78,78,78,78	0
29	MN	X	3330	1/1	0.97	0.06	104,104,104,104	0
29	MN	X	3091	1/1	0.97	0.04	92,92,92,92	0
29	MN	X	3014	1/1	0.98	0.05	53,53,53,53	0
29	MN	X	3035	1/1	0.98	0.06	74,74,74,74	0
29	MN	X	3502	1/1	0.98	0.10	88,88,88,88	0
29	MN	X	3503	1/1	0.98	0.03	68,68,68,68	0
29	MN	X	3017	1/1	0.98	0.11	92,92,92,92	0
29	MN	X	3026	1/1	0.98	0.12	66,66,66,66	0
29	MN	X	3022	1/1	0.98	0.03	92,92,92,92	0
29	MN	X	3127	1/1	0.98	0.03	94,94,94,94	0
29	MN	X	3039	1/1	0.98	0.09	79,79,79,79	0
29	MN	X	3074	1/1	0.98	0.15	113,113,113,113	0
29	MN	X	3169	1/1	0.98	0.08	107,107,107,107	0
29	MN	X	3040	1/1	0.98	0.09	81,81,81,81	0
29	MN	X	3041	1/1	0.98	0.06	77,77,77,77	0
29	MN	X	3172	1/1	0.98	0.03	114,114,114,114	0
29	MN	X	3028	1/1	0.98	0.21	53,53,53,53	0
29	MN	X	3104	1/1	0.98	0.04	94,94,94,94	0
29	MN	X	3079	1/1	0.98	0.08	58,58,58,58	0
29	MN	X	3107	1/1	0.98	0.10	73,73,73,73	0
29	MN	X	3215	1/1	0.98	0.03	87,87,87,87	0
29	MN	X	3029	1/1	0.98	0.09	69,69,69,69	0
29	MN	X	3030	1/1	0.98	0.18	69,69,69,69	0
29	MN	X	3220	1/1	0.98	0.04	103,103,103,103	0
29	MN	X	3031	1/1	0.98	0.09	68,68,68,68	0
29	MN	X	3023	1/1	0.98	0.11	92,92,92,92	0
29	MN	X	3086	1/1	0.98	0.12	92,92,92,92	0
29	MN	X	3062	1/1	0.98	0.05	87,87,87,87	0
30	MG	X	3427	1/1	0.98	0.14	59,59,59,59	0

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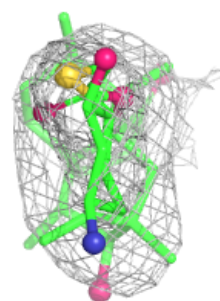
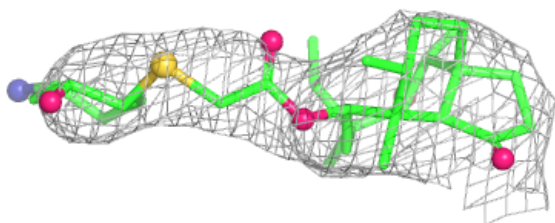
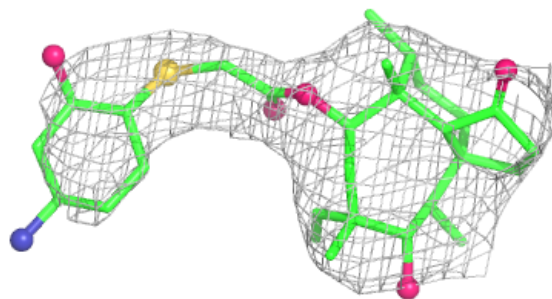
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
30	MG	X	3501	1/1	0.98	0.12	64,64,64,64	0
29	MN	X	3152	1/1	0.98	0.10	75,75,75,75	0
29	MN	X	3063	1/1	0.98	0.12	70,70,70,70	0
29	MN	X	3064	1/1	0.98	0.07	84,84,84,84	0
30	MG	X	3431	1/1	0.98	0.10	55,55,55,55	0
29	MN	X	3047	1/1	0.98	0.04	70,70,70,70	0
29	MN	X	3156	1/1	0.98	0.07	77,77,77,77	0
29	MN	X	3066	1/1	0.98	0.07	80,80,80,80	0
29	MN	X	3048	1/1	0.98	0.11	93,93,93,93	0
29	MN	X	3032	1/1	0.99	0.08	64,64,64,64	0
29	MN	X	3126	1/1	0.99	0.02	74,74,74,74	0
29	MN	X	3145	1/1	0.99	0.05	69,69,69,69	0
29	MN	X	3083	1/1	0.99	0.08	73,73,73,73	0
29	MN	X	3118	1/1	0.99	0.06	65,65,65,65	0
29	MN	X	3015	1/1	0.99	0.04	80,80,80,80	0
29	MN	X	3251	1/1	0.99	0.04	81,81,81,81	0
29	MN	X	3021	1/1	0.99	0.04	91,91,91,91	0
29	MN	X	3106	1/1	0.99	0.04	100,100,100,100	0
29	MN	X	3217	1/1	0.99	0.04	86,86,86,86	0
30	MG	X	3204	1/1	0.99	0.05	100,100,100,100	0
29	MN	X	3075	1/1	0.99	0.08	71,71,71,71	0
29	MN	X	3270	1/1	0.99	0.04	110,110,110,110	0
29	MN	X	3016	1/1	0.99	0.02	75,75,75,75	0
29	MN	X	3201	1/1	0.99	0.05	88,88,88,88	0
29	MN	X	3136	1/1	0.99	0.12	55,55,55,55	0
29	MN	X	3018	1/1	1.00	0.04	86,86,86,86	0
29	MN	X	3085	1/1	1.00	0.07	59,59,59,59	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 62B X 3003:

$2mF_o-DF_c$ (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.