



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 11:49 AM UTC

PDB ID : 1EJX / pdb_00001ejx
Title : CRYSTAL STRUCTURE OF WILD-TYPE KLEBSIELLA AEROGENES
UREASE AT 100K
Authors : Pearson, M.A.; Karplus, P.A.
Deposited on : 2000-03-04
Resolution : 1.60 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

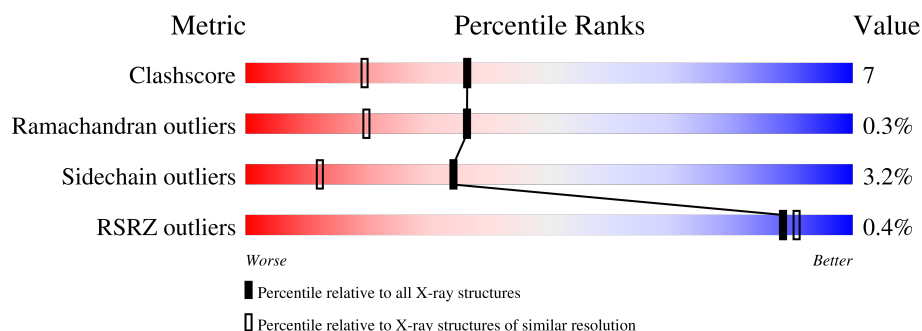
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.60 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	4931 (1.60-1.60)
Ramachandran outliers	187476	4831 (1.60-1.60)
Sidechain outliers	187428	4830 (1.60-1.60)
RSRZ outliers	180081	4672 (1.60-1.60)

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	
2	B	101	
3	A	100	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 6272 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	556	Total	C	N	O	S	0	5	0
			4161	2615	727	796	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	402	Total	O	0	0
			402	402		

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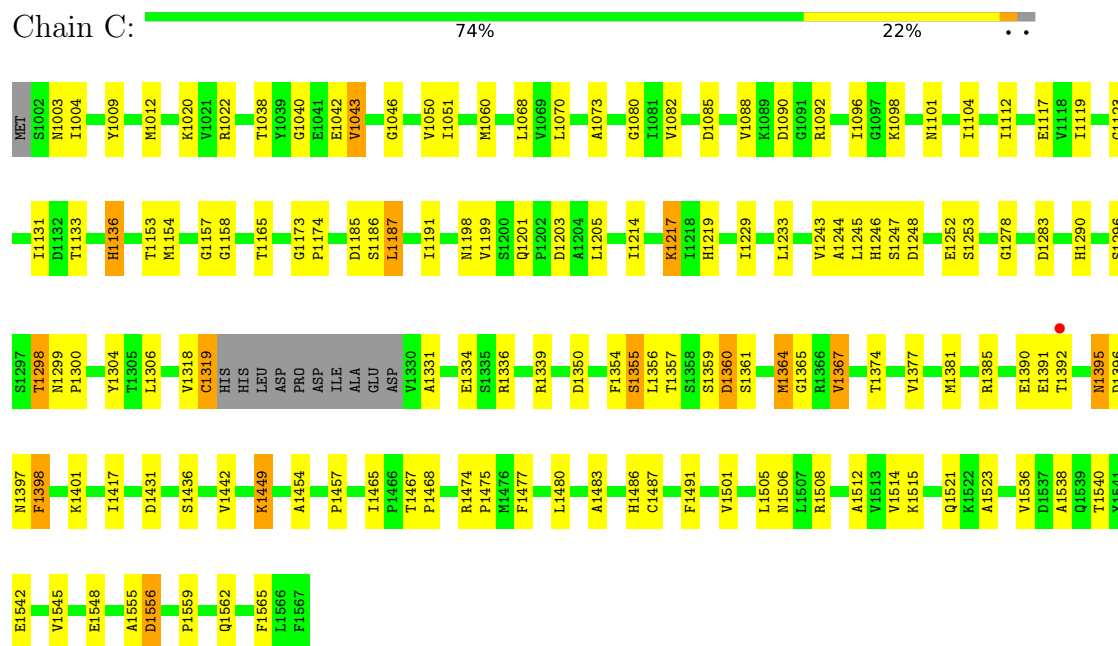
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	76	Total 76	O 76	0	0
5	A	70	Total 70	O 70	0	0

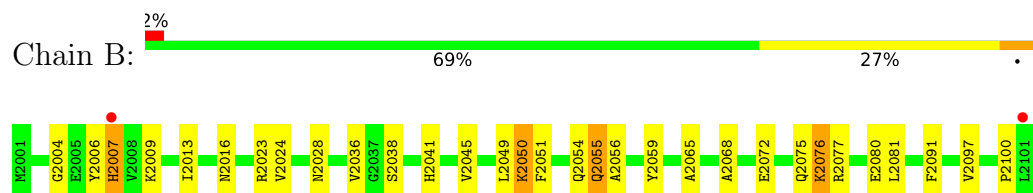
3 Residue-property plots

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.

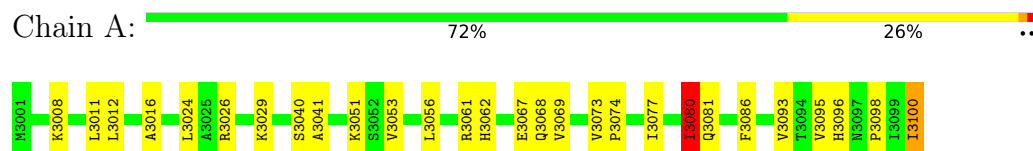
• Molecule 1: UREASE ALPHA SUBUNIT



• 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	168.96Å 168.96Å 168.96Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	10.00 – 1.60 10.00 – 1.60	Depositor EDS
% Data completeness (in resolution range)	(Not available) (10.00-1.60) 92.5 (10.00-1.60)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.19 (at 1.60Å)	Xtriage
Refinement program	TNT	Depositor
R, R_{free}	0.172 , 0.240 0.171 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	18.9	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 92.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.028 for -l,-k,-h	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	6272	wwPDB-VP
Average B, all atoms (Å ²)	24.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.07% 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: NI, KCX

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	1.39	11/4254 (0.3%)	1.72	68/5794 (1.2%)
2	B	1.31	1/805 (0.1%)	1.76	14/1087 (1.3%)
3	A	1.39	1/787 (0.1%)	1.74	16/1061 (1.5%)
All	All	1.38	13/5846 (0.2%)	1.73	98/7942 (1.2%)

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	1377	VAL	CA-C	6.80	1.61	1.52
1	C	1556	ASP	CA-C	6.15	1.60	1.52
1	C	1385	ARG	NE-CZ	5.44	1.39	1.33
1	C	1046	GLY	CA-C	5.42	1.58	1.52
1	C	1253	SER	C-N	5.38	1.38	1.32
1	C	1556	ASP	CB-CG	5.25	1.65	1.52
2	B	2097	VAL	CA-C	-5.24	1.46	1.52
1	C	1556	ASP	CA-CB	5.23	1.61	1.53
1	C	1157	GLY	CA-C	5.21	1.56	1.52
1	C	1474	ARG	NE-CZ	5.14	1.38	1.33
3	A	3074	PRO	C-O	5.07	1.30	1.24
1	C	1101	ASN	CA-C	5.07	1.58	1.52
1	C	1454	ALA	CA-C	5.06	1.59	1.52

All (98) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	1283	ASP	N-CA-C	10.28	126.14	112.88
1	C	1092	ARG	CD-NE-CZ	10.15	138.62	124.40
1	C	1556	ASP	N-CA-CB	-9.66	95.97	109.98
1	C	1555	ALA	CA-C-N	9.50	133.55	120.63
1	C	1555	ALA	C-N-CA	9.50	133.55	120.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	1556	ASP	CA-CB-CG	9.28	121.88	112.60
1	C	1092	ARG	NE-CZ-NH2	-8.94	111.15	119.20
1	C	1247	SER	N-CA-C	8.94	122.06	110.53
1	C	1136	HIS	CA-CB-CG	-8.90	104.90	113.80
1	C	1290	HIS	N-CA-C	8.74	121.08	110.07
3	A	3068	GLN	N-CA-CB	-8.66	97.92	110.56
1	C	1483	ALA	N-CA-C	-8.59	102.00	111.36
1	C	1556	ASP	CA-C-O	8.54	129.69	120.90
2	B	2100	PRO	CA-C-N	8.47	136.95	121.70
2	B	2100	PRO	C-N-CA	8.47	136.95	121.70
1	C	1004	ILE	N-CA-C	-8.46	97.18	108.35
1	C	1299	ASN	N-CA-C	8.30	128.16	109.81
1	C	1436	SER	N-CA-C	-8.17	99.36	109.65
1	C	1442	VAL	N-CA-C	7.61	118.06	111.90
2	B	2038	SER	N-CA-C	7.29	120.16	111.33
1	C	1119	ILE	N-CA-C	-7.29	97.90	108.11
1	C	1477	PHE	N-CA-C	7.14	119.92	111.71
3	A	3073	VAL	N-CA-CB	7.01	115.92	110.45
1	C	1486	HIS	CA-CB-CG	-7.00	106.80	113.80
3	A	3053	VAL	N-CA-C	-6.99	103.71	110.42
1	C	1538	ALA	N-CA-C	6.98	120.68	111.75
3	A	3062	HIS	CA-CB-CG	-6.96	106.84	113.80
1	C	1060	MET	N-CA-C	6.94	120.28	110.50
3	A	3067	GLU	N-CA-C	6.89	120.78	112.38
2	B	2007	HIS	CA-CB-CG	-6.85	106.95	113.80
1	C	1298	THR	N-CA-C	-6.85	100.66	110.59
2	B	2097	VAL	CA-C-N	-6.79	112.89	122.34
2	B	2097	VAL	C-N-CA	-6.79	112.89	122.34
3	A	3024	LEU	N-CA-C	-6.71	104.05	111.36
1	C	1398	PHE	CA-CB-CG	-6.57	107.23	113.80
1	C	1562	GLN	N-CA-C	6.54	120.36	112.38
1	C	1487	CYS	N-CA-C	6.45	121.30	113.17
3	A	3040	SER	CB-CA-C	6.40	121.73	110.85
3	A	3067	GLU	CB-CG-CD	6.39	123.46	112.60
3	A	3086	PHE	N-CA-C	-6.37	102.81	110.13
2	B	2041	HIS	CA-CB-CG	-6.33	107.47	113.80
2	B	2100	PRO	O-C-N	6.32	130.68	123.03
3	A	3080	ILE	N-CA-C	-6.30	99.07	108.46
1	C	1354	PHE	N-CA-C	-6.25	99.01	109.07
1	C	1085	ASP	N-CA-C	-6.25	100.39	110.32
1	C	1092	ARG	CG-CD-NE	-6.21	98.33	112.00
1	C	1244	ALA	N-CA-C	-6.20	99.60	109.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	1133	THR	CA-C-N	-6.07	114.90	123.03
1	C	1133	THR	C-N-CA	-6.07	114.90	123.03
1	C	1050	VAL	N-CA-C	6.06	116.84	110.72
1	C	1392	THR	N-CA-C	6.06	121.34	113.88
1	C	1357	THR	N-CA-C	-5.96	100.43	109.85
1	C	1012	MET	N-CA-C	5.94	118.99	111.69
1	C	1070	LEU	N-CA-C	-5.92	97.52	107.99
1	C	1198	ASN	N-CA-C	5.88	119.06	108.17
2	B	2056	ALA	N-CA-CB	-5.87	100.54	110.41
1	C	1123	GLY	N-CA-C	-5.83	107.28	115.32
1	C	1009	TYR	N-CA-C	-5.82	104.85	111.14
2	B	2065	ALA	CA-C-N	-5.77	114.26	123.31
2	B	2065	ALA	C-N-CA	-5.77	114.26	123.31
1	C	1457	PRO	N-CA-C	-5.75	102.15	111.19
1	C	1374	THR	N-CA-C	-5.75	105.01	111.28
1	C	1245	LEU	N-CA-C	5.73	118.23	108.90
1	C	1501	VAL	CB-CA-C	-5.72	104.42	112.14
1	C	1319	CYS	N-CA-CB	5.70	120.19	110.50
1	C	1248	ASP	CA-CB-CG	5.67	118.27	112.60
1	C	1480	LEU	N-CA-C	5.66	117.96	108.73
1	C	1092	ARG	CB-CG-CD	5.64	124.28	111.30
1	C	1117	GLU	N-CA-C	-5.59	102.24	110.52
1	C	1431	ASP	N-CA-C	-5.58	98.11	107.99
1	C	1545	VAL	N-CA-C	-5.58	99.51	107.77
1	C	1252	GLU	N-CA-C	5.52	116.97	111.07
1	C	1355	SER	N-CA-C	5.49	121.00	113.97
1	C	1367	VAL	N-CA-C	5.44	119.72	111.89
1	C	1396	ASP	CA-CB-CG	-5.44	107.16	112.60
3	A	3093	VAL	N-CA-C	-5.43	100.50	108.11
3	A	3041	ALA	N-CA-C	-5.41	105.46	111.36
2	B	2100	PRO	CA-C-O	-5.41	115.17	121.34
1	C	1336	ARG	N-CA-C	5.37	119.92	112.45
3	A	3073	VAL	O-C-N	5.37	123.86	120.42
1	C	1073	ALA	O-C-N	-5.29	116.99	122.96
1	C	1559	PRO	N-CA-C	-5.24	101.96	110.40
3	A	3026	ARG	N-CA-C	-5.23	106.87	113.20
1	C	1096	ILE	N-CA-C	-5.22	98.97	107.28
1	C	1092	ARG	NE-CZ-NH1	5.21	126.71	121.50
1	C	1038	THR	N-CA-C	-5.21	98.91	108.02
1	C	1185	ASP	CA-CB-CG	5.21	117.81	112.60
3	A	3016	ALA	N-CA-C	-5.18	105.63	111.28
1	C	1331	ALA	N-CA-C	-5.13	105.86	111.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	2006	TYR	CB-CA-C	-5.12	101.35	109.80
1	C	1565	PHE	N-CA-C	5.12	117.59	109.24
3	A	3095	VAL	CB-CA-C	-5.11	104.16	111.31
1	C	1306	LEU	N-CA-C	5.10	117.58	111.71
1	C	1480	LEU	CB-CA-C	-5.09	101.94	110.19
2	B	2091	PHE	CA-CB-CG	-5.07	108.73	113.80
1	C	1536	VAL	N-CA-C	-5.04	100.86	108.12
1	C	1334	GLU	N-CA-C	5.03	117.66	111.82
1	C	1318	VAL	N-CA-C	5.01	115.73	110.62

There are no chirality outliers.

There are no planarity outliers.

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	C	4161	0	4138	53	0
2	B	785	0	772	19	0
3	A	776	0	804	15	0
4	C	2	0	0	0	0
5	A	70	0	0	3	0
5	B	76	0	0	1	0
5	C	402	0	0	3	1
All	All	6272	0	5714	82	1

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 7.

All (82) 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:1043:VAL:HB	1:C:1051[B]:ILE:HD11	1.48	0.94
1:C:1131:ILE:HD13	1:C:1153:THR:HB	1.51	0.92
2:B:2072:GLU:H	2:B:2075:GLN:HE21	0.93	0.92
1:C:1201:GLN:HE21	1:C:1203:ASP:H	1.13	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:2072:GLU:H	2:B:2075:GLN:NE2	1.70	0.89
2:B:2072:GLU:N	2:B:2075:GLN:HE21	1.78	0.81
3:A:3061:ARG:HD3	3:A:3096:HIS:O	1.84	0.77
2:B:2050:LYS:HE2	5:B:558:HOH:O	1.86	0.75
3:A:3080:ILE:HD12	3:A:3098:PRO:HG3	1.70	0.73
1:C:1043:VAL:CB	1:C:1051[B]:ILE:HD11	2.19	0.72
1:C:1361[B]:SER:OG	1:C:1367:VAL:HB	1.89	0.72
2:B:2024:VAL:CG2	2:B:2055:GLN:HG2	2.20	0.71
3:A:3029:LYS:HE3	3:A:3069:VAL:O	1.90	0.71
3:A:3061:ARG:NH1	5:A:576:HOH:O	2.28	0.67
3:A:3012:LEU:C	3:A:3012:LEU:HD23	2.22	0.64
1:C:1090:ASP:HB3	5:C:516:HOH:O	1.99	0.62
3:A:3061:ARG:HD2	5:A:576:HOH:O	1.99	0.61
1:C:1043:VAL:CG1	1:C:1051[B]:ILE:HD11	2.30	0.61
1:C:1296:SER:HB3	1:C:1356:LEU:HB2	1.83	0.60
1:C:1199:VAL:HG12	1:C:1205:LEU:HD21	1.83	0.60
2:B:2076:LYS:HG2	2:B:2076:LYS:O	2.02	0.59
1:C:1304:TYR:OH	1:C:1339:ARG:HG2	2.04	0.58
1:C:1467:THR:OG1	3:A:3081:GLN:NE2	2.33	0.58
1:C:1131:ILE:HD13	1:C:1153:THR:CB	2.32	0.58
1:C:1395:ASN:HD22	1:C:1397:ASN:H	1.51	0.57
1:C:1022:ARG:O	2:B:2004:GLY:HA2	2.03	0.57
1:C:1390:GLU:HB2	1:C:1398:PHE:CD1	2.39	0.57
2:B:2024:VAL:HG21	2:B:2055:GLN:HG2	1.87	0.56
2:B:2024:VAL:HG22	2:B:2055:GLN:OE1	2.06	0.55
1:C:1475:PRO:HB2	5:C:411:HOH:O	2.06	0.55
1:C:1233[B]:LEU:HD12	1:C:1243:VAL:HG21	1.89	0.54
3:A:3008:LYS:O	3:A:3011:LEU:HB2	2.08	0.53
1:C:1003:ASN:HA	2:B:2013:ILE:O	2.08	0.52
1:C:1465:ILE:HG13	1:C:1468:PRO:HD3	1.90	0.52
1:C:1390:GLU:N	1:C:1390:GLU:OE1	2.40	0.52
1:C:1246:HIS:CE1	1:C:1278:GLY:HA3	2.46	0.50
3:A:3100:ILE:HD12	5:A:295:HOH:O	2.12	0.50
1:C:1540:THR:OG1	1:C:1542:GLU:HG3	2.12	0.50
1:C:1355:SER:C	1:C:1356:LEU:HD12	2.37	0.49
3:A:3077:ILE:HG21	3:A:3080:ILE:HD11	1.94	0.49
3:A:3100:ILE:HD12	3:A:3100:ILE:OXT	2.12	0.49
1:C:1080:GLY:HA2	1:C:1401:LYS:HE2	1.95	0.48
1:C:1300:PRO:HG3	1:C:1364:MET:O	2.14	0.48
2:B:2045:VAL:HG21	2:B:2049:LEU:HD12	1.95	0.47
1:C:1505:LEU:O	1:C:1506:ASN:ND2	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1020:LYS:HB2	2:B:2007:HIS:HB3	1.98	0.46
3:A:3051:LYS:HD3	3:A:3056:LEU:HD21	1.96	0.46
1:C:1515:LYS:HD3	5:C:264:HOH:O	2.16	0.45
1:C:1154:MET:O	1:C:1191:ILE:HA	2.16	0.45
1:C:1201:GLN:O	1:C:1201:GLN:HG3	2.17	0.45
1:C:1229:ILE:O	1:C:1233[B]:LEU:HD13	2.17	0.45
1:C:1521:GLN:HG3	1:C:1523:ALA:H	1.82	0.45
1:C:1491:PHE:CD2	1:C:1512:ALA:HB3	2.52	0.45
1:C:1068:LEU:HB3	1:C:1088:VAL:HB	1.99	0.45
1:C:1217:KCX:CX	1:C:1219:HIS:HD2	2.30	0.45
1:C:1395:ASN:ND2	1:C:1397:ASN:H	2.14	0.44
2:B:2036:VAL:O	2:B:2068:ALA:HB1	2.17	0.44
1:C:1098:LYS:HD3	1:C:1098:LYS:C	2.44	0.43
1:C:1449:LYS:HA	1:C:1449:LYS:HD2	1.82	0.43
1:C:1350:ASP:CG	1:C:1381:MET:HB3	2.44	0.43
1:C:1051[B]:ILE:HD12	1:C:1112:ILE:HD12	2.00	0.43
1:C:1417:ILE:CG2	1:C:1514:VAL:HG12	2.49	0.43
1:C:1186:SER:HB2	1:C:1187[A]:LEU:HD22	1.99	0.42
1:C:1246:HIS:CD2	1:C:1246:HIS:C	2.97	0.42
3:A:3061:ARG:HD2	3:A:3061:ARG:HH11	1.60	0.42
2:B:2059:TYR:HB3	2:B:2081:LEU:HB3	2.01	0.42
2:B:2024:VAL:CG1	2:B:2051:PHE:HB2	2.49	0.42
2:B:2023:ARG:NH1	2:B:2080:GLU:OE2	2.53	0.42
3:A:3029:LYS:HE3	3:A:3069:VAL:C	2.44	0.42
1:C:1173:GLY:HA2	1:C:1174:PRO:HD3	1.86	0.41
1:C:1359:SER:O	1:C:1365:GLY:HA3	2.20	0.41
2:B:2024:VAL:HG22	2:B:2055:GLN:HG2	2.01	0.41
1:C:1158:GLY:HA3	1:C:1165:THR:HG23	2.03	0.41
1:C:1298:THR:HB	1:C:1360:ASP:HB2	2.03	0.41
1:C:1040:GLY:HA3	2:B:2016:ASN:ND2	2.36	0.40
1:C:1417:ILE:HG22	1:C:1514:VAL:HG12	2.03	0.40
3:A:3011:LEU:HD23	3:A:3011:LEU:HA	1.97	0.40
1:C:1042:GLU:H	1:C:1042:GLU:CD	2.28	0.40
2:B:2028:ASN:HA	2:B:2049:LEU:HD23	2.04	0.40
1:C:1214:ILE:HB	1:C:1514:VAL:HG11	2.03	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:C:527:HOH:O	5:C:527:HOH:O[15_556]	1.21	0.99

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	556/567 (98%)	525 (94%)	29 (5%)	2 (0%)	30	14
2	B	99/101 (98%)	93 (94%)	6 (6%)	0	100	100
3	A	98/100 (98%)	97 (99%)	1 (1%)	0	100	100
All	All	753/768 (98%)	715 (95%)	36 (5%)	2 (0%)	36	20

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	1364	MET
1	C	1360	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	C	438/443 (99%)	426 (97%)	12 (3%)	39	16
2	B	78/78 (100%)	72 (92%)	6 (8%)	12	2
3	A	85/85 (100%)	83 (98%)	2 (2%)	43	19
All	All	601/606 (99%)	581 (97%)	20 (3%)	34	12

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	1043	VAL

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Mol	Chain	Res	Type
1	C	1082	VAL
1	C	1104	ILE
1	C	1187[A]	LEU
1	C	1187[B]	LEU
1	C	1319	CYS
1	C	1391	GLU
1	C	1395	ASN
1	C	1449	LYS
1	C	1508	ARG
1	C	1548	GLU
1	C	1556	ASP
2	B	2009	LYS
2	B	2050	LYS
2	B	2054	GLN
2	B	2055	GLN
2	B	2076	LYS
2	B	2077	ARG
3	A	3080	ILE
3	A	3100	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	1003	ASN
1	C	1107	ASN
1	C	1142	GLN
1	C	1201	GLN
1	C	1362	GLN
1	C	1395	ASN
1	C	1469	GLN
1	C	1486	HIS
1	C	1531	GLN
2	B	2016	ASN
2	B	2075	GLN
2	B	2087	HIS
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	4,1	10,11,12	1.44	1 (10%)	6,12,14	1.75	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	4,1	-	0/9/10/12	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	1217	KCX	OQ1-CX	3.49	1.28	1.21

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	1217	KCX	OQ1-CX-NZ	-4.04	118.78	124.92

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	C	1217	KCX	1	0

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	555/567 (97%)	-0.60	1 (0%) 91 92	13, 20, 36, 63	5 (0%)
2	B	101/101 (100%)	-0.30	2 (1%) 65 69	19, 25, 51, 64	0
3	A	100/100 (100%)	-0.68	0 100 100	15, 20, 38, 57	0
All	All	756/768 (98%)	-0.57	3 (0%) 88 91	13, 21, 40, 64	5 (0%)

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	1392	THR	2.5
2	B	2101	LEU	2.0
2	B	2007	HIS	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(Å ²)	Q<0.9
1	KCX	C	1217	12/13	0.97	0.05	14,18,22,22	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	0.02	21,21,21,21	0
4	NI	C	4775	1/1	1.00	0.02	20,20,20,20	0

6.5 Other polymers [i](#)

There are no such residues in this entry.