



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 7, 2026 – 11:15 PM UTC

PDB ID : 1EJW / pdb_00001ejw
Title : CRYSTAL STRUCTURE OF WILD-TYPE KLEBSIELLA AEROGENES
UREASE AT 298K
Authors : Pearson, M.A.; Karplus, P.A.
Deposited on : 2000-03-04
Resolution : 1.90 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
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

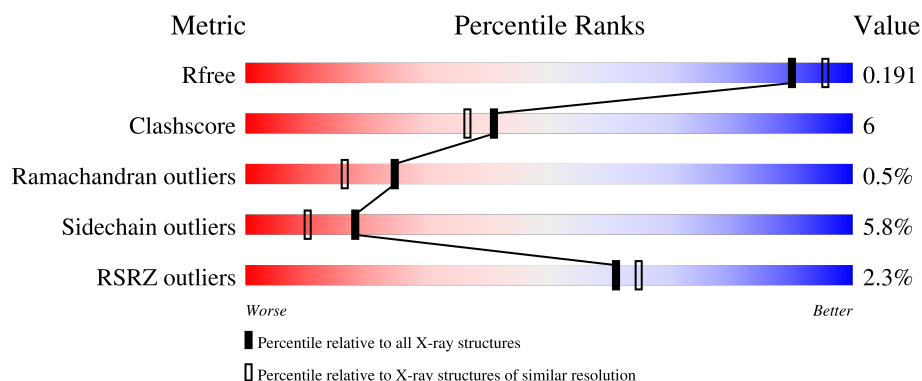
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 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	7789 (1.90-1.90)
Clashscore	190562	8410 (1.90-1.90)
Ramachandran outliers	187476	8333 (1.90-1.90)
Sidechain outliers	187428	8333 (1.90-1.90)
RSRZ outliers	180081	7790 (1.90-1.90)

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	C	567	3% 76% 19% • •
2	B	101	75% 19% 6%
3	A	100	84% 15% •

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 6198 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 UREASE ALPHA SUBUNIT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	C	566	Total	C	N	O	S	0	0	0
			4229	2652	741	813	23			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	1217	KCX	LYS	modified residue	UNP P18314

- Molecule 2 is a protein called UREASE BETA SUBUNIT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	101	Total	C	N	O	S	0	0	0
			785	496	150	136	3			

- Molecule 3 is a protein called UREASE GAMMA SUBUNIT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	A	100	Total	C	N	O	S	0	0	0
			776	491	134	146	5			

- Molecule 4 is NICKEL (II) ION (CCD ID: NI) (formula: Ni).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	C	2	Total	Ni	0	0
			2	2		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	C	307	Total	O	0	0
			307	307		

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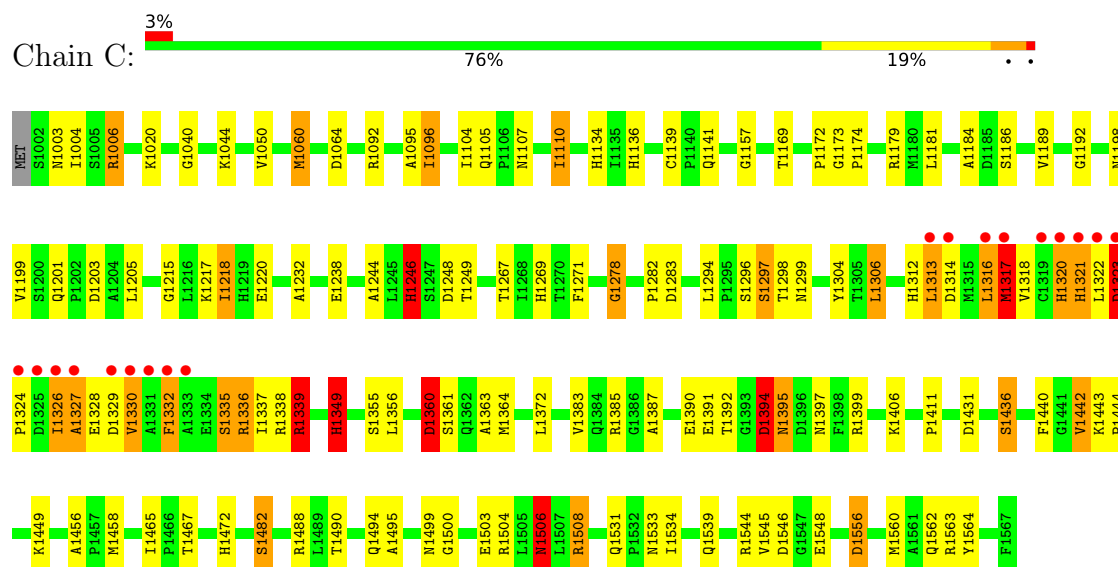
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	46	Total	O	0	0
			46	46		
5	A	53	Total	O	0	0
			53	53		

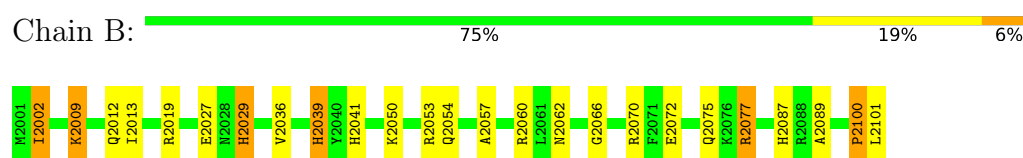
3 Residue-property plots

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.

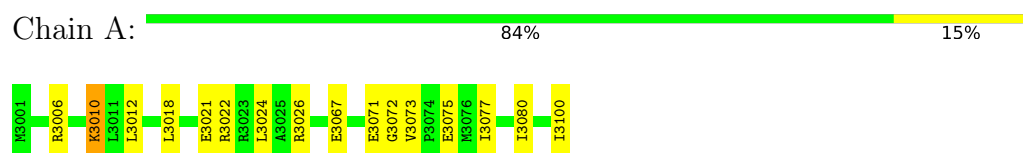
• Molecule 1: UREASE ALPHA SUBUNIT



• Molecule 2: UREASE BETA SUBUNIT



• Molecule 3: UREASE GAMMA SUBUNIT



4 Data and refinement statistics

Property	Value	Source
Space group	I 21 3	Depositor
Cell constants a, b, c, α , β , γ	170.80Å 170.80Å 170.80Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	10.00 – 1.90 10.00 – 1.90	Depositor EDS
% Data completeness (in resolution range)	(Not available) (10.00-1.90) 90.2 (10.00-1.90)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.24 (at 1.60Å)	Xtriage
Refinement program	TNT	Depositor
R, R_{free}	0.144 , 0.200 0.141 , 0.191	Depositor DCC
R_{free} test set	4676 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å ²)	16.6	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.26 , 78.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.019 for -l,-k,-h	Xtriage
F_o, F_c correlation	0.98	EDS
Total number of atoms	6198	wwPDB-VP
Average B, all atoms (Å ²)	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.50% 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: KCX, NI

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	C	1.46	15/4301 (0.3%)	1.79	75/5860 (1.3%)
2	B	1.39	2/805 (0.2%)	1.84	12/1087 (1.1%)
3	A	1.35	0/787	1.75	10/1061 (0.9%)
All	All	1.44	17/5893 (0.3%)	1.79	97/8008 (1.2%)

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	2070	ARG	NE-CZ	6.91	1.40	1.33
1	C	1215	GLY	CA-C	6.40	1.58	1.51
1	C	1337	ILE	CA-CB	6.09	1.61	1.53
1	C	1399	ARG	CA-C	5.86	1.60	1.52
1	C	1157	GLY	CA-C	5.82	1.57	1.51
2	B	2062	ASN	C-N	5.72	1.38	1.33
1	C	1169	THR	CA-CB	5.40	1.59	1.52
1	C	1472	HIS	CE1-NE2	5.40	1.38	1.32
1	C	1392	THR	C-O	5.24	1.30	1.23
1	C	1531	GLN	CA-C	5.23	1.59	1.52
1	C	1472	HIS	CD2-NE2	-5.20	1.32	1.37
1	C	1278	GLY	N-CA	5.20	1.50	1.45
1	C	1220	GLU	CA-C	5.19	1.59	1.52
1	C	1390	GLU	C-N	-5.17	1.26	1.33
1	C	1269	HIS	CA-CB	5.10	1.60	1.53
1	C	1339	ARG	NE-CZ	5.03	1.38	1.33
1	C	1488	ARG	NE-CZ	5.02	1.38	1.33

All (97) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	1312	HIS	N-CA-C	11.94	124.29	111.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	1320	HIS	N-CA-C	11.30	126.33	112.54
1	C	1004	ILE	N-CA-C	-11.26	92.32	108.42
1	C	1323	ASP	CA-C-N	10.35	130.01	119.56
1	C	1323	ASP	C-N-CA	10.35	130.01	119.56
1	C	1314	ASP	N-CA-C	9.72	123.10	111.82
3	A	3006	ARG	CD-NE-CZ	-9.50	111.11	124.40
1	C	1506	ASN	CA-CB-CG	-9.05	103.55	112.60
1	C	1283	ASP	N-CA-C	8.76	124.23	111.87
2	B	2029	HIS	CA-CB-CG	-8.48	105.32	113.80
1	C	1372	LEU	N-CA-CB	-8.40	97.82	110.01
1	C	1238	GLU	CB-CA-C	-8.39	96.58	110.85
1	C	1335	SER	N-CA-C	-7.81	103.88	113.41
1	C	1322	LEU	N-CA-C	7.68	121.75	109.24
2	B	2100	PRO	CA-C-N	7.67	135.50	121.70
2	B	2100	PRO	C-N-CA	7.67	135.50	121.70
1	C	1246	HIS	N-CA-C	-7.55	94.80	108.02
3	A	3024	LEU	N-CA-C	-7.42	103.19	111.28
1	C	1349	HIS	CA-CB-CG	-7.39	106.41	113.80
1	C	1336	ARG	N-CA-C	7.35	120.73	111.69
1	C	1490	THR	CA-CB-OG1	-7.30	98.64	109.60
1	C	1096	ILE	N-CA-C	-7.30	97.09	107.75
1	C	1392	THR	N-CA-C	-7.27	98.01	109.50
1	C	1136	HIS	CA-CB-CG	-7.22	106.58	113.80
1	C	1050	VAL	N-CA-C	7.18	118.83	111.00
1	C	1299	ASN	N-CA-C	7.11	125.52	109.81
1	C	1431	ASP	N-CA-C	-7.04	96.15	108.20
1	C	1181	LEU	N-CA-C	-7.04	103.68	111.36
1	C	1546	ASP	CA-CB-CG	7.00	119.60	112.60
1	C	1105	GLN	O-C-N	6.91	128.27	121.57
1	C	1385	ARG	CD-NE-CZ	6.77	133.88	124.40
1	C	1355	SER	N-CA-C	6.76	121.82	113.50
1	C	1456	ALA	N-CA-C	-6.67	102.22	108.22
1	C	1326	ILE	N-CA-CB	6.66	122.22	111.23
1	C	1172	PRO	CB-CA-C	-6.61	105.38	111.40
1	C	1297	SER	CB-CA-C	-6.60	97.30	109.37
2	B	2009	LYS	CB-CA-C	6.50	120.39	109.67
1	C	1394	ASP	N-CA-CB	6.48	118.44	110.53
2	B	2036	VAL	N-CA-C	6.44	117.19	108.17
1	C	1534	ILE	N-CA-C	6.40	117.13	108.17
1	C	1107	ASN	CB-CA-C	-6.27	101.60	111.51
2	B	2039	HIS	CA-CB-CG	-6.26	107.54	113.80
1	C	1092	ARG	NE-CZ-NH1	-6.22	115.28	121.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	1318	VAL	N-CA-C	6.19	117.68	110.62
1	C	1363	ALA	CA-C-N	6.13	133.25	121.54
1	C	1363	ALA	C-N-CA	6.13	133.25	121.54
1	C	1482	SER	N-CA-CB	-6.11	100.82	110.28
1	C	1192	GLY	N-CA-C	-6.08	101.60	110.90
1	C	1467	THR	N-CA-C	6.07	123.22	109.81
1	C	1361	SER	N-CA-C	6.05	118.97	109.96
2	B	2053	ARG	N-CA-C	6.03	117.86	111.28
1	C	1306	LEU	N-CA-C	6.03	117.85	111.28
1	C	1490	THR	N-CA-C	-5.96	99.47	109.07
1	C	1198	ASN	N-CA-C	5.90	119.08	108.17
1	C	1040	GLY	N-CA-C	-5.87	106.97	114.37
1	C	1436	SER	CA-CB-OG	-5.80	99.50	111.10
1	C	1006	ARG	NE-CZ-NH1	-5.78	115.72	121.50
1	C	1328	GLU	N-CA-C	-5.77	104.96	112.23
3	A	3010	LYS	N-CA-C	-5.75	105.15	111.82
3	A	3073	VAL	N-CA-CB	5.74	114.11	110.50
1	C	1482	SER	CA-CB-OG	-5.72	99.65	111.10
1	C	1186	SER	CB-CA-C	-5.70	99.74	110.01
1	C	1436	SER	N-CA-C	-5.69	102.90	110.07
1	C	1442	VAL	CB-CA-C	-5.69	106.88	111.71
1	C	1110	ILE	CA-C-O	5.64	127.51	119.95
3	A	3080	ILE	CA-CB-CG1	-5.58	100.92	110.40
1	C	1298	THR	N-CA-C	-5.56	101.80	110.42
3	A	3072	GLY	CA-C-N	-5.53	116.76	120.24
3	A	3072	GLY	C-N-CA	-5.53	116.76	120.24
2	B	2036	VAL	CA-CB-CG2	-5.41	101.21	110.40
3	A	3077	ILE	CA-C-O	5.40	127.19	119.95
3	A	3022	ARG	CA-CB-CG	-5.39	103.31	114.10
1	C	1562	GLN	N-CA-C	5.34	118.90	112.38
1	C	1323	ASP	CA-CB-CG	5.34	117.94	112.60
1	C	1564	TYR	N-CA-C	5.30	120.75	113.97
1	C	1494	GLN	OE1-CD-NE2	-5.27	117.33	122.60
1	C	1189	VAL	CA-C-O	-5.25	116.16	121.67
1	C	1321	HIS	CA-C-N	5.25	129.96	122.72
1	C	1321	HIS	C-N-CA	5.25	129.96	122.72
1	C	1387	ALA	N-CA-C	5.22	118.01	110.28
3	A	3026	ARG	CB-CA-C	-5.19	99.57	110.17
1	C	1184	ALA	O-C-N	-5.18	116.16	122.22
2	B	2041	HIS	CA-CB-CG	-5.18	108.62	113.80
1	C	1249	THR	CA-C-N	5.17	128.88	120.60
1	C	1249	THR	C-N-CA	5.17	128.88	120.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	1244	ALA	N-CA-C	-5.16	101.29	109.59
1	C	1092	ARG	CA-CB-CG	-5.14	103.82	114.10
1	C	1248	ASP	N-CA-CB	-5.14	101.80	110.49
2	B	2012	GLN	CB-CG-CD	-5.07	103.98	112.60
1	C	1391	GLU	N-CA-CB	-5.05	102.55	109.97
1	C	1360	ASP	N-CA-C	-5.04	100.06	110.80
2	B	2057	ALA	N-CA-C	5.04	117.47	109.96
1	C	1327	ALA	CB-CA-C	5.03	121.44	110.18
1	C	1458	MET	CA-C-O	-5.03	114.10	120.28
1	C	1060	MET	CG-SD-CE	5.02	111.94	100.90
2	B	2087	HIS	CB-CA-C	-5.02	99.97	109.95
1	C	1444	PRO	N-CA-C	5.01	119.19	111.57

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	4229	0	4176	60	0
2	B	785	0	772	13	0
3	A	776	0	804	5	0
4	C	2	0	0	0	0
5	A	53	0	0	0	0
5	B	46	0	0	2	0
5	C	307	0	0	1	0
All	All	6198	0	5752	75	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 6.

All (75) 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:C:1327:ALA:HA	1:C:1330:VAL:HG22	1.32	1.10

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1508:ARG:HG2	1:C:1508:ARG:HH11	1.25	1.01
1:C:1201:GLN:HE21	1:C:1203:ASP:H	1.12	0.90
1:C:1545:VAL:O	1:C:1548:GLU:HG2	1.81	0.80
1:C:1317:MET:HE1	1:C:1329:ASP:O	1.86	0.76
2:B:2072:GLU:H	2:B:2075:GLN:NE2	1.84	0.75
1:C:1324:PRO:HA	1:C:1330:VAL:CG1	2.18	0.73
2:B:2002:ILE:HD13	3:A:3075:GLU:HG2	1.70	0.73
2:B:2050:LYS:HB2	5:B:143:HOH:O	1.91	0.69
1:C:1323:ASP:HB2	1:C:1326:ILE:HD12	1.75	0.68
1:C:1218:ILE:HD11	1:C:1232:ALA:CB	2.24	0.68
1:C:1506:ASN:O	1:C:1508:ARG:HD2	1.94	0.68
1:C:1508:ARG:HG2	1:C:1508:ARG:NH1	2.03	0.67
1:C:1324:PRO:HA	1:C:1330:VAL:HG11	1.77	0.66
1:C:1304:TYR:OH	1:C:1339:ARG:HD3	1.97	0.64
1:C:1297:SER:OG	1:C:1349:HIS:HE1	1.81	0.63
1:C:1324:PRO:C	1:C:1330:VAL:HG11	2.25	0.62
1:C:1324:PRO:HA	1:C:1330:VAL:HG12	1.83	0.61
1:C:1327:ALA:HA	1:C:1330:VAL:CG2	2.19	0.60
1:C:1306:LEU:HG	1:C:1556:ASP:HA	1.84	0.60
1:C:1442:VAL:HG12	1:C:1443:LYS:HG3	1.84	0.59
1:C:1201:GLN:NE2	1:C:1203:ASP:H	1.92	0.59
1:C:1323:ASP:CB	1:C:1326:ILE:HD12	2.33	0.58
1:C:1323:ASP:O	1:C:1329:ASP:HB2	2.04	0.58
1:C:1316:LEU:HD11	1:C:1336:ARG:CZ	2.35	0.56
1:C:1324:PRO:CA	1:C:1330:VAL:HG11	2.37	0.55
2:B:2072:GLU:HA	2:B:2072:GLU:OE1	2.07	0.54
1:C:1563:ARG:NH1	3:A:3071:GLU:O	2.42	0.53
1:C:1356:LEU:HD21	1:C:1411:PRO:HA	1.90	0.53
1:C:1395:ASN:HD22	1:C:1397:ASN:H	1.57	0.52
1:C:1326:ILE:O	1:C:1330:VAL:HG13	2.08	0.52
1:C:1349:HIS:HD2	1:C:1406:LYS:NZ	2.07	0.52
2:B:2089:ALA:HA	2:B:2100:PRO:HA	1.92	0.51
2:B:2072:GLU:HB2	2:B:2075:GLN:HE21	1.74	0.51
1:C:1246:HIS:CE1	1:C:1278:GLY:HA3	2.45	0.51
2:B:2039:HIS:HA	2:B:2060:ARG:HD2	1.92	0.51
2:B:2027:GLU:HG2	2:B:2029:HIS:CE1	2.47	0.50
1:C:1500:GLY:HA2	1:C:1503:GLU:OE1	2.13	0.49
1:C:1320:HIS:HE1	5:C:501:HOH:O	1.96	0.49
1:C:1395:ASN:HD22	1:C:1395:ASN:C	2.20	0.49
1:C:1508:ARG:HH11	1:C:1508:ARG:CG	2.09	0.48
1:C:1060:MET:HB2	1:C:1064:ASP:HB2	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1201:GLN:O	1:C:1201:GLN:HG3	2.13	0.47
2:B:2054:GLN:HE21	2:B:2054:GLN:HB3	1.42	0.47
1:C:1267:THR:HG23	1:C:1294:LEU:HD21	1.96	0.47
1:C:1095:ALA:HB3	1:C:1110:ILE:HG12	1.97	0.46
1:C:1199:VAL:HG12	1:C:1205:LEU:HD21	1.97	0.46
1:C:1134:HIS:CD2	1:C:1360:ASP:HA	2.50	0.46
1:C:1313:LEU:HD23	1:C:1313:LEU:N	2.30	0.46
3:A:3012:LEU:C	3:A:3012:LEU:HD23	2.40	0.46
1:C:1296:SER:HB3	1:C:1356:LEU:HB2	1.99	0.45
1:C:1440:PHE:O	1:C:1560:MET:HE2	2.16	0.45
1:C:1556:ASP:OD1	1:C:1556:ASP:N	2.43	0.45
1:C:1313:LEU:N	1:C:1313:LEU:CD2	2.79	0.45
1:C:1313:LEU:H	1:C:1313:LEU:HG	1.22	0.45
1:C:1003:ASN:HA	2:B:2013:ILE:O	2.18	0.44
1:C:1326:ILE:O	1:C:1329:ASP:HB2	2.17	0.44
1:C:1020:LYS:HE3	1:C:1394:ASP:O	2.19	0.43
2:B:2027:GLU:HG2	2:B:2029:HIS:ND1	2.33	0.43
1:C:1395:ASN:ND2	1:C:1397:ASN:H	2.15	0.43
2:B:2066:GLY:HA2	5:B:223:HOH:O	2.17	0.43
1:C:1495:ALA:O	1:C:1499:ASN:ND2	2.53	0.42
1:C:1499:ASN:O	1:C:1504:ARG:NH2	2.51	0.42
3:A:3010:LYS:HD3	3:A:3010:LYS:HA	1.80	0.42
1:C:1006:ARG:HH11	1:C:1006:ARG:HD2	1.66	0.41
1:C:1173:GLY:HA2	1:C:1174:PRO:HD3	1.77	0.41
1:C:1332:PHE:O	1:C:1336:ARG:HB2	2.21	0.41
2:B:2077:ARG:HH21	2:B:2077:ARG:HD3	1.74	0.41
1:C:1335:SER:O	1:C:1338:ARG:NH1	2.49	0.41
1:C:1544:ARG:HA	1:C:1548:GLU:O	2.20	0.41
1:C:1134:HIS:CE1	1:C:1271:PHE:CD2	3.09	0.40
1:C:1246:HIS:CD2	1:C:1246:HIS:C	3.00	0.40
1:C:1323:ASP:HB3	1:C:1326:ILE:HB	2.03	0.40
1:C:1139:CYS:HB2	1:C:1141:GLN:OE1	2.22	0.40
3:A:3018:LEU:HA	3:A:3018:LEU:HD23	1.93	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	C	563/567 (99%)	528 (94%)	31 (6%)	4 (1%)	18	10
2	B	99/101 (98%)	95 (96%)	4 (4%)	0	100	100
3	A	98/100 (98%)	97 (99%)	1 (1%)	0	100	100
All	All	760/768 (99%)	720 (95%)	36 (5%)	4 (0%)	24	16

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	1321	HIS
1	C	1360	ASP
1	C	1364	MET
1	C	1317	MET

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	C	442/443 (100%)	415 (94%)	27 (6%)	17	9
2	B	78/78 (100%)	73 (94%)	5 (6%)	16	8
3	A	85/85 (100%)	82 (96%)	3 (4%)	32	24
All	All	605/606 (100%)	570 (94%)	35 (6%)	18	10

All (35) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	1044	LYS
1	C	1096	ILE
1	C	1104	ILE
1	C	1179	ARG
1	C	1218	ILE
1	C	1246	HIS
1	C	1282	PRO
1	C	1313	LEU
1	C	1316	LEU
1	C	1317	MET
1	C	1323	ASP
1	C	1330	VAL
1	C	1332	PHE
1	C	1339	ARG
1	C	1349	HIS
1	C	1383	VAL
1	C	1394	ASP
1	C	1395	ASN
1	C	1436	SER
1	C	1449	LYS
1	C	1465	ILE
1	C	1482	SER
1	C	1506	ASN
1	C	1508	ARG
1	C	1533	ASN
1	C	1539	GLN
1	C	1556	ASP
2	B	2002	ILE
2	B	2009	LYS
2	B	2019	ARG
2	B	2077	ARG
2	B	2101	LEU
3	A	3021	GLU
3	A	3067	GLU
3	A	3100	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	1142	GLN
1	C	1201	GLN
1	C	1349	HIS
1	C	1362	GLN

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Mol	Chain	Res	Type
1	C	1395	ASN
1	C	1469	GLN
2	B	2016	ASN
2	B	2054	GLN
2	B	2075	GLN
3	A	3081	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

1 non-standard protein/DNA/RNA residue is modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
1	KCX	C	1217	1,4	10,11,12	1.64	2 (20%)	6,12,14	2.13	1 (16%)

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	KCX	C	1217	1,4	-	0/9/10/12	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	1217	KCX	OQ1-CX	3.80	1.28	1.21
1	C	1217	KCX	CE-NZ	2.55	1.51	1.46

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	C	1217	KCX	OQ1-CX-NZ	-4.66	117.84	124.92

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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](#)

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	C	565/567 (99%)	-0.90	18 (3%) 50 54	10, 18, 58, 100	0
2	B	101/101 (100%)	-0.56	0 100 100	16, 28, 61, 72	0
3	A	100/100 (100%)	-1.04	0 100 100	12, 19, 50, 60	0
All	All	766/768 (99%)	-0.87	18 (2%) 61 65	10, 19, 59, 100	0

All (18) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	1330	VAL	4.8
1	C	1331	ALA	4.4
1	C	1327	ALA	4.3
1	C	1320	HIS	4.3
1	C	1313	LEU	4.1
1	C	1333	ALA	4.0
1	C	1321	HIS	4.0
1	C	1332	PHE	3.7
1	C	1329	ASP	3.6
1	C	1326	ILE	3.3
1	C	1322	LEU	3.0
1	C	1316	LEU	3.0
1	C	1324	PRO	2.8
1	C	1323	ASP	2.8
1	C	1319	CYS	2.6
1	C	1325	ASP	2.4
1	C	1314	ASP	2.2
1	C	1317	MET	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [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
1	KCX	C	1217	12/13	0.98	0.03	9,13,15,16	0

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	NI	C	4774	1/1	1.00	0.01	18,18,18,18	0
4	NI	C	4775	1/1	1.00	0.01	16,16,16,16	0

6.5 Other polymers [i](#)

There are no such residues in this entry.