Full wwPDB X-ray Structure Validation Report (i)

Jun 12, 2024 – 10:48 PM EDT

PDB ID	:	1EJW
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 (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:

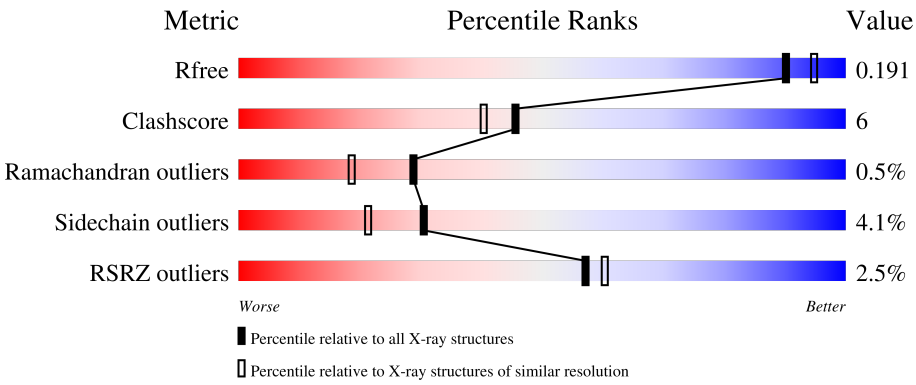
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36.2
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (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 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}	130704	6207 (1.90-1.90)
Clashscore	141614	6847 (1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
Sidechain outliers	138945	6760 (1.90-1.90)
RSRZ outliers	127900	6082 (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 <=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% 84% 13% •
2	B	101	% 77% 20% •
3	A	100	88% 11% •

2 Entry composition (i)

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
			Total	C	N	O	S			
1	C	566	4229	2652	741	813	23	0	0	0

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
			Total	C	N	O	S			
2	B	101	785	496	150	136	3	0	0	0

- Molecule 3 is a protein called UREASE GAMMA SUBUNIT.

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

- Molecule 4 is NICKEL (II) ION (three-letter code: NI) (formula: Ni).

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

- Molecule 5 is water.

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

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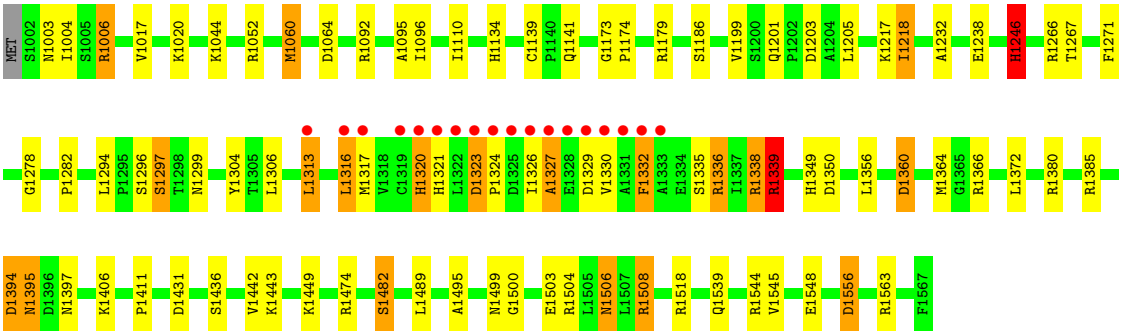
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
5	B	46	46	46	0	0
			Total	O		
5	A	53	53	53	0	0

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 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.

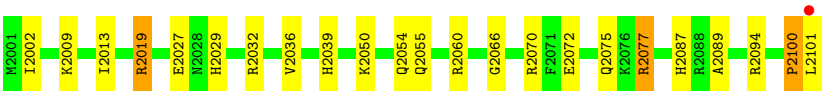
• Molecule 1: UREASE ALPHA SUBUNIT

Chain C:



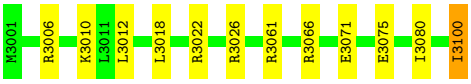
• Molecule 2: UREASE BETA SUBUNIT

Chain B:



• Molecule 3: UREASE GAMMA SUBUNIT

Chain A:



4 Data and refinement statistics (i)

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 54.01 – 1.60	Depositor EDS
% Data completeness (in resolution range)	(Not available) (10.00-1.90) 85.2 (54.01-1.60)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [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)	0.34 , 103.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	0.019 for -l,-k,-h	Xtriage
F_o,F_c correlation	0.97	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.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

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: 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	1.02	0/4301	1.45	28/5860 (0.5%)
2	B	1.04	1/805 (0.1%)	1.53	9/1087 (0.8%)
3	A	0.97	0/787	1.45	9/1061 (0.8%)
All	All	1.02	1/5893 (0.0%)	1.46	46/8008 (0.6%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	2070	ARG	NE-CZ	5.84	1.40	1.33

All (46) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	3006	ARG	NE-CZ-NH2	-10.32	115.14	120.30
2	B	2070	ARG	NE-CZ-NH1	10.06	125.33	120.30
1	C	1092	ARG	NE-CZ-NH1	-10.04	115.28	120.30
1	C	1385	ARG	NE-CZ-NH1	9.51	125.05	120.30
1	C	1006	ARG	NE-CZ-NH1	-9.16	115.72	120.30
1	C	1366	ARG	NE-CZ-NH1	9.11	124.86	120.30
3	A	3006	ARG	CD-NE-CZ	-8.92	111.11	123.60
3	A	3061	ARG	NE-CZ-NH2	-7.83	116.39	120.30
2	B	2032	ARG	NE-CZ-NH1	7.75	124.17	120.30
1	C	1327	ALA	CB-CA-C	7.56	121.44	110.10
1	C	1385	ARG	CD-NE-CZ	7.34	133.88	123.60
1	C	1060	MET	CG-SD-CE	7.34	111.94	100.20
3	A	3006	ARG	NE-CZ-NH1	7.19	123.89	120.30
2	B	2070	ARG	NE-CZ-NH2	-6.95	116.83	120.30
1	C	1004	ILE	N-CA-C	-6.92	92.32	111.00
1	C	1238	GLU	CB-CA-C	-6.91	96.58	110.40
1	C	1380	ARG	NE-CZ-NH1	-6.83	116.89	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	1297	SER	CB-CA-C	-6.74	97.30	110.10
3	A	3066	ARG	NE-CZ-NH1	-6.58	117.01	120.30
2	B	2094	ARG	NE-CZ-NH2	6.56	123.58	120.30
1	C	1266	ARG	NE-CZ-NH1	-6.55	117.03	120.30
2	B	2036	VAL	CA-CB-CG2	-6.46	101.21	110.90
1	C	1482	SER	N-CA-CB	-6.46	100.82	110.50
1	C	1372	LEU	N-CA-CB	-6.29	97.82	110.40
1	C	1052	ARG	NE-CZ-NH1	-6.27	117.16	120.30
1	C	1339	ARG	NE-CZ-NH1	6.17	123.38	120.30
1	C	1246	HIS	N-CA-C	-6.00	94.80	111.00
1	C	1320	HIS	N-CA-C	5.68	126.33	111.00
1	C	1338	ARG	NE-CZ-NH2	-5.65	117.47	120.30
1	C	1017	VAL	CG1-CB-CG2	-5.57	101.99	110.90
2	B	2100	PRO	C-N-CA	5.52	135.50	121.70
1	C	1518	ARG	NE-CZ-NH2	-5.51	117.55	120.30
1	C	1431	ASP	N-CA-C	-5.50	96.15	111.00
1	C	1186	SER	CB-CA-C	-5.45	99.74	110.10
1	C	1350	ASP	CB-CG-OD1	5.43	123.19	118.30
3	A	3026	ARG	CB-CA-C	-5.41	99.57	110.40
3	A	3100	ILE	CA-C-O	-5.41	108.75	120.10
1	C	1299	ASN	N-CA-C	5.38	125.52	111.00
1	C	1474	ARG	NE-CZ-NH2	-5.37	117.62	120.30
2	B	2070	ARG	CD-NE-CZ	5.32	131.05	123.60
3	A	3080	ILE	CA-CB-CG1	-5.30	100.92	111.00
3	A	3022	ARG	NE-CZ-NH2	-5.24	117.68	120.30
2	B	2087	HIS	CB-CA-C	-5.22	99.97	110.40
2	B	2019	ARG	NE-CZ-NH2	-5.21	117.70	120.30
1	C	1489	LEU	CB-CA-C	-5.16	100.41	110.20
1	C	1096	ILE	N-CA-C	-5.15	97.09	111.00

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	4229	0	4175	58	0
2	B	785	0	772	14	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	5751	74	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 (74) 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
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
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: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:1324:PRO:C	1:C:1330:VAL:HG11	2.25	0.57
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
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
1:C:1296:SER:HB3	1:C:1356:LEU:HB2	1.99	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:1395:ASN:HD22	1:C:1395:ASN:C	2.20	0.44
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
2:B:2055:GLN:O	2:B:2055:GLN:HG3	2.17	0.43
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
3:A:3012:LEU:C	3:A:3012:LEU:HD23	2.40	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1349:HIS:HD2	1:C:1406:LYS:HZ2	1.69	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: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 (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	C	563/567 (99%)	528 (94%)	31 (6%)	4 (1%)	22 12
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%)	29 18

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 (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	C	442/443 (100%)	422 (96%)	20 (4%)	27	18
2	B	78/78 (100%)	74 (95%)	4 (5%)	24	14
3	A	85/85 (100%)	84 (99%)	1 (1%)	71	70
All	All	605/606 (100%)	580 (96%)	25 (4%)	30	21

All (25) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	1044	LYS
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	1323	ASP
1	C	1332	PHE
1	C	1336	ARG
1	C	1339	ARG
1	C	1394	ASP
1	C	1395	ASN
1	C	1436	SER
1	C	1449	LYS
1	C	1482	SER
1	C	1506	ASN
1	C	1508	ARG
1	C	1539	GLN
1	C	1556	ASP
2	B	2009	LYS
2	B	2019	ARG
2	B	2077	ARG
2	B	2101	LEU
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	1107	ASN

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Mol	Chain	Res	Type
1	C	1142	GLN
1	C	1201	GLN
1	C	1349	HIS
1	C	1362	GLN
1	C	1395	ASN
1	C	1469	GLN
1	C	1499	ASN
1	C	1533	ASN
2	B	2016	ASN
2	B	2054	GLN
2	B	2075	GLN
3	A	3081	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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	9,11,12	1.70	2 (22%)	5,12,14	2.34	1 (20%)

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	3.77	1.28	1.21
1	C	1217	KCX	CE-NZ	2.51	1.51	1.46

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	1217	KCX	OQ1-CX-NZ	-4.59	117.84	124.96

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 monosaccharides 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%)	-0.79	18 (3%) 47 50	10, 18, 58, 100	0
2	B	101/101 (100%)	-0.31	1 (0%) 82 84	16, 28, 61, 72	0
3	A	100/100 (100%)	-1.08	0 100 100	12, 19, 50, 60	0
All	All	766/768 (99%)	-0.77	19 (2%) 57 60	10, 19, 59, 100	0

All (19) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	1332	PHE	5.6
1	C	1330	VAL	4.6
1	C	1327	ALA	4.4
1	C	1326	ILE	4.3
1	C	1321	HIS	4.1
1	C	1313	LEU	4.1
1	C	1325	ASP	4.0
1	C	1329	ASP	3.9
1	C	1316	LEU	3.5
1	C	1324	PRO	3.3
1	C	1320	HIS	3.2
1	C	1323	ASP	3.2
1	C	1333	ALA	3.1
1	C	1322	LEU	2.8
1	C	1317	MET	2.6
1	C	1331	ALA	2.4
2	B	2101	LEU	2.2
1	C	1319	CYS	2.2
1	C	1328	GLU	2.1

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	0.98	0.04	9,13,15,16	0

6.3 Carbohydrates (i)

There are no monosaccharides 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(Å^2)	Q<0.9
4	NI	C	4774	1/1	1.00	0.02	18,18,18,18	0
4	NI	C	4775	1/1	1.00	0.04	16,16,16,16	0

6.5 Other polymers (i)

There are no such residues in this entry.