



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 12:44 AM UTC

PDB ID : 1FV9 / pdb_00001fv9
Title : Crystal structure of human microurokinase in complex with 2-amino-5-hydroxy-benzimidazole
Authors : Nienaber, V.
Deposited on : 2000-09-19
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)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

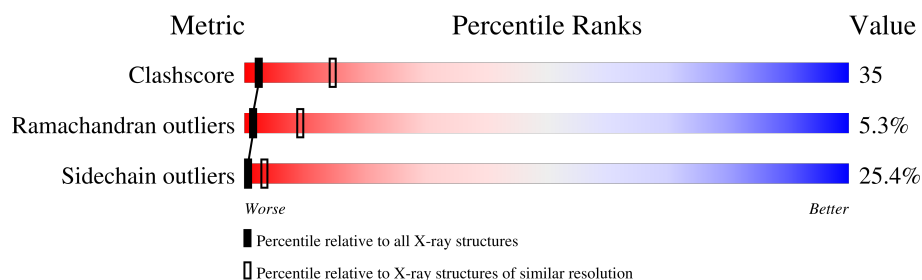
1 Overall quality at a glance

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))
Clashscore	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (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 $\leq 5\%$

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	245	

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 1949 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 UROKINASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	245	1933	1218	338	361	16	0	0	0

There is a discrepancy between the modelled and reference sequences:

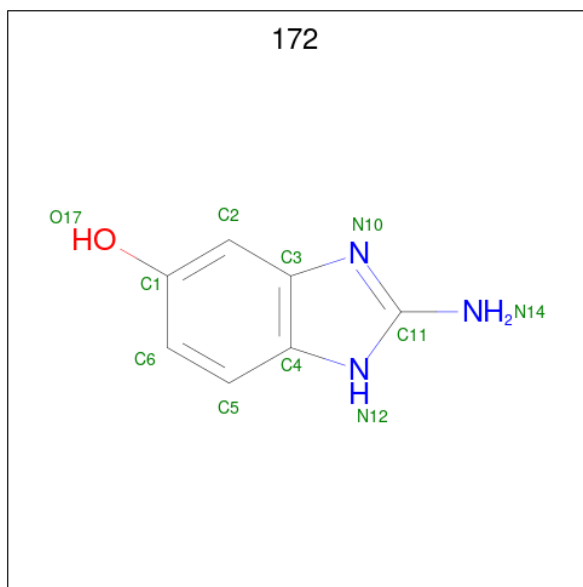
Chain	Residue	Modelled	Actual	Comment	Reference
A	120	ALA	CYS	conflict	UNP P00749

- Molecule 2 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	O	S		
2	A	1	5	4	1	0	0

- Molecule 3 is 2-AMINO-5-HYDROXY-BENZIMIDAZOLE (CCD ID: 172) (formula: C₇H₇N₃O).



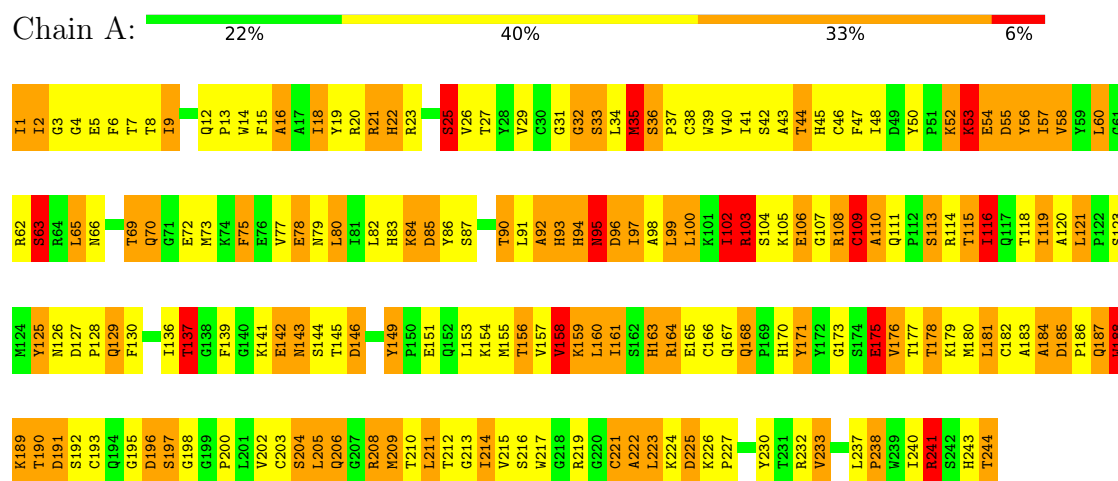
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			11	7	3	1		

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. 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. 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.

Note EDS was not executed.

• Molecule 1: UROKINASE



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	55.16Å 53.00Å 82.30Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	10.00 – 3.00	Depositor
% Data completeness (in resolution range)	(Not available) (10.00-3.00)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR 98.0	Depositor
R, R_{free}	0.248 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	1949	wwPDB-VP
Average B, all atoms (Å ²)	11.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: SO4, 172

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	1.70	41/1982 (2.1%)	2.18	109/2684 (4.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	4

All (41) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	99	LEU	CA-C	9.93	1.65	1.52
1	A	127	ASP	CA-C	-8.39	1.46	1.52
1	A	163	HIS	CA-C	8.33	1.63	1.52
1	A	116	ILE	CA-C	7.85	1.62	1.52
1	A	241	ARG	NE-CZ	7.81	1.41	1.33
1	A	170	HIS	C-N	7.49	1.44	1.33
1	A	185	ASP	CA-C	-7.24	1.44	1.52
1	A	171	TYR	N-CA	7.15	1.55	1.46
1	A	206	GLN	CA-C	6.71	1.61	1.52
1	A	93	HIS	CA-C	-6.60	1.45	1.52
1	A	137	THR	C-N	-6.53	1.25	1.33
1	A	158	VAL	N-CA	-6.52	1.38	1.46
1	A	170	HIS	CA-C	6.37	1.61	1.52
1	A	90	THR	CA-C	-6.29	1.44	1.52
1	A	205	LEU	N-CA	6.16	1.54	1.46
1	A	219	ARG	NE-CZ	6.00	1.39	1.33
1	A	42	SER	CA-C	-5.96	1.48	1.53
1	A	98	ALA	N-CA	5.90	1.53	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	200	PRO	N-CA	-5.83	1.39	1.47
1	A	53	LYS	N-CA	-5.83	1.38	1.46
1	A	9	ILE	N-CA	-5.80	1.39	1.46
1	A	103	ARG	CA-C	-5.80	1.45	1.52
1	A	206	GLN	N-CA	5.78	1.53	1.46
1	A	121	LEU	C-N	5.70	1.40	1.33
1	A	163	HIS	N-CA	5.70	1.53	1.46
1	A	100	LEU	CA-C	-5.69	1.45	1.52
1	A	142	GLU	CA-C	-5.67	1.45	1.52
1	A	180	MET	SD-CE	5.57	1.93	1.79
1	A	204	SER	C-N	5.56	1.41	1.33
1	A	115	THR	N-CA	-5.56	1.39	1.46
1	A	151	GLU	CA-C	5.49	1.60	1.52
1	A	222	ALA	N-CA	5.48	1.53	1.46
1	A	171	TYR	CA-C	5.39	1.59	1.52
1	A	20	ARG	CA-C	-5.28	1.46	1.52
1	A	18	ILE	CA-C	5.26	1.59	1.52
1	A	94	HIS	CA-C	-5.25	1.46	1.52
1	A	8	THR	C-N	-5.19	1.27	1.34
1	A	243	HIS	N-CA	5.18	1.51	1.46
1	A	164	ARG	NE-CZ	5.04	1.38	1.33
1	A	102	ILE	CA-C	-5.02	1.46	1.52
1	A	85	ASP	CA-C	5.00	1.59	1.52

All (109) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	196	ASP	CA-CB-CG	19.51	132.11	112.60
1	A	55	ASP	CA-CB-CG	17.37	129.97	112.60
1	A	143	ASN	CA-CB-CG	15.10	127.70	112.60
1	A	196	ASP	N-CA-C	-12.64	98.83	114.75
1	A	63	SER	CA-CB-OG	12.12	135.34	111.10
1	A	92	ALA	N-CA-C	11.74	127.60	110.10
1	A	189	LYS	N-CA-C	11.46	128.64	113.97
1	A	85	ASP	CA-CB-CG	11.06	123.66	112.60
1	A	110	ALA	N-CA-C	10.62	126.17	110.46
1	A	54	GLU	N-CA-C	10.57	125.56	112.87
1	A	180	MET	N-CA-C	-10.39	91.39	109.06
1	A	2	ILE	N-CA-C	-10.18	102.50	112.17
1	A	191	ASP	CA-CB-CG	10.09	122.69	112.60
1	A	94	HIS	N-CA-C	9.20	123.89	109.07
1	A	139	PHE	N-CA-C	-9.16	98.20	111.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	168	GLN	N-CA-C	-8.90	96.66	109.48
1	A	114	ARG	N-CA-C	-8.80	102.12	113.12
1	A	75	PHE	N-CA-C	8.68	123.43	108.76
1	A	187	GLN	N-CA-C	8.50	128.90	110.80
1	A	70	GLN	N-CA-C	8.26	128.38	110.80
1	A	185	ASP	N-CA-C	-8.14	97.53	109.50
1	A	209	MET	N-CA-C	-8.13	98.44	110.23
1	A	127	ASP	CA-CB-CG	-8.08	104.52	112.60
1	A	91	LEU	CA-CB-CG	7.93	144.07	116.30
1	A	105	LYS	CA-C-N	7.83	136.55	122.38
1	A	105	LYS	C-N-CA	7.83	136.55	122.38
1	A	25	SER	CA-CB-OG	-7.72	95.66	111.10
1	A	208	ARG	N-CA-C	7.65	121.44	109.96
1	A	233	VAL	N-CA-C	7.57	119.25	110.62
1	A	113	SER	CA-C-N	7.51	136.94	122.53
1	A	113	SER	C-N-CA	7.51	136.94	122.53
1	A	35	MET	N-CA-C	7.36	120.75	111.69
1	A	22	HIS	N-CA-C	7.34	121.52	110.14
1	A	238	PRO	CA-C-N	7.25	130.32	120.38
1	A	238	PRO	C-N-CA	7.25	130.32	120.38
1	A	146	ASP	CA-CB-CG	7.18	119.78	112.60
1	A	170	HIS	CA-C-N	7.15	135.19	121.54
1	A	170	HIS	C-N-CA	7.15	135.19	121.54
1	A	188	TRP	CA-C-N	-7.07	110.51	122.11
1	A	188	TRP	C-N-CA	-7.07	110.51	122.11
1	A	87	SER	CA-CB-OG	7.04	125.19	111.10
1	A	98	ALA	N-CA-C	6.98	119.95	108.99
1	A	32	GLY	CA-C-N	-6.98	109.66	121.94
1	A	32	GLY	C-N-CA	-6.98	109.66	121.94
1	A	36	SER	N-CA-C	-6.82	94.75	109.81
1	A	16	ALA	N-CA-C	6.78	120.98	107.62
1	A	121	LEU	O-C-N	-6.64	114.56	121.60
1	A	46	CYS	CA-CB-SG	6.55	129.47	114.40
1	A	175	GLU	CA-C-N	-6.50	110.26	121.97
1	A	175	GLU	C-N-CA	-6.50	110.26	121.97
1	A	106	GLU	N-CA-C	6.48	121.19	113.16
1	A	50	TYR	O-C-N	-6.40	114.97	121.31
1	A	86	TYR	N-CA-C	6.39	119.50	110.23
1	A	184	ALA	CA-C-N	6.38	129.22	120.67
1	A	184	ALA	C-N-CA	6.38	129.22	120.67
1	A	57	ILE	N-CA-C	-6.37	96.08	109.34
1	A	160	LEU	CA-C-N	-6.28	113.41	122.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	160	LEU	C-N-CA	-6.28	113.41	122.45
1	A	151	GLU	CA-C-N	-6.13	112.08	123.05
1	A	151	GLU	C-N-CA	-6.13	112.08	123.05
1	A	72	GLU	N-CA-C	-6.05	102.52	110.33
1	A	187	GLN	CA-C-N	6.01	133.02	121.54
1	A	187	GLN	C-N-CA	6.01	133.02	121.54
1	A	188	TRP	N-CA-C	6.01	123.60	110.80
1	A	6	PHE	N-CA-C	-5.99	99.94	109.76
1	A	5	GLU	N-CA-C	5.93	119.33	110.14
1	A	120	ALA	N-CA-C	5.91	119.02	110.28
1	A	80	LEU	N-CA-C	-5.90	99.28	108.90
1	A	185	ASP	CA-CB-CG	5.83	118.43	112.60
1	A	66	ASN	CB-CG-ND2	5.79	125.08	116.40
1	A	18	ILE	N-CA-C	5.74	116.37	107.99
1	A	39	TRP	N-CA-C	5.70	118.75	109.06
1	A	216	SER	N-CA-C	5.58	122.69	110.80
1	A	13	PRO	N-CA-C	-5.58	108.88	114.68
1	A	42	SER	CA-C-N	-5.56	114.17	122.74
1	A	42	SER	C-N-CA	-5.56	114.17	122.74
1	A	214	ILE	CA-C-N	-5.56	113.18	120.91
1	A	214	ILE	C-N-CA	-5.56	113.18	120.91
1	A	21	ARG	CA-C-N	-5.52	113.21	122.92
1	A	21	ARG	C-N-CA	-5.52	113.21	122.92
1	A	108	ARG	CG-CD-NE	-5.44	100.03	112.00
1	A	208	ARG	CD-NE-CZ	5.41	131.97	124.40
1	A	176	VAL	N-CA-C	-5.40	98.11	109.34
1	A	9	ILE	N-CA-C	5.38	117.78	111.05
1	A	149	TYR	CA-C-N	5.35	125.29	119.78
1	A	149	TYR	C-N-CA	5.35	125.29	119.78
1	A	145	THR	N-CA-C	-5.34	106.26	112.89
1	A	65	LEU	N-CA-C	5.34	122.17	110.80
1	A	128	PRO	CA-C-N	5.31	132.74	122.07
1	A	128	PRO	C-N-CA	5.31	132.74	122.07
1	A	62	ARG	NE-CZ-NH2	-5.30	114.43	119.20
1	A	79	ASN	CA-C-N	5.26	130.41	122.99
1	A	79	ASN	C-N-CA	5.26	130.41	122.99
1	A	62	ARG	N-CA-C	-5.22	101.19	109.96
1	A	21	ARG	N-CA-C	-5.21	101.78	110.17
1	A	20	ARG	CG-CD-NE	-5.20	100.57	112.00
1	A	243	HIS	N-CA-C	-5.20	105.23	112.30
1	A	110	ALA	CA-C-N	-5.18	113.75	121.83
1	A	110	ALA	C-N-CA	-5.18	113.75	121.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	96	ASP	CA-CB-CG	5.17	117.77	112.60
1	A	95	ASN	N-CA-C	-5.14	103.92	111.17
1	A	16	ALA	CB-CA-C	-5.13	102.39	111.22
1	A	237	LEU	N-CA-C	5.13	121.14	109.81
1	A	221	CYS	N-CA-C	-5.04	100.19	108.41
1	A	168	GLN	CA-C-N	5.03	125.10	119.87
1	A	168	GLN	C-N-CA	5.03	125.10	119.87
1	A	91	LEU	N-CA-C	-5.02	100.10	110.80
1	A	87	SER	N-CA-C	5.00	117.49	108.48
1	A	109	CYS	CA-CB-SG	-5.00	102.89	114.40

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	186	PRO	Peptide
1	A	25	SER	Peptide
1	A	53	LYS	Mainchain
1	A	56	TYR	Sidechain

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	1933	0	1881	136	0
2	A	5	0	0	0	0
3	A	11	0	6	1	0
All	All	1949	0	1887	136	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 (136) 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:63:SER:HB2	1:A:69:THR:HG21	1.49	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:181:LEU:HG	1:A:232:ARG:HE	1.44	0.83
1:A:75:PHE:CD2	1:A:102:ILE:HB	2.18	0.78
1:A:37:PRO:C	1:A:109:CYS:HB3	2.09	0.76
1:A:103:ARG:HD3	1:A:107:GLY:HA2	1.71	0.72
1:A:73:MET:HE3	1:A:116:ILE:HD12	1.72	0.72
1:A:21:ARG:HA	1:A:26:VAL:HG22	1.71	0.72
1:A:2:ILE:HD11	1:A:193:CYS:SG	2.30	0.72
1:A:119:ILE:H	1:A:119:ILE:HD12	1.56	0.69
1:A:166:CYS:HA	1:A:171:TYR:HD2	1.58	0.69
1:A:158:VAL:HG22	1:A:184:ALA:HA	1.75	0.69
1:A:32:GLY:HA2	1:A:198:GLY:O	1.94	0.67
1:A:78:GLU:HG2	1:A:103:ARG:HH11	1.58	0.67
1:A:188:TRP:HD1	1:A:222:ALA:O	1.77	0.67
1:A:47:PHE:CD2	1:A:80:LEU:HD11	2.30	0.66
1:A:165:GLU:O	1:A:168:GLN:HG2	1.97	0.65
1:A:75:PHE:CZ	1:A:110:ALA:HB2	2.33	0.64
1:A:44:THR:HB	1:A:82:LEU:HD22	1.79	0.64
1:A:19:TYR:HB3	1:A:26:VAL:HG13	1.81	0.63
1:A:1:ILE:HG22	1:A:3:GLY:H	1.65	0.62
1:A:142:GLU:HG2	1:A:154:LYS:HZ3	1.64	0.61
1:A:142:GLU:HG2	1:A:154:LYS:NZ	2.16	0.60
1:A:119:ILE:HA	1:A:208:ARG:NH2	2.17	0.59
1:A:3:GLY:HA3	1:A:190:THR:OG1	2.03	0.59
1:A:197:SER:HA	1:A:215:VAL:HB	1.83	0.59
1:A:21:ARG:HG3	1:A:57:ILE:HD11	1.84	0.59
1:A:167:GLN:HG2	1:A:173:GLY:O	2.02	0.59
1:A:208:ARG:HD2	1:A:209:MET:N	2.17	0.58
1:A:73:MET:HE3	1:A:116:ILE:CD1	2.33	0.58
1:A:208:ARG:NH1	1:A:209:MET:HB2	2.17	0.58
1:A:215:VAL:HG22	1:A:230:TYR:CE1	2.38	0.58
1:A:63:SER:CB	1:A:69:THR:HG21	2.28	0.58
1:A:12:GLN:HG3	1:A:137:THR:HG21	1.86	0.58
1:A:241:ARG:HH11	1:A:241:ARG:CA	2.16	0.57
1:A:176:VAL:HG11	1:A:182:CYS:SG	2.44	0.57
1:A:143:ASN:O	1:A:146:ASP:HB2	2.05	0.57
1:A:240:ILE:O	1:A:244:THR:HB	2.05	0.57
1:A:75:PHE:HZ	1:A:110:ALA:HB2	1.69	0.56
1:A:211:LEU:O	1:A:233:VAL:HG21	2.06	0.56
1:A:19:TYR:HB3	1:A:26:VAL:CG1	2.36	0.56
1:A:9:ILE:HD12	1:A:12:GLN:HB2	1.88	0.55
1:A:41:ILE:HG21	1:A:211:LEU:HD21	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:241:ARG:NH1	1:A:241:ARG:O	2.40	0.55
1:A:18:ILE:O	1:A:29:VAL:HB	2.07	0.55
1:A:22:HIS:HE1	1:A:27:THR:OG1	1.90	0.54
1:A:92:ALA:HA	1:A:217:TRP:CD2	2.42	0.54
1:A:241:ARG:NH1	1:A:244:THR:HG22	2.22	0.54
1:A:175:GLU:HA	1:A:175:GLU:OE1	2.07	0.54
1:A:213:GLY:HA2	1:A:233:VAL:HG23	1.89	0.53
1:A:159:LYS:O	1:A:184:ALA:N	2.42	0.53
1:A:161:ILE:CG2	1:A:166:CYS:HB2	2.38	0.53
1:A:95:ASN:HD22	1:A:95:ASN:N	2.05	0.53
1:A:7:THR:HB	1:A:155:MET:HG2	1.91	0.53
1:A:52:LYS:O	1:A:53:LYS:C	2.52	0.53
1:A:41:ILE:HD11	1:A:240:ILE:HD11	1.92	0.52
1:A:52:LYS:HB3	1:A:52:LYS:NZ	2.24	0.52
1:A:241:ARG:HH11	1:A:241:ARG:HA	1.75	0.51
1:A:75:PHE:HD2	1:A:102:ILE:HB	1.71	0.51
1:A:53:LYS:HD2	1:A:77:VAL:O	2.11	0.50
1:A:181:LEU:CD2	1:A:232:ARG:HH21	2.24	0.50
1:A:208:ARG:HG3	1:A:209:MET:O	2.12	0.49
1:A:14:TRP:CE3	1:A:119:ILE:HG23	2.48	0.49
1:A:53:LYS:HE2	1:A:54:GLU:OE2	2.13	0.49
1:A:136:ILE:CG1	1:A:156:THR:HG22	2.42	0.49
1:A:7:THR:HG23	1:A:153:LEU:HD23	1.94	0.49
1:A:141:LYS:HE2	1:A:146:ASP:O	2.13	0.48
1:A:177:THR:HG23	1:A:178:THR:N	2.27	0.48
1:A:43:ALA:HB1	1:A:96:ASP:OD2	2.13	0.48
1:A:36:SER:O	1:A:38:CYS:N	2.47	0.48
1:A:136:ILE:HG13	1:A:156:THR:HG22	1.95	0.48
1:A:163:HIS:NE2	1:A:167:GLN:OE1	2.45	0.48
1:A:161:ILE:HG21	1:A:166:CYS:HB2	1.95	0.47
1:A:110:ALA:HA	1:A:111:GLN:NE2	2.29	0.47
1:A:83:HIS:CD2	1:A:85:ASP:HB2	2.49	0.47
1:A:83:HIS:CD2	1:A:85:ASP:H	2.33	0.47
1:A:225:ASP:O	1:A:227:PRO:HD3	2.16	0.46
1:A:2:ILE:HD11	1:A:193:CYS:HB2	1.97	0.46
1:A:215:VAL:HG22	1:A:230:TYR:HE1	1.78	0.46
1:A:104:SER:O	1:A:106:GLU:N	2.49	0.45
1:A:33:SER:O	1:A:40:VAL:HA	2.16	0.45
1:A:73:MET:HE1	1:A:111:GLN:HB2	1.98	0.45
1:A:19:TYR:O	1:A:56:TYR:HA	2.16	0.45
1:A:32:GLY:CA	1:A:198:GLY:O	2.65	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:119:ILE:HA	1:A:208:ARG:HH22	1.82	0.45
1:A:1:ILE:O	1:A:142:GLU:HA	2.17	0.45
1:A:34:LEU:HD22	1:A:60:LEU:HD13	1.99	0.44
1:A:149:TYR:CE1	1:A:195:GLY:HA3	2.52	0.44
1:A:136:ILE:O	1:A:155:MET:HA	2.18	0.44
1:A:160:LEU:HD12	1:A:183:ALA:HB2	1.98	0.44
1:A:38:CYS:N	1:A:109:CYS:HB3	2.31	0.44
1:A:95:ASN:N	1:A:95:ASN:ND2	2.66	0.44
1:A:16:ALA:O	1:A:31:GLY:HA2	2.17	0.44
1:A:2:ILE:HD11	1:A:193:CYS:CB	2.46	0.44
1:A:37:PRO:O	1:A:109:CYS:HB3	2.17	0.44
1:A:15:PHE:CE1	1:A:31:GLY:HA3	2.53	0.43
1:A:77:VAL:HG21	1:A:100:LEU:HD23	1.99	0.43
1:A:35:MET:C	1:A:118:THR:HG22	2.43	0.43
1:A:93:HIS:H	1:A:217:TRP:NE1	2.17	0.43
1:A:155:MET:HE2	1:A:155:MET:HB2	1.82	0.43
1:A:53:LYS:HG3	1:A:54:GLU:N	2.32	0.43
1:A:163:HIS:CD2	1:A:167:GLN:HG3	2.54	0.43
1:A:163:HIS:NE2	1:A:167:GLN:CD	2.77	0.43
1:A:14:TRP:CZ3	1:A:119:ILE:HG23	2.54	0.43
1:A:190:THR:O	1:A:191:ASP:HB2	2.17	0.43
1:A:57:ILE:HD13	1:A:57:ILE:HG21	1.82	0.42
1:A:93:HIS:HD2	1:A:217:TRP:HB3	1.83	0.42
1:A:103:ARG:CD	1:A:107:GLY:HA2	2.44	0.42
1:A:53:LYS:O	1:A:55:ASP:N	2.52	0.42
1:A:226:LYS:HD3	1:A:226:LYS:HA	1.64	0.42
1:A:1:ILE:HG12	1:A:196:ASP:OD2	2.20	0.42
1:A:22:HIS:HB2	1:A:25:SER:O	2.20	0.42
1:A:75:PHE:HD2	1:A:103:ARG:H	1.67	0.42
1:A:77:VAL:CG2	1:A:100:LEU:HD23	2.49	0.42
1:A:93:HIS:H	1:A:217:TRP:CD1	2.36	0.42
1:A:215:VAL:CG1	3:A:246:172:HC5	2.50	0.42
1:A:58:VAL:HG11	1:A:100:LEU:HD22	2.00	0.42
1:A:208:ARG:HD2	1:A:209:MET:H	1.85	0.42
1:A:223:LEU:HB2	1:A:226:LYS:HB2	2.01	0.42
1:A:240:ILE:O	1:A:244:THR:CB	2.68	0.42
1:A:97:ILE:O	1:A:97:ILE:HG23	2.20	0.42
1:A:2:ILE:HG13	1:A:221:CYS:HB3	2.00	0.42
1:A:44:THR:HG22	1:A:97:ILE:O	2.20	0.42
1:A:78:GLU:HG2	1:A:103:ARG:NH1	2.30	0.42
1:A:40:VAL:HG12	1:A:41:ILE:N	2.35	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:104:SER:OG	1:A:106:GLU:HB2	2.19	0.42
1:A:223:LEU:O	1:A:224:LYS:C	2.63	0.42
1:A:129:GLN:O	1:A:129:GLN:HG2	2.20	0.41
1:A:129:GLN:O	1:A:130:PHE:C	2.63	0.41
1:A:203:CYS:SG	1:A:212:THR:HG21	2.59	0.41
1:A:34:LEU:O	1:A:118:THR:HA	2.20	0.41
1:A:149:TYR:CZ	1:A:195:GLY:HA3	2.56	0.41
1:A:12:GLN:HG3	1:A:153:LEU:HD21	2.03	0.41
1:A:97:ILE:HD13	1:A:214:ILE:HD12	2.03	0.41
1:A:94:HIS:C	1:A:95:ASN:HD22	2.29	0.41
1:A:224:LYS:O	1:A:225:ASP:HB2	2.21	0.40
1:A:166:CYS:HA	1:A:171:TYR:CD2	2.47	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	243/245 (99%)	190 (78%)	40 (16%)	13 (5%)	1 9

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	187	GLN
1	A	4	GLY
1	A	65	LEU
1	A	70	GLN
1	A	84	LYS
1	A	125	TYR
1	A	103	ARG
1	A	113	SER
1	A	211	LEU

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Mol	Chain	Res	Type
1	A	225	ASP
1	A	109	CYS
1	A	116	ILE
1	A	238	PRO

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	213/213 (100%)	159 (75%)	54 (25%)	0 3

All (54) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	ILE
1	A	23	ARG
1	A	33	SER
1	A	35	MET
1	A	44	THR
1	A	45	HIS
1	A	48	ILE
1	A	52	LYS
1	A	58	VAL
1	A	60	LEU
1	A	63	SER
1	A	69	THR
1	A	78	GLU
1	A	84	LYS
1	A	90	THR
1	A	95	ASN
1	A	97	ILE
1	A	99	LEU
1	A	102	ILE
1	A	103	ARG
1	A	108	ARG
1	A	115	THR

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Mol	Chain	Res	Type
1	A	119	ILE
1	A	121	LEU
1	A	123	SER
1	A	125	TYR
1	A	126	ASN
1	A	129	GLN
1	A	137	THR
1	A	144	SER
1	A	156	THR
1	A	157	VAL
1	A	158	VAL
1	A	159	LYS
1	A	161	ILE
1	A	164	ARG
1	A	175	GLU
1	A	178	THR
1	A	179	LYS
1	A	181	LEU
1	A	185	ASP
1	A	188	TRP
1	A	189	LYS
1	A	190	THR
1	A	192	SER
1	A	197	SER
1	A	202	VAL
1	A	204	SER
1	A	205	LEU
1	A	206	GLN
1	A	210	THR
1	A	223	LEU
1	A	241	ARG
1	A	244	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	11	ASN
1	A	22	HIS
1	A	66	ASN
1	A	94	HIS
1	A	95	ASN
1	A	111	GLN

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Mol	Chain	Res	Type
1	A	117	GLN
1	A	243	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 ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

2 ligands are 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$
3	172	A	246	-	12,12,12	3.54	5 (41%)	17,17,17	2.69	7 (41%)
2	SO4	A	245	-	4,4,4	0.43	0	6,6,6	0.61	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	172	A	246	-	-	-	0/2/2/2

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	246	172	C4-C3	-9.83	1.26	1.40
3	A	246	172	C11-N10	4.24	1.41	1.34
3	A	246	172	C2-C3	-3.09	1.35	1.40
3	A	246	172	C11-N12	2.83	1.42	1.36
3	A	246	172	C5-C4	-2.82	1.35	1.39

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	246	172	C3-C4-N12	5.67	112.53	105.71
3	A	246	172	C4-C3-N10	4.10	115.03	109.42
3	A	246	172	C4-N12-C11	-3.95	100.16	107.39
3	A	246	172	C2-C3-N10	-3.92	120.87	129.31
3	A	246	172	C5-C4-N12	-3.67	123.41	130.83
3	A	246	172	C3-N10-C11	-2.80	99.51	104.19
3	A	246	172	C2-C3-C4	2.56	124.08	120.50

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	246	172	1	0

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

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.