



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 03:56 PM UTC

PDB ID : 6J33 / pdb_00006j33
Title : Crystal structure of ligand-free of PulA from *Klebsiella pneumoniae*
Authors : Saka, N.; Iwamoto, H.; Takahashi, N.; Mizutani, K.; Mikami, B.
Deposited on : 2019-01-09
Resolution : 1.30 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

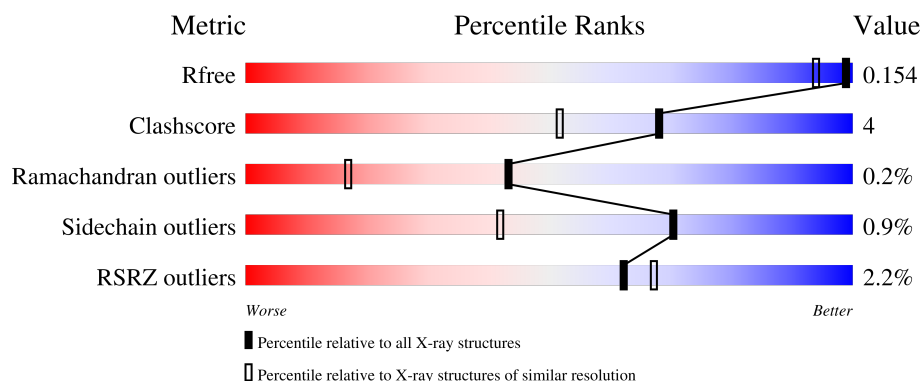
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

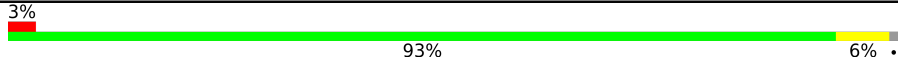
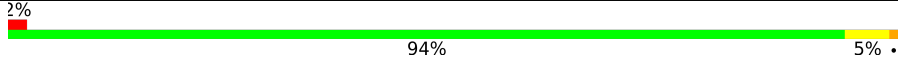
The reported resolution of this entry is 1.30 Å.

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	1553 (1.30-1.30)
Clashscore	190562	1595 (1.30-1.30)
Ramachandran outliers	187476	1551 (1.30-1.30)
Sidechain outliers	187428	1551 (1.30-1.30)
RSRZ outliers	180081	1549 (1.30-1.30)

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	A	1053	
1	B	1053	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 20463 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 pullulanase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1045	Total	C	N	O	S	0	70	0
			8553	5313	1469	1744	27			
1	B	1053	Total	C	N	O	S	0	84	0
			8723	5409	1500	1787	27			

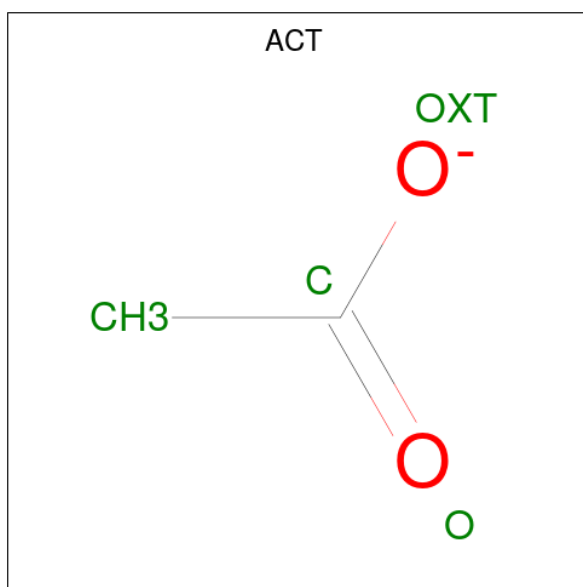
There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	31	MET	-	initiating methionine	UNP W9BQ28
A	229	SER	ASN	see sequence details	UNP W9BQ28
B	31	MET	-	initiating methionine	UNP W9BQ28
B	229	SER	ASN	see sequence details	UNP W9BQ28

- Molecule 2 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	12	Total	Mg	0	0
			12	12		
2	B	10	Total	Mg	0	0
			10	10		

- Molecule 3 is ACETATE ION (CCD ID: ACT) (formula: C₂H₃O₂).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 4 2 2	0	0
3	A	1	Total C O 4 2 2	0	0
3	A	1	Total C O 4 2 2	0	0
3	B	1	Total C O 4 2 2	0	0
3	B	1	Total C O 4 2 2	0	0
3	B	1	Total C O 4 2 2	0	0
3	B	1	Total C O 4 2 2	0	0
3	B	1	Total C O 4 2 2	0	0

- Molecule 4 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	1	Total Ca 1 1	0	0

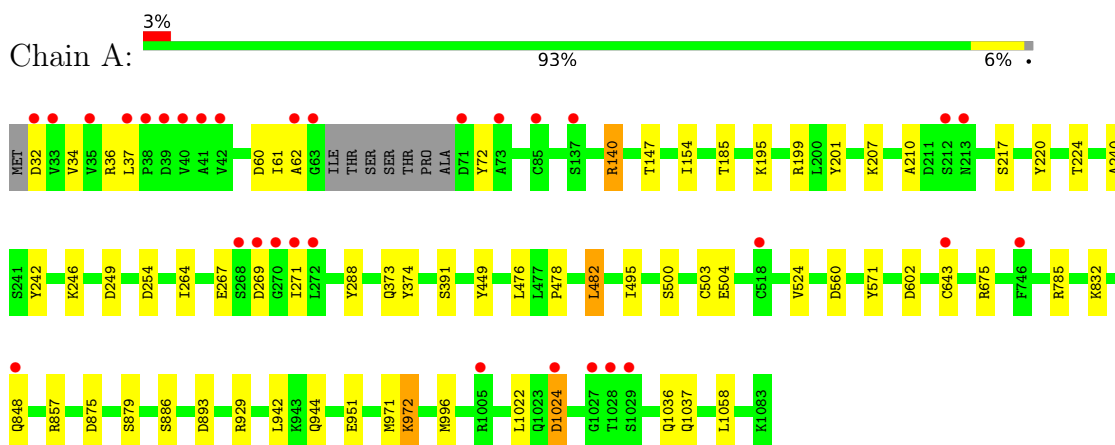
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1527	Total 1527	O 1527	0	0
5	B	1605	Total 1605	O 1605	0	0

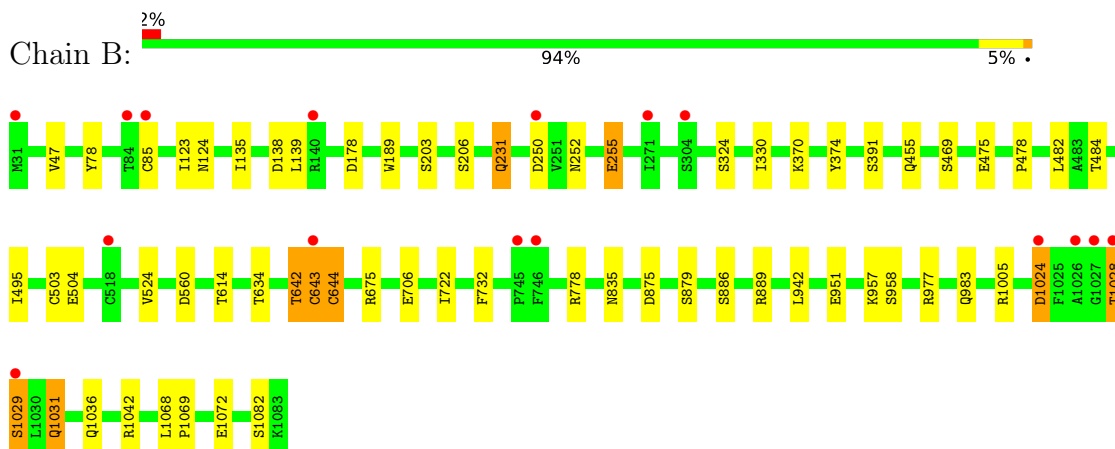
3 Residue-property plots [i](#)

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: pullulanase



• Molecule 1: pullulanase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	60.36Å 80.28Å 127.74Å 96.70° 102.30° 112.10°	Depositor
Resolution (Å)	39.26 – 1.30 39.26 – 1.30	Depositor EDS
% Data completeness (in resolution range)	94.4 (39.26-1.30) 94.4 (39.26-1.30)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.49 (at 1.30Å)	Xtriage
Refinement program	PHENIX (1.10.1_2155: ???)	Depositor
R, R_{free}	0.128 , 0.154 0.128 , 0.154	Depositor DCC
R_{free} test set	24855 reflections (4.73%)	wwPDB-VP
Wilson B-factor (Å ²)	15.0	Xtriage
Anisotropy	0.173	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 55.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.064 for h,-h-k,-h-l	Xtriage
F_o, F_c correlation	0.98	EDS
Total number of atoms	20463	wwPDB-VP
Average B, all atoms (Å ²)	23.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.26% 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: ACT, MG, CA

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	0.47	9/8723 (0.1%)	0.55	4/11856 (0.0%)
1	B	0.37	6/8897 (0.1%)	0.54	5/12097 (0.0%)
All	All	0.42	15/17620 (0.1%)	0.54	9/23953 (0.0%)

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	893[A]	ASP	CA-C	9.02	1.64	1.52
1	A	893[B]	ASP	CA-C	9.02	1.64	1.52
1	B	503	CYS	C-O	-6.31	1.16	1.24
1	B	642	THR	CA-C	-6.18	1.44	1.52
1	A	503	CYS	C-O	-5.83	1.17	1.24
1	A	476	LEU	C-O	-5.83	1.17	1.24
1	A	242	TYR	C-O	-5.43	1.17	1.23
1	A	1022	LEU	C-O	-5.35	1.17	1.24
1	B	644	CYS	C-O	-5.25	1.17	1.24
1	A	34	VAL	C-O	-5.22	1.18	1.24
1	B	135	ILE	C-O	-5.20	1.18	1.24
1	B	78	TYR	C-O	-5.15	1.17	1.24
1	A	60	ASP	C-O	-5.13	1.18	1.23
1	B	1028	THR	C-O	-5.11	1.17	1.24
1	A	971	MET	C-O	-5.10	1.17	1.24

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	1029	SER	N-CA-C	7.62	121.91	111.39
1	B	138	ASP	N-CA-C	-6.39	98.13	108.41
1	B	1028	THR	N-CA-C	6.36	123.15	113.61
1	B	642	THR	O-C-N	6.17	129.86	122.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1024	ASP	N-CA-C	6.14	120.46	113.15
1	A	72	TYR	N-CA-C	5.72	119.98	112.89
1	A	217	SER	N-CA-C	5.55	120.16	113.17
1	B	139	LEU	N-CA-C	5.13	118.31	110.20
1	A	240	ALA	N-CA-C	5.02	117.48	111.71

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	A	8553	0	8168	52	0
1	B	8723	0	8304	66	0
2	A	12	0	0	0	0
2	B	10	0	0	0	0
3	A	12	0	9	1	0
3	B	20	0	15	0	0
4	B	1	0	0	0	0
5	A	1527	0	0	31	0
5	B	1605	0	0	28	0
All	All	20463	0	16496	119	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 4.

All (119) 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)
3:A:1113:ACT:H2	5:A:1794:HOH:O	1.47	1.13
1:A:36[B]:ARG:HH21	1:A:271:ILE:HG22	1.25	1.01
1:B:504[A]:GLU:HG2	5:B:1555:HOH:O	1.62	1.00
1:A:560:ASP:HB2	5:A:1888:HOH:O	1.64	0.95
1:B:1082[B]:SER:HB2	5:B:1268:HOH:O	1.70	0.91
1:B:614[A]:THR:HG22	5:B:1813:HOH:O	1.71	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:36[B]:ARG:NH2	1:A:271:ILE:HG22	1.91	0.84
1:B:977:ARG:NH1	1:B:1024[B]:ASP:HB3	1.95	0.82
1:A:942[A]:LEU:HD21	5:A:1995:HOH:O	1.84	0.78
1:B:675:ARG:NH2	1:B:706:GLU:HG3	1.98	0.78
1:A:482[A]:LEU:HB2	5:A:1888:HOH:O	1.83	0.77
1:A:373[B]:GLN:HG3	5:A:2120:HOH:O	1.88	0.73
1:B:942[A]:LEU:HD21	5:B:1882:HOH:O	1.88	0.73
1:A:972[A]:LYS:HD2	5:A:2281:HOH:O	1.89	0.73
1:B:977:ARG:HH11	1:B:1024[B]:ASP:HB3	1.55	0.72
1:A:675:ARG:HH21	1:A:832[B]:LYS:HZ1	1.36	0.71
1:A:254[B]:ASP:HB2	5:A:1558:HOH:O	1.88	0.71
1:B:675:ARG:HD2	1:B:732:PHE:HE2	1.56	0.71
1:A:785[B]:ARG:NH1	5:A:1201:HOH:O	2.23	0.70
1:A:942[A]:LEU:CD2	5:A:1995:HOH:O	2.38	0.70
1:A:675:ARG:HH21	1:A:832[B]:LYS:NZ	1.90	0.70
1:B:1031[B]:GLN:OE1	1:B:1069:PRO:CG	2.40	0.69
1:A:1058:LEU:HD22	5:A:2307:HOH:O	1.92	0.69
1:B:675:ARG:HD2	1:B:732:PHE:CE2	2.28	0.68
1:B:1031[B]:GLN:OE1	1:B:1069:PRO:HG2	1.95	0.67
1:A:972[A]:LYS:CD	5:A:2281:HOH:O	2.43	0.65
1:A:269:ASP:OD1	1:A:271:ILE:HG23	1.96	0.65
1:A:848:GLN:NE2	5:A:1205:HOH:O	2.30	0.65
1:A:1058:LEU:HD13	5:A:2307:HOH:O	1.95	0.65
1:A:1037[B]:GLN:NE2	5:A:1204:HOH:O	2.30	0.64
1:B:1082[A]:SER:HA	5:B:2107:HOH:O	1.95	0.64
1:B:942[A]:LEU:CD2	5:B:1882:HOH:O	2.44	0.63
1:A:929[A]:ARG:HD2	5:A:2229:HOH:O	1.98	0.62
1:A:972[A]:LYS:CG	5:A:2281:HOH:O	2.46	0.62
1:B:47[A]:VAL:HG23	5:B:2423:HOH:O	1.99	0.61
1:A:207[A]:LYS:HE3	5:A:1311:HOH:O	2.00	0.61
1:B:977:ARG:NH1	1:B:1024[A]:ASP:HB2	2.16	0.61
1:B:370[B]:LYS:HE3	5:B:2133:HOH:O	2.00	0.61
1:B:1031[B]:GLN:OE1	1:B:1069:PRO:HG3	2.01	0.60
1:A:1058:LEU:HB3	5:A:2307:HOH:O	2.02	0.60
1:B:1028:THR:HG22	1:B:1068:LEU:HD21	1.84	0.60
1:B:675:ARG:HH22	1:B:706:GLU:HG3	1.64	0.59
1:A:944:GLN:NE2	5:A:1207:HOH:O	2.34	0.59
1:A:996:MET:HE3	5:A:2626:HOH:O	2.02	0.59
1:B:958:SER:O	1:B:1005[A]:ARG:NH1	2.31	0.59
1:B:634[B]:THR:HG21	5:B:1837:HOH:O	2.02	0.58
1:A:951[A]:GLU:HG3	5:A:1648:HOH:O	2.04	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:644:CYS:HB3	5:B:2049:HOH:O	2.04	0.58
1:B:504[B]:GLU:HG3	5:B:1555:HOH:O	2.04	0.57
1:B:203[B]:SER:OG	1:B:206[B]:SER:O	2.20	0.57
1:A:147:THR:HG23	5:A:1216:HOH:O	2.04	0.57
1:A:972[A]:LYS:HG3	5:A:2281:HOH:O	2.05	0.57
1:B:675:ARG:HH22	1:B:706:GLU:CD	2.13	0.57
1:B:1082[B]:SER:HA	5:B:2107:HOH:O	2.03	0.57
1:A:195:LYS:HE3	1:A:267:GLU:OE2	2.05	0.56
1:A:36[B]:ARG:NH2	1:A:271:ILE:CG2	2.67	0.56
1:B:835:ASN:ND2	5:B:1215:HOH:O	2.40	0.55
1:A:246[A]:LYS:NZ	5:A:1214:HOH:O	2.40	0.55
1:B:643:CYS:SG	1:B:644:CYS:N	2.81	0.53
1:B:889[A]:ARG:NH2	5:B:1203:HOH:O	2.30	0.53
1:B:1005[A]:ARG:CZ	5:B:1283:HOH:O	2.57	0.52
1:B:675:ARG:HH22	1:B:706:GLU:CG	2.22	0.52
1:B:231[A]:GLN:H	1:B:231[A]:GLN:CD	2.17	0.52
1:A:61:ILE:HG13	1:A:154:ILE:HD13	1.91	0.51
1:A:929[A]:ARG:CD	5:A:2229:HOH:O	2.57	0.51
1:B:778[A]:ARG:NH2	1:B:983:GLN:O	2.43	0.51
1:A:875:ASP:OD2	1:A:879:SER:HB2	2.11	0.50
1:B:1042:ARG:HD2	5:B:1273:HOH:O	2.10	0.50
1:B:1028:THR:CG2	1:B:1068:LEU:HD21	2.40	0.50
1:B:889[A]:ARG:NH1	5:B:1238:HOH:O	2.44	0.49
1:A:224[B]:THR:HG23	5:A:1813:HOH:O	2.12	0.49
1:A:36[B]:ARG:HG2	1:A:37:LEU:O	2.12	0.49
1:A:37:LEU:HD21	1:A:210:ALA:CB	2.42	0.49
1:B:469[A]:SER:HB2	5:B:1359:HOH:O	2.13	0.49
1:B:1024[A]:ASP:OD1	1:B:1024[A]:ASP:N	2.39	0.49
1:B:484:THR:OG1	1:B:560[B]:ASP:OD2	2.28	0.48
1:B:951[A]:GLU:OE2	1:B:1036:GLN:HG2	2.13	0.48
1:B:875:ASP:OD2	1:B:879:SER:HB2	2.14	0.48
1:B:495:ILE:HA	1:B:524:VAL:HB	1.96	0.48
1:A:482[B]:LEU:HB3	5:A:1888:HOH:O	2.13	0.47
1:A:254[B]:ASP:OD2	1:A:288:TYR:OH	2.29	0.47
1:B:722:ILE:HG13	5:B:2213:HOH:O	2.14	0.47
1:B:1028:THR:HG22	1:B:1068:LEU:CD2	2.45	0.47
1:A:495:ILE:HA	1:A:524:VAL:HB	1.97	0.47
1:A:207[B]:LYS:HE2	5:A:1655:HOH:O	2.15	0.47
1:B:1028:THR:HG22	1:B:1028:THR:O	2.14	0.47
1:A:199:ARG:HD3	1:A:220:TYR:CD1	2.50	0.46
1:B:252:ASN:O	1:B:255:GLU:HB2	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:889[A]:ARG:NH1	5:B:1203:HOH:O	2.40	0.46
1:B:324:SER:HB3	1:B:330[B]:ILE:HD11	1.97	0.46
1:B:675:ARG:CZ	5:B:1938:HOH:O	2.64	0.45
1:A:32:ASP:N	5:A:1242:HOH:O	2.48	0.45
1:B:475:GLU:OE2	1:B:675:ARG:HD3	2.16	0.45
1:A:951[A]:GLU:OE2	1:A:1036:GLN:HG2	2.16	0.45
1:B:123:ILE:HA	5:B:2189:HOH:O	2.16	0.45
1:B:1082[A]:SER:CB	5:B:1268:HOH:O	2.65	0.44
1:B:957[A]:LYS:NZ	5:B:1209:HOH:O	2.36	0.44
1:B:675:ARG:NH2	1:B:706:GLU:CG	2.76	0.43
1:A:602[A]:ASP:OD1	1:A:675:ARG:HD2	2.18	0.43
1:B:1082[A]:SER:HB3	5:B:1268:HOH:O	2.19	0.43
1:B:85:CYS:HB2	1:B:124:ASN:ND2	2.34	0.43
1:B:1005[A]:ARG:HE	1:B:1005[A]:ARG:HB2	1.66	0.42
1:A:500:SER:O	1:A:504[A]:GLU:HG3	2.19	0.42
1:A:1024:ASP:OD1	1:A:1024:ASP:N	2.48	0.42
1:A:185:THR:O	1:A:246[B]:LYS:HA	2.20	0.42
1:B:178[B]:ASP:OD1	1:B:189:TRP:NE1	2.51	0.42
1:B:250[A]:ASP:OD1	1:B:250[A]:ASP:N	2.53	0.42
1:A:246[B]:LYS:NZ	1:A:249:ASP:OD1	2.53	0.41
1:A:449:TYR:CZ	1:A:571:TYR:HB2	2.55	0.41
1:A:857[B]:ARG:NH1	5:A:1254:HOH:O	2.51	0.41
1:B:675:ARG:HH21	1:B:706:GLU:HG3	1.81	0.41
1:B:1028:THR:CG2	1:B:1028:THR:O	2.69	0.40
1:A:140[B]:ARG:NH1	5:A:1217:HOH:O	2.40	0.40
1:B:642:THR:O	1:B:643:CYS:HB3	2.22	0.40
1:B:560[B]:ASP:HA	5:B:1910:HOH:O	2.21	0.40
1:B:1005[A]:ARG:NE	5:B:1283:HOH:O	2.54	0.40
1:B:1072[B]:GLU:H	1:B:1072[B]:GLU:HG3	1.72	0.40
1:A:201:TYR:CD1	1:A:264:ILE:HD12	2.56	0.40
1:B:455:GLN:HG2	5:B:2653:HOH:O	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1111/1053 (106%)	1092 (98%)	16 (1%)	3 (0%)	36	15
1	B	1136/1053 (108%)	1111 (98%)	23 (2%)	2 (0%)	43	17
All	All	2247/2106 (107%)	2203 (98%)	39 (2%)	5 (0%)	43	17

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	643	CYS
1	B	643	CYS
1	A	62	ALA
1	A	478	PRO
1	B	478	PRO

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	928/866 (107%)	918 (99%)	10 (1%)	65	33
1	B	950/866 (110%)	936 (98%)	14 (2%)	57	21
All	All	1878/1732 (108%)	1854 (99%)	24 (1%)	70	26

All (24) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	140[A]	ARG
1	A	140[B]	ARG
1	A	374	TYR
1	A	391[A]	SER
1	A	391[B]	SER
1	A	482[A]	LEU
1	A	482[B]	LEU
1	A	886	SER

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Mol	Chain	Res	Type
1	A	972[A]	LYS
1	A	972[B]	LYS
1	B	231[A]	GLN
1	B	231[B]	GLN
1	B	255	GLU
1	B	374	TYR
1	B	391[A]	SER
1	B	391[B]	SER
1	B	482[A]	LEU
1	B	482[B]	LEU
1	B	886	SER
1	B	1024[A]	ASP
1	B	1024[B]	ASP
1	B	1029	SER
1	B	1031[A]	GLN
1	B	1031[B]	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	124	ASN
1	A	277	GLN
1	A	712	GLN
1	B	712	GLN
1	B	1049	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 31 ligands modelled in this entry, 23 are monoatomic - leaving 8 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	ACT	B	1116	-	3,3,3	0.96	0	3,3,3	1.08	0
3	ACT	A	1113	-	3,3,3	0.64	0	3,3,3	1.57	1 (33%)
3	ACT	B	1113	-	3,3,3	1.24	1 (33%)	3,3,3	0.93	0
3	ACT	B	1114	-	3,3,3	1.56	1 (33%)	3,3,3	0.73	0
3	ACT	A	1114	-	3,3,3	0.87	0	3,3,3	1.14	0
3	ACT	A	1112	-	3,3,3	0.60	0	3,3,3	1.46	1 (33%)
3	ACT	B	1115	-	3,3,3	1.17	1 (33%)	3,3,3	0.91	0
3	ACT	B	1112	-	3,3,3	0.74	0	3,3,3	1.11	0

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1114	ACT	OXT-C	-2.65	1.18	1.30
3	B	1113	ACT	OXT-C	-2.11	1.21	1.30
3	B	1115	ACT	OXT-C	-2.00	1.21	1.30

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1112	ACT	O-C-CH3	-2.24	113.35	122.53
3	A	1113	ACT	OXT-C-O	2.20	130.20	122.03

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
3	A	1113	ACT	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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	A	1045/1053 (99%)	-0.05	31 (2%)	52	58	6, 16, 40, 81	71 (6%)
1	B	1053/1053 (100%)	-0.11	16 (1%)	72	76	5, 16, 33, 65	84 (7%)
All	All	2098/2106 (99%)	-0.08	47 (2%)	62	67	5, 16, 36, 81	155 (7%)

All (47) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	63	GLY	6.8
1	A	85	CYS	5.8
1	B	746[A]	PHE	5.1
1	B	85	CYS	4.9
1	A	40	VAL	4.4
1	A	73	ALA	3.7
1	A	270	GLY	3.3
1	B	1024[A]	ASP	3.2
1	A	1028[A]	THR	3.1
1	A	518	CYS	3.0
1	A	1027[A]	GLY	3.0
1	B	140[A]	ARG	3.0
1	A	41	ALA	3.0
1	B	518	CYS	3.0
1	A	746[A]	PHE	2.9
1	B	745	PRO	2.9
1	A	1029[A]	SER	2.9
1	A	39	ASP	2.9
1	A	62	ALA	2.9
1	A	271	ILE	2.8
1	B	643	CYS	2.8
1	A	269	ASP	2.7
1	B	1027	GLY	2.7
1	A	643	CYS	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	1028	THR	2.6
1	A	42	VAL	2.5
1	A	33	VAL	2.5
1	B	250[A]	ASP	2.5
1	A	38	PRO	2.4
1	B	1029	SER	2.4
1	A	212	SER	2.3
1	A	71	ASP	2.3
1	B	1026	ALA	2.3
1	A	213	ASN	2.3
1	A	272	LEU	2.3
1	A	35	VAL	2.3
1	A	1024	ASP	2.2
1	B	271	ILE	2.2
1	A	32	ASP	2.1
1	A	137	SER	2.1
1	B	31	MET	2.1
1	A	37	LEU	2.1
1	A	848	GLN	2.1
1	A	1005[A]	ARG	2.0
1	A	268	SER	2.0
1	B	304	SER	2.0
1	B	84	THR	2.0

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

There are no non-standard protein/DNA/RNA residues in this entry.

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.

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	ACT	A	1114	4/4	0.86	0.15	39,41,42,44	0
3	ACT	B	1116	4/4	0.87	0.12	56,56,56,57	0
3	ACT	B	1115	4/4	0.88	0.12	36,39,39,40	0
2	MG	B	1105	1/1	0.92	0.10	50,50,50,50	0
3	ACT	A	1113	4/4	0.93	0.12	19,20,21,23	4
2	MG	A	1109	1/1	0.93	0.09	35,35,35,35	1
3	ACT	A	1112	4/4	0.94	0.09	20,24,26,26	4
3	ACT	B	1112	4/4	0.94	0.11	19,21,22,25	4
3	ACT	B	1113	4/4	0.95	0.09	21,22,22,22	4
2	MG	A	1107	1/1	0.95	0.12	38,38,38,38	1
2	MG	B	1109	1/1	0.95	0.10	32,32,32,32	1
2	MG	A	1104	1/1	0.96	0.11	38,38,38,38	0
2	MG	A	1108	1/1	0.96	0.06	36,36,36,36	1
3	ACT	B	1114	4/4	0.96	0.06	22,23,24,24	4
2	MG	B	1106	1/1	0.96	0.08	32,32,32,32	1
2	MG	B	1107	1/1	0.96	0.10	30,30,30,30	1
2	MG	A	1110	1/1	0.97	0.10	26,26,26,26	1
2	MG	B	1110	1/1	0.97	0.06	38,38,38,38	1
2	MG	B	1108	1/1	0.98	0.04	28,28,28,28	1
4	CA	B	1111	1/1	0.98	0.06	18,18,18,18	0
2	MG	A	1103	1/1	0.99	0.10	29,29,29,29	0
2	MG	A	1101	1/1	0.99	0.03	20,20,20,20	0
2	MG	A	1111	1/1	0.99	0.13	28,28,28,28	0
2	MG	B	1102	1/1	0.99	0.04	22,22,22,22	0
2	MG	B	1103	1/1	0.99	0.07	25,25,25,25	0
2	MG	A	1106	1/1	1.00	0.02	11,11,11,11	0
2	MG	A	1102	1/1	1.00	0.02	18,18,18,18	0
2	MG	B	1104	1/1	1.00	0.03	17,17,17,17	0
2	MG	A	1105	1/1	1.00	0.06	11,11,11,11	0
2	MG	A	1115	1/1	1.00	0.10	19,19,19,19	0
2	MG	B	1101	1/1	1.00	0.02	10,10,10,10	0

6.5 Other polymers ⓘ

There are no such residues in this entry.