Full wwPDB X-ray Structure Validation Report (i)

Jun 12, 2024 – 03:19 PM EDT

PDB ID	:	1FV9
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 (i) 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 (i)) were used in the production of this report:

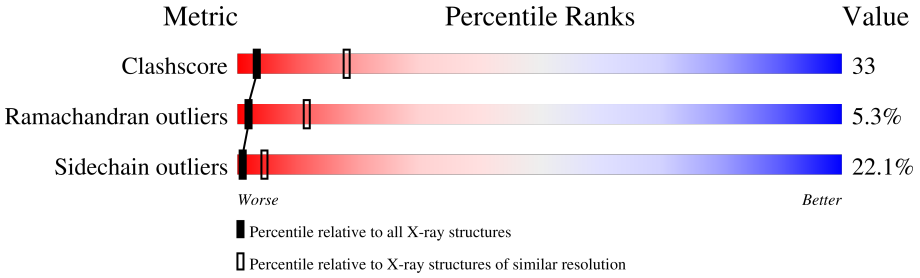
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

1 Overall quality at a glance (i)

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	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (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 <=5%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	245	32% 43% 21% •

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.

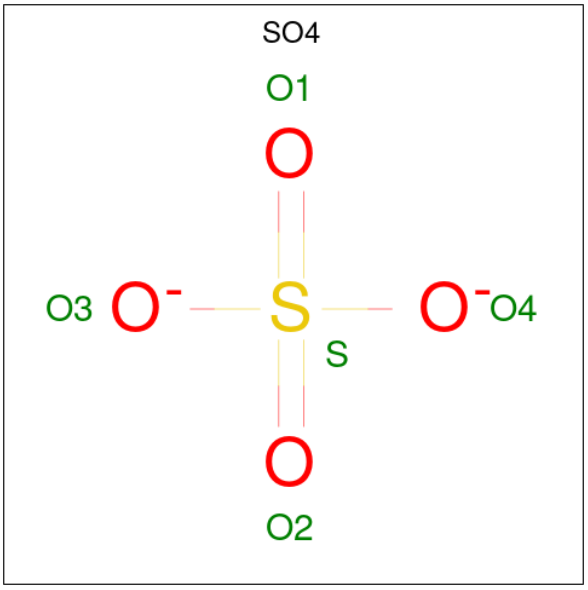
- Molecule 1 is a protein called UROKINASE.

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:

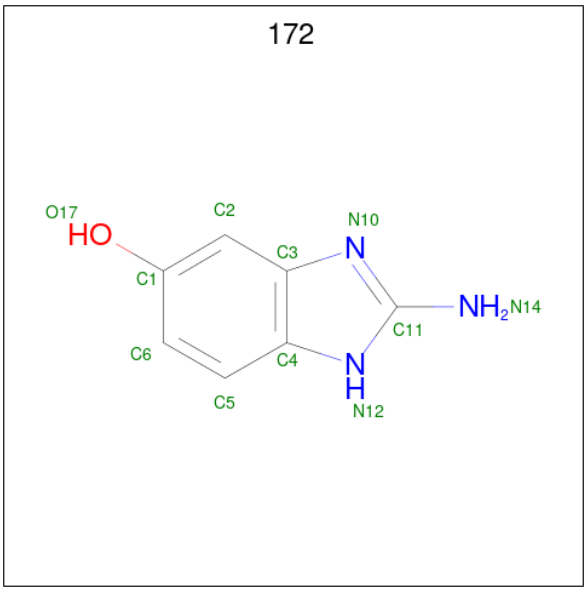
Chain	Residue	Modelled	Actual	Comment	Reference
A	120	ALA	CYS	CONFLICT	UNP P00749

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



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 (three-letter code: 172) (formula: $C_7H_7N_3O$).



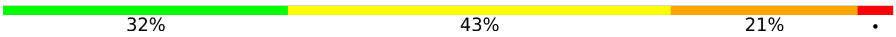
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
3	A	1	11	7	3	1	0	0

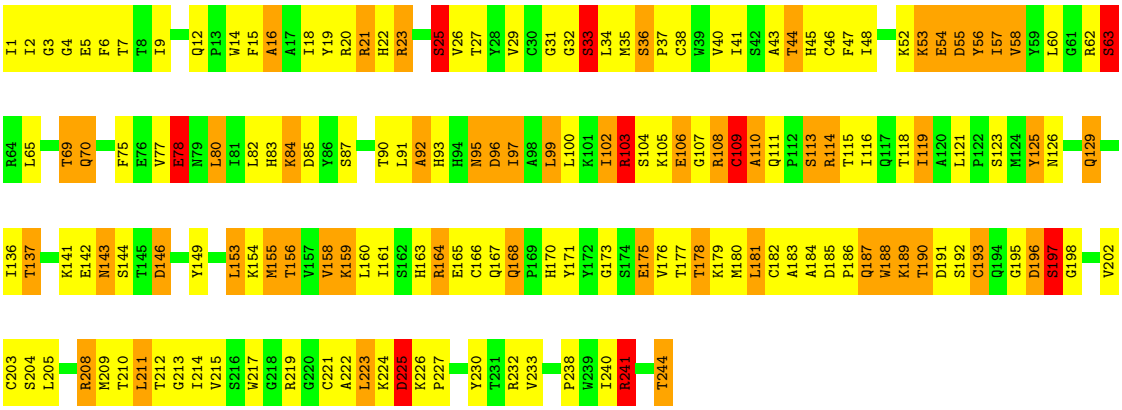
3 Residue-property plots (i)

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. 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

Chain A: 



4 Data and refinement statistics (i)

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 (i)

5.1 Standard geometry (i)

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

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	1.20	8/1982 (0.4%)	1.69	57/2684 (2.1%)

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 (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	33	SER	CB-OG	6.73	1.50	1.42
1	A	197	SER	CB-OG	-6.67	1.33	1.42
1	A	241	ARG	NE-CZ	6.61	1.41	1.33
1	A	78	GLU	CG-CD	6.08	1.61	1.51
1	A	5	GLU	CG-CD	5.14	1.59	1.51
1	A	106	GLU	CG-CD	5.12	1.59	1.51
1	A	219	ARG	NE-CZ	5.08	1.39	1.33
1	A	175	GLU	CG-CD	5.00	1.59	1.51

All (57) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	91	LEU	CA-CB-CG	12.51	144.07	115.30
1	A	62	ARG	NE-CZ-NH2	-11.74	114.43	120.30
1	A	96	ASP	CB-CG-OD1	11.44	128.59	118.30
1	A	225	ASP	CB-CG-OD2	-11.28	108.14	118.30
1	A	208	ARG	NE-CZ-NH2	-10.72	114.94	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	225	ASP	CB-CG-OD1	10.70	127.93	118.30
1	A	208	ARG	NE-CZ-NH1	10.50	125.55	120.30
1	A	96	ASP	CB-CG-OD2	-10.45	108.90	118.30
1	A	62	ARG	NE-CZ-NH1	9.88	125.24	120.30
1	A	219	ARG	NE-CZ-NH2	-9.77	115.41	120.30
1	A	241	ARG	NE-CZ-NH1	9.76	125.18	120.30
1	A	196	ASP	CB-CG-OD1	-8.98	110.22	118.30
1	A	63	SER	CA-CB-OG	8.94	135.34	111.20
1	A	219	ARG	NE-CZ-NH1	8.61	124.60	120.30
1	A	46	CYS	CA-CB-SG	8.59	129.47	114.00
1	A	196	ASP	CA-CB-CG	8.50	132.11	113.40
1	A	241	ARG	NE-CZ-NH2	-7.92	116.34	120.30
1	A	21	ARG	NE-CZ-NH1	7.85	124.23	120.30
1	A	114	ARG	NE-CZ-NH1	7.64	124.12	120.30
1	A	21	ARG	NE-CZ-NH2	-7.60	116.50	120.30
1	A	55	ASP	CA-CB-CG	7.53	129.97	113.40
1	A	23	ARG	NE-CZ-NH2	-7.53	116.54	120.30
1	A	180	MET	N-CA-C	-7.26	91.39	111.00
1	A	91	LEU	CB-CG-CD1	-7.16	98.83	111.00
1	A	114	ARG	NE-CZ-NH2	-6.93	116.83	120.30
1	A	187	GLN	N-CA-C	6.63	128.90	111.00
1	A	91	LEU	CB-CG-CD2	6.61	122.24	111.00
1	A	189	LYS	N-CA-C	6.53	128.64	111.00
1	A	143	ASN	CA-CB-CG	6.50	127.70	113.40
1	A	70	GLN	N-CA-C	6.44	128.38	111.00
1	A	181	LEU	CA-CB-CG	6.33	129.87	115.30
1	A	23	ARG	NE-CZ-NH1	6.19	123.39	120.30
1	A	109	CYS	CA-CB-SG	-6.17	102.89	114.00
1	A	92	ALA	N-CA-C	6.15	127.60	111.00
1	A	113	SER	C-N-CA	6.10	136.94	121.70
1	A	36	SER	N-CA-C	-6.02	94.75	111.00
1	A	99	LEU	CB-CG-CD1	-5.99	100.82	111.00
1	A	208	ARG	CD-NE-CZ	5.98	131.97	123.60
1	A	105	LYS	C-N-CA	5.94	136.55	121.70
1	A	25	SER	CA-CB-OG	-5.76	95.66	111.20
1	A	80	LEU	CA-CB-CG	5.67	128.35	115.30
1	A	110	ALA	N-CA-C	5.62	126.17	111.00
1	A	108	ARG	CG-CD-NE	-5.60	100.03	111.80
1	A	164	ARG	NE-CZ-NH2	-5.55	117.52	120.30
1	A	57	ILE	N-CA-C	-5.53	96.08	111.00
1	A	146	ASP	CB-CG-OD1	-5.47	113.38	118.30
1	A	223	LEU	CB-CG-CD1	-5.46	101.72	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	170	HIS	C-N-CA	5.39	135.19	121.70
1	A	54	GLU	N-CA-C	5.39	125.56	111.00
1	A	193	CYS	CA-CB-SG	-5.37	104.34	114.00
1	A	20	ARG	CG-CD-NE	-5.35	100.57	111.80
1	A	168	GLN	N-CA-C	-5.31	96.66	111.00
1	A	153	LEU	CB-CG-CD2	-5.22	102.13	111.00
1	A	87	SER	CA-CB-OG	5.18	125.19	111.20
1	A	16	ALA	CB-CA-C	-5.14	102.39	110.10
1	A	78	GLU	OE1-CD-OE2	-5.12	117.16	123.30
1	A	97	ILE	CG1-CB-CG2	-5.04	100.32	111.40

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 (i)

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	128	0
2	A	5	0	0	0	0
3	A	11	0	6	1	0
All	All	1949	0	1887	128	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 33.

All (128) 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:103:ARG:HD3	1:A:107:GLY:HA2	1.71	0.72
1:A:37:PRO:C	1:A:109:CYS:HB3	2.09	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: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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:52:LYS:HB3	1:A:52:LYS:HZ3	1.77	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:142:GLU:HG2	1:A:154:LYS:HZ3	1.78	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:52:LYS:O	1:A:53:LYS:C	2.52	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:171:TYR:HA	1:A:226:LYS:HZ3	1.82	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
1:A:119:ILE:HA	1:A:208:ARG:HH22	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1:ILE:O	1:A:142:GLU:HA	2.17	0.45
1:A:53:LYS:HG3	1:A:54:GLU:N	2.32	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:190:THR:O	1:A:191:ASP:HB2	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:163:HIS:CD2	1:A:167:GLN:HG3	2.54	0.43
1:A:14:TRP:CZ3	1:A:119:ILE:HG23	2.54	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: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
1:A:104:SER:OG	1:A:106:GLU:HB2	2.19	0.42
1:A:129:GLN:O	1:A:129:GLN:HG2	2.20	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:142:GLU:HG2	1:A:154:LYS:HZ2	1.85	0.41
1:A:149:TYR:CZ	1:A:195:GLY:HA3	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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 (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	243/245 (99%)	190 (78%)	40 (16%)	13 (5%)	2 11

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
1	A	225	ASP
1	A	109	CYS
1	A	116	ILE
1	A	238	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	213/213 (100%)	166 (78%)	47 (22%)	1 4

All (47) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	PHE
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	58	VAL
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	99	LEU
1	A	102	ILE
1	A	103	ARG
1	A	108	ARG
1	A	114	ARG
1	A	115	THR
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	155	MET
1	A	156	THR

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Mol	Chain	Res	Type
1	A	158	VAL
1	A	159	LYS
1	A	164	ARG
1	A	178	THR
1	A	179	LYS
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	210	THR
1	A	241	ARG
1	A	244	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	22	HIS
1	A	79	ASN
1	A	94	HIS
1	A	95	ASN
1	A	111	GLN
1	A	243	HIS

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 monosaccharides in this entry.

5.6 Ligand geometry (i)

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	3.14	6 (50%)	10,17,17	2.96	6 (60%)
2	SO4	A	245	-	4,4,4	0.38	0	6,6,6	0.75	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 (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	246	172	C11-N12	5.61	1.42	1.34
3	A	246	172	C4-C3	-4.78	1.26	1.42
3	A	246	172	C11-N10	4.57	1.41	1.34
3	A	246	172	C2-C3	-4.22	1.35	1.41
3	A	246	172	C5-C4	-3.87	1.35	1.41
3	A	246	172	C5-C6	2.09	1.41	1.36

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	246	172	C11-N10-C3	-5.22	99.51	106.73
3	A	246	172	C11-N12-C4	-4.75	100.16	106.73
3	A	246	172	C2-C3-N10	-3.48	120.87	130.83
3	A	246	172	C6-C5-C4	-3.38	116.58	120.84
3	A	246	172	C5-C4-N12	-2.54	123.41	130.78
3	A	246	172	C1-C2-C3	-2.22	116.94	119.29

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 (i)

6.1 Protein, DNA and RNA chains (i)

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates (i)

EDS was not executed - this section is therefore empty.

6.4 Ligands (i)

EDS was not executed - this section is therefore empty.

6.5 Other polymers (i)

EDS was not executed - this section is therefore empty.