Full wwPDB EM Validation Report ⓘ

Nov 6, 2023 – 08:00 pm GMT

PDB ID	:	7ZZ6
EMDB ID	:	EMD-15036
Title	:	Cryo-EM structure of "CT-CT dimer" of Lactococcus lactis pyruvate carboxylase with acetyl-CoA
Authors	:	Lopez-Alonso, J.P.; Lazaro, M.; Gil, D.; Choi, P.H.; Tong, L.; Valle, M.
Deposited on	:	2022-05-25
Resolution	:	2.15 Å(reported)
Based on initial model	:	5VYW

This is a Full wwPDB EM 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/EMValidationReportHelp
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:

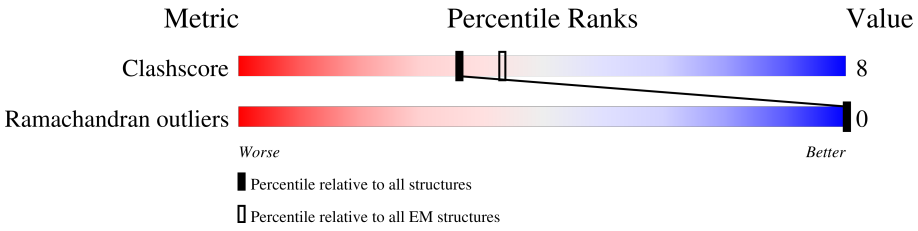
EMDB validation analysis	:	0.0.1.dev70
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	FAILED
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 2.15 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)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the 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%

Mol	Chain	Length	Quality of chain
1	A	1143	35% 10% 56%
1	D	1143	35% 10% 55%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	PYR	A	1203	-	X	-	-
4	PYR	D	1203	-	X	-	-

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 8257 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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 Pyruvate carboxylase.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	D	509	Total 4047	C 2574	N 685	O 770	S 18	0	0
1	A	508	Total 4037	C 2568	N 682	O 769	S 18	0	0

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	-5	VAL	-	expression tag	UNP A0A2A9IR05
D	-4	PRO	-	expression tag	UNP A0A2A9IR05
D	-3	ARG	-	expression tag	UNP A0A2A9IR05
D	-2	GLY	-	expression tag	UNP A0A2A9IR05
D	-1	SER	-	expression tag	UNP A0A2A9IR05
D	0	HIS	-	expression tag	UNP A0A2A9IR05
D	1055	ALA	THR	conflict	UNP A0A2A9IR05
A	-5	VAL	-	expression tag	UNP A0A2A9IR05
A	-4	PRO	-	expression tag	UNP A0A2A9IR05
A	-3	ARG	-	expression tag	UNP A0A2A9IR05
A	-2	GLY	-	expression tag	UNP A0A2A9IR05
A	-1	SER	-	expression tag	UNP A0A2A9IR05
A	0	HIS	-	expression tag	UNP A0A2A9IR05
A	1055	ALA	THR	conflict	UNP A0A2A9IR05

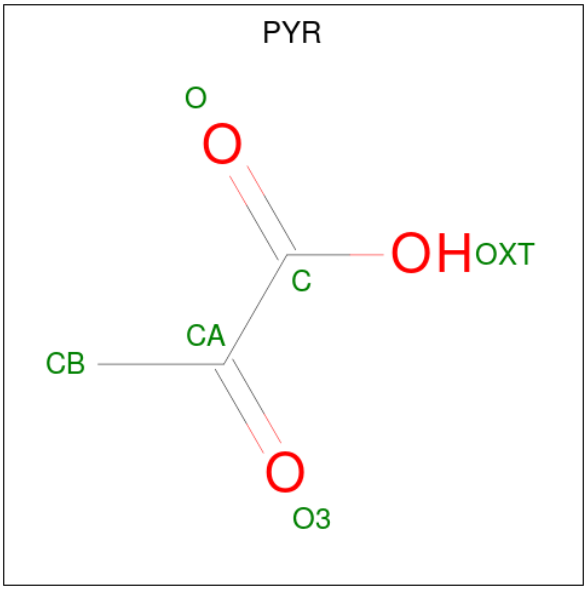
- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
2	D	1	Total 1	Mg 1	0
2	A	1	Total 1	Mg 1	0

- Molecule 3 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

Mol	Chain	Residues	Atoms	AltConf
3	D	1	Total Mn 1 1	0
3	A	1	Total Mn 1 1	0

- Molecule 4 is PYRUVIC ACID (three-letter code: PYR) (formula: $C_3H_4O_3$).



Mol	Chain	Residues	Atoms	AltConf
4	D	1	Total C O 6 3 3	0
4	A	1	Total C O 6 3 3	0

- Molecule 5 is water.

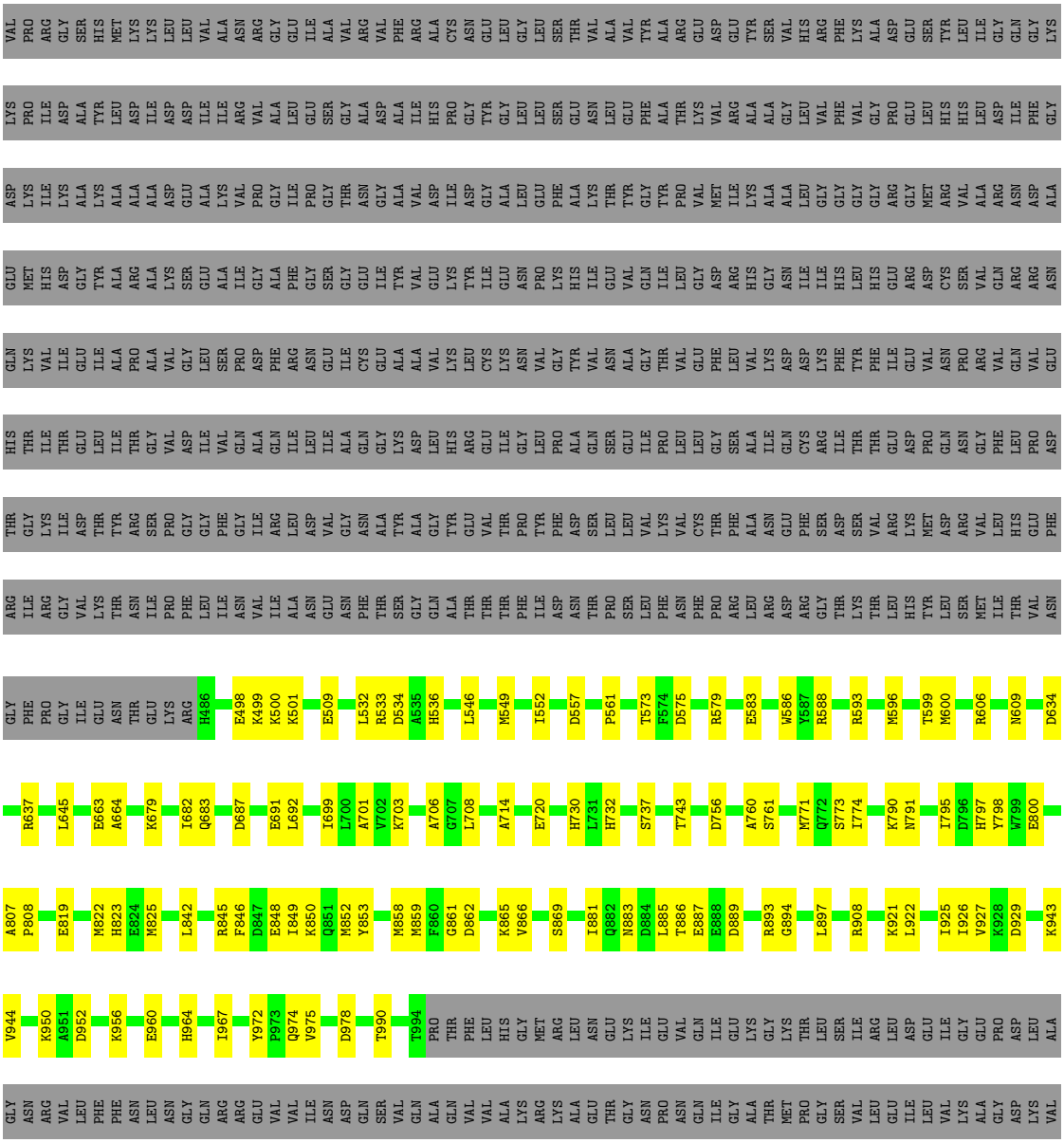
Mol	Chain	Residues	Atoms	AltConf
5	D	99	Total O 99 99	0
5	A	58	Total O 58 58	0

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. 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. 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.

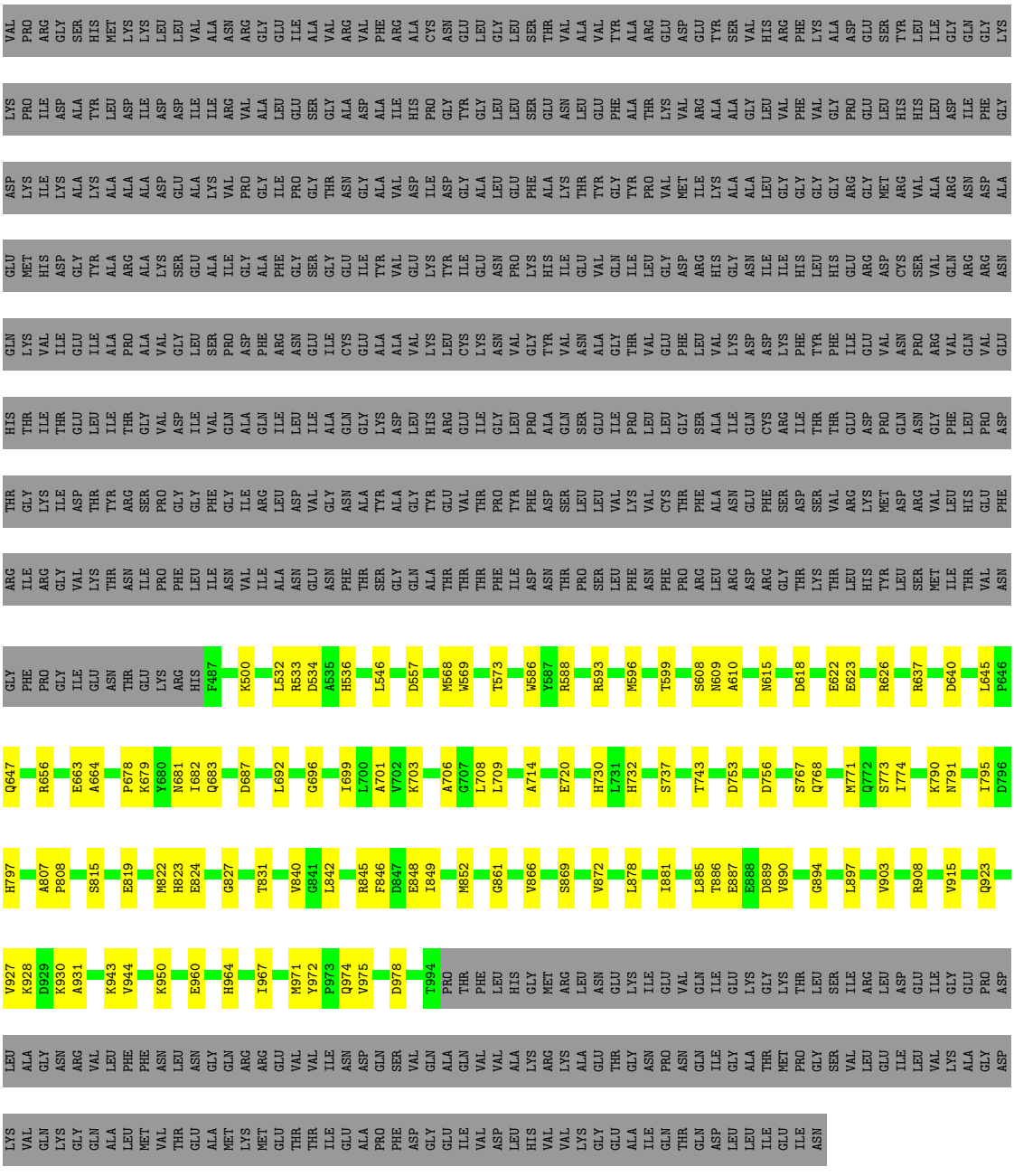
- Molecule 1: Pyruvate carboxylase

Chain D:



• Molecule 1: Pyruvate carboxylase

Chain A: 35% 10% 56%



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	1369092	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	48	Depositor
Minimum defocus (nm)	900	Depositor
Maximum defocus (nm)	2400	Depositor
Magnification	81000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: KCX, PYR, MN, MG

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	0.32	0/4111	0.44	0/5565
1	D	0.33	0/4122	0.46	0/5580
All	All	0.33	0/8233	0.45	0/11145

There are no bond length outliers.

There are no bond angle outliers.

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	A	4037	0	3980	73	0
1	D	4047	0	3987	69	0
2	A	1	0	0	1	0
2	D	1	0	0	0	0
3	A	1	0	0	0	0
3	D	1	0	0	0	0
4	A	6	0	0	0	0
4	D	6	0	0	0	0
5	A	58	0	0	1	0
5	D	99	0	0	0	0
All	All	8257	0	7967	135	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 8.

All (135) 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:D:532:LEU:HD22	1:D:549:MET:HG2	1.68	0.76
1:A:840:VAL:HG23	1:A:842:LEU:HD23	1.71	0.71
1:D:819:GLU:OE2	1:A:797:HIS:NE2	2.24	0.68
1:A:894:GLY:HA2	1:A:897:LEU:HD12	1.74	0.68
1:A:753:ASP:OD2	2:A:1201:MG:MG	1.38	0.66
1:A:679:LYS:NZ	1:A:861:GLY:O	2.27	0.66
1:A:753:ASP:OD2	5:A:1301:HOH:O	2.14	0.65
1:D:797:HIS:NE2	1:A:819:GLU:OE2	2.25	0.64
1:D:683:GLN:NE2	1:D:687:ASP:OD1	2.30	0.64
1:D:679:LYS:NZ	1:D:861:GLY:O	2.30	0.64
1:D:952:ASP:OD1	1:D:956:LYS:NZ	2.30	0.63
1:D:885:LEU:HD12	1:D:889:ASP:HB3	1.80	0.62
1:D:825:MET:HG2	1:D:853:TYR:CE1	2.34	0.61
1:A:885:LEU:HD12	1:A:889:ASP:HB3	1.83	0.60
1:A:683:GLN:NE2	1:A:687:ASP:OD1	2.34	0.59
1:D:637:ARG:HA	1:D:663:GLU:HB3	1.84	0.59
1:A:664:ALA:HB1	1:A:692:LEU:HD22	1.82	0.59
1:D:730:HIS:NE2	1:D:756:ASP:OD1	2.32	0.58
1:A:663:GLU:HG3	1:A:699:ILE:HB	1.85	0.58
1:A:972:TYR:HB3	1:A:975:VAL:HB	1.86	0.58
1:A:532:LEU:O	1:A:536:HIS:NE2	2.36	0.57
1:D:791:ASN:O	1:D:795:ILE:HG12	2.06	0.56
1:A:730:HIS:NE2	1:A:756:ASP:OD1	2.34	0.56
1:D:664:ALA:HB1	1:D:692:LEU:HD22	1.85	0.56
1:D:886:THR:OG1	1:D:887:GLU:N	2.38	0.56
1:D:501:LYS:NZ	1:D:509:GLU:OE2	2.38	0.56
1:A:823:HIS:ND1	1:A:823:HIS:O	2.39	0.56
1:D:950:LYS:NZ	1:D:960:GLU:OE2	2.39	0.56
1:D:974:GLN:NE2	1:D:978:ASP:OD1	2.39	0.56
1:A:791:ASN:O	1:A:795:ILE:HG12	2.06	0.56
1:A:609:ASN:N	1:A:609:ASN:OD1	2.39	0.56
1:D:894:GLY:HA2	1:D:897:LEU:HD23	1.88	0.55
1:D:498:GLU:OE1	1:D:500:LYS:NZ	2.39	0.55
1:A:950:LYS:NZ	1:A:960:GLU:OE2	2.36	0.55
1:A:656:ARG:NH1	1:A:696:GLY:O	2.38	0.55
1:D:773:SER:OG	1:A:737:SER:O	2.24	0.54
1:A:974:GLN:NE2	1:A:978:ASP:OD1	2.39	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:606:ARG:HB2	1:D:609:ASN:O	2.08	0.53
1:A:586:TRP:CD2	1:A:964:HIS:HB2	2.43	0.53
1:A:878:LEU:HD12	1:A:881:ILE:HD11	1.90	0.53
1:A:886:THR:OG1	1:A:887:GLU:N	2.41	0.53
1:A:637:ARG:HA	1:A:663:GLU:HB3	1.91	0.52
1:A:846:PHE:HA	1:A:849:ILE:HB	1.92	0.52
1:D:593:ARG:NH1	1:D:599:THR:O	2.33	0.52
1:D:586:TRP:CD2	1:D:964:HIS:HB2	2.44	0.52
1:A:663:GLU:HG2	1:A:701:ALA:HB2	1.91	0.52
1:D:557:ASP:HB2	1:D:596:MET:HG2	1.91	0.52
1:D:822:MET:SD	1:A:790:LYS:NZ	2.83	0.52
1:D:823:HIS:ND1	1:D:823:HIS:O	2.42	0.52
1:D:846:PHE:HA	1:D:849:ILE:HB	1.92	0.51
1:A:645:LEU:HD13	1:A:692:LEU:HD23	1.93	0.51
1:D:532:LEU:O	1:D:536:HIS:NE2	2.43	0.51
1:A:623:GLU:OE2	1:A:626:ARG:NH2	2.42	0.50
1:D:972:TYR:HB3	1:D:975:VAL:HB	1.92	0.50
1:A:771:MET:O	1:A:774:ILE:HG22	2.11	0.50
1:A:923:GLN:O	1:A:927:VAL:HG22	2.12	0.50
1:A:682:ILE:HG12	1:A:720:GLU:HG3	1.94	0.50
1:D:866:VAL:O	1:D:869:SER:N	2.45	0.49
1:A:845:ARG:HB2	1:A:848:GLU:HG2	1.93	0.49
1:D:929:ASP:N	1:D:929:ASP:OD1	2.45	0.49
1:A:852:MET:HG2	1:A:881:ILE:HG23	1.93	0.49
1:A:706:ALA:HB3	1:A:708:LEU:HG	1.94	0.49
1:D:943:LYS:HD2	1:D:944:VAL:H	1.78	0.48
1:A:866:VAL:O	1:A:869:SER:N	2.46	0.48
1:D:586:TRP:CE2	1:D:964:HIS:HB2	2.49	0.48
1:D:921:LYS:O	1:D:925:ILE:HG12	2.14	0.48
1:D:575:ASP:OD1	1:D:579:ARG:NH1	2.41	0.47
1:D:922:LEU:O	1:D:926:ILE:HG12	2.14	0.47
1:D:663:GLU:HG2	1:D:701:ALA:HB2	1.96	0.47
1:D:771:MET:O	1:D:774:ILE:HG22	2.13	0.47
1:A:533:ARG:HG2	1:A:573:THR:HG21	1.96	0.47
1:D:889:ASP:O	1:D:893:ARG:HB3	2.15	0.47
1:A:640:ASP:OD1	1:A:647:GLN:NE2	2.48	0.47
1:D:858:MET:HE3	1:D:858:MET:HA	1.96	0.47
1:D:645:LEU:HD13	1:D:692:LEU:HD23	1.96	0.46
1:A:943:LYS:HD2	1:A:944:VAL:H	1.80	0.46
1:D:600:MET:HG2	1:D:634:ASP:HB2	1.97	0.46
1:D:546:LEU:HD13	1:D:588:ARG:HG3	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:499:LYS:HB3	1:D:499:LYS:HE3	1.68	0.46
1:D:737:SER:O	1:A:773:SER:OG	2.32	0.46
1:A:593:ARG:NH1	1:A:599:THR:O	2.37	0.46
1:A:908:ARG:HD2	1:A:931:ALA:O	2.16	0.45
1:D:583:GLU:HB3	1:D:990:THR:HB	1.98	0.45
1:D:842:LEU:HD11	1:D:845:ARG:HH11	1.81	0.45
1:A:894:GLY:O	1:A:928:LYS:NZ	2.49	0.45
1:D:845:ARG:HD2	1:D:848:GLU:OE2	2.17	0.45
1:A:546:LEU:HD13	1:A:588:ARG:HG3	1.98	0.45
1:D:852:MET:HG2	1:D:881:ILE:HG23	1.99	0.44
1:A:534:ASP:OD2	1:A:732:HIS:HE1	2.00	0.44
1:D:682:ILE:HG12	1:D:720:GLU:HG3	1.99	0.44
1:D:687:ASP:O	1:D:691:GLU:HG3	2.17	0.44
1:D:858:MET:HE3	1:D:862:ASP:HB2	2.00	0.44
1:D:908:ARG:HG2	1:D:927:VAL:HG11	1.99	0.44
1:D:533:ARG:HG2	1:D:573:THR:HG21	2.00	0.44
1:D:967:ILE:HA	1:D:967:ILE:HD13	1.73	0.44
1:A:872:VAL:HG13	1:A:903:VAL:HA	1.98	0.44
1:D:706:ALA:HB3	1:D:708:LEU:HG	2.00	0.43
1:A:678:PRO:O	1:A:681:ASN:ND2	2.46	0.43
1:D:761:SER:OG	1:D:800:GLU:HB2	2.19	0.43
1:D:774:ILE:HD12	1:D:774:ILE:HA	1.83	0.43
1:A:568:MET:O	1:A:568:MET:HE2	2.19	0.42
1:A:714:ALA:HB2	1:A:743:THR:HG23	2.01	0.42
1:A:894:GLY:HA2	1:A:897:LEU:CD1	2.44	0.42
1:D:853:TYR:CE1	1:D:865:LYS:HD2	2.55	0.42
1:A:679:LYS:HE2	1:A:915:VAL:HG13	2.02	0.42
1:D:663:GLU:HG3	1:D:699:ILE:HB	2.00	0.42
1:A:827:GLY:O	1:A:831:THR:HG23	2.20	0.42
1:A:823:HIS:O	1:A:823:HIS:CG	2.73	0.42
1:D:883:ASN:HB2	1:D:885:LEU:CD2	2.50	0.41
1:D:500:LYS:HD2	1:D:561:PRO:HG2	2.02	0.41
1:A:586:TRP:CE2	1:A:964:HIS:HB2	2.55	0.41
1:D:760:ALA:O	1:A:815:SER:HB3	2.21	0.41
1:D:823:HIS:CD2	1:D:850:LYS:HD2	2.55	0.41
1:A:767:SER:OG	1:A:768:GLN:N	2.54	0.41
1:A:807:ALA:N	1:A:808:PRO:HD2	2.36	0.41
1:A:845:ARG:NE	1:A:848:GLU:OE1	2.34	0.41
1:A:878:LEU:HD12	1:A:878:LEU:HA	1.91	0.41
1:A:500:LYS:HB3	1:A:500:LYS:HE3	1.80	0.41
1:A:610:ALA:HB3	1:A:971:MET:SD	2.61	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:890:VAL:O	1:A:894:GLY:HA3	2.21	0.41
1:A:908:ARG:HG2	1:A:927:VAL:HG12	2.03	0.41
1:A:908:ARG:HD3	1:A:930:LYS:HB3	2.03	0.41
1:A:557:ASP:HB2	1:A:596:MET:HG2	2.02	0.40
1:D:534:ASP:OD2	1:D:732:HIS:HE1	2.04	0.40
1:D:807:ALA:N	1:D:808:PRO:HD2	2.37	0.40
1:A:709:LEU:HG	1:A:714:ALA:HB2	2.04	0.40
1:D:714:ALA:HB2	1:D:743:THR:HG23	2.04	0.40
1:A:568:MET:SD	1:A:569:TRP:HB2	2.62	0.40
1:D:552:ILE:HB	1:D:798:TYR:CE1	2.56	0.40
1:D:859:MET:SD	1:D:887:GLU:HG3	2.62	0.40
1:A:967:ILE:HD13	1:A:967:ILE:HA	1.73	0.40
1:D:790:LYS:NZ	1:A:822:MET:SD	2.95	0.40
1:A:608:SER:HB2	1:A:615:ASN:ND2	2.37	0.40
1:A:618:ASP:O	1:A:622:GLU:HG3	2.22	0.40
1:A:708:LEU:HD11	1:A:824:GLU:HB3	2.04	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 PDB entries followed by that with respect to all EM entries.

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	505/1143 (44%)	489 (97%)	16 (3%)	0	100	100
1	D	506/1143 (44%)	492 (97%)	14 (3%)	0	100	100
All	All	1011/2286 (44%)	981 (97%)	30 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

There are no protein residues with a non-rotameric sidechain to report in this entry.

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

2 non-standard protein/DNA/RNA residues are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
1	KCX	A	703	3,1	9,11,12	0.82	0	5,12,14	1.67	1 (20%)
1	KCX	D	703	3,1	9,11,12	0.79	0	5,12,14	1.49	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	A	703	3,1	-	0/9/10/12	-
1	KCX	D	703	3,1	-	0/9/10/12	-

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	703	KCX	OQ1-CX-NZ	-3.22	119.96	124.96
1	D	703	KCX	OQ1-CX-NZ	-2.96	120.37	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 6 ligands modelled in this entry, 4 are monoatomic - leaving 2 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	$\#\|Z\| > 2$
4	PYR	D	1203	-	5,5,5	2.84	3 (60%)	3,6,6	1.69	1 (33%)
4	PYR	A	1203	-	5,5,5	2.88	3 (60%)	3,6,6	1.56	1 (33%)

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
4	PYR	D	1203	-	-	2/4/4/4	-
4	PYR	A	1203	-	-	3/4/4/4	-

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1203	PYR	CA-C	-4.17	1.39	1.54
4	D	1203	PYR	CA-C	-4.06	1.39	1.54
4	A	1203	PYR	O3-CA	3.70	1.31	1.23
4	D	1203	PYR	O3-CA	3.64	1.31	1.23
4	D	1203	PYR	O-C	3.24	1.31	1.22
4	A	1203	PYR	O-C	3.21	1.31	1.22

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	D	1203	PYR	OXT-C-CA	2.38	120.49	113.97
4	A	1203	PYR	OXT-C-CA	2.18	119.95	113.97

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	D	1203	PYR	OXT-C-CA-CB
4	A	1203	PYR	O-C-CA-CB
4	A	1203	PYR	OXT-C-CA-CB
4	D	1203	PYR	O-C-CA-CB
4	A	1203	PYR	OXT-C-CA-O3

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 Map visualisation

This section contains visualisations of the EMDB entry EMD-15036. These allow visual inspection of the internal detail of the map and identification of artifacts.

Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

This section was not generated.

6.2 Central slices

This section was not generated.

6.3 Largest variance slices

This section was not generated.

6.4 Orthogonal standard-deviation projections (False-color)

This section was not generated.

6.5 Orthogonal surface views

This section was not generated.

6.6 Mask visualisation

This section was not generated. No masks/segmentation were deposited.

7 Map analysis

This section contains the results of statistical analysis of the map.

7.1 Map-value distribution

This section was not generated.

7.2 Volume estimate versus contour level

This section was not generated.

7.3 Rotationally averaged power spectrum

This section was not generated. The rotationally averaged power spectrum had issues being displayed.

8 Fourier-Shell correlation (i)

This section was not generated. No FSC curve or half-maps provided.

9 Map-model fit

This section was not generated.