



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 23, 2018 – 07:57 PM EST

PDB ID : 1D7K
Title : CRYSTAL STRUCTURE OF HUMAN ORNITHINE DECARBOXYLASE
AT 2.1 ANGSTROMS RESOLUTION
Authors : Almrud, J.J.; Oliveira, M.A.; Kern, A.D.; Grishin, N.V.; Phillips, M.A.; Hackert, M.L.
Deposited on : 1999-10-18
Resolution : 2.10 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

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity	:	4.02b-467
Mogul	:	1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20030736

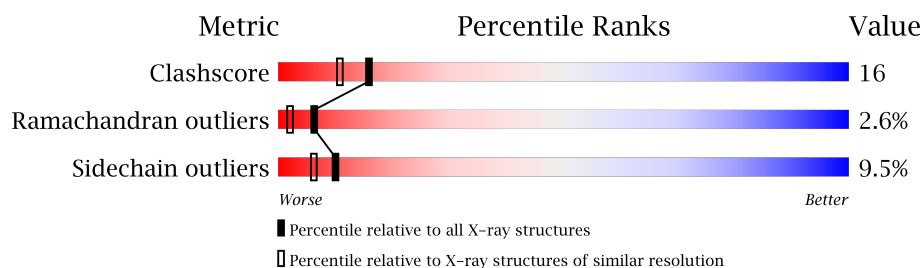
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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	112137	4788 (2.10-2.10)
Ramachandran outliers	110173	4740 (2.10-2.10)
Sidechain outliers	110143	4741 (2.10-2.10)

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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	421	
1	B	421	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 6824 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 HUMAN ORNITHINE DECARBOXYLASE.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	412	Total	C	N	O	P	S	0	0	0
			3242	2073	537	610	1	21			
1	B	407	Total	C	N	O	P	S	0	0	0
			3181	2037	531	591	1	21			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	349	ARG	LYS	CONFLICT	UNP P11926
A	415	GLN	GLU	CONFLICT	UNP P11926
B	349	ARG	LYS	CONFLICT	UNP P11926
B	415	GLN	GLU	CONFLICT	UNP P11926

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	219	Total	O	0	0
			219	219		
2	B	182	Total	O	0	0
			182	182		

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	61.68 Å 107.45 Å 139.71 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.50 – 2.10	Depositor
% Data completeness (in resolution range)	(Not available) (30.50-2.10)	Depositor
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	REFMAC	Depositor
R, R_{free}	0.212 , 0.288	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	6824	wwPDB-VP
Average B, all atoms (Å ²)	26.0	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: LLP

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	0.80	0/3291	1.78	57/4458 (1.3%)
1	B	0.78	0/3226	1.84	76/4367 (1.7%)
All	All	0.79	0/6517	1.81	133/8825 (1.5%)

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	24
1	B	0	15
All	All	0	39

There are no bond length outliers.

All (133) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	61	ARG	CD-NE-CZ	34.11	171.35	123.60
1	B	35	ASP	CB-CG-OD1	17.21	133.79	118.30
1	A	61	ARG	NE-CZ-NH1	16.90	128.75	120.30
1	B	61	ARG	NE-CZ-NH1	13.85	127.23	120.30
1	A	425	PHE	CB-CG-CD1	13.07	129.95	120.80
1	A	144	ARG	NE-CZ-NH1	13.06	126.83	120.30
1	B	107	ARG	NE-CZ-NH2	-12.45	114.08	120.30
1	A	365	ARG	CD-NE-CZ	12.03	140.44	123.60
1	B	47	ASP	CB-CG-OD2	11.17	128.36	118.30
1	A	144	ARG	CD-NE-CZ	11.16	139.22	123.60
1	A	54	ARG	NE-CZ-NH1	-11.12	114.74	120.30
1	B	107	ARG	NE-CZ-NH1	10.58	125.59	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	61	ARG	CD-NE-CZ	10.40	138.16	123.60
1	A	202	CYS	CA-CB-SG	10.08	132.14	114.00
1	B	320	ASP	CB-CG-OD1	10.02	127.31	118.30
1	A	61	ARG	NE-CZ-NH2	-10.00	115.30	120.30
1	A	140	MET	CA-CB-CG	9.86	130.06	113.30
1	B	165	ARG	CD-NE-CZ	9.85	137.39	123.60
1	A	47	ASP	CB-CG-OD2	9.72	127.05	118.30
1	B	365	ARG	NE-CZ-NH1	-9.29	115.65	120.30
1	A	277	ARG	NE-CZ-NH2	8.68	124.64	120.30
1	A	10	ASP	CB-CG-OD2	8.68	126.11	118.30
1	B	175	ARG	CD-NE-CZ	8.60	135.64	123.60
1	A	154	ARG	NE-CZ-NH2	-8.51	116.04	120.30
1	A	299	GLU	CA-CB-CG	8.51	132.12	113.40
1	B	28	ILE	CA-CB-CG2	8.50	127.91	110.90
1	A	132	THR	N-CA-CB	-8.41	94.31	110.30
1	B	381	MET	CA-CB-CG	8.39	127.57	113.30
1	B	16	GLU	CA-C-N	8.13	132.46	116.20
1	B	54	ARG	NE-CZ-NH2	8.11	124.35	120.30
1	A	216	ARG	NE-CZ-NH1	8.06	124.33	120.30
1	B	110	TYR	CB-CG-CD1	8.00	125.80	121.00
1	A	88	ASP	CB-CG-OD1	7.90	125.41	118.30
1	B	10	ASP	CA-CB-CG	7.80	130.57	113.40
1	B	38	ASP	CB-CG-OD1	7.80	125.32	118.30
1	B	88	ASP	CB-CG-OD2	7.75	125.27	118.30
1	A	17	GLY	C-N-CA	7.63	140.76	121.70
1	A	233	ASP	CB-CG-OD2	-7.60	111.46	118.30
1	B	384	GLU	OE1-CD-OE2	-7.53	114.26	123.30
1	B	369	ARG	NE-CZ-NH2	-7.53	116.53	120.30
1	B	220	ASP	CB-CG-OD1	7.20	124.78	118.30
1	B	365	ARG	NH1-CZ-NH2	7.16	127.27	119.40
1	A	371	ASP	CB-CG-OD2	7.14	124.72	118.30
1	A	110	TYR	CA-CB-CG	7.13	126.96	113.40
1	B	332	ASP	CB-CG-OD1	7.12	124.70	118.30
1	B	35	ASP	OD1-CG-OD2	-7.10	109.81	123.30
1	B	365	ARG	CD-NE-CZ	7.09	133.52	123.60
1	A	426	PRO	N-CA-C	7.08	130.52	112.10
1	A	143	ALA	O-C-N	-7.08	111.37	122.70
1	A	365	ARG	NE-CZ-NH1	7.02	123.81	120.30
1	A	277	ARG	NE-CZ-NH1	-6.96	116.82	120.30
1	B	35	ASP	N-CA-CB	6.94	123.10	110.60
1	B	360	CYS	CA-CB-SG	-6.93	101.52	114.00
1	A	132	THR	OG1-CB-CG2	6.92	125.91	110.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	270	ARG	NE-CZ-NH2	-6.86	116.87	120.30
1	A	425	PHE	CB-CG-CD2	-6.73	116.09	120.80
1	B	16	GLU	O-C-N	-6.69	111.83	123.20
1	A	421	GLN	N-CA-CB	6.62	122.52	110.60
1	A	381	MET	CA-CB-CG	6.59	124.51	113.30
1	B	347	ASP	CB-CA-C	6.52	123.43	110.40
1	B	365	ARG	NE-CZ-NH2	-6.47	117.06	120.30
1	B	27	LYS	CD-CE-NZ	6.47	126.58	111.70
1	A	154	ARG	NH1-CZ-NH2	6.46	126.50	119.40
1	B	134	ASP	CB-CG-OD2	-6.46	112.49	118.30
1	B	10	ASP	N-CA-CB	6.43	122.17	110.60
1	A	165	ARG	CG-CD-NE	6.42	125.29	111.80
1	B	34	SER	N-CA-C	6.39	128.26	111.00
1	B	183	ARG	NE-CZ-NH2	-6.33	117.13	120.30
1	B	368	GLU	OE1-CD-OE2	-6.31	115.73	123.30
1	B	277	ARG	NE-CZ-NH1	6.23	123.41	120.30
1	B	379	ASP	CB-CG-OD1	6.21	123.89	118.30
1	A	425	PHE	CG-CD2-CE2	6.13	127.55	120.80
1	A	221	MET	CA-CB-CG	6.12	123.71	113.30
1	A	208	PHE	CB-CG-CD1	6.09	125.06	120.80
1	B	349	ARG	N-CA-CB	-6.08	99.65	110.60
1	B	93	THR	O-C-N	-6.04	113.05	122.70
1	B	31	VAL	CA-C-O	6.00	132.71	120.10
1	B	154	ARG	NE-CZ-NH2	-6.00	117.30	120.30
1	B	346	PRO	O-C-N	-6.00	113.10	122.70
1	A	154	ARG	NE-CZ-NH1	-5.97	117.32	120.30
1	A	110	TYR	CB-CG-CD2	5.95	124.57	121.00
1	A	175	ARG	CD-NE-CZ	5.94	131.92	123.60
1	B	50	LYS	CA-CB-CG	5.93	126.45	113.40
1	B	347	ASP	CA-C-N	-5.93	104.15	117.20
1	A	54	ARG	NE-CZ-NH2	5.93	123.27	120.30
1	A	231	LEU	CA-CB-CG	-5.88	101.78	115.30
1	A	391	VAL	CG1-CB-CG2	-5.80	101.61	110.90
1	A	166	LEU	CA-CB-CG	5.75	128.52	115.30
1	B	35	ASP	CA-CB-CG	5.75	126.05	113.40
1	B	260	ASP	CB-CG-OD2	5.75	123.47	118.30
1	B	369	ARG	NH1-CZ-NH2	5.75	125.72	119.40
1	A	203	THR	CA-CB-CG2	5.74	120.44	112.40
1	B	347	ASP	CA-C-O	5.72	132.11	120.10
1	A	218	VAL	O-C-N	-5.71	113.57	122.70
1	B	116	GLN	CA-CB-CG	5.67	125.88	113.40
1	A	252	THR	CA-CB-CG2	-5.59	104.57	112.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	61	ARG	NE-CZ-NH2	-5.57	117.52	120.30
1	B	215	ALA	CB-CA-C	-5.56	101.75	110.10
1	B	110	TYR	CB-CG-CD2	-5.55	117.67	121.00
1	B	36	ASP	CA-C-O	5.53	131.72	120.10
1	B	311	GLU	CB-CA-C	-5.53	99.34	110.40
1	A	107	ARG	NE-CZ-NH2	5.52	123.06	120.30
1	B	33	SER	CA-C-N	5.49	129.28	117.20
1	B	401	GLN	O-C-N	-5.49	113.92	122.70
1	B	363	LEU	N-CA-CB	-5.45	99.50	110.40
1	A	320	ASP	CB-CG-OD1	5.45	123.21	118.30
1	A	318	VAL	O-C-N	-5.44	113.99	122.70
1	A	404	THR	O-C-N	-5.44	114.00	122.70
1	B	343	ARG	NE-CZ-NH1	5.43	123.02	120.30
1	A	88	ASP	OD1-CG-OD2	-5.40	113.04	123.30
1	B	310	SER	O-C-N	-5.39	114.07	122.70
1	B	72	ASP	CB-CG-OD2	5.38	123.14	118.30
1	B	339	LEU	CA-CB-CG	5.37	127.66	115.30
1	B	27	LYS	CG-CD-CE	5.37	128.01	111.90
1	B	35	ASP	CB-CA-C	5.36	121.11	110.40
1	A	216	ARG	CG-CD-NE	5.33	123.00	111.80
1	B	311	GLU	CA-CB-CG	5.33	125.12	113.40
1	B	371	ASP	CB-CG-OD1	5.27	123.04	118.30
1	A	133	PHE	O-C-N	5.19	131.01	122.70
1	B	41	TYR	CB-CG-CD2	-5.16	117.90	121.00
1	A	144	ARG	NH1-CZ-NH2	-5.15	113.73	119.40
1	B	50	LYS	CD-CE-NZ	5.15	123.54	111.70
1	B	112	ASN	N-CA-CB	-5.15	101.33	110.60
1	B	378	GLY	N-CA-C	5.15	125.97	113.10
1	B	228	SER	N-CA-CB	-5.14	102.79	110.50
1	B	369	ARG	NE-CZ-NH1	-5.14	117.73	120.30
1	B	270	ARG	NE-CZ-NH2	-5.10	117.75	120.30
1	A	16	GLU	CA-C-N	5.07	126.33	116.20
1	A	110	TYR	O-C-N	-5.06	114.61	122.70
1	B	323	TYR	CB-CG-CD1	5.02	124.01	121.00
1	A	339	LEU	CB-CA-C	-5.02	100.66	110.20
1	B	88	ASP	OD1-CG-OD2	-5.02	113.76	123.30
1	B	28	ILE	O-C-N	-5.02	114.67	122.70

There are no chirality outliers.

All (39) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	124	ALA	Mainchain
1	A	143	ALA	Mainchain
1	A	158	ASP	Peptide
1	A	16	GLU	Peptide
1	A	160	SER	Peptide
1	A	161	LYS	Peptide
1	A	165	ARG	Peptide
1	A	201	GLY	Peptide
1	A	208	PHE	Mainchain
1	A	26	GLN	Peptide
1	A	271	ILE	Mainchain
1	A	274	GLU	Mainchain
1	A	29	ASN	Mainchain
1	A	297	LEU	Peptide
1	A	342	LYS	Peptide
1	A	343	ARG	Peptide
1	A	35	ASP	Peptide
1	A	421	GLN	Peptide
1	A	422	ASN	Peptide
1	A	424	ASP	Peptide
1	A	425	PHE	Peptide
1	A	50	LYS	Mainchain
1	A	7	GLU	Peptide
1	A	99	GLN	Mainchain
1	B	101	LEU	Peptide
1	B	104	PRO	Mainchain
1	B	160	SER	Peptide
1	B	164	CYS	Peptide
1	B	165	ARG	Peptide
1	B	172	ALA	Peptide
1	B	241	SER	Mainchain
1	B	297	LEU	Peptide
1	B	320	ASP	Mainchain
1	B	34	SER	Peptide
1	B	341	GLN	Peptide
1	B	342	LYS	Peptide
1	B	346	PRO	Peptide
1	B	347	ASP	Peptide
1	B	417	MET	Peptide

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	3242	0	3185	104	0
1	B	3181	0	3133	112	0
2	A	219	0	0	9	0
2	B	182	0	0	10	0
All	All	6824	0	6318	208	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 16.

All (208) 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:426:PRO:CB	1:A:427:PRO:HD3	1.77	1.13
1:A:426:PRO:HB2	1:A:427:PRO:HD3	1.18	1.11
1:A:79:THR:HG23	1:A:417:MET:HE2	1.29	1.11
1:A:15:ASP:O	1:A:16:GLU:O	1.71	1.06
1:B:173:THR:HB	1:B:175:ARG:HD3	1.43	1.01
1:A:426:PRO:HB2	1:A:427:PRO:CD	1.97	0.95
1:A:217:CYS:HB2	2:A:612:HOH:O	1.72	0.90
1:A:343:ARG:O	1:A:344:PRO:O	1.90	0.89
1:A:84:GLY:HA2	1:A:422:ASN:ND2	1.91	0.85
1:B:410:SER:HB2	1:B:412:PRO:HD2	1.59	0.85
1:B:345:LYS:HB2	1:B:348:GLU:HG3	1.60	0.83
1:A:426:PRO:CB	1:A:427:PRO:CD	2.54	0.81
1:A:322:VAL:HB	1:A:330:LEU:HD11	1.67	0.77
1:A:35:ASP:HB2	1:A:37:LYS:HG3	1.67	0.77
1:B:341:GLN:HB3	2:B:506:HOH:O	1.85	0.76
1:A:282:SER:HA	1:A:385:ASN:HD22	1.50	0.76
1:B:218:VAL:HG22	1:B:221:MET:HE3	1.67	0.75
1:B:159:ASP:HB2	1:B:207:THR:HG21	1.68	0.75
1:B:173:THR:OG1	1:B:176:THR:HB	1.87	0.75
1:A:165:ARG:HD2	1:A:166:LEU:CD1	2.17	0.74
1:A:137:VAL:HA	1:A:140:MET:HG3	1.69	0.74
1:B:205:PRO:HB2	1:B:254:VAL:HG21	1.67	0.74
1:A:165:ARG:HD2	1:A:166:LEU:HD12	1.72	0.71

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:404:THR:HG22	2:B:445:HOH:O	1.91	0.71
1:A:202:CYS:HB3	2:A:561:HOH:O	1.90	0.70
1:B:298:LYS:HE2	1:B:313:THR:HG21	1.74	0.70
1:A:218:VAL:HA	1:A:221:MET:HE2	1.74	0.69
1:A:348:GLU:O	1:A:349:ARG:HB3	1.91	0.69
1:A:79:THR:HG23	1:A:417:MET:CE	2.16	0.69
1:B:345:LYS:HB3	1:B:346:PRO:HD2	1.74	0.69
1:B:82:ALA:HB1	1:B:421:GLN:HG3	1.75	0.68
1:A:218:VAL:HG22	1:A:221:MET:HE1	1.76	0.68
1:B:53:LEU:HD11	1:B:416:LEU:HD11	1.75	0.68
1:B:159:ASP:OD2	1:B:202:CYS:HA	1.94	0.67
1:A:165:ARG:HA	1:A:165:ARG:HH11	1.60	0.66
1:A:424:ASP:O	1:A:425:PHE:HB2	1.96	0.65
1:B:183:ARG:O	1:B:187:LEU:HG	1.98	0.64
1:B:24:LEU:HD12	1:B:40:PHE:CE1	2.32	0.64
1:A:163:VAL:HG22	1:A:164:CYS:H	1.62	0.64
1:B:117:VAL:HG22	1:B:141:LYS:HG2	1.78	0.64
1:A:175:ARG:H	1:A:175:ARG:HD2	1.64	0.62
1:A:372:LEU:HD13	1:A:375:MET:CE	2.28	0.62
1:B:298:LYS:HG2	1:B:313:THR:HG23	1.82	0.62
1:B:345:LYS:HB3	1:B:346:PRO:CD	2.29	0.62
1:A:148:LYS:HA	1:A:148:LYS:HE2	1.81	0.62
1:B:24:LEU:HD12	1:B:40:PHE:HE1	1.65	0.62
1:B:257:PRO:HA	1:B:260:ASP:HB2	1.81	0.61
1:A:165:ARG:HG2	1:B:368:GLU:OE2	2.00	0.61
1:A:165:ARG:HD3	1:A:166:LEU:N	2.15	0.61
1:A:175:ARG:H	1:A:175:ARG:CD	2.13	0.61
1:A:165:ARG:CG	1:A:166:LEU:H	2.14	0.60
1:A:404:THR:HG22	2:A:544:HOH:O	2.01	0.60
1:A:348:GLU:O	1:A:349:ARG:CB	2.48	0.60
1:B:130:MET:HA	1:B:150:LYS:O	2.03	0.59
1:B:185:LYS:HD3	1:B:227:PHE:CE2	2.38	0.58
1:B:82:ALA:O	1:B:421:GLN:HA	2.03	0.58
1:A:270:ARG:NH2	2:A:444:HOH:O	2.37	0.58
1:A:426:PRO:HB3	1:A:427:PRO:HD3	1.81	0.57
1:B:117:VAL:HG23	2:B:534:HOH:O	2.04	0.57
2:A:584:HOH:O	1:B:93:THR:HG23	2.05	0.57
1:A:15:ASP:O	1:A:16:GLU:C	2.42	0.57
1:A:165:ARG:CD	1:A:166:LEU:H	2.18	0.57
1:A:178:ARG:HH11	1:A:221:MET:HB3	1.70	0.56
1:A:411:GLY:N	1:A:412:PRO:CD	2.69	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:216:ARG:O	1:B:217:CYS:O	2.24	0.56
1:B:174:LEU:H	1:B:174:LEU:HD12	1.71	0.55
1:B:159:ASP:CB	1:B:207:THR:HG21	2.35	0.55
1:B:298:LYS:O	1:B:299:GLU:CB	2.53	0.55
1:B:344:PRO:HD3	2:B:442:HOH:O	2.06	0.55
1:B:33:SER:O	1:B:34:SER:CB	2.52	0.55
1:B:311:GLU:HG3	1:B:314:PHE:HZ	1.72	0.55
1:A:165:ARG:HG3	1:A:166:LEU:H	1.72	0.54
1:B:117:VAL:HG12	1:B:121:LYS:HE2	1.88	0.54
1:A:37:LYS:NZ	1:A:378:GLY:O	2.41	0.54
1:B:183:ARG:NH2	1:B:186:GLU:OE1	2.41	0.53
1:A:292:ALA:HB3	1:A:317:TYR:HB2	1.91	0.53
1:B:92:LYS:O	1:B:96:GLN:HG3	2.09	0.53
1:B:159:ASP:HB2	1:B:207:THR:CG2	2.38	0.53
1:B:259:LEU:HD22	1:B:271:ILE:HD13	1.90	0.53
1:A:353:SER:HB2	1:A:370:CYS:O	2.08	0.53
1:B:132:THR:HG21	2:B:542:HOH:O	2.09	0.53
1:B:128:VAL:O	1:B:146:HIS:HE1	1.91	0.53
1:B:29:ASN:O	1:B:32:SER:HB2	2.09	0.52
1:A:341:GLN:HE21	1:A:342:LYS:N	2.07	0.52
1:B:147:PRO:HD2	2:B:475:HOH:O	2.10	0.52
1:B:297:LEU:HD21	1:B:310:SER:O	2.10	0.52
1:A:84:GLY:HA2	1:A:422:ASN:HD22	1.70	0.52
1:B:69:LLP:H6	1:B:274:GLU:O	2.10	0.52
1:A:355:ILE:HD13	1:A:381:MET:SD	2.50	0.51
1:B:298:LYS:HG2	1:B:313:THR:CG2	2.40	0.51
1:A:132:THR:HG21	2:A:447:HOH:O	2.10	0.51
1:A:165:ARG:HD2	1:A:166:LEU:CG	2.41	0.51
1:A:93:THR:HG23	2:B:502:HOH:O	2.11	0.51
1:A:24:LEU:HD21	1:A:382:LEU:HD13	1.92	0.51
1:B:282:SER:HA	1:B:385:ASN:HD22	1.74	0.51
1:A:401:GLN:NE2	1:B:93:THR:HG21	2.25	0.51
1:B:33:SER:O	1:B:34:SER:HB2	2.10	0.51
1:A:421:GLN:O	1:A:423:PRO:HD2	2.11	0.51
1:B:251:ILE:O	1:B:254:VAL:HG22	2.11	0.51
1:A:295:ILE:HG12	1:A:314:PHE:CE1	2.46	0.51
1:B:216:ARG:O	1:B:217:CYS:C	2.48	0.51
1:B:121:LYS:HG2	1:B:145:ALA:HB1	1.93	0.50
1:B:196:PHE:CZ	1:B:234:ILE:HG22	2.47	0.50
1:B:175:ARG:CD	1:B:175:ARG:H	2.24	0.50
1:A:35:ASP:CB	1:A:37:LYS:HG3	2.40	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:205:PRO:HB2	1:A:254:VAL:HG21	1.94	0.50
1:A:340:LEU:HD11	1:A:375:MET:SD	2.52	0.50
1:B:173:THR:OG1	1:B:176:THR:N	2.44	0.49
1:B:83:THR:HG22	1:B:85:THR:HG23	1.94	0.49
1:A:166:LEU:HD11	1:B:368:GLU:HG2	1.94	0.49
1:A:218:VAL:HA	1:A:221:MET:CE	2.42	0.49
1:A:28:ILE:HD12	1:A:28:ILE:O	2.12	0.49
1:A:165:ARG:HD2	1:A:166:LEU:HG	1.94	0.48
1:A:366:ILE:HG22	1:A:367:VAL:HG23	1.94	0.48
1:A:298:LYS:HA	1:A:298:LYS:HE2	1.95	0.48
1:A:165:ARG:CD	1:A:166:LEU:N	2.75	0.48
1:A:243:ASP:OD2	1:A:337:LYS:HE3	2.13	0.48
1:A:35:ASP:O	1:A:36:ASP:HB2	2.14	0.48
1:B:246:LEU:HG	1:B:251:ILE:HD11	1.95	0.48
1:A:111:ALA:HA	1:A:132:THR:HB	1.96	0.48
1:A:294:LYS:HD2	1:A:315:MET:CE	2.43	0.48
1:B:163:VAL:O	1:B:164:CYS:C	2.52	0.48
1:A:342:LYS:HB2	2:A:559:HOH:O	2.14	0.47
1:A:93:THR:HG21	1:B:401:GLN:NE2	2.29	0.47
1:B:366:ILE:HG22	1:B:367:VAL:HG23	1.96	0.47
1:B:35:ASP:O	1:B:36:ASP:C	2.53	0.47
1:A:159:ASP:HB3	1:A:207:THR:HG21	1.97	0.47
1:A:21:LYS:HD2	2:A:464:HOH:O	2.14	0.47
1:B:175:ARG:HD2	1:B:175:ARG:H	1.78	0.47
1:A:165:ARG:CG	1:A:166:LEU:N	2.78	0.47
1:B:158:ASP:O	1:B:159:ASP:HB3	2.15	0.47
1:A:297:LEU:O	1:A:312:GLN:HB2	2.15	0.47
1:B:96:GLN:HG2	1:B:122:TYR:OH	2.13	0.47
1:B:165:ARG:HA	1:B:165:ARG:HD3	1.69	0.46
1:B:329:ILE:HG13	1:B:330:LEU:HD12	1.97	0.46
1:B:178:ARG:HA	1:B:178:ARG:HD2	1.73	0.46
1:B:214:ASP:O	1:B:217:CYS:HB3	2.14	0.46
1:A:166:LEU:CD1	1:B:368:GLU:HG2	2.46	0.46
1:B:297:LEU:HD23	1:B:297:LEU:HA	1.77	0.46
1:A:37:LYS:HD3	1:A:289:ASN:ND2	2.30	0.45
1:B:142:VAL:O	1:B:143:ALA:C	2.54	0.45
1:B:138:GLU:O	1:B:142:VAL:HG23	2.17	0.45
1:A:376:HIS:O	1:A:377:VAL:C	2.54	0.45
1:A:410:SER:HB2	1:A:412:PRO:HD2	1.99	0.45
1:A:16:GLU:O	1:A:18:PHE:N	2.35	0.45
1:A:41:TYR:CE1	1:A:286:LEU:HB2	2.52	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:248:PHE:O	1:B:252:THR:HG23	2.15	0.45
1:A:417:MET:O	1:A:421:GLN:N	2.49	0.45
1:A:37:LYS:HD3	1:A:289:ASN:HD21	1.82	0.45
1:A:21:LYS:HG3	2:A:585:HOH:O	2.16	0.44
1:A:425:PHE:CD2	1:A:425:PHE:C	2.91	0.44
1:A:373:PRO:O	1:A:374:GLU:C	2.55	0.44
1:B:294:LYS:HB2	1:B:315:MET:HB2	1.98	0.44
1:B:206:GLU:OE2	1:B:209:VAL:HG21	2.17	0.44
1:A:312:GLN:OE1	1:A:312:GLN:HA	2.16	0.44
1:A:165:ARG:HA	1:A:165:ARG:NH1	2.29	0.44
1:B:164:CYS:O	1:B:165:ARG:HB2	2.17	0.44
1:A:372:LEU:HD13	1:A:375:MET:HE1	1.98	0.44
1:A:351:TYR:N	1:A:372:LEU:O	2.47	0.43
1:B:166:LEU:O	1:B:167:SER:HB3	2.18	0.43
1:A:424:ASP:O	1:A:425:PHE:CB	2.65	0.43
1:A:25:ASP:O	1:A:26:GLN:C	2.55	0.43
1:B:204:ASP:HA	1:B:205:PRO:HD2	1.90	0.43
1:B:28:ILE:HD12	1:B:28:ILE:C	2.38	0.43
1:B:27:LYS:NZ	2:B:604:HOH:O	2.40	0.43
1:A:93:THR:HG21	1:B:401:GLN:HE21	1.82	0.43
1:B:343:ARG:HA	1:B:344:PRO:HD3	1.77	0.43
1:A:221:MET:HE2	1:A:221:MET:HB2	1.84	0.43
1:B:124:ALA:HB2	1:B:146:HIS:CG	2.54	0.43
1:B:157:THR:CG2	1:B:196:PHE:HB2	2.49	0.43
1:B:375:MET:HE1	1:B:381:MET:HE1	2.02	0.42
1:B:411:GLY:N	1:B:412:PRO:CD	2.82	0.42
1:B:83:THR:CG2	1:B:85:THR:HG23	2.49	0.42
1:B:104:PRO:O	1:B:105:PRO:C	2.58	0.42
1:B:183:ARG:O	1:B:186:GLU:HB2	2.20	0.42
1:A:421:GLN:HG3	1:A:422:ASN:H	1.84	0.42
1:B:220:ASP:O	1:B:223:ALA:HB3	2.20	0.42
1:A:346:PRO:O	1:A:347:ASP:HB3	2.19	0.42
1:B:122:TYR:O	1:B:126:ASN:ND2	2.37	0.42
1:B:195:SER:HB3	1:B:233:ASP:HB3	2.01	0.42
1:B:142:VAL:HG12	1:B:146:HIS:O	2.20	0.42
1:B:185:LYS:HA	1:B:185:LYS:HD2	1.90	0.42
1:B:381:MET:HG2	1:B:383:PHE:CE1	2.55	0.42
1:A:409:MET:HE1	1:A:417:MET:HE3	2.02	0.41
1:B:146:HIS:CG	1:B:149:ALA:HB2	2.55	0.41
1:A:36:ASP:HA	1:B:118:SER:HB3	2.02	0.41
1:B:195:SER:CB	1:B:233:ASP:HB3	2.50	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:176:THR:O	1:B:180:LEU:HG	2.21	0.41
1:B:222:GLY:O	1:B:225:VAL:HG22	2.20	0.41
1:B:254:VAL:O	1:B:257:PRO:HD2	2.20	0.41
1:A:148:LYS:CA	1:A:148:LYS:HE2	2.48	0.41
1:A:411:GLY:N	1:A:412:PRO:HD2	2.35	0.41
1:B:103:VAL:HG13	1:B:104:PRO:HD2	2.02	0.41
1:A:165:ARG:CD	1:B:368:GLU:OE2	2.68	0.41
1:B:46:GLY:HA3	2:B:435:HOH:O	2.21	0.41
1:A:165:ARG:CD	1:A:166:LEU:HG	2.50	0.41
1:A:261:LYS:HE2	1:A:262:TYR:CZ	2.55	0.41
1:A:372:LEU:HD13	1:A:375:MET:HE2	2.00	0.41
1:B:290:ILE:HD11	1:B:375:MET:HE3	2.03	0.41
1:B:53:LEU:CD1	1:B:416:LEU:HD11	2.49	0.41
1:B:164:CYS:O	1:B:165:ARG:NH1	2.54	0.41
1:B:24:LEU:HD13	1:B:42:VAL:CG2	2.51	0.41
1:B:113:PRO:HD3	2:B:542:HOH:O	2.21	0.41
1:A:153:LEU:HD23	1:A:153:LEU:C	2.42	0.40
1:A:345:LYS:O	1:A:348:GLU:HB2	2.21	0.40
1:B:222:GLY:O	1:B:227:PHE:HB2	2.21	0.40
1:B:166:LEU:O	1:B:167:SER:CB	2.70	0.40
1:A:49:LEU:HB3	1:A:416:LEU:HD23	2.03	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	407/421 (97%)	371 (91%)	23 (6%)	13 (3%)	5	1
1	B	402/421 (96%)	362 (90%)	32 (8%)	8 (2%)	9	4
All	All	809/842 (96%)	733 (91%)	55 (7%)	21 (3%)	6	2

All (21) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	16	GLU
1	A	160	SER
1	A	312	GLN
1	A	344	PRO
1	A	360	CYS
1	A	423	PRO
1	A	425	PHE
1	A	426	PRO
1	B	35	ASP
1	B	173	THR
1	A	299	GLU
1	B	36	ASP
1	B	269	VAL
1	B	299	GLU
1	B	419	GLN
1	A	34	SER
1	A	346	PRO
1	B	105	PRO
1	B	343	ARG
1	A	71	ASN
1	A	35	ASP

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	348/358 (97%)	315 (90%)	33 (10%)	10	6
1	B	337/358 (94%)	305 (90%)	32 (10%)	10	6
All	All	685/716 (96%)	620 (90%)	65 (10%)	10	6

All (65) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	GLU
1	A	16	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	31	VAL
1	A	36	ASP
1	A	50	LYS
1	A	53	LEU
1	A	93	THR
1	A	110	TYR
1	A	132	THR
1	A	140	MET
1	A	146	HIS
1	A	158	ASP
1	A	159	ASP
1	A	160	SER
1	A	165	ARG
1	A	166	LEU
1	A	167	SER
1	A	168	VAL
1	A	175	ARG
1	A	203	THR
1	A	265	SER
1	A	296	VAL
1	A	298	LYS
1	A	299	GLU
1	A	339	LEU
1	A	340	LEU
1	A	341	GLN
1	A	345	LYS
1	A	349	ARG
1	A	353	SER
1	A	369	ARG
1	A	398	ASN
1	A	426	PRO
1	B	10	ASP
1	B	16	GLU
1	B	27	LYS
1	B	28	ILE
1	B	31	VAL
1	B	32	SER
1	B	34	SER
1	B	49	LEU
1	B	50	LYS
1	B	74	LYS
1	B	83	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	93	THR
1	B	99	GLN
1	B	105	PRO
1	B	125	ASN
1	B	132	THR
1	B	140	MET
1	B	165	ARG
1	B	175	ARG
1	B	192	VAL
1	B	203	THR
1	B	225	VAL
1	B	266	ASP
1	B	339	LEU
1	B	343	ARG
1	B	349	ARG
1	B	363	LEU
1	B	398	ASN
1	B	404	THR
1	B	414	TRP
1	B	420	PHE
1	B	421	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	96	GLN
1	A	125	ASN
1	A	385	ASN
1	A	422	ASN
1	B	125	ASN
1	B	146	HIS
1	B	188	ASN
1	B	385	ASN
1	B	419	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

2 non-standard protein/DNA/RNA residues 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
1	LLP	A	69	1	24,24,25	1.38	4 (16%)	28,32,34	2.66	11 (39%)
1	LLP	B	69	1	24,24,25	1.15	2 (8%)	28,32,34	2.70	14 (50%)

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
1	LLP	A	69	1	-	0/15/17/19	0/1/1/1
1	LLP	B	69	1	-	0/15/17/19	0/1/1/1

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	69	LLP	P-OP3	-2.27	1.45	1.54
1	B	69	LLP	P-OP3	-2.16	1.45	1.54
1	B	69	LLP	C5'-C5	2.02	1.56	1.50
1	A	69	LLP	C3-C2	2.22	1.42	1.40
1	A	69	LLP	C2'-C2	2.26	1.54	1.50
1	A	69	LLP	CA-C	3.66	1.55	1.50

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	69	LLP	CB-CA-C	-7.49	99.30	111.65
1	A	69	LLP	CB-CA-C	-6.11	101.59	111.65
1	B	69	LLP	C3-C2-N1	-4.00	115.49	120.75
1	A	69	LLP	O-C-CA	-3.94	114.13	125.02
1	B	69	LLP	C5'-C5-C4	-3.74	115.12	121.66

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	69	LLP	C5'-C5-C4	-3.48	115.58	121.66
1	A	69	LLP	OP3-P-OP4	-3.34	97.84	106.73
1	A	69	LLP	C5-C6-N1	-3.22	118.42	123.87
1	B	69	LLP	C5-C6-N1	-3.12	118.59	123.87
1	B	69	LLP	O-C-CA	-2.54	118.00	125.02
1	B	69	LLP	C3-C4-C5	-2.47	116.36	118.24
1	A	69	LLP	OP3-P-OP1	2.01	118.36	110.50
1	A	69	LLP	O3-C3-C4	2.12	125.41	119.59
1	B	69	LLP	C5'-C5-C6	2.35	123.37	119.33
1	B	69	LLP	CG-CD-CE	2.47	123.09	113.59
1	B	69	LLP	OP3-P-OP1	2.60	120.69	110.50
1	A	69	LLP	C5'-C5-C6	2.70	123.97	119.33
1	B	69	LLP	C2'-C2-C3	2.79	124.30	120.96
1	A	69	LLP	C6-N1-C2	2.93	124.90	119.26
1	A	69	LLP	CD-CE-NZ	2.98	117.47	110.88
1	B	69	LLP	C6-N1-C2	3.39	125.79	119.26
1	B	69	LLP	C4-C3-C2	3.41	122.25	120.15
1	B	69	LLP	CD-CE-NZ	3.94	119.59	110.88
1	B	69	LLP	CE-NZ-C4'	3.95	130.50	119.03
1	A	69	LLP	CE-NZ-C4'	7.62	141.17	119.03

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
1	B	69	LLP	1	0

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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.