



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 20, 2026 – 05:11 AM UTC

PDB ID : 4YZN / pdb_00004yzn
Title : Humanized Roco4 bound to Compound 19
Authors : Gilsbach, B.K.; Messias, A.C.; Ito, G.; Sattler, M.; Alessi, D.R.; Wittinghofer, A.; Kortholt, A.
Deposited on : 2015-03-25
Resolution : 1.55 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

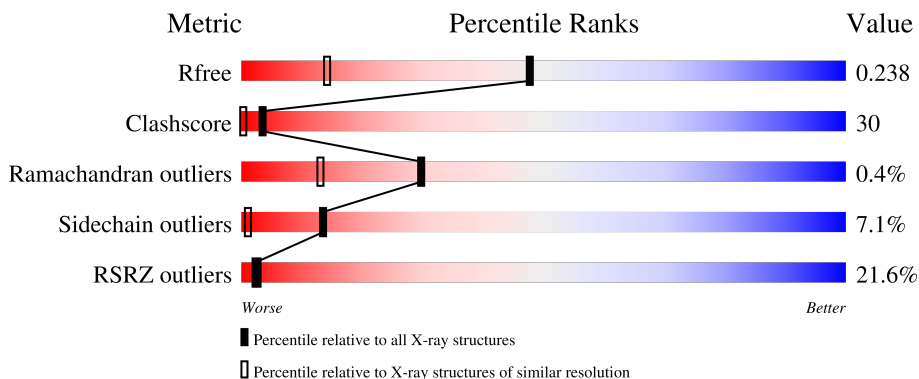
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.55 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	2145 (1.56-1.56)
Clashscore	190562	2189 (1.56-1.56)
Ramachandran outliers	187476	2153 (1.56-1.56)
Sidechain outliers	187428	2150 (1.56-1.56)
RSRZ outliers	180081	2146 (1.56-1.56)

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	20% 39% 41% 11% 6%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 2473 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.

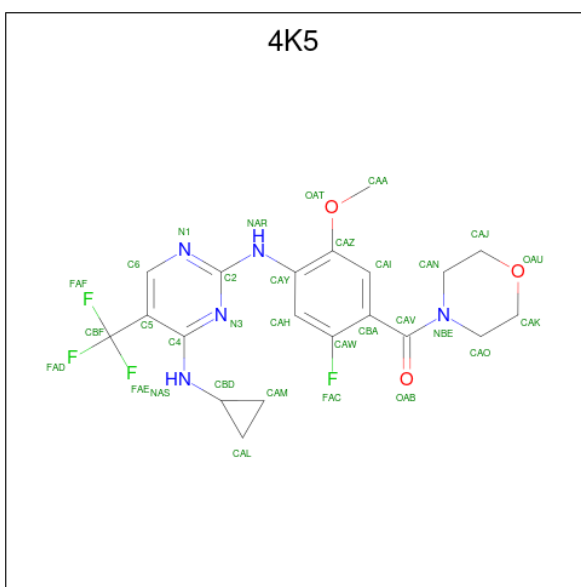
- Molecule 1 is a protein called Probable serine/threonine-protein kinase roco4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	269	Total	C	N	O	S	0	13	0
			2227	1439	369	404	15			

There are 15 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

- Molecule 2 is (4-{[4-(cyclopropylamino)-5-(trifluoromethyl)pyrimidin-2-yl]amino}-2-fluoro-5-methoxyphenyl)(morpholin-4-yl)methanone (CCD ID: 4K5) (formula: C₂₀H₂₁F₄N₅O₃).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	F	N	O	0	0
			32	20	4	5	3		

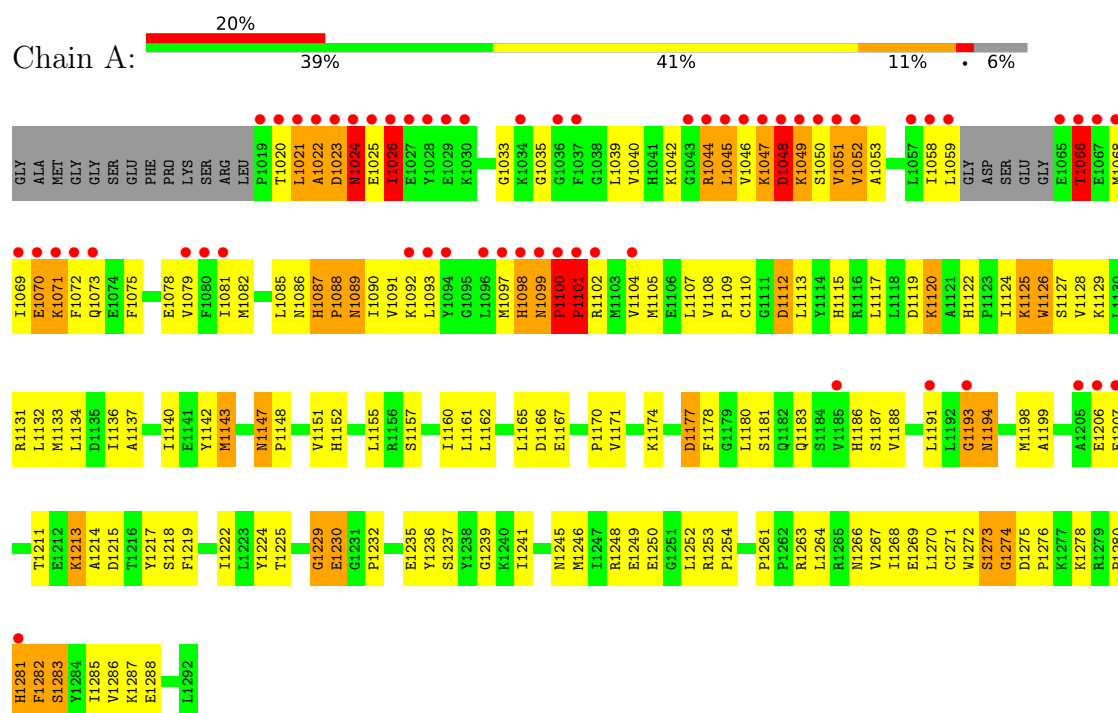
- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	214	Total O 214 214	0	0

3 Residue-property plots [i](#)

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

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



4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α , β , γ	42.40Å 42.40Å 326.90Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	37.64 – 1.55 37.64 – 1.55	Depositor EDS
% Data completeness (in resolution range)	99.9 (37.64-1.55) 99.9 (37.64-1.55)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.61 (at 1.55Å)	Xtriage
Refinement program	REFMAC 5.6.0093	Depositor
R, R_{free}	0.187 , 0.216 0.215 , 0.238	Depositor DCC
R_{free} test set	2262 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	18.3	Xtriage
Anisotropy	0.003	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 38.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	2473	wwPDB-VP
Average B, all atoms (Å ²)	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.45% 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: 4K5

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	3.10	157/2317 (6.8%)	1.50	47/3125 (1.5%)

All (157) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1070	GLU	C-N	-23.96	1.02	1.33
1	A	1026	ILE	C-N	18.64	1.59	1.33
1	A	1230[A]	GLU	N-CA	17.83	1.67	1.45
1	A	1230[B]	GLU	N-CA	17.83	1.67	1.45
1	A	1143[A]	MET	N-CA	17.70	1.67	1.46
1	A	1143[B]	MET	N-CA	17.70	1.67	1.46
1	A	1283[A]	SER	N-CA	17.59	1.67	1.46
1	A	1283[B]	SER	N-CA	17.59	1.67	1.46
1	A	1125[A]	LYS	CA-C	17.16	1.73	1.52
1	A	1125[B]	LYS	CA-C	17.16	1.73	1.52
1	A	1287[A]	LYS	N-CA	17.12	1.66	1.46
1	A	1287[B]	LYS	N-CA	17.12	1.66	1.46
1	A	1071	LYS	C-N	-17.06	1.12	1.33
1	A	1222[A]	ILE	N-CA	16.48	1.65	1.46
1	A	1222[B]	ILE	N-CA	16.48	1.65	1.46
1	A	1283[A]	SER	CA-C	16.13	1.74	1.52
1	A	1283[B]	SER	CA-C	16.13	1.74	1.52
1	A	1281[A]	HIS	CA-C	16.10	1.73	1.52
1	A	1281[B]	HIS	CA-C	16.10	1.73	1.52
1	A	1273[A]	SER	CA-C	15.85	1.72	1.52
1	A	1273[B]	SER	CA-C	15.85	1.72	1.52
1	A	1181[A]	SER	N-CA	15.68	1.65	1.45
1	A	1181[B]	SER	N-CA	15.68	1.65	1.45
1	A	1222[A]	ILE	CA-C	15.36	1.71	1.52
1	A	1222[B]	ILE	CA-C	15.36	1.71	1.52
1	A	1213[A]	LYS	N-CA	15.03	1.65	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1213[B]	LYS	N-CA	15.03	1.65	1.46
1	A	1273[A]	SER	N-CA	14.97	1.65	1.46
1	A	1273[B]	SER	N-CA	14.97	1.65	1.46
1	A	1287[A]	LYS	CA-C	14.64	1.71	1.52
1	A	1287[B]	LYS	CA-C	14.64	1.71	1.52
1	A	1213[A]	LYS	CA-C	14.62	1.73	1.52
1	A	1213[B]	LYS	CA-C	14.62	1.73	1.52
1	A	1120[A]	LYS	CA-C	14.48	1.72	1.52
1	A	1120[B]	LYS	CA-C	14.48	1.72	1.52
1	A	1125[A]	LYS	N-CA	14.31	1.64	1.46
1	A	1125[B]	LYS	N-CA	14.31	1.64	1.46
1	A	1177[A]	ASP	CA-C	14.29	1.72	1.52
1	A	1177[B]	ASP	CA-C	14.29	1.72	1.52
1	A	1181[A]	SER	CA-C	13.47	1.70	1.52
1	A	1181[B]	SER	CA-C	13.47	1.70	1.52
1	A	1090[A]	ILE	N-CA	13.05	1.63	1.46
1	A	1090[B]	ILE	N-CA	13.05	1.63	1.46
1	A	1143[A]	MET	CA-C	12.57	1.69	1.52
1	A	1143[B]	MET	CA-C	12.57	1.69	1.52
1	A	1120[A]	LYS	N-CA	12.29	1.61	1.46
1	A	1120[B]	LYS	N-CA	12.29	1.61	1.46
1	A	1177[A]	ASP	N-CA	12.19	1.61	1.46
1	A	1177[B]	ASP	N-CA	12.19	1.61	1.46
1	A	1090[A]	ILE	CA-C	11.36	1.67	1.52
1	A	1090[B]	ILE	CA-C	11.36	1.67	1.52
1	A	1281[A]	HIS	N-CA	10.01	1.58	1.46
1	A	1281[B]	HIS	N-CA	10.01	1.58	1.46
1	A	1230[A]	GLU	CA-C	9.50	1.64	1.52
1	A	1230[B]	GLU	CA-C	9.50	1.64	1.52
1	A	1253	ARG	C-O	-9.16	1.14	1.24
1	A	1092	LYS	C-N	-8.90	1.21	1.33
1	A	1147	ASN	C-O	-8.77	1.17	1.25
1	A	1100	PRO	CA-C	8.57	1.60	1.52
1	A	1160	ILE	C-O	-8.11	1.15	1.24
1	A	1120[A]	LYS	C-O	-8.05	1.14	1.24
1	A	1120[B]	LYS	C-O	-8.05	1.14	1.24
1	A	1157	SER	C-O	-8.04	1.17	1.24
1	A	1215	ASP	C-O	-7.58	1.15	1.24
1	A	1213[A]	LYS	C-O	-7.58	1.14	1.24
1	A	1213[B]	LYS	C-O	-7.58	1.14	1.24
1	A	1091	VAL	C-O	-7.44	1.15	1.24
1	A	1112	ASP	C-O	-7.34	1.15	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1261	PRO	C-O	-7.31	1.16	1.24
1	A	1270	LEU	C-O	-7.12	1.15	1.24
1	A	1222[A]	ILE	C-O	-6.92	1.16	1.24
1	A	1222[B]	ILE	C-O	-6.92	1.16	1.24
1	A	1134	LEU	C-O	-6.83	1.16	1.24
1	A	1268	ILE	C-O	-6.79	1.16	1.24
1	A	1199	ALA	C-O	-6.71	1.15	1.23
1	A	1217	TYR	C-O	-6.71	1.16	1.24
1	A	1254	PRO	C-O	-6.66	1.15	1.23
1	A	1143[A]	MET	C-O	-6.57	1.16	1.24
1	A	1143[B]	MET	C-O	-6.57	1.16	1.24
1	A	1171	VAL	C-O	-6.56	1.17	1.24
1	A	1136	ILE	C-O	-6.42	1.16	1.24
1	A	1218	SER	C-O	-6.42	1.16	1.24
1	A	1087	HIS	C-O	-6.39	1.16	1.24
1	A	1131	ARG	C-O	-6.35	1.16	1.24
1	A	1099	ASN	C-N	6.30	1.40	1.33
1	A	1276	PRO	C-O	-6.28	1.16	1.24
1	A	1267	VAL	C-O	-6.22	1.16	1.24
1	A	1129	LYS	C-O	-6.18	1.16	1.24
1	A	1128	VAL	C-O	-6.16	1.16	1.24
1	A	1224	TYR	C-O	-6.14	1.17	1.24
1	A	1281[A]	HIS	C-O	-6.08	1.16	1.23
1	A	1281[B]	HIS	C-O	-6.08	1.16	1.23
1	A	1264	LEU	C-O	-6.04	1.17	1.24
1	A	1225	THR	C-O	-6.01	1.17	1.24
1	A	1274	GLY	C-O	-6.01	1.16	1.23
1	A	1249	GLU	C-O	-6.01	1.16	1.24
1	A	1245	ASN	C-O	-5.97	1.17	1.24
1	A	1155	LEU	C-O	-5.95	1.16	1.24
1	A	1266	ASN	C-O	-5.93	1.17	1.24
1	A	1165	LEU	C-O	-5.91	1.15	1.24
1	A	1252	LEU	C-O	-5.90	1.16	1.23
1	A	1132	LEU	C-O	-5.89	1.17	1.24
1	A	1170	PRO	C-O	-5.79	1.16	1.24
1	A	1033	GLY	C-O	-5.73	1.17	1.23
1	A	1275	ASP	C-O	-5.71	1.17	1.24
1	A	1286	VAL	C-O	-5.71	1.17	1.24
1	A	1174	LYS	C-O	-5.70	1.17	1.23
1	A	1108	VAL	C-O	-5.63	1.17	1.24
1	A	1246	MET	C-O	-5.63	1.17	1.24
1	A	1137	ALA	C-O	-5.61	1.17	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1232	PRO	C-O	-5.56	1.17	1.23
1	A	1126	TRP	C-O	-5.54	1.17	1.24
1	A	1273[A]	SER	C-O	-5.52	1.17	1.23
1	A	1273[B]	SER	C-O	-5.52	1.17	1.23
1	A	1271	CYS	C-O	-5.52	1.17	1.24
1	A	1124	ILE	C-O	-5.51	1.18	1.24
1	A	1166	ASP	C-O	-5.47	1.17	1.24
1	A	1125[A]	LYS	C-O	-5.47	1.17	1.23
1	A	1125[B]	LYS	C-O	-5.47	1.17	1.23
1	A	1263	ARG	C-O	-5.46	1.17	1.24
1	A	1133	MET	C-O	-5.44	1.17	1.24
1	A	1280	PRO	C-O	-5.44	1.17	1.23
1	A	1188	VAL	N-CA	-5.43	1.39	1.45
1	A	1235	GLU	C-O	-5.42	1.17	1.24
1	A	1198	MET	C-O	-5.38	1.17	1.23
1	A	1088	PRO	C-O	-5.38	1.17	1.24
1	A	1285	ILE	C-O	-5.35	1.18	1.24
1	A	1024	ASN	C-O	-5.34	1.19	1.24
1	A	1089	ASN	C-O	-5.33	1.17	1.24
1	A	1250	GLU	C-O	-5.29	1.17	1.24
1	A	1040	VAL	C-O	-5.29	1.18	1.24
1	A	1287[A]	LYS	C-O	-5.29	1.18	1.24
1	A	1287[B]	LYS	C-O	-5.29	1.18	1.24
1	A	1269	GLU	C-O	-5.26	1.18	1.24
1	A	1151	VAL	C-O	-5.25	1.18	1.24
1	A	1127	SER	C-O	-5.24	1.18	1.24
1	A	1086	ASN	C-O	-5.24	1.17	1.23
1	A	1288	GLU	C-O	-5.23	1.18	1.24
1	A	1177[A]	ASP	C-O	-5.23	1.17	1.24
1	A	1177[B]	ASP	C-O	-5.23	1.17	1.24
1	A	1241	ILE	C-O	-5.23	1.18	1.24
1	A	1070	GLU	C-O	-5.22	1.18	1.24
1	A	1113	LEU	C-O	-5.21	1.18	1.24
1	A	1282	PHE	C-O	-5.21	1.17	1.24
1	A	1122	HIS	C-O	-5.21	1.18	1.24
1	A	1167	GLU	C-O	-5.20	1.17	1.24
1	A	1161	LEU	C-O	-5.19	1.17	1.23
1	A	1237	SER	C-O	-5.18	1.18	1.23
1	A	1211	THR	C-O	-5.14	1.17	1.24
1	A	1117	LEU	C-O	-5.11	1.17	1.24
1	A	1236	TYR	C-O	-5.10	1.17	1.23
1	A	1183	GLN	CA-C	-5.07	1.48	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1214	ALA	C-O	-5.06	1.18	1.24
1	A	1193	GLY	C-O	-5.05	1.18	1.23
1	A	1219	PHE	C-O	-5.05	1.17	1.24
1	A	1101	PRO	N-CD	5.03	1.54	1.47
1	A	1194	ASN	C-O	-5.01	1.17	1.23

All (47) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1070	GLU	O-C-N	-13.78	107.76	122.09
1	A	1100	PRO	N-CA-C	13.54	127.22	110.70
1	A	1024	ASN	N-CA-C	-12.11	92.57	108.19
1	A	1099	ASN	N-CA-C	9.19	126.21	113.16
1	A	1023	ASP	CB-CA-C	9.07	125.79	110.74
1	A	1099	ASN	CB-CA-C	-8.89	95.06	112.05
1	A	1109	PRO	N-CA-C	8.48	124.87	113.84
1	A	1048	ASP	N-CA-C	-8.14	103.95	114.04
1	A	1119	ASP	CA-C-N	8.06	131.88	120.28
1	A	1119	ASP	C-N-CA	8.06	131.88	120.28
1	A	1066	THR	N-CA-C	7.86	121.63	110.23
1	A	1045	LEU	CA-C-N	7.64	130.93	120.46
1	A	1045	LEU	C-N-CA	7.64	130.93	120.46
1	A	1248	ARG	N-CA-C	6.97	118.67	111.14
1	A	1147	ASN	C-N-CD	6.24	134.32	120.60
1	A	1090[A]	ILE	CA-C-O	-5.97	114.18	120.39
1	A	1090[B]	ILE	CA-C-O	-5.97	114.18	120.39
1	A	1280	PRO	CA-C-N	5.91	129.10	120.71
1	A	1280	PRO	C-N-CA	5.91	129.10	120.71
1	A	1098	HIS	N-CA-C	5.90	122.32	114.12
1	A	1100	PRO	CA-C-O	-5.89	112.02	120.56
1	A	1089	ASN	CA-C-N	5.71	130.69	123.10
1	A	1089	ASN	C-N-CA	5.71	130.69	123.10
1	A	1085	LEU	N-CA-C	5.67	119.49	109.96
1	A	1287[A]	LYS	N-CA-C	-5.66	105.02	111.07
1	A	1287[B]	LYS	N-CA-C	-5.66	105.02	111.07
1	A	1283[A]	SER	N-CA-C	-5.65	104.33	111.11
1	A	1283[B]	SER	N-CA-C	-5.65	104.33	111.11
1	A	1052	VAL	N-CA-C	5.58	117.10	108.44
1	A	1198	MET	N-CA-C	5.56	118.79	109.95
1	A	1239	GLY	N-CA-C	-5.48	105.53	112.54
1	A	1022	ALA	CA-C-N	5.33	128.82	120.82
1	A	1022	ALA	C-N-CA	5.33	128.82	120.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1120[A]	LYS	N-CA-C	-5.33	105.58	111.71
1	A	1120[B]	LYS	N-CA-C	-5.33	105.58	111.71
1	A	1222[A]	ILE	N-CA-C	-5.21	105.42	110.42
1	A	1222[B]	ILE	N-CA-C	-5.21	105.42	110.42
1	A	1180	LEU	CA-C-N	5.14	129.01	120.94
1	A	1180	LEU	C-N-CA	5.14	129.01	120.94
1	A	1024	ASN	CA-C-N	-5.09	118.87	126.86
1	A	1024	ASN	C-N-CA	-5.09	118.87	126.86
1	A	1229	GLY	CA-C-O	5.09	125.34	119.13
1	A	1273[A]	SER	N-CA-C	-5.08	103.08	110.24
1	A	1273[B]	SER	N-CA-C	-5.08	103.08	110.24
1	A	1081	ILE	N-CA-C	5.05	115.28	110.53
1	A	1101	PRO	N-CA-C	5.05	125.22	112.10
1	A	1193	GLY	N-CA-C	-5.02	103.72	112.55

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	2227	0	2287	134	9
2	A	32	0	21	0	0
3	A	214	0	0	8	1
All	All	2473	0	2308	134	10

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 30.

All (134) 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:1045:LEU:O	1:A:1049:LYS:CA	1.64	1.45
1:A:1024:ASN:ND2	1:A:1025:GLU:H	1.06	1.43
1:A:1026:ILE:HD13	1:A:1097:MET:CE	1.61	1.29

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1045:LEU:O	1:A:1049:LYS:N	1.69	1.24
1:A:1024:ASN:ND2	1:A:1025:GLU:N	1.88	1.21
1:A:1044:ARG:HD3	1:A:1049:LYS:O	1.40	1.20
1:A:1045:LEU:O	1:A:1049:LYS:HA	1.22	1.13
1:A:1021:LEU:HD13	1:A:1021:LEU:N	1.62	1.11
1:A:1026:ILE:CD1	1:A:1097:MET:CE	2.29	1.11
1:A:1021:LEU:HD13	1:A:1021:LEU:H	1.13	1.09
1:A:1026:ILE:HD13	1:A:1097:MET:HE3	1.22	1.08
1:A:1099:ASN:HB3	1:A:1100:PRO:HD3	1.43	1.00
1:A:1099:ASN:HB3	1:A:1100:PRO:CD	1.98	0.94
1:A:1026:ILE:CD1	1:A:1097:MET:HE3	1.95	0.94
1:A:1044:ARG:CD	1:A:1049:LYS:O	2.16	0.92
1:A:1021:LEU:HG	1:A:1098:HIS:NE2	1.85	0.92
1:A:1021:LEU:N	1:A:1021:LEU:CD1	2.29	0.90
1:A:1044:ARG:HG3	1:A:1044:ARG:HH11	1.37	0.89
1:A:1024:ASN:HD22	1:A:1025:GLU:H	0.99	0.89
1:A:1099:ASN:CB	1:A:1102:ARG:NH2	2.39	0.86
1:A:1099:ASN:HB2	1:A:1102:ARG:NH2	1.93	0.84
1:A:1047:LYS:HG3	1:A:1048:ASP:OD1	1.78	0.83
1:A:1026:ILE:HD13	1:A:1097:MET:HE1	1.60	0.83
1:A:1082:MET:HE1	1:A:1105:MET:HE2	1.63	0.79
1:A:1281[A]:HIS:HE1	3:A:1497:HOH:O	1.68	0.76
1:A:1087:HIS:HD2	1:A:1089:ASN:H	1.32	0.76
1:A:1048:ASP:HB2	1:A:1050:SER:H	1.50	0.75
1:A:1021:LEU:H	1:A:1021:LEU:CD1	1.80	0.74
1:A:1143[A]:MET:HE3	1:A:1178:PHE:HE2	1.52	0.74
1:A:1066:THR:HG22	1:A:1069:ILE:HG13	1.70	0.74
1:A:1112:ASP:OD1	1:A:1115:HIS:HD2	1.71	0.72
1:A:1177[B]:ASP:OD1	3:A:1402:HOH:O	2.06	0.72
1:A:1046:VAL:HG13	1:A:1047:LYS:N	2.04	0.72
1:A:1099:ASN:HB3	1:A:1102:ARG:NH2	2.03	0.71
1:A:1024:ASN:CG	1:A:1025:GLU:N	2.47	0.71
1:A:1026:ILE:HD12	1:A:1097:MET:CE	2.22	0.70
1:A:1087:HIS:CD2	1:A:1089:ASN:H	2.08	0.70
1:A:1026:ILE:HD12	1:A:1097:MET:HE2	1.75	0.69
1:A:1026:ILE:CD1	1:A:1097:MET:HE2	2.22	0.69
1:A:1048:ASP:OD1	1:A:1048:ASP:N	2.25	0.69
1:A:1047:LYS:O	1:A:1047:LYS:HD3	1.94	0.68
1:A:1282:PHE:C	1:A:1283[A]:SER:CA	2.63	0.68
1:A:1282:PHE:C	1:A:1283[B]:SER:CA	2.63	0.67
1:A:1059:LEU:HB3	1:A:1068:MET:HE2	1.76	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1099:ASN:CB	1:A:1102:ARG:HH21	2.09	0.66
1:A:1186:HIS:HD2	1:A:1187:SER:O	1.78	0.66
1:A:1142:TYR:C	1:A:1143[B]:MET:CA	2.64	0.65
1:A:1082:MET:HE2	1:A:1093:LEU:HB2	1.78	0.65
1:A:1052:VAL:HG21	1:A:1104:VAL:CG1	2.26	0.65
1:A:1024:ASN:HD22	1:A:1025:GLU:N	1.72	0.65
1:A:1142:TYR:C	1:A:1143[A]:MET:CA	2.64	0.65
1:A:1140:ILE:HA	1:A:1143[B]:MET:HE3	1.80	0.64
1:A:1024:ASN:C	1:A:1025:GLU:HG3	2.23	0.64
1:A:1125[A]:LYS:CA	1:A:1126:TRP:N	2.56	0.64
1:A:1273[B]:SER:CA	1:A:1274:GLY:N	2.57	0.64
1:A:1042:LYS:HZ3	1:A:1051:VAL:CG2	2.12	0.63
1:A:1097:MET:HB2	1:A:1102:ARG:HB2	1.79	0.62
1:A:1044:ARG:HH11	1:A:1044:ARG:CG	2.12	0.62
1:A:1045:LEU:C	1:A:1049:LYS:HA	2.19	0.62
1:A:1052:VAL:HG22	1:A:1053:ALA:N	2.15	0.62
1:A:1066:THR:HG23	1:A:1068:MET:N	2.15	0.61
1:A:1048:ASP:O	1:A:1049:LYS:HG2	1.99	0.61
1:A:1099:ASN:CB	1:A:1100:PRO:HD3	2.25	0.61
1:A:1024:ASN:O	1:A:1025:GLU:HG3	2.01	0.61
1:A:1281[A]:HIS:CD2	1:A:1283[A]:SER:OG	2.53	0.60
1:A:1042:LYS:NZ	1:A:1051:VAL:CG2	2.65	0.60
1:A:1021:LEU:HG	1:A:1098:HIS:CD2	2.37	0.59
1:A:1281[A]:HIS:CA	1:A:1282:PHE:N	2.58	0.59
1:A:1048:ASP:O	1:A:1049:LYS:CG	2.51	0.58
1:A:1047:LYS:HD3	1:A:1047:LYS:C	2.28	0.58
1:A:1046:VAL:HG13	1:A:1047:LYS:H	1.67	0.58
1:A:1272:TRP:C	1:A:1273[A]:SER:CA	2.68	0.58
1:A:1066:THR:HG23	1:A:1068:MET:H	1.69	0.58
1:A:1100:PRO:HD2	1:A:1102:ARG:NE	2.19	0.57
1:A:1099:ASN:HB2	1:A:1102:ARG:HH22	1.67	0.57
1:A:1051:VAL:HG22	1:A:1107:LEU:HD22	1.86	0.57
1:A:1281[A]:HIS:ND1	3:A:1403:HOH:O	2.23	0.56
1:A:1052:VAL:HG22	1:A:1053:ALA:H	1.71	0.55
1:A:1024:ASN:O	1:A:1025:GLU:CB	2.55	0.55
1:A:1026:ILE:HG13	1:A:1045:LEU:HD23	1.90	0.54
1:A:1048:ASP:O	1:A:1049:LYS:CB	2.55	0.53
1:A:1125[B]:LYS:NZ	1:A:1125[B]:LYS:CB	2.71	0.53
1:A:1026:ILE:HG13	1:A:1045:LEU:CD2	2.39	0.53
1:A:1281[A]:HIS:ND1	1:A:1282:PHE:N	2.57	0.53
1:A:1044:ARG:CG	1:A:1044:ARG:NH1	2.70	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1052:VAL:HG21	1:A:1104:VAL:HG12	1.90	0.51
1:A:1046:VAL:CG1	1:A:1047:LYS:N	2.73	0.50
1:A:1024:ASN:O	1:A:1025:GLU:CG	2.59	0.50
1:A:1044:ARG:HG3	1:A:1044:ARG:NH1	2.13	0.50
1:A:1035:GLY:HA3	3:A:1546:HOH:O	2.12	0.50
1:A:1278:LYS:NZ	3:A:1404:HOH:O	2.45	0.50
1:A:1193:GLY:HA2	3:A:1410:HOH:O	2.12	0.49
1:A:1052:VAL:HG23	1:A:1105:MET:O	2.14	0.48
1:A:1281[A]:HIS:HD2	1:A:1283[A]:SER:OG	1.96	0.48
1:A:1078:GLU:HG3	1:A:1082:MET:SD	2.54	0.47
1:A:1087:HIS:CG	1:A:1088:PRO:HD2	2.49	0.47
1:A:1101:PRO:C	1:A:1102:ARG:HG3	2.39	0.47
1:A:1143[A]:MET:HE3	1:A:1178:PHE:CE2	2.39	0.47
1:A:1047:LYS:C	1:A:1047:LYS:CD	2.86	0.46
1:A:1052:VAL:HG21	1:A:1104:VAL:HG13	1.97	0.46
1:A:1087:HIS:CD2	1:A:1088:PRO:HD2	2.51	0.46
1:A:1099:ASN:H	1:A:1102:ARG:HH21	1.63	0.46
1:A:1059:LEU:HD22	1:A:1068:MET:HB3	1.97	0.45
1:A:1066:THR:CG2	1:A:1069:ILE:H	2.29	0.45
1:A:1143[A]:MET:HE1	1:A:1152:HIS:HB2	1.97	0.45
1:A:1120[B]:LYS:NZ	1:A:1229:GLY:O	2.49	0.45
1:A:1066:THR:HG22	1:A:1069:ILE:CG1	2.43	0.45
1:A:1066:THR:CG2	1:A:1069:ILE:HG13	2.43	0.45
1:A:1120[A]:LYS:NZ	1:A:1230[A]:GLU:OE2	2.48	0.45
1:A:1075:PHE:O	1:A:1079:VAL:HG23	2.17	0.44
1:A:1082:MET:CE	1:A:1105:MET:HE2	2.42	0.44
1:A:1281[A]:HIS:HD1	1:A:1282:PHE:H	1.67	0.43
1:A:1042:LYS:HZ3	1:A:1051:VAL:HG22	1.84	0.43
1:A:1058:ILE:O	1:A:1071:LYS:HE2	2.18	0.42
1:A:1070:GLU:O	1:A:1071:LYS:C	2.59	0.42
1:A:1193:GLY:CA	3:A:1410:HOH:O	2.67	0.42
1:A:1213[B]:LYS:HD3	1:A:1213[B]:LYS:HA	1.79	0.42
1:A:1059:LEU:HB3	1:A:1068:MET:CE	2.47	0.42
1:A:1110:CYS:HB2	1:A:1162:LEU:O	2.19	0.42
1:A:1022:ALA:O	1:A:1097:MET:HG2	2.19	0.41
1:A:1147:ASN:HA	1:A:1148:PRO:HA	1.82	0.41
1:A:1066:THR:HG22	1:A:1069:ILE:H	1.85	0.41
1:A:1194:ASN:N	3:A:1410:HOH:O	2.54	0.40

All (10) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1072:PHE:CE2	1:A:1072:PHE:CZ[7_555]	0.51	1.69
1:A:1072:PHE:CE2	1:A:1072:PHE:CE2[7_555]	0.87	1.33
1:A:1047:LYS:CE	1:A:1047:LYS:CE[7_465]	1.13	1.07
1:A:1072:PHE:CD2	1:A:1072:PHE:CZ[7_555]	1.19	1.01
1:A:1047:LYS:CE	1:A:1047:LYS:NZ[7_465]	1.33	0.87
3:A:1591:HOH:O	3:A:1592:HOH:O[1_455]	1.60	0.60
1:A:1072:PHE:CD2	1:A:1072:PHE:CE1[7_555]	1.64	0.56
1:A:1072:PHE:CE1	1:A:1072:PHE:CE2[7_555]	1.74	0.46
1:A:1072:PHE:CZ	1:A:1072:PHE:CZ[7_555]	1.89	0.31
1:A:1072:PHE:CD2	1:A:1072:PHE:CE2[7_555]	2.01	0.19

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	278/287 (97%)	269 (97%)	8 (3%)	1 (0%)	30 13

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1100	PRO

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	254/253 (100%)	237 (93%)	17 (7%)	15 1

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1020	THR
1	A	1021	LEU
1	A	1023	ASP
1	A	1024	ASN
1	A	1026	ILE
1	A	1039	LEU
1	A	1044	ARG
1	A	1047	LYS
1	A	1048	ASP
1	A	1049	LYS
1	A	1051	VAL
1	A	1066	THR
1	A	1073	GLN
1	A	1101	PRO
1	A	1191	LEU
1	A	1206	GLU
1	A	1207	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1024	ASN
1	A	1084	ASN
1	A	1087	HIS
1	A	1115	HIS
1	A	1146	GLN
1	A	1147	ASN
1	A	1186	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

1 ligand is modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	4K5	A	1301	-	35,35,35	1.85	7 (20%)	49,51,51	2.21	13 (26%)

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 Torsions and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	4K5	A	1301	-	-	0/24/34/34	0/4/4/4

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1301	4K5	CBA-CAV	-5.47	1.42	1.50
2	A	1301	4K5	CBF-C5	-4.64	1.40	1.50
2	A	1301	4K5	CAN-NBE	2.95	1.52	1.47
2	A	1301	4K5	OAT-CAA	2.89	1.50	1.42
2	A	1301	4K5	C2-NAR	-2.19	1.31	1.36
2	A	1301	4K5	CAM-CBD	2.07	1.53	1.48
2	A	1301	4K5	CBD-NAS	2.03	1.50	1.46

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1301	4K5	N1-C2-N3	-8.16	118.53	126.42
2	A	1301	4K5	C4-NAS-CBD	-6.12	113.85	124.18

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1301	4K5	CAO-NBE-CAN	4.31	121.48	112.68
2	A	1301	4K5	CBA-CAV-NBE	4.20	124.76	118.24
2	A	1301	4K5	C2-N3-C4	3.58	125.16	116.36
2	A	1301	4K5	C5-C4-N3	-3.04	117.47	122.02
2	A	1301	4K5	C6-N1-C2	3.03	119.97	115.81
2	A	1301	4K5	CAH-CAY-NAR	2.48	126.21	121.12
2	A	1301	4K5	FAD-CBF-C5	2.39	116.89	112.65
2	A	1301	4K5	NAR-C2-N3	2.31	124.84	116.90
2	A	1301	4K5	OAB-CAV-NBE	-2.29	118.74	122.35
2	A	1301	4K5	CBF-C5-C4	2.19	122.86	120.06
2	A	1301	4K5	FAE-CBF-C5	2.18	116.50	112.65

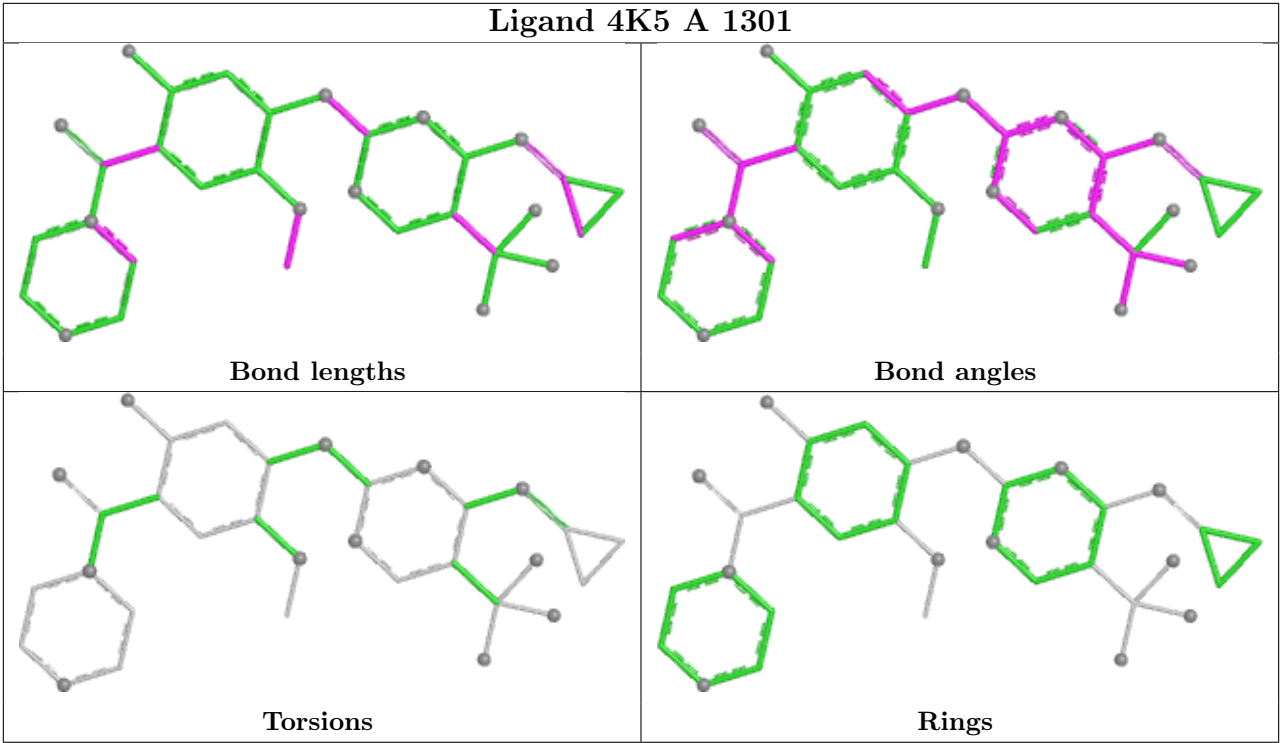
There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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 ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	2

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	1071:LYS	C	1072:PHE	N	1.12
1	A	1070:GLU	C	1071:LYS	N	1.02

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	269/287 (93%)	1.17	58 (21%) 2 3	7, 19, 48, 78	13 (4%)

All (58) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1072	PHE	12.4
1	A	1023	ASP	10.5
1	A	1022	ALA	10.3
1	A	1020	THR	9.8
1	A	1205	ALA	8.8
1	A	1099	ASN	8.6
1	A	1046	VAL	8.2
1	A	1100	PRO	7.6
1	A	1059	LEU	7.5
1	A	1047	LYS	7.4
1	A	1026	ILE	6.9
1	A	1206	GLU	6.3
1	A	1045	LEU	6.0
1	A	1080	PHE	5.5
1	A	1021	LEU	5.1
1	A	1027	GLU	5.0
1	A	1058	ILE	4.9
1	A	1066	THR	4.9
1	A	1207	GLU	4.9
1	A	1024	ASN	4.8
1	A	1025	GLU	4.6
1	A	1049	LYS	4.6
1	A	1052	VAL	4.5
1	A	1067	GLU	4.5
1	A	1096	LEU	4.5
1	A	1019	PRO	4.2
1	A	1028	TYR	3.9

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Mol	Chain	Res	Type	RSRZ
1	A	1098	HIS	3.9
1	A	1101	PRO	3.9
1	A	1070	GLU	3.7
1	A	1065	GLU	3.7
1	A	1193	GLY	3.6
1	A	1051	VAL	3.6
1	A	1036	GLY	3.5
1	A	1093	LEU	3.5
1	A	1185	VAL	3.3
1	A	1043	GLY	3.1
1	A	1073	GLN	3.0
1	A	1044	ARG	2.9
1	A	1037	PHE	2.9
1	A	1097	MET	2.8
1	A	1050	SER	2.7
1	A	1048	ASP	2.6
1	A	1030	LYS	2.5
1	A	1057	LEU	2.5
1	A	1104	VAL	2.5
1	A	1081	ILE	2.5
1	A	1094	TYR	2.5
1	A	1034	LYS	2.4
1	A	1191	LEU	2.4
1	A	1092	LYS	2.4
1	A	1102	ARG	2.3
1	A	1071	LYS	2.3
1	A	1079	VAL	2.3
1	A	1281[A]	HIS	2.2
1	A	1029	GLU	2.1
1	A	1069	ILE	2.1
1	A	1068	MET	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](#)

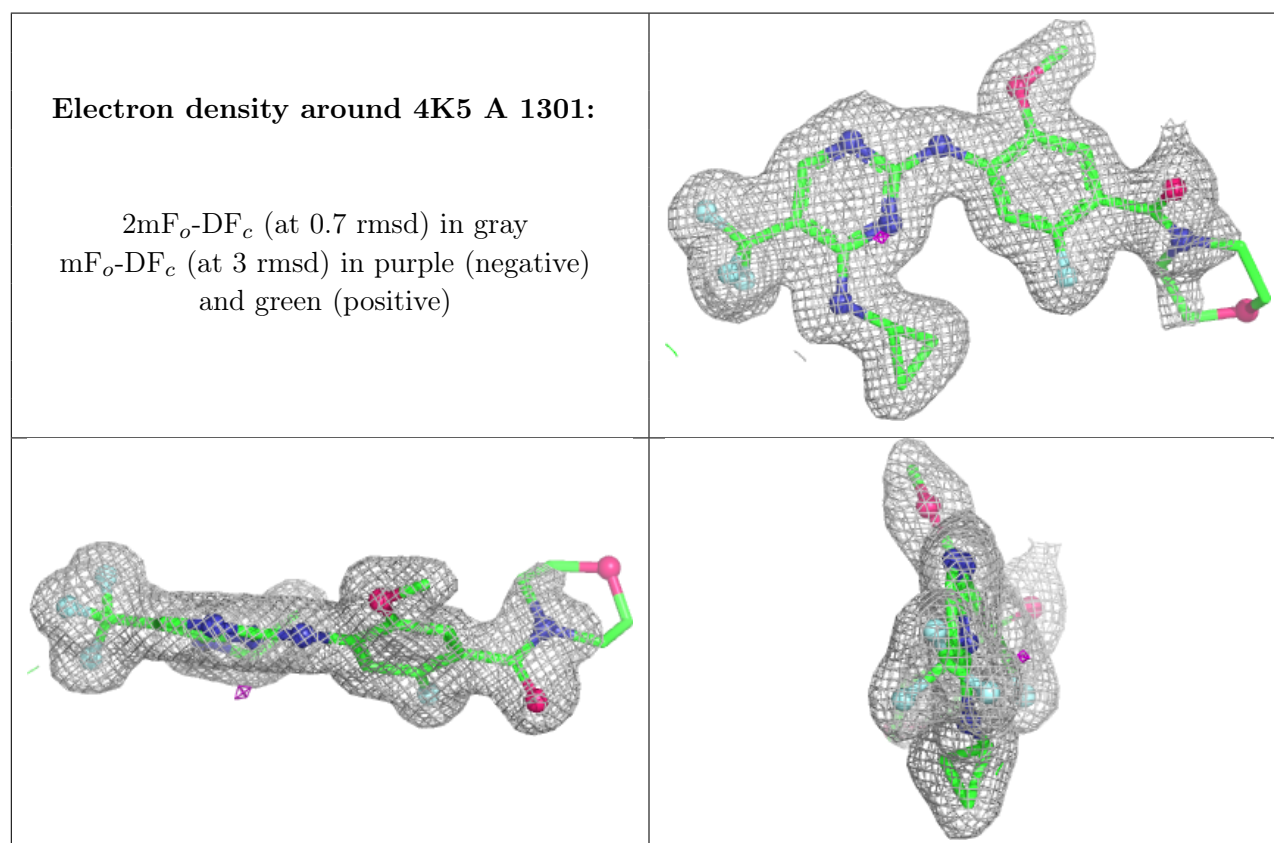
There are no oligosaccharides in this entry.

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
2	4K5	A	1301	32/32	0.95	0.09	17,25,56,60	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.



6.5 Other polymers [i](#)

There are no such residues in this entry.