



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 02:22 AM UTC

PDB ID : 6G6Z / pdb_00006g6z
Title : Eg5-inhibitor complex
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Deposited on : 2018-04-04
Resolution : 2.80 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

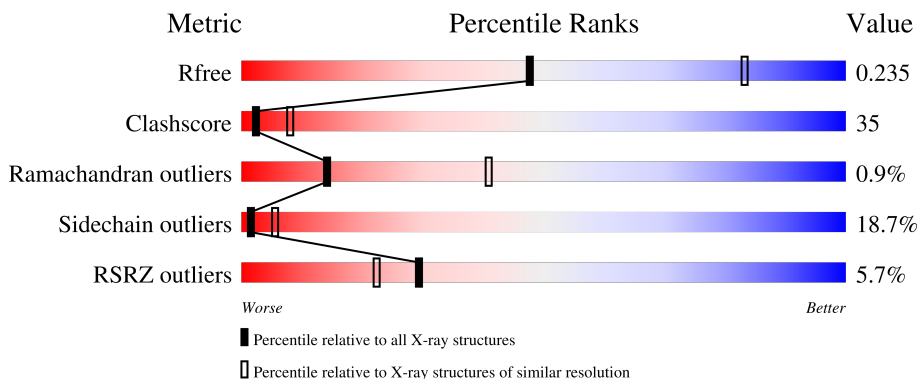
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 Å.

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



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

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

Mol	Chain	Length	Quality of chain
1	A	370	5% 24% 39% 22% 5% 10%

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 2654 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.

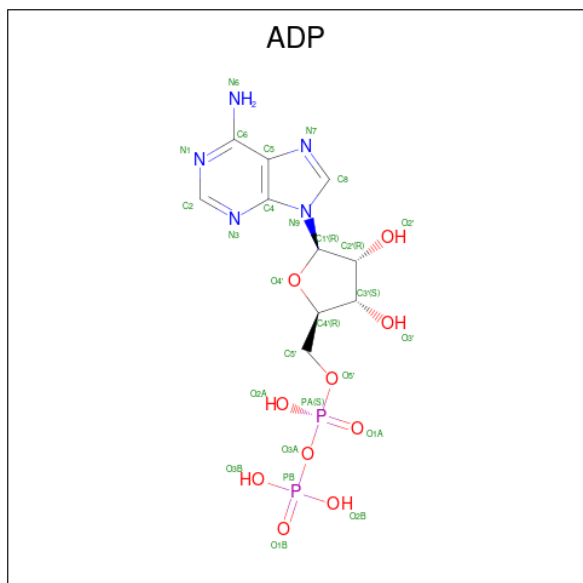
- Molecule 1 is a protein called Kinesin-like protein KIF11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	333	2566	1612	441	503	10	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

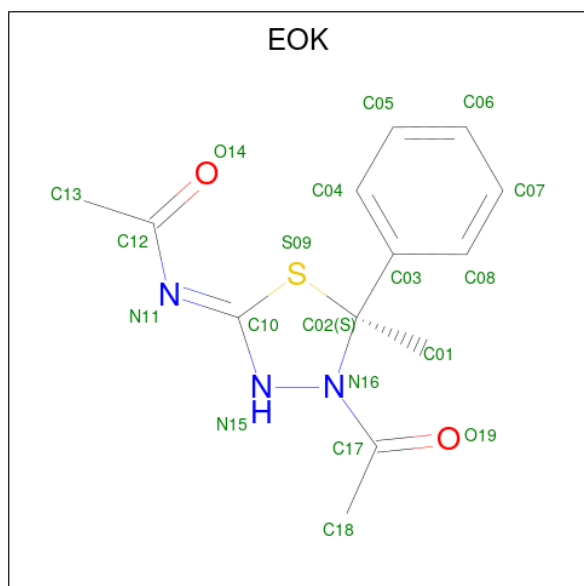
Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLY	-	expression tag	UNP P52732
A	0	PRO	-	expression tag	UNP P52732

- Molecule 2 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



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

- Molecule 4 is ({N} {Z})- {N}-[(5 {S})-4-ethanoyl-5-methyl-5-phenyl-1,3,4-thiadiazolidin-2-ylidene]ethanamide (CCD ID: EOK) (formula: C₁₃H₁₅N₃O₂S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	S	0	0
			19	13	3	2	1		

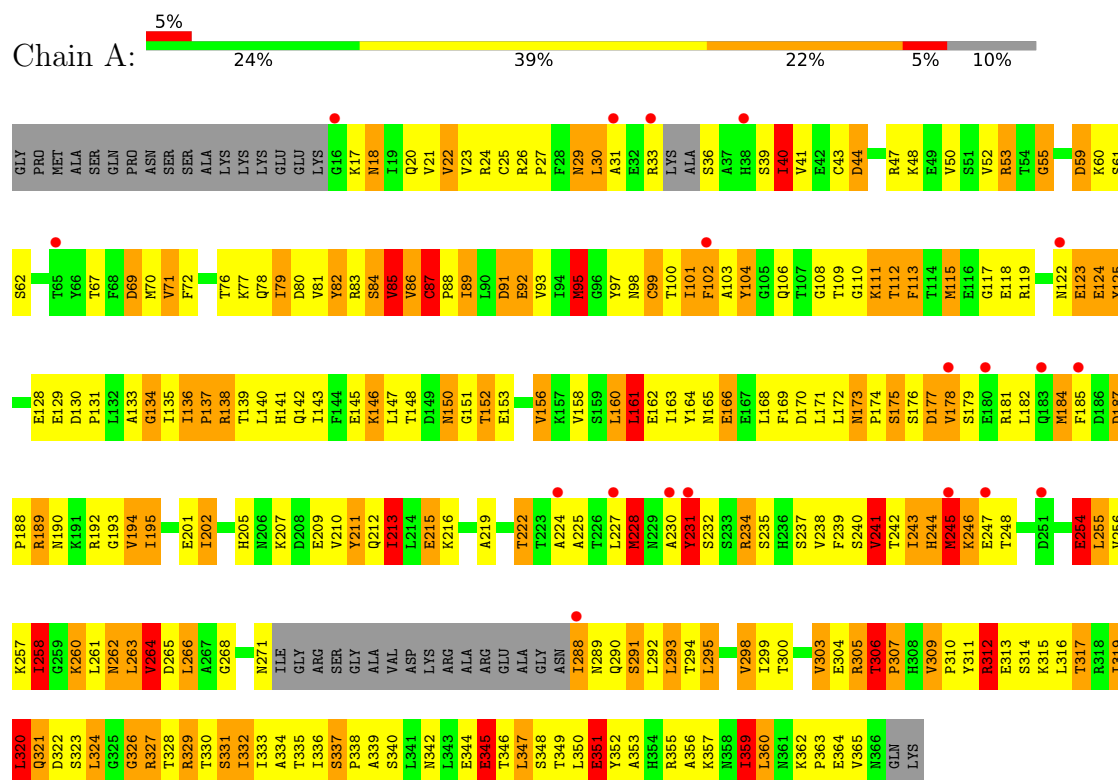
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	41	Total	O	0	0
			41	41		

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: Kinesin-like protein KIF11



4 Data and refinement statistics

Property	Value	Source
Space group	P 65 2 2	Depositor
Cell constants a, b, c, α , β , γ	100.30Å 100.30Å 185.37Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	48.41 – 2.80 48.41 – 2.80	Depositor EDS
% Data completeness (in resolution range)	99.4 (48.41-2.80) 94.0 (48.41-2.80)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.65 (at 2.81Å)	Xtriage
Refinement program	PHENIX (1.13_2998: ???)	Depositor
R, R_{free}	0.219 , 0.287 (Not available) , 0.235	Depositor DCC
R_{free} test set	759 reflections (5.33%)	wwPDB-VP
Wilson B-factor (Å ²)	80.2	Xtriage
Anisotropy	0.213	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 51.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	2654	wwPDB-VP
Average B, all atoms (Å ²)	77.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.22% 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: MG, EOK, ADP

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	2.83	158/2604 (6.1%)	2.34	50/3528 (1.4%)

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

All (158) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	245	MET	CA-C	40.39	2.01	1.52
1	A	23	VAL	C-O	-9.48	1.14	1.24
1	A	139	THR	C-O	-8.04	1.14	1.24
1	A	59	ASP	CA-C	-7.99	1.44	1.52
1	A	71	VAL	C-O	-7.72	1.16	1.24
1	A	21	VAL	C-O	-7.56	1.16	1.24
1	A	332	ILE	C-O	-7.51	1.16	1.24
1	A	82	TYR	C-O	-7.24	1.15	1.24
1	A	130	ASP	CA-C	-7.24	1.44	1.53
1	A	85	VAL	C-O	-7.15	1.16	1.23
1	A	134	GLY	C-O	-7.12	1.17	1.23
1	A	24	ARG	C-O	-7.00	1.16	1.24
1	A	244	HIS	C-O	-6.97	1.15	1.24
1	A	156	VAL	C-O	-6.75	1.17	1.24
1	A	91	ASP	C-O	-6.65	1.16	1.24
1	A	80	ASP	C-O	-6.64	1.16	1.24
1	A	141	HIS	C-O	-6.52	1.16	1.24
1	A	143	ILE	C-O	-6.50	1.16	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	125	TYR	CA-C	-6.46	1.45	1.52
1	A	87	CYS	C-O	-6.43	1.18	1.24
1	A	152	THR	CA-C	-6.39	1.44	1.52
1	A	25	CYS	C-O	-6.37	1.16	1.24
1	A	351	GLU	C-O	-6.35	1.16	1.24
1	A	111	LYS	C-O	-6.33	1.16	1.24
1	A	258	ILE	C-O	-6.25	1.17	1.24
1	A	93	VAL	CA-C	-6.22	1.44	1.52
1	A	101	ILE	C-O	-6.19	1.17	1.24
1	A	83	ARG	C-O	-6.19	1.16	1.24
1	A	238	VAL	C-O	-6.16	1.17	1.24
1	A	139	THR	CA-C	-6.14	1.44	1.52
1	A	345	GLU	C-O	-6.14	1.16	1.24
1	A	333	ILE	C-O	-6.13	1.17	1.24
1	A	238	VAL	CA-CB	-6.11	1.46	1.54
1	A	93	VAL	C-O	-6.10	1.17	1.24
1	A	264	VAL	C-O	-6.10	1.17	1.24
1	A	78	GLN	CA-C	-6.10	1.44	1.52
1	A	351	GLU	CA-C	-6.08	1.45	1.52
1	A	104	TYR	C-O	-6.06	1.17	1.24
1	A	260	LYS	C-O	-6.04	1.17	1.24
1	A	81	VAL	C-O	-6.04	1.17	1.24
1	A	342	ASN	C-O	-6.04	1.16	1.24
1	A	92	GLU	C-O	-6.01	1.17	1.24
1	A	67	THR	C-O	-6.01	1.16	1.24
1	A	261	LEU	C-O	-5.99	1.16	1.24
1	A	44	ASP	C-O	-5.98	1.17	1.24
1	A	124	GLU	CA-C	-5.91	1.45	1.52
1	A	86	VAL	C-O	-5.91	1.16	1.24
1	A	321	GLN	CA-C	-5.89	1.45	1.52
1	A	235	SER	C-O	-5.88	1.16	1.23
1	A	321	GLN	C-O	-5.88	1.17	1.24
1	A	112	THR	C-O	-5.88	1.17	1.24
1	A	362	LYS	C-O	-5.86	1.17	1.24
1	A	130	ASP	C-O	-5.85	1.16	1.24
1	A	89	ILE	C-O	-5.85	1.16	1.24
1	A	352	TYR	C-O	-5.84	1.17	1.24
1	A	353	ALA	C-O	-5.83	1.17	1.24
1	A	99	CYS	C-O	-5.80	1.16	1.23
1	A	22	VAL	C-O	-5.79	1.17	1.23
1	A	164	TYR	CA-C	-5.78	1.45	1.52
1	A	262	ASN	C-O	-5.78	1.17	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	211	TYR	CA-C	-5.78	1.45	1.52
1	A	111	LYS	CA-C	-5.77	1.45	1.52
1	A	339	ALA	C-O	-5.76	1.17	1.23
1	A	344	GLU	C-O	-5.76	1.17	1.24
1	A	77	LYS	C-O	-5.76	1.16	1.23
1	A	113	PHE	CA-C	-5.75	1.45	1.52
1	A	330	THR	CA-C	-5.75	1.45	1.52
1	A	138	ARG	C-O	-5.74	1.17	1.24
1	A	263	LEU	C-O	-5.73	1.17	1.24
1	A	100	THR	C-O	-5.72	1.17	1.24
1	A	255	LEU	CA-C	-5.69	1.45	1.52
1	A	316	LEU	C-O	-5.66	1.17	1.24
1	A	309	VAL	C-O	-5.65	1.18	1.24
1	A	347	LEU	C-O	-5.65	1.17	1.24
1	A	52	VAL	C-O	-5.64	1.18	1.24
1	A	266	LEU	C-O	-5.64	1.16	1.23
1	A	97	TYR	C-O	-5.63	1.16	1.23
1	A	124	GLU	C-O	-5.61	1.17	1.24
1	A	346	THR	C-O	-5.61	1.17	1.24
1	A	334	ALA	C-O	-5.61	1.17	1.24
1	A	266	LEU	CA-C	-5.58	1.45	1.53
1	A	146	LYS	C-O	-5.58	1.17	1.24
1	A	136	ILE	C-O	-5.57	1.17	1.24
1	A	348	SER	C-O	-5.57	1.17	1.24
1	A	135	ILE	N-CA	-5.55	1.40	1.46
1	A	350	LEU	C-O	-5.55	1.16	1.24
1	A	254	GLU	C-O	-5.54	1.17	1.23
1	A	50	VAL	C-O	-5.53	1.18	1.24
1	A	69	ASP	CA-C	-5.52	1.45	1.52
1	A	242	THR	C-O	-5.51	1.17	1.24
1	A	352	TYR	CA-C	-5.51	1.45	1.52
1	A	268	GLY	C-O	-5.51	1.18	1.23
1	A	83	ARG	CA-C	-5.50	1.45	1.52
1	A	195	ILE	C-O	-5.49	1.18	1.24
1	A	130	ASP	C-N	-5.46	1.28	1.33
1	A	324	LEU	C-O	-5.46	1.17	1.23
1	A	145	GLU	C-O	-5.46	1.17	1.24
1	A	72	PHE	C-O	-5.46	1.17	1.24
1	A	143	ILE	CA-C	-5.43	1.46	1.52
1	A	237	SER	C-O	-5.42	1.17	1.24
1	A	256	VAL	CA-CB	-5.42	1.47	1.54
1	A	293	LEU	CA-C	-5.41	1.45	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	23	VAL	CA-C	-5.41	1.46	1.52
1	A	248	THR	C-O	-5.41	1.17	1.24
1	A	337	SER	C-O	-5.40	1.17	1.24
1	A	319	ILE	C-O	-5.38	1.17	1.24
1	A	201	GLU	C-O	-5.37	1.17	1.24
1	A	133	ALA	CA-C	-5.37	1.46	1.52
1	A	163	ILE	C-O	-5.34	1.18	1.24
1	A	246	LYS	C-O	-5.31	1.17	1.23
1	A	239	PHE	C-O	-5.30	1.17	1.24
1	A	53	ARG	C-O	-5.29	1.17	1.24
1	A	141	HIS	CA-C	-5.29	1.46	1.52
1	A	194	VAL	CA-CB	-5.29	1.47	1.55
1	A	360	LEU	CA-C	-5.28	1.46	1.52
1	A	295	LEU	C-O	-5.28	1.18	1.24
1	A	81	VAL	CA-C	-5.27	1.46	1.52
1	A	262	ASN	CA-C	-5.26	1.46	1.52
1	A	268	GLY	CA-C	-5.26	1.47	1.52
1	A	41	VAL	C-O	-5.25	1.18	1.24
1	A	320	LEU	CA-C	-5.24	1.45	1.52
1	A	255	LEU	C-O	-5.22	1.17	1.24
1	A	118	GLU	C-O	-5.22	1.17	1.23
1	A	103	ALA	C-O	-5.21	1.17	1.24
1	A	291	SER	C-O	-5.21	1.18	1.24
1	A	326	GLY	C-O	-5.20	1.18	1.24
1	A	124	GLU	N-CA	-5.20	1.40	1.46
1	A	211	TYR	C-O	-5.20	1.18	1.24
1	A	110	GLY	C-O	-5.18	1.17	1.24
1	A	80	ASP	CA-C	-5.18	1.46	1.52
1	A	212	GLN	C-O	-5.17	1.18	1.24
1	A	349	THR	C-O	-5.17	1.18	1.24
1	A	82	TYR	CA-C	-5.16	1.46	1.52
1	A	160	LEU	C-O	-5.16	1.18	1.23
1	A	336	ILE	C-O	-5.15	1.17	1.23
1	A	102	PHE	C-O	-5.14	1.17	1.23
1	A	243	ILE	CA-CB	-5.13	1.48	1.54
1	A	131	PRO	C-O	-5.13	1.18	1.24
1	A	298	VAL	C-O	-5.13	1.18	1.24
1	A	137	PRO	C-O	-5.12	1.17	1.24
1	A	115	MET	C-O	-5.12	1.18	1.24
1	A	202	ILE	C-O	-5.12	1.18	1.24
1	A	216	LYS	C-O	-5.11	1.18	1.24
1	A	161	LEU	C-O	-5.11	1.17	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	359	ILE	C-O	-5.11	1.17	1.24
1	A	69	ASP	N-CA	-5.09	1.40	1.46
1	A	95	MET	C-O	-5.09	1.17	1.24
1	A	128	GLU	C-O	-5.08	1.17	1.24
1	A	213	ILE	C-O	-5.08	1.18	1.24
1	A	347	LEU	CA-C	-5.08	1.46	1.52
1	A	79	ILE	C-O	-5.08	1.18	1.24
1	A	265	ASP	C-O	-5.07	1.18	1.23
1	A	108	GLY	C-O	-5.06	1.17	1.24
1	A	133	ALA	C-O	-5.04	1.17	1.23
1	A	365	VAL	C-O	-5.04	1.17	1.24
1	A	360	LEU	C-O	-5.03	1.17	1.23
1	A	135	ILE	CA-C	-5.02	1.46	1.52
1	A	335	THR	C-O	-5.01	1.17	1.24

All (50) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	245	MET	CA-C-O	-98.83	12.66	120.38
1	A	187	ASP	CA-C-N	19.14	140.30	119.05
1	A	187	ASP	C-N-CA	19.14	140.30	119.05
1	A	173	ASN	CA-C-N	17.90	138.16	119.19
1	A	173	ASN	C-N-CA	17.90	138.16	119.19
1	A	337	SER	CA-C-N	16.30	137.21	119.28
1	A	337	SER	C-N-CA	16.30	137.21	119.28
1	A	55	GLY	N-CA-C	10.06	126.33	114.16
1	A	177	ASP	N-CA-C	-8.19	94.32	108.56
1	A	39	SER	N-CA-C	7.83	121.86	110.28
1	A	245	MET	N-CA-C	7.75	121.54	109.07
1	A	110	GLY	N-CA-C	7.65	126.81	115.64
1	A	84	SER	N-CA-C	7.56	119.31	111.14
1	A	86	VAL	N-CA-C	7.07	119.93	111.09
1	A	312	ARG	N-CA-C	6.98	121.05	112.54
1	A	30	LEU	N-CA-C	-6.87	103.72	111.07
1	A	210	VAL	N-CA-C	6.71	116.87	110.42
1	A	241	VAL	CB-CA-C	-6.70	100.71	110.63
1	A	243	ILE	CB-CA-C	-6.62	100.66	110.33
1	A	228	MET	N-CA-C	6.13	118.17	108.79
1	A	178	VAL	N-CA-C	6.09	116.27	110.42
1	A	40	ILE	CB-CA-C	-6.07	104.15	111.85
1	A	44	ASP	CA-C-N	5.85	125.54	119.05
1	A	44	ASP	C-N-CA	5.85	125.54	119.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	163	ILE	CB-CA-C	-5.79	103.15	111.19
1	A	306	THR	CA-C-N	5.77	125.62	119.28
1	A	306	THR	C-N-CA	5.77	125.62	119.28
1	A	313	GLU	N-CA-C	5.70	119.85	113.01
1	A	310	PRO	N-CA-C	5.66	120.12	112.48
1	A	76	THR	N-CA-C	5.65	118.74	109.76
1	A	101	ILE	CB-CA-C	-5.60	102.16	110.33
1	A	362	LYS	CA-C-N	5.57	125.75	119.90
1	A	362	LYS	C-N-CA	5.57	125.75	119.90
1	A	210	VAL	CB-CA-C	-5.51	104.92	111.97
1	A	365	VAL	N-CA-C	5.45	116.83	108.71
1	A	102	PHE	N-CA-C	5.45	117.46	109.24
1	A	264	VAL	N-CA-C	5.41	116.28	108.48
1	A	333	ILE	CB-CA-C	-5.40	103.07	110.96
1	A	135	ILE	CB-CA-C	-5.39	104.87	112.14
1	A	84	SER	CA-C-N	-5.31	117.51	122.66
1	A	84	SER	C-N-CA	-5.31	117.51	122.66
1	A	307	PRO	CA-C-N	-5.31	115.52	123.00
1	A	307	PRO	C-N-CA	-5.31	115.52	123.00
1	A	205	HIS	N-CA-C	5.22	119.70	113.23
1	A	228	MET	CA-C-N	5.21	128.17	120.82
1	A	228	MET	C-N-CA	5.21	128.17	120.82
1	A	18	ASN	N-CA-C	5.19	121.86	110.80
1	A	23	VAL	CB-CA-C	-5.05	103.16	110.63
1	A	178	VAL	CB-CA-C	-5.03	105.53	111.97
1	A	243	ILE	N-CA-C	5.00	115.32	108.12

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	245	MET	Mainchain

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	2566	0	2547	183	0
2	A	27	0	12	0	0
3	A	1	0	0	0	0
4	A	19	0	0	1	0
5	A	41	0	0	9	0
All	All	2654	0	2559	183	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 35.

All (183) 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:102:PHE:HB3	1:A:264:VAL:HG22	1.18	1.14
1:A:153:GLU:OE1	1:A:246:LYS:HE3	1.45	1.13
1:A:20:GLN:NE2	1:A:331:SER:OG	1.86	1.08
1:A:322:ASP:O	1:A:326:GLY:HA3	1.55	1.07
1:A:219:ALA:O	1:A:222:THR:OG1	1.71	1.06
1:A:227:LEU:O	1:A:228:MET:HG2	1.59	1.01
1:A:153:GLU:OE1	1:A:246:LYS:CE	2.10	0.99
1:A:102:PHE:CB	1:A:264:VAL:HG22	1.93	0.98
1:A:271:ASN:HB3	1:A:289:ASN:ND2	1.77	0.97
1:A:244:HIS:CE1	1:A:258:ILE:CD1	2.50	0.95
1:A:312:ARG:HH11	1:A:312:ARG:HG2	1.33	0.93
1:A:153:GLU:OE1	1:A:246:LYS:HD2	1.68	0.92
1:A:112:THR:OG1	5:A:501:HOH:O	1.83	0.91
1:A:244:HIS:ND1	1:A:258:ILE:HD13	1.86	0.90
1:A:153:GLU:OE1	1:A:246:LYS:CD	2.20	0.88
1:A:184:MET:C	1:A:185:PHE:HD2	1.81	0.88
1:A:244:HIS:CE1	1:A:258:ILE:HD13	2.08	0.88
1:A:184:MET:O	1:A:185:PHE:HD2	1.56	0.86
1:A:87:CYS:HB3	1:A:88:PRO:HD3	1.58	0.84
1:A:299:ILE:O	1:A:303:VAL:CG1	2.25	0.84
1:A:134:GLY:O	1:A:138:ARG:HG3	1.77	0.84
1:A:70:MET:HE1	1:A:85:VAL:HG12	1.60	0.84
1:A:299:ILE:O	1:A:303:VAL:HG13	1.76	0.84
1:A:40:ILE:HG22	1:A:53:ARG:HB2	1.62	0.82
1:A:184:MET:C	1:A:185:PHE:CD2	2.57	0.81
1:A:151:GLY:O	1:A:152:THR:OG1	1.97	0.81
1:A:161:LEU:HD12	1:A:161:LEU:O	1.82	0.80
1:A:304:GLU:O	1:A:305:ARG:HB2	1.81	0.80
1:A:300:THR:OG1	1:A:355:ARG:NH2	2.14	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:243:ILE:HB	1:A:245:MET:CE	2.12	0.79
1:A:112:THR:OG1	5:A:502:HOH:O	2.00	0.79
1:A:314:SER:OG	1:A:317:THR:OG1	2.00	0.79
1:A:187:ASP:O	1:A:190:ASN:O	2.00	0.78
1:A:20:GLN:HE21	1:A:331:SER:HG	1.30	0.77
1:A:290:GLN:O	1:A:294:THR:OG1	2.03	0.76
1:A:70:MET:CE	1:A:85:VAL:HG12	2.16	0.76
1:A:224:ALA:O	1:A:231:TYR:CE2	2.40	0.75
1:A:192:ARG:HH11	1:A:192:ARG:HG3	1.52	0.75
1:A:240:SER:OG	1:A:262:ASN:OD1	2.05	0.74
1:A:311:TYR:CG	1:A:321:GLN:HG3	2.22	0.74
1:A:209:GLU:O	1:A:213:ILE:HD12	1.87	0.74
1:A:173:ASN:OD1	1:A:174:PRO:HD2	1.89	0.72
1:A:119:ARG:NH2	1:A:125:TYR:O	2.22	0.72
1:A:44:ASP:OD1	1:A:47:ARG:HG3	1.89	0.72
1:A:59:ASP:OD2	1:A:62:SER:OG	2.05	0.72
1:A:311:TYR:CD1	1:A:321:GLN:HG3	2.25	0.72
1:A:322:ASP:O	1:A:326:GLY:CA	2.36	0.71
1:A:345:GLU:OE2	1:A:345:GLU:HA	1.89	0.71
1:A:271:ASN:HB3	1:A:289:ASN:HD21	1.52	0.70
1:A:337:SER:HB2	1:A:338:PRO:HD2	1.73	0.69
1:A:244:HIS:ND1	1:A:258:ILE:CD1	2.53	0.69
1:A:98:ASN:HB2	1:A:328:THR:HG22	1.72	0.69
1:A:247:GLU:OE1	5:A:503:HOH:O	2.11	0.68
1:A:168:LEU:HD11	1:A:184:MET:HE2	1.75	0.68
1:A:82:TYR:OH	1:A:142:GLN:HG3	1.94	0.67
1:A:153:GLU:CD	1:A:246:LYS:HD2	2.19	0.67
1:A:228:MET:HB2	1:A:231:TYR:HE2	1.60	0.67
1:A:319:ILE:C	1:A:320:LEU:HD23	2.20	0.66
1:A:43:CYS:HB3	1:A:71:VAL:CG1	2.25	0.66
1:A:59:ASP:O	1:A:61:SER:N	2.28	0.65
1:A:161:LEU:HD12	1:A:161:LEU:C	2.21	0.64
1:A:102:PHE:CB	1:A:264:VAL:CG2	2.74	0.64
1:A:189:ARG:HD2	1:A:189:ARG:N	2.13	0.64
1:A:227:LEU:C	1:A:228:MET:HG2	2.23	0.64
1:A:243:ILE:O	1:A:245:MET:HE3	1.97	0.63
1:A:356:ALA:O	1:A:359:ILE:HG13	1.98	0.63
1:A:192:ARG:HG3	1:A:192:ARG:NH1	2.14	0.62
1:A:48:LYS:HD3	1:A:69:ASP:O	1.99	0.62
1:A:327:ARG:CG	1:A:327:ARG:HH11	2.12	0.62
1:A:288:ILE:HD12	1:A:288:ILE:O	1.99	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:327:ARG:HH11	1:A:327:ARG:HG3	1.64	0.62
1:A:87:CYS:HB3	1:A:88:PRO:CD	2.28	0.62
1:A:254:GLU:C	1:A:255:LEU:HD23	2.26	0.61
1:A:228:MET:HB2	1:A:231:TYR:CE2	2.35	0.61
1:A:20:GLN:NE2	1:A:331:SER:HG	1.89	0.61
1:A:298:VAL:HG21	1:A:317:THR:HG21	1.83	0.60
1:A:289:ASN:O	1:A:293:LEU:HG	2.02	0.60
1:A:312:ARG:HH11	1:A:312:ARG:CG	2.09	0.59
1:A:224:ALA:HA	1:A:227:LEU:HB2	1.84	0.59
1:A:299:ILE:HG23	1:A:359:ILE:HD11	1.84	0.59
1:A:122:ASN:O	1:A:124:GLU:N	2.35	0.58
1:A:136:ILE:N	1:A:137:PRO:HD2	2.18	0.58
1:A:319:ILE:O	1:A:319:ILE:HG22	2.03	0.58
1:A:92:GLU:HA	1:A:95:MET:HG3	1.85	0.58
1:A:243:ILE:HB	1:A:245:MET:HE2	1.85	0.57
1:A:243:ILE:HB	1:A:245:MET:HE3	1.84	0.57
1:A:187:ASP:HB2	1:A:195:ILE:HG13	1.87	0.57
1:A:337:SER:CB	1:A:338:PRO:HD2	2.31	0.57
1:A:211:TYR:HE2	1:A:215:GLU:OE1	1.87	0.57
1:A:211:TYR:CE2	1:A:215:GLU:OE1	2.58	0.57
1:A:184:MET:O	1:A:185:PHE:CD2	2.48	0.55
1:A:112:THR:OG1	5:A:504:HOH:O	2.18	0.55
1:A:150:ASN:ND2	1:A:150:ASN:C	2.65	0.55
1:A:55:GLY:HA3	1:A:59:ASP:HB3	1.89	0.55
1:A:91:ASP:OD1	1:A:146:LYS:NZ	2.38	0.55
1:A:166:GLU:HA	1:A:166:GLU:OE2	2.07	0.54
1:A:299:ILE:O	1:A:303:VAL:HG12	2.04	0.54
1:A:185:PHE:CD2	1:A:185:PHE:N	2.73	0.54
1:A:172:LEU:O	1:A:174:PRO:HD3	2.06	0.54
1:A:169:PHE:HE1	1:A:179:SER:HB3	1.72	0.54
1:A:165:ASN:O	1:A:166:GLU:HB2	2.07	0.54
1:A:175:SER:OG	1:A:177:ASP:HB2	2.07	0.53
1:A:182:LEU:CD2	5:A:514:HOH:O	2.55	0.53
1:A:327:ARG:CG	1:A:327:ARG:NH1	2.72	0.52
1:A:225:ALA:HA	1:A:231:TYR:CG	2.44	0.52
1:A:109:THR:HG22	1:A:337:SER:HB3	1.92	0.52
1:A:113:PHE:O	1:A:117:GLY:HA2	2.09	0.52
1:A:319:ILE:O	1:A:320:LEU:HD23	2.08	0.52
1:A:87:CYS:CB	1:A:88:PRO:CD	2.88	0.52
1:A:150:ASN:ND2	1:A:152:THR:OG1	2.43	0.52
1:A:181:ARG:O	1:A:182:LEU:HD23	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:29:ASN:HB2	1:A:31:ALA:HB3	1.92	0.51
1:A:123:GLU:O	1:A:124:GLU:C	2.52	0.50
1:A:43:CYS:HB3	1:A:71:VAL:HG11	1.93	0.50
1:A:158:VAL:HG12	1:A:241:VAL:HG13	1.94	0.50
1:A:357:LYS:HG2	5:A:518:HOH:O	2.11	0.50
1:A:106:GLN:O	1:A:109:THR:OG1	2.20	0.50
1:A:161:LEU:C	1:A:161:LEU:CD1	2.85	0.50
1:A:247:GLU:HB3	1:A:255:LEU:HB2	1.94	0.50
1:A:337:SER:CB	1:A:338:PRO:CD	2.87	0.50
1:A:151:GLY:C	1:A:152:THR:HG1	2.04	0.49
1:A:106:GLN:NE2	1:A:345:GLU:HG3	2.28	0.49
1:A:244:HIS:CE1	1:A:258:ILE:HD12	2.46	0.49
1:A:102:PHE:HB3	1:A:264:VAL:CG2	2.12	0.49
1:A:312:ARG:CG	1:A:312:ARG:NH1	2.71	0.49
1:A:86:VAL:O	1:A:86:VAL:HG12	2.11	0.49
1:A:30:LEU:O	1:A:33:ARG:HB2	2.12	0.49
1:A:255:LEU:HD23	1:A:255:LEU:N	2.28	0.49
1:A:87:CYS:CB	1:A:88:PRO:HD3	2.36	0.49
1:A:115:MET:CE	1:A:263:LEU:HB3	2.43	0.49
1:A:104:TYR:HD1	1:A:266:LEU:HD12	1.79	0.48
1:A:351:GLU:OE1	1:A:351:GLU:HA	2.13	0.48
1:A:140:LEU:HA	1:A:140:LEU:HD23	1.49	0.48
1:A:363:PRO:C	1:A:364:GLU:HG3	2.38	0.48
1:A:98:ASN:O	1:A:328:THR:HB	2.13	0.47
1:A:323:SER:HA	1:A:328:THR:OG1	2.14	0.47
1:A:320:LEU:HD23	1:A:320:LEU:N	2.30	0.47
1:A:102:PHE:CE1	1:A:332:ILE:HG12	2.49	0.47
1:A:173:ASN:HA	1:A:174:PRO:HD3	1.36	0.47
1:A:337:SER:HA	1:A:338:PRO:HD3	1.61	0.47
1:A:187:ASP:HA	1:A:188:PRO:HD2	1.24	0.46
1:A:228:MET:O	1:A:231:TYR:HD2	1.97	0.46
1:A:181:ARG:C	1:A:182:LEU:HD23	2.41	0.46
1:A:95:MET:O	1:A:257:LYS:HE3	2.15	0.46
1:A:101:ILE:HG21	1:A:101:ILE:HD13	1.65	0.46
1:A:306:THR:HA	1:A:307:PRO:HD3	1.80	0.46
1:A:29:ASN:OD1	1:A:29:ASN:N	2.43	0.46
1:A:193:GLY:C	1:A:194:VAL:CG1	2.89	0.46
1:A:193:GLY:C	1:A:194:VAL:HG13	2.41	0.46
1:A:295:LEU:O	1:A:299:ILE:HG13	2.16	0.45
1:A:225:ALA:HA	1:A:231:TYR:CD2	2.51	0.45
1:A:26:ARG:HB2	1:A:27:PRO:HD2	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:18:ASN:H	1:A:360:LEU:HD23	1.82	0.45
1:A:168:LEU:HD11	1:A:184:MET:CE	2.45	0.45
1:A:112:THR:CB	5:A:501:HOH:O	2.57	0.44
1:A:147:LEU:HA	1:A:147:LEU:HD23	1.52	0.44
1:A:148:THR:O	1:A:148:THR:HG22	2.15	0.44
1:A:243:ILE:C	1:A:245:MET:HE3	2.42	0.44
1:A:182:LEU:HD23	5:A:514:HOH:O	2.16	0.44
1:A:305:ARG:HA	1:A:305:ARG:HD2	1.65	0.44
1:A:230:ALA:O	1:A:234:ARG:HB2	2.18	0.44
1:A:347:LEU:HD23	1:A:347:LEU:HA	1.57	0.44
1:A:20:GLN:HB3	1:A:331:SER:OG	2.17	0.44
1:A:40:ILE:H	1:A:40:ILE:HG13	1.57	0.44
1:A:162:GLU:OE1	1:A:231:TYR:HE1	2.00	0.44
1:A:119:ARG:HB2	4:A:403:EOK:O19	2.18	0.43
1:A:243:ILE:CB	1:A:245:MET:HE2	2.48	0.43
1:A:332:ILE:HG21	1:A:332:ILE:HD13	1.76	0.43
1:A:184:MET:HE3	1:A:315:LYS:HD2	2.01	0.43
1:A:171:LEU:HA	1:A:171:LEU:HD23	1.84	0.42
1:A:92:GLU:H	1:A:92:GLU:HG2	1.60	0.42
1:A:99:CYS:SG	1:A:329:ARG:HG3	2.60	0.42
1:A:160:LEU:HG	1:A:171:LEU:HD12	2.01	0.42
1:A:182:LEU:HD22	5:A:514:HOH:O	2.18	0.41
1:A:219:ALA:C	1:A:222:THR:OG1	2.57	0.41
1:A:70:MET:CE	1:A:85:VAL:CG1	2.95	0.41
1:A:111:LYS:HE2	1:A:111:LYS:HB2	1.75	0.41
1:A:243:ILE:CB	1:A:245:MET:CE	2.91	0.41
1:A:123:GLU:OE1	1:A:123:GLU:N	2.53	0.40
1:A:320:LEU:O	1:A:324:LEU:HD12	2.21	0.40
1:A:59:ASP:OD2	1:A:62:SER:CB	2.69	0.40
1:A:243:ILE:CG2	1:A:245:MET:HE2	2.52	0.40
1:A:170:ASP:OD2	1:A:173:ASN:N	2.54	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	321/370 (87%)	311 (97%)	7 (2%)	3 (1%)	14	41

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	60	LYS
1	A	123	GLU
1	A	231	TYR

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	283/323 (88%)	230 (81%)	53 (19%)	1	5

All (53) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	17	LYS
1	A	22	VAL
1	A	29	ASN
1	A	36	SER
1	A	40	ILE
1	A	79	ILE
1	A	84	SER
1	A	85	VAL
1	A	87	CYS
1	A	89	ILE
1	A	95	MET
1	A	129	GLU
1	A	150	ASN
1	A	156	VAL
1	A	161	LEU
1	A	166	GLU

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Mol	Chain	Res	Type
1	A	175	SER
1	A	176	SER
1	A	178	VAL
1	A	184	MET
1	A	189	ARG
1	A	202	ILE
1	A	207	LYS
1	A	213	ILE
1	A	215	GLU
1	A	222	THR
1	A	228	MET
1	A	231	TYR
1	A	232	SER
1	A	234	ARG
1	A	241	VAL
1	A	245	MET
1	A	254	GLU
1	A	258	ILE
1	A	260	LYS
1	A	264	VAL
1	A	288	ILE
1	A	291	SER
1	A	292	LEU
1	A	303	VAL
1	A	305	ARG
1	A	306	THR
1	A	309	VAL
1	A	312	ARG
1	A	317	THR
1	A	320	LEU
1	A	327	ARG
1	A	329	ARG
1	A	331	SER
1	A	340	SER
1	A	345	GLU
1	A	351	GLU
1	A	359	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	20	GLN

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Mol	Chain	Res	Type
1	A	150	ASN
1	A	205	HIS
1	A	342	ASN
1	A	358	ASN

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 3 ligands modelled in this entry, 1 is 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	ADP	A	401	3	28,29,29	1.64	4 (14%)	43,45,45	1.80	9 (20%)
4	EOK	A	403	-	16,20,20	5.11	7 (43%)	15,29,29	1.83	4 (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 Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	ADP	A	401	3	-	2/16/32/32	0/3/3/3
4	EOK	A	403	-	-	2/14/29/29	0/2/2/2

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	403	EOK	C02-S09	-11.54	1.62	1.86
4	A	403	EOK	C10-N11	10.72	1.49	1.32
4	A	403	EOK	N15-N16	10.56	1.56	1.41
4	A	403	EOK	C10-S09	-5.55	1.69	1.75
2	A	401	ADP	C5-C4	5.36	1.48	1.39
4	A	403	EOK	C12-N11	3.42	1.45	1.38
2	A	401	ADP	PA-O3A	3.15	1.62	1.59
2	A	401	ADP	C5-C6	2.91	1.49	1.41
4	A	403	EOK	C13-C12	2.88	1.53	1.49
2	A	401	ADP	C8-N7	2.60	1.36	1.31
4	A	403	EOK	O14-C12	-2.07	1.18	1.23

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	401	ADP	C5-C4-N3	-5.67	118.91	126.72
4	A	403	EOK	C13-C12-N11	4.80	121.95	114.84
2	A	401	ADP	N3-C4-N9	4.62	135.03	127.17
2	A	401	ADP	C4-C5-N7	-3.73	106.32	110.58
2	A	401	ADP	C4-N9-C8	3.10	109.00	105.74
2	A	401	ADP	C2-N3-C4	2.78	118.61	111.83
2	A	401	ADP	C5-N7-C8	2.69	107.67	103.45
4	A	403	EOK	O14-C12-N11	-2.57	118.72	123.63
4	A	403	EOK	C12-N11-C10	2.43	122.89	117.26
2	A	401	ADP	O2A-PA-O3A	2.37	113.69	107.27
4	A	403	EOK	S09-C10-N15	-2.32	106.73	108.22
2	A	401	ADP	N9-C8-N7	-2.09	110.97	113.94
2	A	401	ADP	O2B-PB-O1B	2.01	118.68	110.83

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	401	ADP	C5'-O5'-PA-O1A
4	A	403	EOK	N16-C02-C03-C04
4	A	403	EOK	N16-C02-C03-C08

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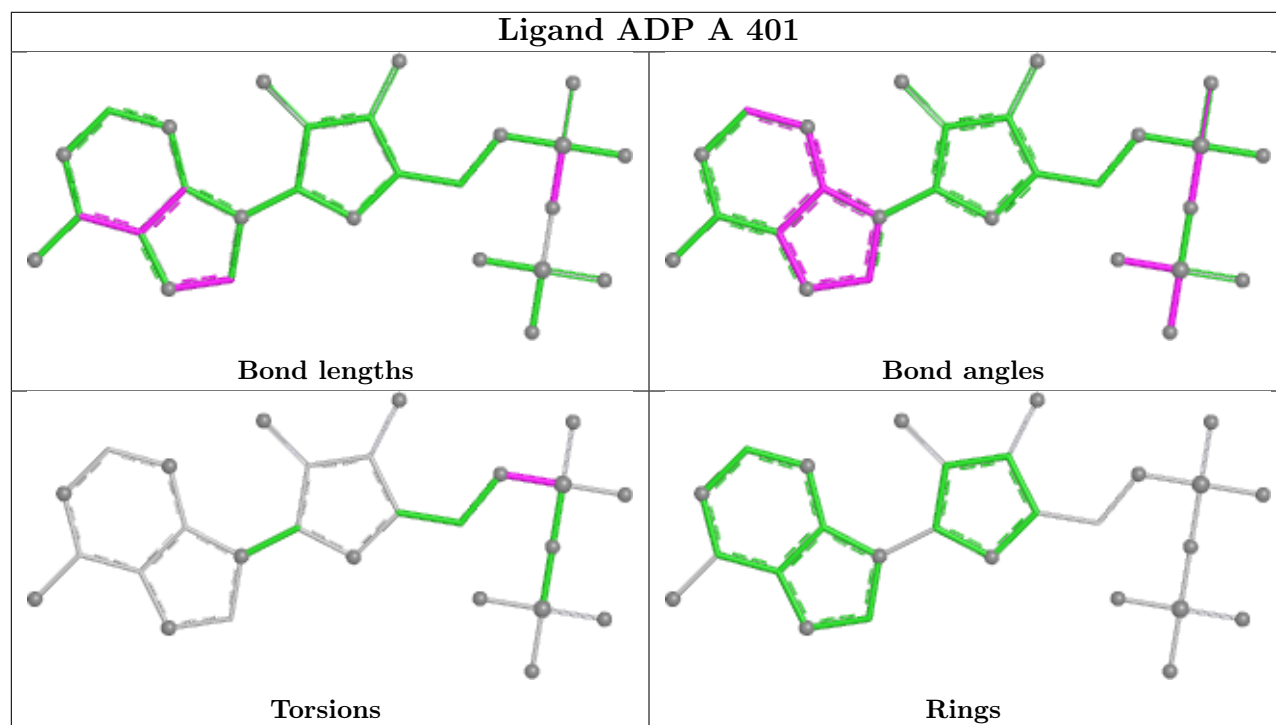
Mol	Chain	Res	Type	Atoms
2	A	401	ADP	C5'-O5'-PA-O2A

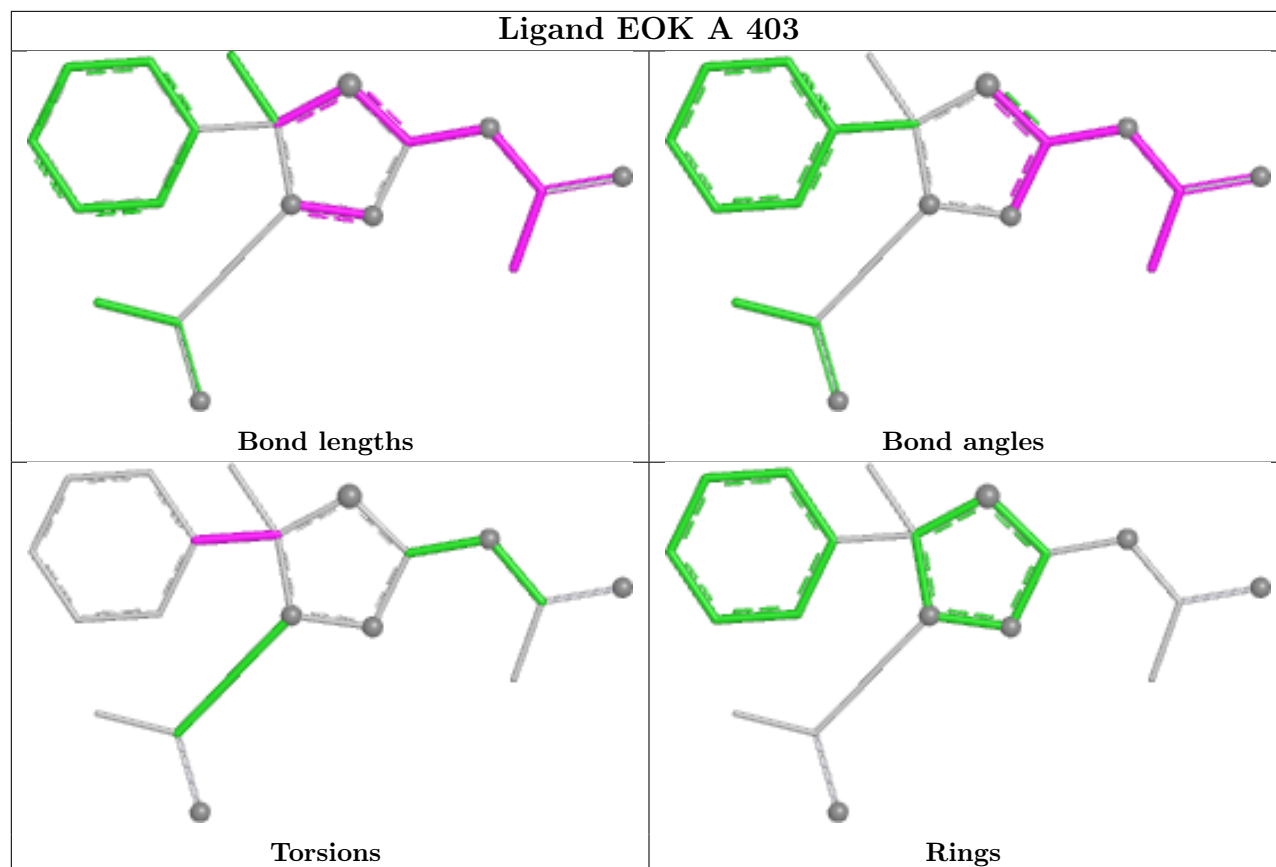
There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	403	EOK	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





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	333/370 (90%)	0.50	19 (5%)	29 22	51, 72, 112, 149	0

All (19) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	231	TYR	5.3
1	A	16	GLY	4.1
1	A	245	MET	4.0
1	A	122	ASN	3.3
1	A	224	ALA	3.0
1	A	102	PHE	2.8
1	A	251	ASP	2.6
1	A	288	ILE	2.4
1	A	180	GLU	2.4
1	A	178	VAL	2.4
1	A	38	HIS	2.3
1	A	33	ARG	2.3
1	A	185	PHE	2.3
1	A	230	ALA	2.2
1	A	183	GLN	2.2
1	A	31	ALA	2.2
1	A	65	THR	2.1
1	A	247	GLU	2.1
1	A	227	LEU	2.0

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

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

6.3 Carbohydrates [i](#)

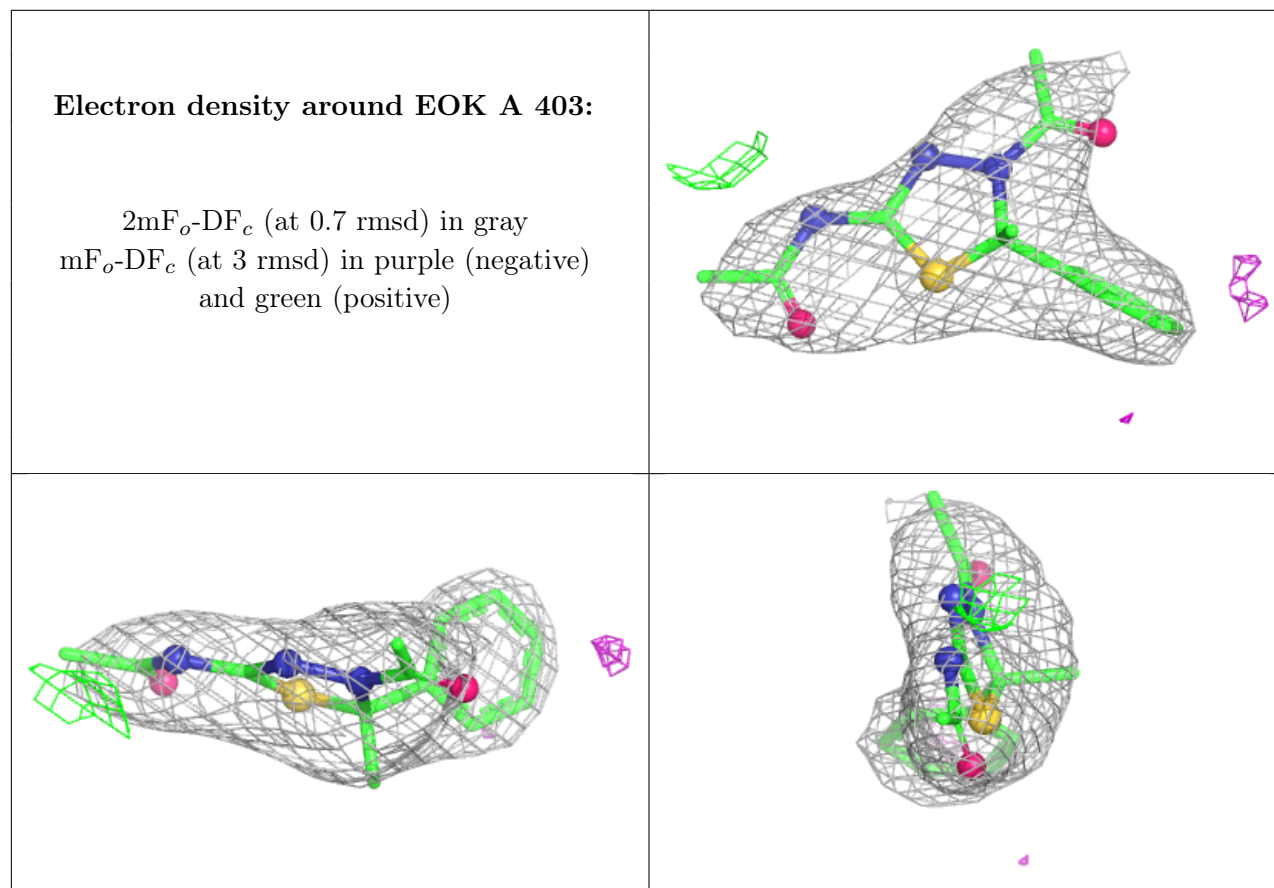
There are no oligosaccharides in this entry.

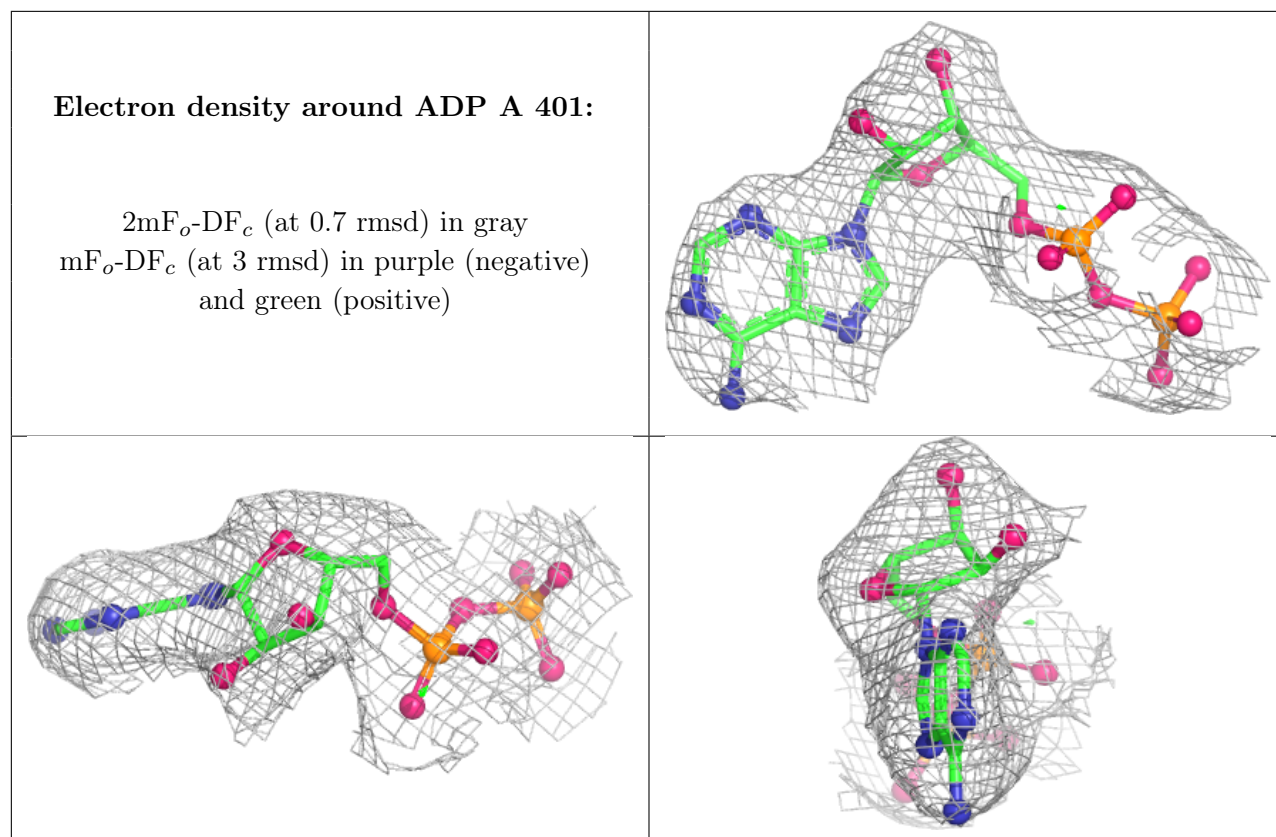
6.4 Ligands [i](#)

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
4	EOK	A	403	19/19	0.93	0.14	67,76,87,90	0
3	MG	A	402	1/1	0.94	0.07	65,65,65,65	0
2	ADP	A	401	27/27	0.97	0.09	55,66,70,74	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.