



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 02:22 PM UTC

PDB ID : 4YZM / pdb_00004yzm
Title : Humanized Roco4 bound to LRRK2-In1
Authors : Gilsbach, B.K.; Messias, A.C.; Ito, G.; Sattler, M.; Alessi, D.R.; Wittinghofer, A.; Kortholt, A.
Deposited on : 2015-03-25
Resolution : 3.00 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

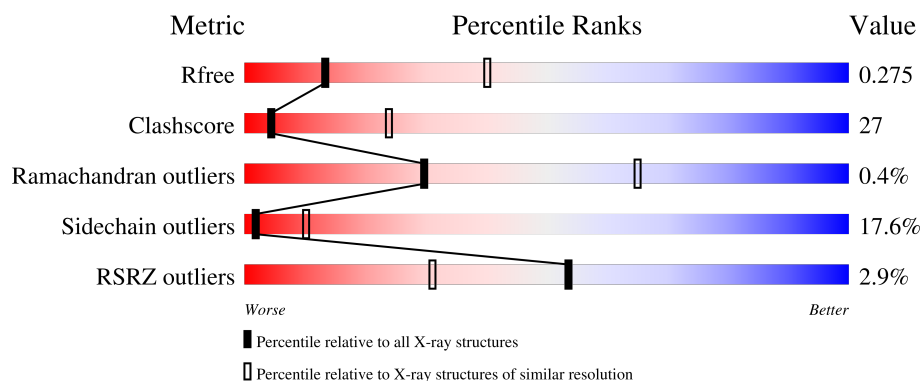
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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	2672 (3.00-3.00)
Clashscore	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)
RSRZ outliers	180081	2671 (3.00-3.00)

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	287	2% 34% 38% 16% • 9%
1	B	287	3% 38% 35% 16% • 9%

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 4330 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 Probable serine/threonine-protein kinase roco4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	260	Total	C	N	O	S	0	0	0
			2098	1352	355	377	14			
1	B	262	Total	C	N	O	S	0	1	0
			2110	1359	356	381	14			

There are 30 discrepancies between the modelled and reference sequences:

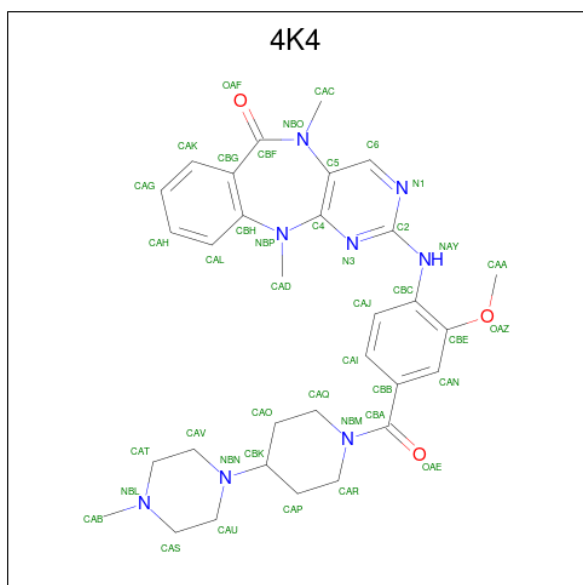
Chain	Residue	Modelled	Actual	Comment	Reference
A	1006	GLY	-	expression tag	UNP Q6XHB2
A	1007	ALA	-	expression tag	UNP Q6XHB2
A	1008	MET	-	expression tag	UNP Q6XHB2
A	1009	GLY	-	expression tag	UNP Q6XHB2
A	1010	GLY	-	expression tag	UNP Q6XHB2
A	1011	SER	-	expression tag	UNP Q6XHB2
A	1012	GLU	-	expression tag	UNP Q6XHB2
A	1013	PHE	-	expression tag	UNP Q6XHB2
A	1014	PRO	-	expression tag	UNP Q6XHB2
A	1015	LYS	-	expression tag	UNP Q6XHB2
A	1016	SER	-	expression tag	UNP Q6XHB2
A	1017	ARG	-	expression tag	UNP Q6XHB2
A	1018	LEU	-	expression tag	UNP Q6XHB2
A	1107	LEU	PHE	engineered mutation	UNP Q6XHB2
A	1161	LEU	PHE	engineered mutation	UNP Q6XHB2
B	1006	GLY	-	expression tag	UNP Q6XHB2
B	1007	ALA	-	expression tag	UNP Q6XHB2
B	1008	MET	-	expression tag	UNP Q6XHB2
B	1009	GLY	-	expression tag	UNP Q6XHB2
B	1010	GLY	-	expression tag	UNP Q6XHB2
B	1011	SER	-	expression tag	UNP Q6XHB2
B	1012	GLU	-	expression tag	UNP Q6XHB2
B	1013	PHE	-	expression tag	UNP Q6XHB2
B	1014	PRO	-	expression tag	UNP Q6XHB2
B	1015	LYS	-	expression tag	UNP Q6XHB2

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Chain	Residue	Modelled	Actual	Comment	Reference
B	1016	SER	-	expression tag	UNP Q6XHB2
B	1017	ARG	-	expression tag	UNP Q6XHB2
B	1018	LEU	-	expression tag	UNP Q6XHB2
B	1107	LEU	PHE	engineered mutation	UNP Q6XHB2
B	1161	LEU	PHE	engineered mutation	UNP Q6XHB2

- Molecule 2 is 2-[(2-methoxy-4-{[4-(4-methylpiperazin-1-yl)piperidin-1-yl]carbonyl}phenyl)amino]-5,11-dimethyl-5,11-dihydro-6H-pyrimido[4,5-b][1,4]benzodiazepin-6-one (CCD ID: 4K4) (formula: C₃₁H₃₈N₈O₃).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			42	31	8	3		
2	B	1	Total	C	N	O	0	0
			42	31	8	3		

- Molecule 3 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Mg	0	0
			1	1		
3	B	1	Total	Mg	0	0
			1	1		

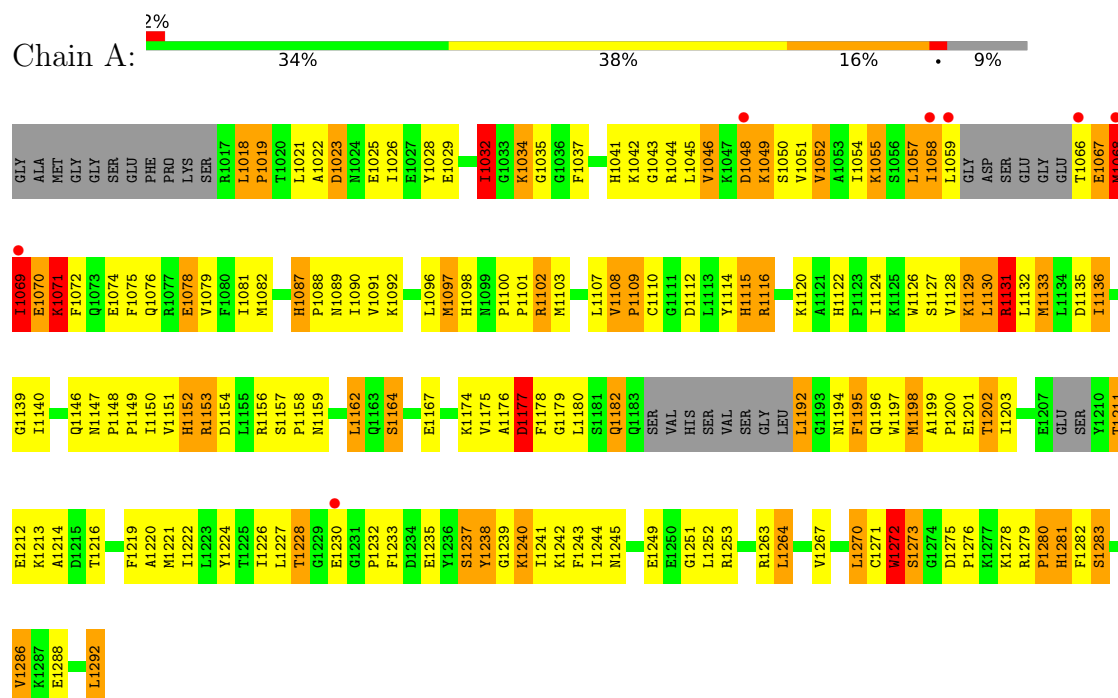
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	13	Total 13	O 13	0	0
4	B	23	Total 23	O 23	0	0

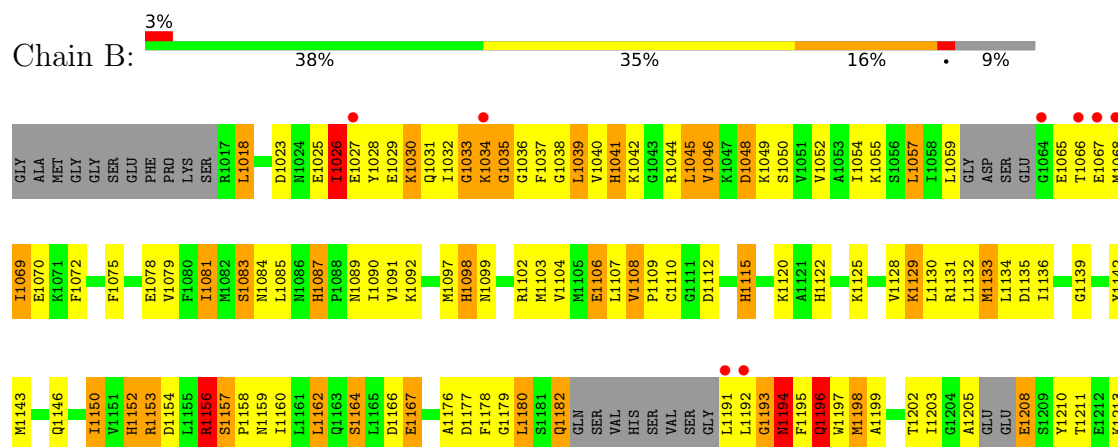
3 Residue-property plots

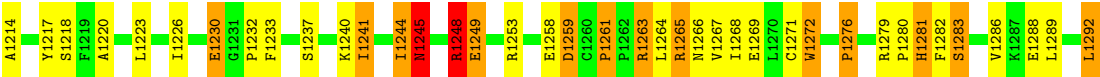
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Probable serine/threonine-protein kinase roco4



- Molecule 1: Probable serine/threonine-protein kinase roco4





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	43.03Å 89.07Å 177.71Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	44.43 – 3.00 44.43 – 3.00	Depositor EDS
% Data completeness (in resolution range)	99.9 (44.43-3.00) 99.9 (44.43-3.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.21 (at 3.01Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.196 , 0.282 0.225 , 0.275	Depositor DCC
R_{free} test set	719 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	47.1	Xtriage
Anisotropy	0.045	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 52.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	4330	wwPDB-VP
Average B, all atoms (Å ²)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 17.52% 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: MG, 4K4

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	2.09	47/2145 (2.2%)	1.46	34/2895 (1.2%)
1	B	2.19	52/2160 (2.4%)	1.61	44/2917 (1.5%)
All	All	2.14	99/4305 (2.3%)	1.54	78/5812 (1.3%)

All (99) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	1261	PRO	CA-C	-9.09	1.46	1.52
1	B	1245[A]	ASN	N-CA	8.36	1.56	1.46
1	B	1245[B]	ASN	N-CA	8.36	1.56	1.46
1	B	1122	HIS	CG-ND1	-7.71	1.29	1.38
1	B	1035	GLY	CA-C	-7.15	1.44	1.52
1	A	1122	HIS	CG-ND1	-7.09	1.30	1.38
1	B	1152	HIS	CG-ND1	-7.02	1.30	1.38
1	A	1152	HIS	CG-ND1	-7.01	1.30	1.38
1	B	1087	HIS	CG-ND1	-6.93	1.30	1.38
1	A	1087	HIS	CG-ND1	-6.86	1.30	1.38
1	B	1041	HIS	CA-C	-6.70	1.44	1.52
1	B	1115	HIS	CG-ND1	-6.66	1.30	1.38
1	B	1157	SER	C-O	-6.65	1.18	1.24
1	B	1035	GLY	N-CA	-6.60	1.38	1.45
1	B	1261	PRO	C-O	-6.54	1.19	1.24
1	B	1288	GLU	C-O	-6.49	1.16	1.24
1	B	1135	ASP	C-O	-6.46	1.16	1.24
1	B	1281	HIS	CA-C	-6.31	1.44	1.52
1	A	1136	ILE	C-O	-6.28	1.16	1.24
1	B	1122	HIS	CA-C	-6.24	1.46	1.52
1	A	1122	HIS	CA-C	-6.19	1.45	1.52
1	B	1136	ILE	C-O	-6.18	1.16	1.24
1	B	1261	PRO	CA-CB	-6.13	1.48	1.54
1	A	1152	HIS	CD2-NE2	-6.12	1.31	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	1132	LEU	C-O	-6.12	1.16	1.24
1	A	1098	HIS	CG-ND1	-6.10	1.31	1.38
1	B	1156	ARG	CA-C	-6.10	1.45	1.52
1	A	1157	SER	C-O	-6.09	1.19	1.24
1	A	1133	MET	C-O	-6.08	1.17	1.24
1	B	1087	HIS	CD2-NE2	-6.02	1.31	1.37
1	A	1131	ARG	C-O	-6.00	1.17	1.24
1	B	1122	HIS	CD2-NE2	-5.94	1.31	1.37
1	B	1281	HIS	CG-ND1	-5.85	1.31	1.38
1	A	1156	ARG	C-O	-5.84	1.17	1.23
1	B	1218	SER	C-O	-5.83	1.17	1.24
1	A	1162	LEU	C-O	-5.80	1.17	1.24
1	B	1133	MET	C-O	-5.80	1.17	1.24
1	A	1288	GLU	C-O	-5.73	1.17	1.24
1	B	1288	GLU	CA-C	-5.73	1.45	1.52
1	B	1128	VAL	C-O	-5.72	1.17	1.24
1	B	1160	ILE	C-O	-5.71	1.18	1.24
1	B	1129	LYS	C-O	-5.69	1.17	1.24
1	A	1041	HIS	CA-C	-5.69	1.45	1.52
1	A	1139	GLY	C-O	-5.67	1.17	1.23
1	A	1108	VAL	CA-C	-5.66	1.48	1.53
1	A	1197	TRP	NE1-CE2	-5.65	1.31	1.37
1	B	1156	ARG	C-O	-5.62	1.17	1.23
1	A	1126	TRP	NE1-CE2	-5.61	1.31	1.37
1	A	1237	SER	C-O	-5.61	1.17	1.24
1	B	1266	ASN	CA-C	-5.60	1.45	1.52
1	B	1041	HIS	CG-ND1	-5.58	1.32	1.38
1	B	1272	TRP	NE1-CE2	-5.58	1.31	1.37
1	A	1122	HIS	N-CA	-5.56	1.41	1.46
1	A	1115	HIS	CG-ND1	-5.54	1.32	1.38
1	B	1152	HIS	CD2-NE2	-5.54	1.31	1.37
1	B	1223	LEU	C-O	-5.46	1.17	1.24
1	A	1251	GLY	C-O	-5.46	1.17	1.24
1	B	1130	LEU	C-O	-5.45	1.17	1.24
1	A	1272	TRP	CA-C	-5.42	1.46	1.53
1	B	1281	HIS	CD2-NE2	-5.42	1.31	1.37
1	A	1129	LYS	C-O	-5.41	1.17	1.24
1	A	1135	ASP	C-O	-5.40	1.17	1.24
1	B	1196	GLN	C-O	-5.37	1.17	1.24
1	A	1214	ALA	C-O	-5.34	1.18	1.24
1	A	1122	HIS	CD2-NE2	-5.34	1.31	1.37
1	A	1219	PHE	C-O	-5.33	1.17	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	1197	TRP	NE1-CE2	-5.32	1.31	1.37
1	B	1035	GLY	C-N	-5.30	1.25	1.33
1	B	1268	ILE	C-O	-5.29	1.18	1.24
1	A	1221	MET	C-O	-5.26	1.17	1.24
1	A	1176	ALA	C-O	-5.25	1.17	1.23
1	A	1216	THR	C-O	-5.25	1.18	1.24
1	B	1098	HIS	CG-ND1	-5.23	1.32	1.38
1	B	1253	ARG	CA-C	-5.21	1.47	1.52
1	A	1164	SER	C-O	-5.20	1.17	1.23
1	B	1106	GLU	C-O	-5.20	1.17	1.23
1	A	1041	HIS	CG-ND1	-5.20	1.32	1.38
1	B	1230	GLU	C-O	-5.20	1.17	1.23
1	A	1087	HIS	CD2-NE2	-5.19	1.32	1.37
1	A	1239	GLY	C-O	-5.19	1.16	1.23
1	A	1286	VAL	C-O	-5.18	1.18	1.24
1	A	1130	LEU	C-O	-5.17	1.18	1.24
1	B	1164	SER	C-O	-5.17	1.17	1.23
1	A	1124	ILE	C-O	-5.16	1.18	1.24
1	A	1264	LEU	C-O	-5.16	1.18	1.24
1	B	1098	HIS	CA-C	-5.15	1.46	1.52
1	A	1222	ILE	C-O	-5.14	1.18	1.24
1	B	1078	GLU	C-O	-5.14	1.18	1.24
1	B	1131	ARG	C-O	-5.14	1.18	1.24
1	A	1270	LEU	C-O	-5.13	1.18	1.24
1	A	1078	GLU	C-O	-5.13	1.18	1.24
1	A	1043	GLY	C-O	-5.12	1.18	1.23
1	A	1281	HIS	CG-ND1	-5.12	1.32	1.38
1	A	1098	HIS	CD2-NE2	-5.06	1.32	1.37
1	B	1135	ASP	CA-C	-5.04	1.46	1.52
1	B	1276	PRO	C-O	-5.04	1.18	1.24
1	A	1272	TRP	NE1-CE2	-5.02	1.31	1.37
1	B	1035	GLY	C-O	-5.02	1.19	1.23
1	A	1200	PRO	C-O	-5.00	1.17	1.24

All (78) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	1035	GLY	N-CA-C	-24.23	80.69	111.70
1	A	1195	PHE	N-CA-CB	-15.84	83.72	110.49
1	B	1176	ALA	N-CA-C	15.25	133.93	114.56
1	A	1195	PHE	N-CA-C	14.76	142.24	110.80
1	B	1244	ILE	CA-C-N	14.25	139.78	120.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	1244	ILE	C-N-CA	14.25	139.78	120.54
1	B	1065	GLU	N-CA-C	13.99	130.63	112.72
1	A	1177	ASP	N-CA-C	13.32	130.16	111.52
1	A	1098	HIS	N-CA-C	12.49	129.24	113.88
1	A	1068	MET	N-CA-C	-12.09	98.24	113.23
1	B	1066	THR	N-CA-C	-11.40	96.52	113.61
1	B	1034	LYS	N-CA-C	-10.82	98.20	111.40
1	B	1046	VAL	N-CA-C	10.06	120.88	110.72
1	A	1179	GLY	N-CA-C	-9.13	91.53	113.18
1	B	1241	ILE	N-CA-C	8.86	119.66	110.62
1	A	1178	PHE	N-CA-C	8.60	123.10	113.21
1	B	1179	GLY	N-CA-C	-8.58	92.84	113.18
1	B	1048	ASP	N-CA-C	-8.57	94.94	109.24
1	A	1048	ASP	N-CA-C	-8.48	96.47	109.95
1	B	1198	MET	N-CA-C	8.39	122.70	110.28
1	B	1280	PRO	N-CA-C	8.22	123.74	111.41
1	B	1281	HIS	N-CA-C	-7.68	99.11	110.48
1	A	1109	PRO	N-CA-C	7.64	123.64	113.40
1	A	1049	LYS	N-CA-C	-7.61	104.41	112.93
1	A	1280	PRO	N-CA-C	7.51	121.74	111.22
1	A	1019	PRO	N-CA-C	7.01	122.35	111.21
1	B	1178	PHE	N-CA-C	6.97	121.09	112.59
1	B	1065	GLU	CB-CA-C	-6.83	99.17	110.37
1	A	1071	LYS	N-CA-C	-6.81	104.45	112.89
1	A	1211	THR	N-CA-C	-6.74	99.42	109.86
1	A	1281	HIS	N-CA-C	-6.67	100.65	110.52
1	B	1037	PHE	N-CA-C	-6.64	105.71	113.88
1	B	1195	PHE	N-CA-C	6.41	120.20	112.38
1	A	1029	GLU	N-CA-C	6.39	120.69	112.12
1	A	1227	LEU	N-CA-C	6.35	118.00	111.14
1	B	1108	VAL	CA-C-N	6.33	126.02	119.56
1	B	1108	VAL	C-N-CA	6.33	126.02	119.56
1	A	1110	CYS	N-CA-C	6.30	120.97	113.16
1	A	1032	ILE	N-CA-C	6.15	116.31	110.53
1	A	1239	GLY	N-CA-C	-6.13	103.13	112.51
1	B	1162	LEU	N-CA-C	5.87	118.23	108.20
1	A	1074	GLU	N-CA-C	-5.81	104.94	111.28
1	B	1108	VAL	CA-C-O	5.76	122.55	119.15
1	B	1109	PRO	N-CA-C	5.73	121.29	113.84
1	A	1249	GLU	N-CA-C	5.70	120.37	112.45
1	A	1238	TYR	N-CA-C	-5.66	100.69	109.24
1	B	1033	GLY	N-CA-C	5.64	126.56	113.18

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1098	HIS	CA-C-N	-5.59	115.14	122.74
1	A	1098	HIS	C-N-CA	-5.59	115.14	122.74
1	A	1150	ILE	CB-CA-C	-5.58	103.34	110.98
1	A	1202	THR	N-CA-C	5.56	117.42	111.36
1	B	1245[A]	ASN	N-CA-C	5.55	117.77	111.11
1	B	1245[B]	ASN	N-CA-C	5.55	117.77	111.11
1	B	1153	ARG	N-CA-CB	-5.52	107.87	114.17
1	A	1081	ILE	N-CA-C	5.51	116.24	110.62
1	A	1214	ALA	N-CA-C	-5.50	105.19	111.14
1	B	1214	ALA	N-CA-C	-5.50	105.36	111.36
1	B	1180	LEU	N-CA-C	5.50	119.22	110.70
1	A	1128	VAL	N-CA-C	5.47	116.25	110.72
1	A	1198	MET	N-CA-C	5.46	118.71	109.76
1	B	1036	GLY	N-CA-C	-5.44	100.29	113.18
1	B	1193	GLY	N-CA-C	-5.42	104.28	112.84
1	B	1108	VAL	CB-CA-C	5.39	116.47	110.71
1	B	1042	LYS	N-CA-C	-5.38	100.93	109.96
1	B	1018	LEU	CA-C-N	-5.25	114.53	119.89
1	B	1018	LEU	C-N-CA	-5.25	114.53	119.89
1	A	1092	LYS	N-CA-C	5.25	118.30	109.95
1	B	1084	ASN	N-CA-C	5.22	117.88	111.82
1	B	1194	ASN	N-CA-C	5.20	116.19	108.60
1	B	1026	ILE	N-CA-C	5.13	117.42	108.95
1	B	1035	GLY	CA-C-N	5.13	131.46	121.41
1	B	1035	GLY	C-N-CA	5.13	131.46	121.41
1	B	1134	LEU	N-CA-C	5.09	116.91	111.36
1	B	1248	ARG	N-CA-C	5.09	116.91	111.36
1	B	1034	LYS	CA-C-N	5.08	130.89	122.65
1	B	1034	LYS	C-N-CA	5.08	130.89	122.65
1	A	1153	ARG	N-CA-CB	-5.04	106.00	114.27
1	A	1070	GLU	CB-CA-C	5.01	119.08	111.02

There are no chirality outliers.

There are no planarity outliers.

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	2098	0	2119	119	0
1	B	2110	0	2130	106	0
2	A	42	0	38	4	0
2	B	42	0	38	2	0
3	A	1	0	0	0	0
3	B	1	0	0	1	0
4	A	13	0	0	0	0
4	B	23	0	0	7	0
All	All	4330	0	4325	229	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 27.

All (229) 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)
1:A:1192:LEU:CD2	1:A:1196:GLN:HE21	1.50	1.24
1:B:1035:GLY:HA3	1:B:1038:GLY:O	1.36	1.20
1:A:1058:ILE:O	1:A:1071:LYS:NZ	1.78	1.16
1:A:1199:ALA:O	1:A:1202:THR:OG1	1.67	1.12
1:B:1075:PHE:O	1:B:1079:VAL:HG23	1.47	1.10
1:A:1192:LEU:CD2	1:A:1196:GLN:NE2	2.17	1.07
1:B:1248:ARG:HH11	1:B:1248:ARG:HB2	1.18	1.07
1:A:1192:LEU:HD22	1:A:1196:GLN:HE21	1.15	1.05
1:B:1112:ASP:OD2	1:B:1115:HIS:HD2	1.43	1.02
1:A:1154:ASP:O	1:A:1159:ASN:ND2	1.93	1.01
1:A:1087:HIS:HD2	1:A:1089:ASN:H	1.09	0.93
1:B:1048:ASP:OD1	1:B:1050:SER:OG	1.86	0.93
1:B:1129:LYS:HE2	1:B:1226:ILE:O	1.70	0.92
1:A:1025:GLU:O	1:A:1046:VAL:HG22	1.69	0.92
1:A:1192:LEU:HD23	1:A:1196:GLN:NE2	1.82	0.91
1:B:1156:ARG:HB2	1:B:1158:PRO:HD2	1.51	0.91
1:A:1067:GLU:O	1:A:1070:GLU:HG2	1.69	0.91
1:B:1092:LYS:N	1:B:1106:GLU:OE2	2.06	0.88
1:A:1087:HIS:CD2	1:A:1089:ASN:H	1.90	0.88
1:A:1068:MET:C	1:A:1070:GLU:H	1.83	0.87
1:A:1075:PHE:O	1:A:1079:VAL:HG23	1.76	0.86
1:A:1068:MET:O	1:A:1070:GLU:N	2.08	0.86
1:A:1025:GLU:O	1:A:1046:VAL:CG2	2.23	0.86
1:A:1224:TYR:O	1:A:1228:THR:OG1	1.93	0.86
1:B:1248:ARG:HH11	1:B:1248:ARG:CB	1.88	0.85
1:B:1033:GLY:HA3	1:B:1040:VAL:H	1.40	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1035:GLY:CA	1:B:1038:GLY:O	2.23	0.84
1:A:1232:PRO:O	1:A:1233:PHE:HB2	1.77	0.84
1:A:1112:ASP:OD1	1:A:1115:HIS:HD2	1.62	0.82
1:B:1112:ASP:OD2	1:B:1115:HIS:CD2	2.32	0.81
1:A:1032:ILE:HD13	1:A:1042:LYS:HB2	1.62	0.81
1:A:1100:PRO:HG2	1:A:1102:ARG:HD3	1.61	0.81
1:A:1273:SER:O	1:A:1279:ARG:NH2	2.13	0.81
1:A:1132:LEU:O	1:A:1136:ILE:HG13	1.79	0.81
1:B:1232:PRO:O	1:B:1233:PHE:HB2	1.80	0.80
1:B:1030:LYS:HG2	1:B:1031:GLN:N	1.94	0.79
1:A:1282:PHE:O	1:A:1286:VAL:HG23	1.82	0.79
1:B:1167:GLU:CG	4:B:1408:HOH:O	2.31	0.79
1:B:1167:GLU:HG2	4:B:1408:HOH:O	1.84	0.78
1:A:1058:ILE:HG23	1:A:1071:LYS:HZ1	1.49	0.78
1:B:1097:MET:HE2	1:B:1104:VAL:HG22	1.63	0.78
1:A:1152:HIS:O	1:A:1153:ARG:HB2	1.84	0.77
1:A:1045:LEU:N	1:A:1045:LEU:HD22	2.00	0.76
1:A:1058:ILE:HG23	1:A:1071:LYS:NZ	2.01	0.76
1:A:1129:LYS:O	1:A:1133:MET:HG3	1.85	0.76
1:A:1087:HIS:HB3	1:A:1090:ILE:HG12	1.69	0.74
1:B:1208:GLU:O	1:B:1208:GLU:HG3	1.86	0.74
1:B:1182:GLN:NE2	1:B:1192:LEU:O	2.21	0.74
1:B:1120:LYS:NZ	1:B:1230:GLU:OE2	2.20	0.74
1:A:1153:ARG:O	1:A:1182:GLN:HG2	1.88	0.73
1:A:1159:ASN:OD1	1:A:1177:ASP:OD2	2.08	0.72
1:B:1194:ASN:HB3	1:B:1196:GLN:OE1	1.90	0.72
1:B:1282:PHE:O	1:B:1286:VAL:HG23	1.90	0.71
1:A:1032:ILE:CD1	1:A:1042:LYS:HB2	2.21	0.71
1:A:1087:HIS:HD2	1:A:1089:ASN:N	1.87	0.70
1:A:1151:VAL:O	1:A:1180:LEU:HD22	1.92	0.70
1:A:1159:ASN:CG	1:A:1177:ASP:OD2	2.36	0.69
1:B:1265:ARG:O	1:B:1269:GLU:HG3	1.92	0.69
1:A:1035:GLY:O	1:A:1055:LYS:HE2	1.92	0.69
1:A:1034:LYS:O	1:A:1034:LYS:HG3	1.93	0.68
1:A:1025:GLU:C	1:A:1046:VAL:HG22	2.17	0.68
1:B:1067:GLU:HA	1:B:1070:GLU:HG3	1.76	0.68
1:A:1025:GLU:C	1:A:1046:VAL:CG2	2.66	0.68
1:B:1240:LYS:O	1:B:1244:ILE:HG13	1.94	0.67
1:A:1270:LEU:O	1:A:1273:SER:OG	2.12	0.67
1:A:1045:LEU:HD21	1:A:1052:VAL:CG2	2.25	0.67
1:A:1070:GLU:OE1	1:A:1070:GLU:HA	1.94	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1044:ARG:NH1	1:A:1049:LYS:O	2.27	0.67
1:B:1057:LEU:HD21	1:B:1072:PHE:HD1	1.59	0.67
1:B:1248:ARG:HB2	1:B:1248:ARG:NH1	2.03	0.67
1:B:1281:HIS:ND1	1:B:1283:SER:OG	2.27	0.66
1:B:1129:LYS:O	1:B:1133:MET:HG3	1.96	0.65
1:A:1112:ASP:OD1	1:A:1115:HIS:CD2	2.50	0.64
1:B:1079:VAL:O	1:B:1083:SER:OG	2.14	0.64
1:A:1114:TYR:HB2	1:A:1158:PRO:HD3	1.80	0.64
1:A:1087:HIS:HB3	1:A:1090:ILE:CG1	2.28	0.63
1:B:1081:ILE:O	1:B:1085:LEU:HG	1.98	0.63
1:A:1058:ILE:HD12	1:A:1059:LEU:N	2.13	0.63
1:A:1037:PHE:HZ	1:A:1103:MET:HE1	1.63	0.62
1:A:1088:PRO:O	1:A:1174:LYS:HE3	1.97	0.62
1:A:1240:LYS:O	1:A:1244:ILE:HG12	1.98	0.62
1:B:1248:ARG:HH11	1:B:1248:ARG:CG	2.12	0.62
1:B:1110:CYS:HB2	1:B:1162:LEU:O	1.99	0.62
1:B:1263:ARG:O	1:B:1267:VAL:HG23	1.99	0.62
1:A:1058:ILE:HD12	1:A:1058:ILE:C	2.24	0.62
1:B:1097:MET:HE2	1:B:1104:VAL:CG2	2.30	0.62
1:B:1157:SER:OG	1:B:1158:PRO:HD3	2.00	0.62
1:B:1035:GLY:HA3	1:B:1038:GLY:C	2.22	0.61
1:A:1097:MET:HB2	1:A:1102:ARG:HB2	1.82	0.61
1:B:1033:GLY:N	1:B:1040:VAL:O	2.34	0.61
1:A:1018:LEU:HD22	1:A:1019:PRO:HD2	1.83	0.60
1:A:1023:ASP:OD1	1:A:1023:ASP:N	2.32	0.60
1:A:1068:MET:C	1:A:1070:GLU:N	2.48	0.60
1:B:1068:MET:CB	4:B:1421:HOH:O	2.49	0.60
1:B:1177:ASP:OD2	3:B:1302:MG:MG	1.44	0.60
1:A:1213:LYS:HD2	1:A:1276:PRO:O	2.02	0.59
1:A:1264:LEU:HB2	1:A:1292:LEU:HD21	1.85	0.59
1:A:1057:LEU:HD21	1:A:1075:PHE:CD2	2.38	0.59
1:B:1153:ARG:NH1	1:B:1180:LEU:O	2.36	0.59
1:A:1263:ARG:HB3	1:A:1292:LEU:HD11	1.84	0.59
1:B:1152:HIS:O	1:B:1153:ARG:HB2	2.03	0.59
1:A:1045:LEU:HD21	1:A:1052:VAL:HG21	1.84	0.59
1:B:1030:LYS:HG2	1:B:1031:GLN:H	1.68	0.59
1:B:1199:ALA:O	1:B:1202:THR:OG1	2.21	0.59
1:A:1263:ARG:O	1:A:1267:VAL:HG23	2.03	0.58
1:A:1037:PHE:HZ	1:A:1103:MET:CE	2.16	0.58
1:B:1069:ILE:HG13	1:B:1070:GLU:N	2.17	0.58
1:B:1143:MET:HB3	1:B:1150:ILE:HB	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1042:LYS:HG3	1:A:1107:LEU:HD22	1.86	0.57
1:B:1034:LYS:HD3	1:B:1035:GLY:O	2.05	0.57
1:B:1068:MET:HB3	4:B:1421:HOH:O	2.05	0.57
1:B:1205:ALA:C	1:B:1208:GLU:HA	2.30	0.56
1:B:1081:ILE:HG22	1:B:1085:LEU:HD11	1.87	0.56
1:B:1039:LEU:HD23	1:B:1041:HIS:CE1	2.41	0.55
1:A:1037:PHE:CD1	1:A:1037:PHE:C	2.86	0.54
1:A:1045:LEU:HD22	1:A:1045:LEU:H	1.71	0.54
1:A:1087:HIS:CD2	1:A:1089:ASN:HB2	2.42	0.54
1:B:1213:LYS:HD2	1:B:1276:PRO:O	2.07	0.54
1:A:1263:ARG:HB3	1:A:1292:LEU:CD1	2.38	0.54
1:A:1018:LEU:HD22	1:A:1019:PRO:CD	2.37	0.54
1:B:1081:ILE:HG22	1:B:1085:LEU:CD1	2.38	0.54
1:B:1087:HIS:CD2	1:B:1089:ASN:H	2.26	0.54
1:B:1091:VAL:HG13	1:B:1106:GLU:HG2	1.90	0.53
1:A:1025:GLU:O	1:A:1046:VAL:HG23	2.06	0.53
1:A:1078:GLU:OE2	1:A:1082:MET:HE3	2.07	0.53
1:A:1281:HIS:ND1	1:A:1283:SER:OG	2.38	0.53
1:A:1108:VAL:HG13	1:A:1109:PRO:HD2	1.90	0.53
1:A:1116:ARG:HD2	1:A:1116:ARG:O	2.09	0.53
1:A:1022:ALA:N	1:A:1025:GLU:OE1	2.37	0.52
1:B:1230:GLU:HB3	4:B:1403:HOH:O	2.08	0.52
1:B:1108:VAL:O	2:B:1301:4K4:H27	2.10	0.52
1:B:1033:GLY:HA3	1:B:1040:VAL:N	2.19	0.52
1:B:1033:GLY:HA2	1:B:1040:VAL:HB	1.91	0.52
1:B:1248:ARG:NH1	1:B:1248:ARG:CG	2.71	0.52
1:B:1027:GLU:HG3	1:B:1046:VAL:HG22	1.92	0.52
1:B:1153:ARG:HG2	1:B:1210:TYR:CD2	2.44	0.52
1:B:1045:LEU:O	1:B:1049:LYS:HA	2.11	0.51
1:B:1153:ARG:HG2	1:B:1210:TYR:CE2	2.45	0.51
1:A:1177:ASP:O	1:A:1177:ASP:CG	2.54	0.51
1:B:1259:ASP:OD1	1:B:1259:ASP:N	2.44	0.51
1:B:1045:LEU:O	1:B:1048:ASP:O	2.29	0.51
1:A:1045:LEU:N	1:A:1045:LEU:CD2	2.73	0.50
1:B:1196:GLN:CD	1:B:1196:GLN:H	2.20	0.50
1:B:1081:ILE:CG2	1:B:1085:LEU:HD11	2.42	0.49
1:B:1075:PHE:O	1:B:1079:VAL:CG2	2.40	0.49
1:A:1177:ASP:O	1:A:1177:ASP:OD1	2.29	0.49
1:A:1018:LEU:HD12	1:A:1096:LEU:HG	1.95	0.49
1:B:1026:ILE:HD11	1:B:1028:TYR:CE1	2.47	0.49
1:A:1072:PHE:O	1:A:1075:PHE:HB3	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1037:PHE:CZ	1:A:1103:MET:HE1	2.47	0.49
1:A:1203:ILE:HG21	1:A:1244:ILE:HD12	1.95	0.48
1:B:1057:LEU:HD21	1:B:1072:PHE:CD1	2.45	0.48
1:A:1018:LEU:CD1	1:A:1096:LEU:HG	2.43	0.48
1:B:1281:HIS:CE1	1:B:1283:SER:OG	2.67	0.48
1:B:1033:GLY:CA	1:B:1040:VAL:H	2.20	0.48
1:A:1182:GLN:NE2	1:A:1182:GLN:C	2.72	0.47
1:B:1026:ILE:HG22	1:B:1045:LEU:HD12	1.95	0.47
1:A:1108:VAL:CG1	1:A:1109:PRO:HD2	2.45	0.47
1:B:1241:ILE:O	1:B:1245[A]:ASN:HB2	2.14	0.47
1:B:1154:ASP:O	1:B:1159:ASN:ND2	2.48	0.47
1:A:1026:ILE:HD11	1:A:1028:TYR:CE1	2.50	0.47
1:A:1198:MET:HE2	1:A:1198:MET:HB3	1.70	0.47
1:A:1136:ILE:O	1:A:1140:ILE:HG13	2.14	0.46
1:B:1289:LEU:HA	1:B:1292:LEU:HD23	1.97	0.46
1:A:1034:LYS:HE3	1:A:1034:LYS:HB2	1.79	0.46
1:B:1182:GLN:NE2	1:B:1182:GLN:C	2.73	0.46
1:A:1066:THR:O	1:A:1067:GLU:HG2	2.16	0.46
1:A:1054:ILE:HA	1:A:1103:MET:O	2.16	0.46
1:B:1034:LYS:HB3	1:B:1035:GLY:O	2.15	0.46
1:B:1087:HIS:HD2	1:B:1089:ASN:H	1.63	0.46
1:B:1097:MET:HB2	1:B:1102:ARG:HB2	1.96	0.46
1:B:1157:SER:N	1:B:1158:PRO:CD	2.79	0.46
1:B:1199:ALA:HA	1:B:1217:TYR:CD1	2.50	0.46
1:A:1130:LEU:HD23	1:A:1130:LEU:HA	1.77	0.46
1:A:1220:ALA:HB2	1:A:1271:CYS:HB2	1.99	0.45
1:B:1198:MET:HB3	1:B:1198:MET:HE2	1.62	0.45
1:A:1058:ILE:O	1:A:1058:ILE:HG23	2.16	0.45
1:B:1032:ILE:CD1	1:B:1107:LEU:HD11	2.47	0.45
1:B:1264:LEU:HD12	1:B:1264:LEU:O	2.17	0.45
1:A:1192:LEU:HD22	1:A:1196:GLN:NE2	2.00	0.45
2:A:1301:4K4:H19	2:A:1301:4K4:CAI	2.47	0.44
1:A:1129:LYS:HE2	1:A:1226:ILE:O	2.17	0.44
1:A:1252:LEU:C	1:A:1253:ARG:HG2	2.43	0.44
1:A:1059:LEU:O	1:A:1069:ILE:HG23	2.17	0.44
1:B:1194:ASN:O	1:B:1198:MET:HG3	2.18	0.44
1:A:1272:TRP:CD1	1:A:1272:TRP:C	2.95	0.44
1:A:1069:ILE:O	1:A:1070:GLU:OE1	2.36	0.44
1:A:1101:PRO:O	1:A:1102:ARG:HG3	2.18	0.44
1:A:1048:ASP:C	1:A:1050:SER:H	2.26	0.43
1:B:1046:VAL:O	1:B:1046:VAL:HG12	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1087:HIS:HB3	1:B:1090:ILE:HG12	2.01	0.43
1:B:1068:MET:HB2	4:B:1421:HOH:O	2.18	0.43
1:A:1045:LEU:HD21	1:A:1052:VAL:HG23	1.98	0.43
1:A:1087:HIS:CG	1:A:1088:PRO:HD2	2.54	0.42
1:A:1097:MET:HB3	1:A:1102:ARG:NH2	2.33	0.42
1:A:1146:GLN:O	1:A:1148:PRO:C	2.62	0.42
1:A:1112:ASP:OD2	1:A:1114:TYR:HB3	2.19	0.42
2:A:1301:4K4:N3	2:A:1301:4K4:CAJ	2.80	0.42
1:A:1131:ARG:HA	1:A:1131:ARG:HD2	1.58	0.42
1:A:1279:ARG:HA	1:A:1280:PRO:HD3	1.81	0.42
1:B:1194:ASN:HD22	1:B:1194:ASN:HA	1.63	0.42
1:B:1220:ALA:HB2	1:B:1271:CYS:HB2	2.00	0.42
1:A:1057:LEU:CD2	1:A:1075:PHE:CD2	3.01	0.42
1:B:1156:ARG:CZ	1:B:1193:GLY:HA2	2.50	0.42
1:B:1166:ASP:OD1	1:B:1167:GLU:N	2.52	0.42
2:B:1301:4K4:H17	2:B:1301:4K4:H2	1.85	0.42
1:A:1201:GLU:H	1:A:1201:GLU:CD	2.27	0.42
1:B:1028:TYR:OH	1:B:1102:ARG:HD2	2.19	0.42
1:B:1098:HIS:O	1:B:1099:ASN:HB2	2.19	0.42
1:A:1275:ASP:HB3	1:A:1278:LYS:HG3	2.00	0.42
1:B:1139:GLY:O	1:B:1142:TYR:HB3	2.20	0.42
1:B:1203:ILE:O	1:B:1248:ARG:NH2	2.53	0.42
1:A:1108:VAL:HG12	1:A:1162:LEU:O	2.19	0.42
1:A:1177:ASP:HB3	2:A:1301:4K4:H36	2.02	0.41
1:B:1087:HIS:HB3	1:B:1090:ILE:CG1	2.51	0.41
1:A:1120:LYS:NZ	1:A:1230:GLU:OE2	2.53	0.41
1:A:1238:TYR:HB2	1:A:1243:PHE:CD2	2.56	0.41
1:A:1292:LEU:HA	1:A:1292:LEU:HD12	1.86	0.41
1:B:1220:ALA:HB2	1:B:1271:CYS:CB	2.50	0.41
1:B:1276:PRO:O	1:B:1279:ARG:HB2	2.21	0.41
2:A:1301:4K4:CAI	2:A:1301:4K4:CAR	2.99	0.41
1:A:1091:VAL:HG23	1:A:1175:VAL:O	2.21	0.41
1:B:1167:GLU:HG3	4:B:1408:HOH:O	2.07	0.41
1:A:1067:GLU:O	1:A:1070:GLU:CG	2.55	0.41
1:A:1272:TRP:CD1	1:A:1272:TRP:O	2.74	0.41
1:B:1034:LYS:CG	1:B:1035:GLY:O	2.69	0.41
1:B:1055:LYS:HD3	1:B:1103:MET:HE3	2.02	0.40
1:B:1035:GLY:HA2	1:B:1040:VAL:HG23	2.02	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	252/287 (88%)	240 (95%)	10 (4%)	2 (1%)	16	50
1	B	255/287 (89%)	252 (99%)	3 (1%)	0	100	100
All	All	507/574 (88%)	492 (97%)	13 (3%)	2 (0%)	30	65

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1069	ILE
1	A	1195	PHE

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	232/253 (92%)	190 (82%)	42 (18%)	2	9
1	B	234/253 (92%)	193 (82%)	41 (18%)	2	10
All	All	466/506 (92%)	383 (82%)	83 (18%)	2	10

All (83) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1018	LEU
1	A	1021	LEU
1	A	1023	ASP
1	A	1032	ILE

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Mol	Chain	Res	Type
1	A	1034	LYS
1	A	1046	VAL
1	A	1051	VAL
1	A	1052	VAL
1	A	1055	LYS
1	A	1057	LEU
1	A	1058	ILE
1	A	1067	GLU
1	A	1068	MET
1	A	1069	ILE
1	A	1071	LYS
1	A	1076	GLN
1	A	1097	MET
1	A	1102	ARG
1	A	1116	ARG
1	A	1127	SER
1	A	1131	ARG
1	A	1147	ASN
1	A	1149	PRO
1	A	1164	SER
1	A	1167	GLU
1	A	1177	ASP
1	A	1182	GLN
1	A	1192	LEU
1	A	1194	ASN
1	A	1211	THR
1	A	1212	GLU
1	A	1228	THR
1	A	1235	GLU
1	A	1237	SER
1	A	1240	LYS
1	A	1241	ILE
1	A	1242	LYS
1	A	1245	ASN
1	A	1272	TRP
1	A	1273	SER
1	A	1283	SER
1	A	1292	LEU
1	B	1018	LEU
1	B	1023	ASP
1	B	1025	GLU
1	B	1026	ILE

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Mol	Chain	Res	Type
1	B	1029	GLU
1	B	1030	LYS
1	B	1039	LEU
1	B	1044	ARG
1	B	1045	LEU
1	B	1052	VAL
1	B	1054	ILE
1	B	1057	LEU
1	B	1059	LEU
1	B	1069	ILE
1	B	1081	ILE
1	B	1083	SER
1	B	1125	LYS
1	B	1146	GLN
1	B	1150	ILE
1	B	1156	ARG
1	B	1164	SER
1	B	1167	GLU
1	B	1182	GLN
1	B	1191	LEU
1	B	1194	ASN
1	B	1196	GLN
1	B	1208	GLU
1	B	1211	THR
1	B	1237	SER
1	B	1245[A]	ASN
1	B	1245[B]	ASN
1	B	1248	ARG
1	B	1249	GLU
1	B	1258	GLU
1	B	1259	ASP
1	B	1261	PRO
1	B	1263	ARG
1	B	1265	ARG
1	B	1272	TRP
1	B	1283	SER
1	B	1292	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1041	HIS

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Mol	Chain	Res	Type
1	A	1087	HIS
1	A	1099	ASN
1	A	1115	HIS
1	A	1182	GLN
1	A	1196	GLN
1	B	1041	HIS
1	B	1087	HIS
1	B	1115	HIS
1	B	1194	ASN
1	B	1196	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 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
2	4K4	B	1301	-	45,47,47	2.35	7 (15%)	60,68,68	2.42	18 (30%)
2	4K4	A	1301	-	45,47,47	2.53	9 (20%)	60,68,68	2.41	19 (31%)

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
2	4K4	B	1301	-	-	3/18/38/38	0/6/6/6
2	4K4	A	1301	-	-	4/18/38/38	0/6/6/6

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1301	4K4	CBH-NBP	-11.30	1.33	1.43
2	B	1301	4K4	CBH-NBP	-8.88	1.35	1.43
2	B	1301	4K4	CBG-CBF	-7.65	1.38	1.50
2	A	1301	4K4	CBG-CBF	-5.54	1.41	1.50
2	B	1301	4K4	CBB-CBA	-5.14	1.41	1.50
2	A	1301	4K4	CAC-NBO	4.91	1.54	1.46
2	A	1301	4K4	CBB-CBA	-4.76	1.41	1.50
2	B	1301	4K4	C6-N1	4.21	1.43	1.34
2	A	1301	4K4	CAR-NBM	3.08	1.52	1.47
2	A	1301	4K4	C6-N1	2.79	1.40	1.34
2	B	1301	4K4	CAR-NBM	2.58	1.51	1.47
2	A	1301	4K4	CBC-NAY	-2.47	1.33	1.39
2	B	1301	4K4	CAQ-NBM	2.43	1.51	1.47
2	B	1301	4K4	C5-NBO	-2.38	1.36	1.42
2	A	1301	4K4	CAQ-NBM	2.32	1.51	1.47
2	A	1301	4K4	OAZ-CBE	2.19	1.40	1.37

All (37) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1301	4K4	C5-C4-NBP	9.23	126.08	120.14
2	B	1301	4K4	CAD-NBP-CBH	8.32	122.04	115.95
2	A	1301	4K4	N1-C2-N3	-6.79	119.85	126.42
2	B	1301	4K4	CBB-CBA-NBM	6.34	126.58	118.66
2	A	1301	4K4	CAL-CBH-NBP	-6.32	110.78	120.66
2	B	1301	4K4	C5-C4-NBP	6.20	124.12	120.14
2	B	1301	4K4	N1-C2-N3	-5.12	121.47	126.42
2	A	1301	4K4	CAV-NBN-CAU	5.10	118.84	109.13
2	A	1301	4K4	C6-N1-C2	4.39	121.83	115.81
2	B	1301	4K4	CAQ-NBM-CAR	3.86	120.56	112.68
2	B	1301	4K4	OAE-CBA-CBB	-3.76	112.83	120.29
2	B	1301	4K4	CAA-OAZ-CBE	3.76	123.03	117.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1301	4K4	CBB-CBA-NBM	3.76	123.35	118.66
2	B	1301	4K4	CAC-NBO-C5	-3.45	112.97	118.38
2	B	1301	4K4	CAK-CBG-CBH	3.39	122.70	118.81
2	B	1301	4K4	OAF-CBF-CBG	-3.35	114.36	119.94
2	B	1301	4K4	CAO-CAQ-NBM	3.24	117.01	110.66
2	A	1301	4K4	CAT-CAV-NBN	3.14	116.14	110.61
2	B	1301	4K4	CAL-CBH-NBP	-3.11	115.81	120.66
2	B	1301	4K4	CAT-NBL-CAS	2.88	114.12	109.54
2	B	1301	4K4	CAK-CBG-CBF	-2.74	110.64	116.22
2	A	1301	4K4	CAP-CAR-NBM	2.61	115.78	110.66
2	B	1301	4K4	C6-N1-C2	2.57	119.33	115.81
2	A	1301	4K4	CAQ-NBM-CAR	2.57	117.92	112.68
2	A	1301	4K4	CAO-CAQ-NBM	2.54	115.63	110.66
2	B	1301	4K4	CAP-CAR-NBM	2.52	115.60	110.66
2	A	1301	4K4	CAL-CBH-CBG	2.51	123.01	119.16
2	A	1301	4K4	CAU-NBN-CBK	2.43	118.96	112.79
2	A	1301	4K4	OAE-CBA-CBB	-2.28	115.77	120.29
2	A	1301	4K4	CAH-CAG-CAK	2.23	123.00	120.24
2	A	1301	4K4	C6-C5-NBO	-2.23	115.35	118.99
2	B	1301	4K4	C2-N3-C4	2.21	121.08	113.99
2	A	1301	4K4	C2-N3-C4	2.11	120.77	113.99
2	A	1301	4K4	CBG-CBH-NBP	2.10	126.12	121.74
2	B	1301	4K4	CAQ-NBM-CBA	-2.09	116.33	122.79
2	A	1301	4K4	CAJ-CBC-CBE	2.07	121.71	119.02
2	A	1301	4K4	CBC-NAY-C2	-2.06	122.94	129.22

There are no chirality outliers.

All (7) torsion outliers are listed below:

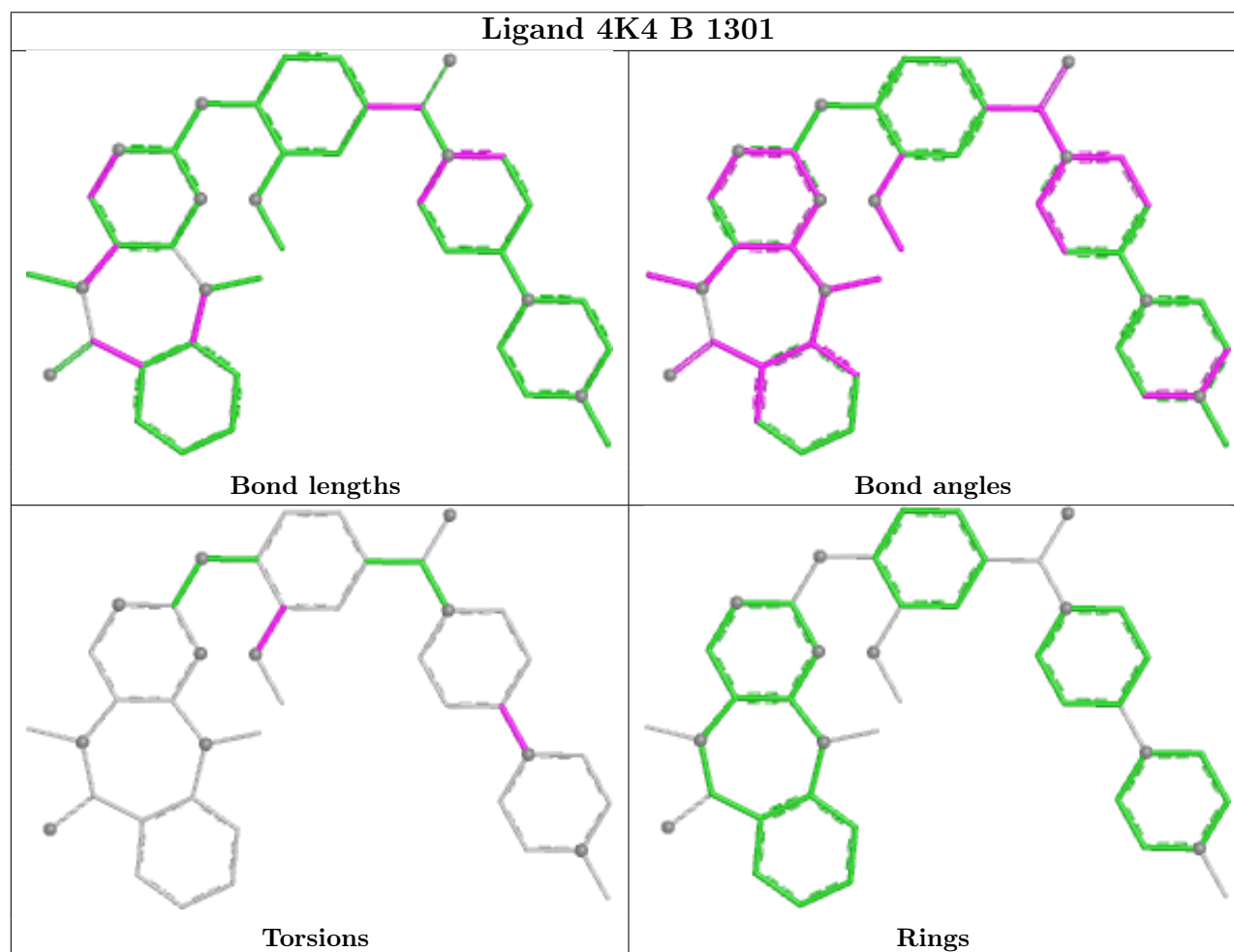
Mol	Chain	Res	Type	Atoms
2	A	1301	4K4	CAO-CBK-NBN-CAV
2	A	1301	4K4	CBC-CBE-OAZ-CAA
2	B	1301	4K4	CBC-CBE-OAZ-CAA
2	A	1301	4K4	CAN-CBE-OAZ-CAA
2	B	1301	4K4	CAN-CBE-OAZ-CAA
2	A	1301	4K4	CAP-CBK-NBN-CAV
2	B	1301	4K4	CAP-CBK-NBN-CAU

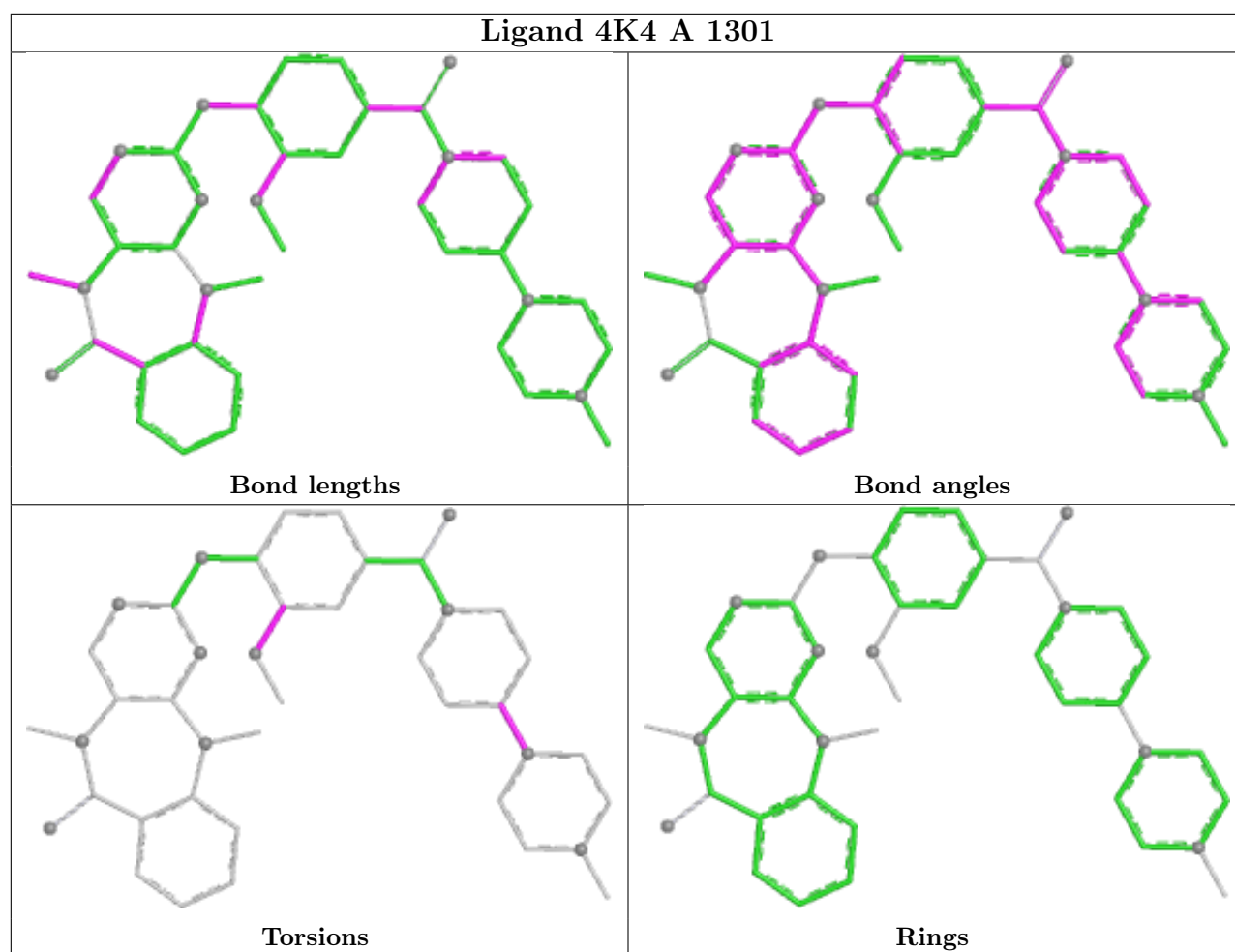
There are no ring outliers.

2 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	1301	4K4	2	0
2	A	1301	4K4	4	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	260/287 (90%)	-0.09	7 (2%) 56 33	21, 32, 69, 93	0
1	B	262/287 (91%)	-0.04	8 (3%) 51 30	17, 32, 62, 94	1 (0%)
All	All	522/574 (90%)	-0.06	15 (2%) 53 31	17, 32, 64, 94	1 (0%)

All (15) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	1068	MET	4.5
1	A	1066	THR	3.8
1	B	1191	LEU	3.7
1	B	1192	LEU	3.6
1	B	1067	GLU	3.4
1	B	1066	THR	3.3
1	B	1034	LYS	2.9
1	B	1027	GLU	2.9
1	A	1059	LEU	2.8
1	A	1069	ILE	2.5
1	A	1230	GLU	2.4
1	A	1058	ILE	2.4
1	B	1064	GLY	2.3
1	A	1068	MET	2.2
1	A	1048	ASP	2.1

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](#)

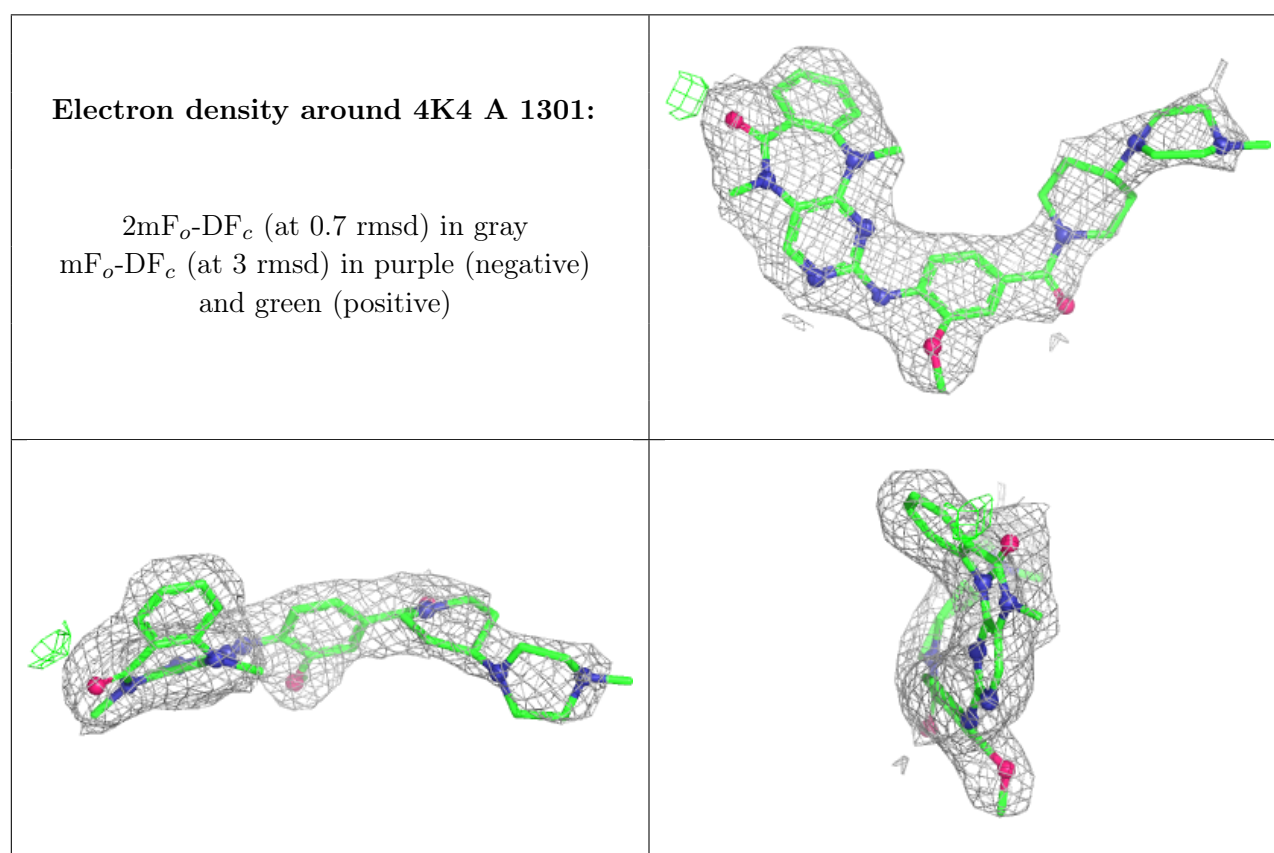
There are no oligosaccharides in this entry.

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.

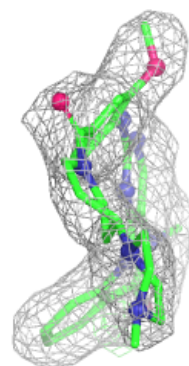
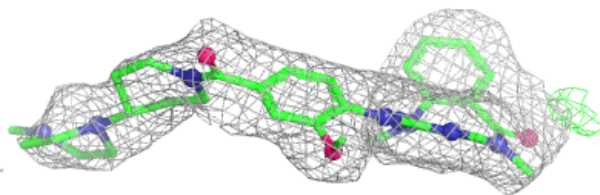
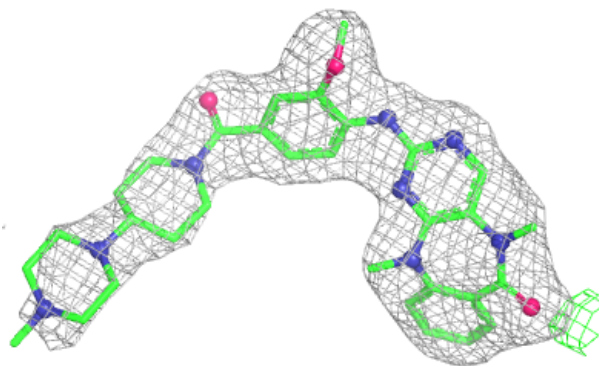
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	MG	A	1302	1/1	0.87	0.18	26,26,26,26	0
3	MG	B	1302	1/1	0.91	0.16	33,33,33,33	0
2	4K4	A	1301	42/42	0.93	0.12	24,37,98,102	0
2	4K4	B	1301	42/42	0.94	0.10	24,30,71,72	0

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 4K4 B 1301:

$2mF_o-DF_c$ (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.