



wwPDB X-ray Structure Validation Summary Report

Mar 1, 2014 – 01:24 AM GMT

PDB ID : 3DV0
Title : Snapshots of catalysis in the E1 subunit of the pyruvate dehydrogenase multi-enzyme complex
Authors : Pei, X.Y.; Titman, C.M.; Frank, R.A.W.; Leeper, F.J.; Luisi, B.F.
Deposited on : 2008-07-18
Resolution : 2.50 Å(reported)

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We welcome your comments at validation@mail.wwpdb.org
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

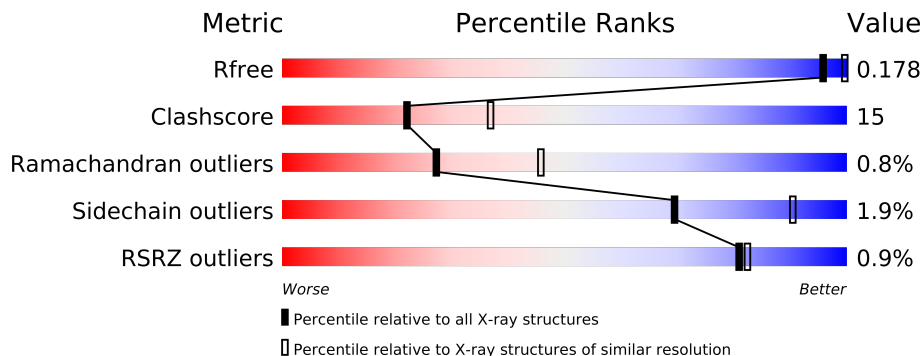
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

The reported resolution of this entry is 2.50 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}	66092	2784 (2.50-2.50)
Clashscore	79885	3562 (2.50-2.50)
Ramachandran outliers	78287	3480 (2.50-2.50)
Sidechain outliers	78261	3482 (2.50-2.50)
RSRZ outliers	66119	2785 (2.50-2.50)

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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	369	
1	C	369	
1	E	369	
1	G	369	
2	B	325	
2	D	325	
2	F	325	
2	H	325	
3	I	428	
3	J	428	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
4	MG	B	1326	-	X
4	MG	C	1368	-	X
4	MG	G	1326	-	X
7	PYR	B	502	-	X
7	PYR	D	502	-	X

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 22633 atoms, of which 0 are hydrogen and 0 are deuterium.

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 Pyruvate dehydrogenase E1 component subunit alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	349	Total	C	N	O	S	0	0	0
			2764	1772	466	519	7			
1	C	351	Total	C	N	O	S	0	0	0
			2776	1779	468	522	7			
1	E	344	Total	C	N	O	S	0	0	0
			2698	1728	456	507	7			
1	G	352	Total	C	N	O	S	0	0	0
			2758	1765	466	520	7			

- Molecule 2 is a protein called Pyruvate dehydrogenase E1 component subunit beta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	324	Total	C	N	O	S	0	0	0
			2488	1586	424	470	8			
2	D	324	Total	C	N	O	S	0	0	0
			2488	1586	424	470	8			
2	F	324	Total	C	N	O	S	0	0	0
			2488	1586	424	470	8			
2	H	324	Total	C	N	O	S	0	0	0
			2489	1586	424	471	8			

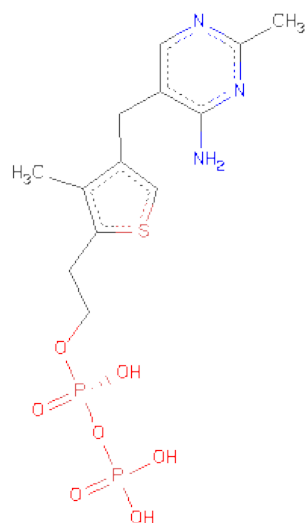
- Molecule 3 is a protein called Dihydrolipoyllysine-residueacetyltransferase component of pyruvate dehydrogenase complex.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	I	43	Total	C	N	O	S	0	0	1
			299	188	54	56	1			
3	J	41	Total	C	N	O	S	0	0	0
			269	165	52	51	1			

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	G	2	Total Mg 2 2	0	0
4	B	1	Total Mg 1 1	0	0
4	A	1	Total Mg 1 1	0	0
4	C	1	Total Mg 1 1	0	0
4	E	1	Total Mg 1 1	0	0

- Molecule 5 is 2-{4-[(4-AMINO-2-METHYLPYRIMIDIN-5-YL)METHYL]-3-METHYLTHIOPHEN-2-YL}ETHYLTRIHYPHROGEN DIPHOSPHATE (three-letter code: TPW) (formula: C₁₃H₁₉N₃O₇P₂S).

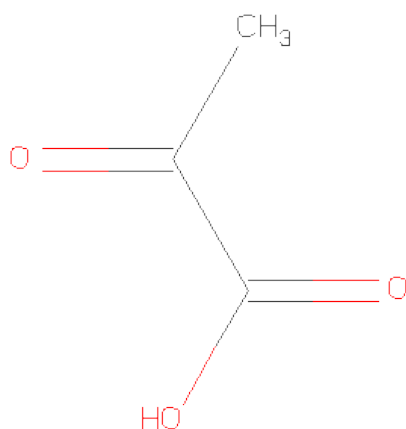


Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
5	A	1	Total 26	C 13	N 3	O 7	P 2	S 1	0	0
5	C	1	Total 26	C 13	N 3	O 7	P 2	S 1	0	0
5	E	1	Total 26	C 13	N 3	O 7	P 2	S 1	0	0
5	G	1	Total 26	C 13	N 3	O 7	P 2	S 1	0	0

- Molecule 6 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	H	1	Total K 1 1	0	0
6	B	1	Total K 1 1	0	0
6	D	1	Total K 1 1	0	0
6	F	1	Total K 1 1	0	0

- Molecule 7 is PYRUVIC ACID (three-letter code: PYR) (formula: $C_3H_4O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	B	1	Total C O 6 3 3	0	0
7	D	1	Total C O 6 3 3	0	0

- Molecule 8 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	125	Total O 125 125	0	0
8	B	143	Total O 143 143	0	0
8	C	146	Total O 146 146	0	0
8	D	151	Total O 151 151	0	0

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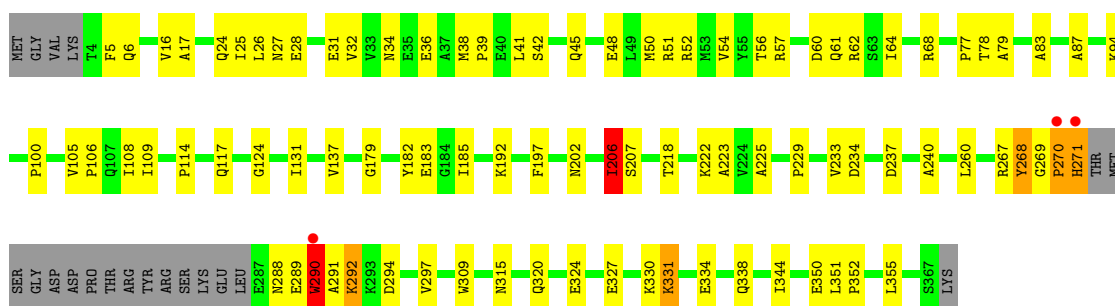
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	E	76	Total 76	O 76	0	0
8	F	87	Total 87	O 87	0	0
8	G	101	Total 101	O 101	0	0
8	H	127	Total 127	O 127	0	0
8	I	19	Total 19	O 19	0	0
8	J	15	Total 15	O 15	0	0

3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

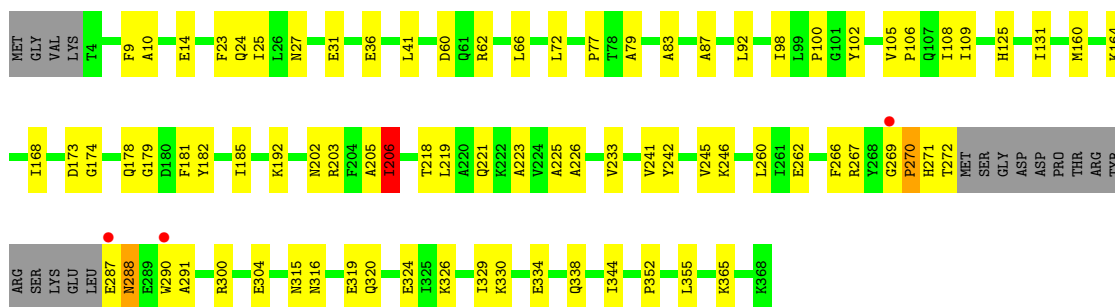
- Molecule 1: Pyruvate dehydrogenase E1 component subunit alpha

Chain A: 



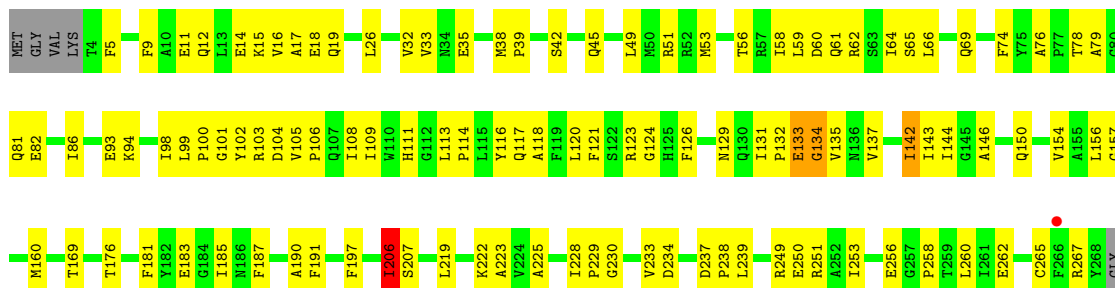
- Molecule 1: Pyruvate dehydrogenase E1 component subunit alpha

Chain C: 

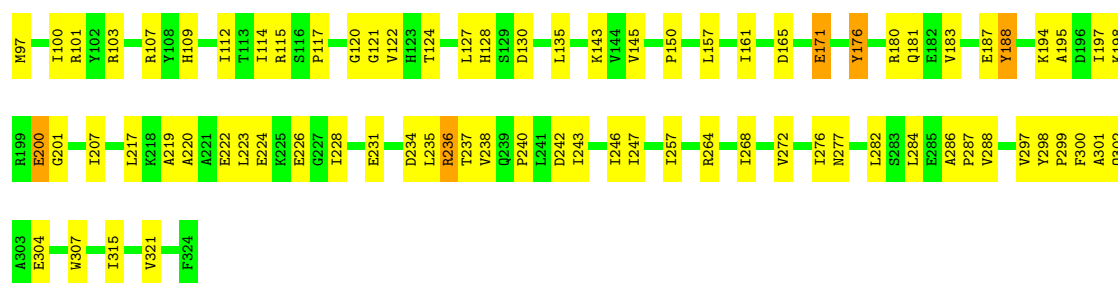


- Molecule 1: Pyruvate dehydrogenase E1 component subunit alpha

Chain E: 

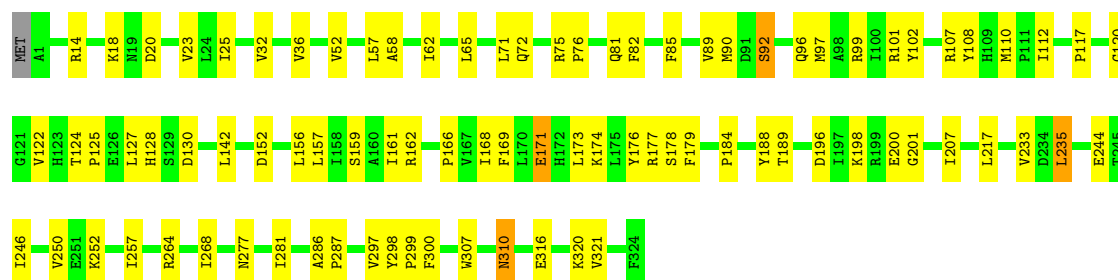






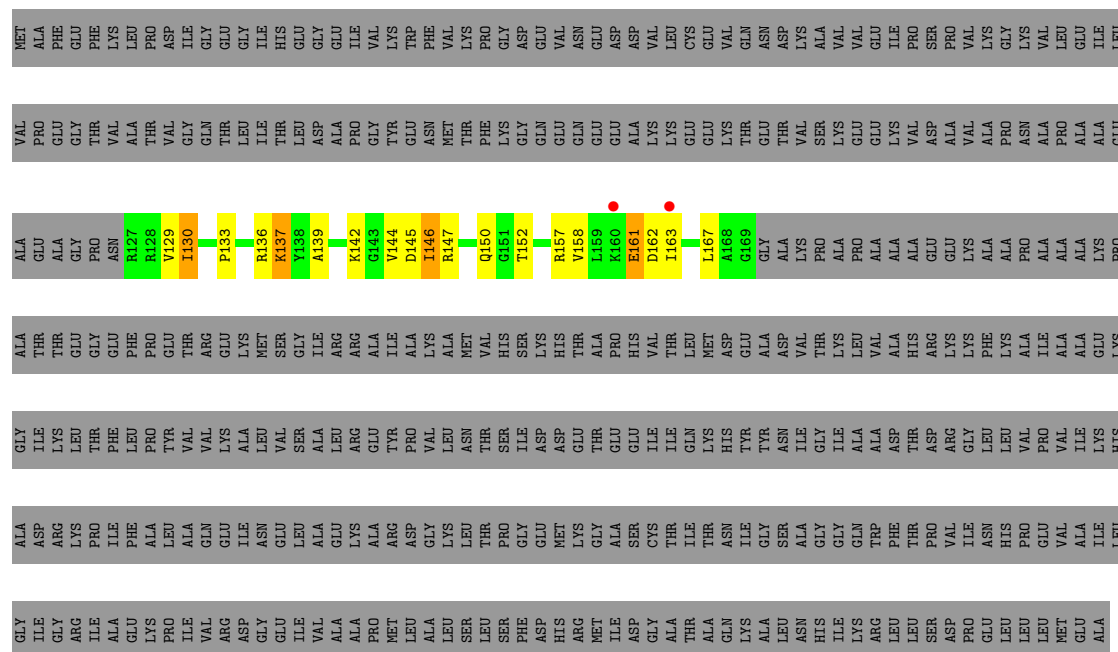
- Molecule 2: Pyruvate dehydrogenase E1 component subunit beta

Chain H:



- Molecule 3: Dihydrolipoyllysine-residueacetyltransferase component of pyruvate dehydrogenase complex

Chain I:



- Molecule 3: Dihydrolipoyllysine-residueacetyltransferase component of pyruvate dehydrogenase complex

Chain J:

[illegible]

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	68.31Å 232.82Å 92.00Å 90.00° 91.83° 90.00°	Depositor
Resolution (Å)	72.17 – 2.50 72.16 – 2.30	Depositor EDS
% Data completeness (in resolution range)	96.2 (72.17-2.50) 87.3 (72.16-2.30)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	0.11	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.26 (at 2.29Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.173 , 0.241 0.177 , 0.178	Depositor DCC
R_{free} test set	4807 reflections (5.32%)	DCC
Wilson B-factor (Å ²)	25.9	Xtriage
Anisotropy	0.424	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 31.4	EDS
Estimated twinning fraction	0.056 for h,-k,-l	Xtriage
L-test for twinning	$\langle L \rangle = 0.42$, $\langle L^2 \rangle = 0.25$	Xtriage
Outliers	0 of 110687 reflections	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	22633	wwPDB-VP
Average B, all atoms (Å ²)	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.73% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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	0.36	0/2824	0.57	1/3816 (0.0%)
1	C	0.35	0/2836	0.56	1/3833 (0.0%)
1	E	0.32	0/2754	0.52	1/3719 (0.0%)
1	G	0.33	0/2815	0.55	1/3803 (0.0%)
2	B	0.35	0/2534	0.64	1/3437 (0.0%)
2	D	0.36	0/2534	0.66	2/3437 (0.1%)
2	F	0.32	0/2534	0.59	0/3437
2	H	0.35	0/2535	0.61	1/3437 (0.0%)
3	I	0.33	0/300	0.55	0/401
3	J	0.33	0/271	0.54	0/363
All	All	0.34	0/21937	0.59	8/29683 (0.0%)

There are no bond length outliers.

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	206	ILE	N-CA-C	-9.09	86.47	111.00
1	C	206	ILE	N-CA-C	-6.92	92.33	111.00
2	D	236	ARG	CB-CA-C	-6.68	97.04	110.40
2	D	237	THR	N-CA-CB	6.43	122.53	110.30
1	A	206	ILE	N-CA-C	-5.82	95.29	111.00

There are no chirality outliers.

There are no planarity outliers.

5.2 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 hydrogens

added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2764	0	2736	74	0
1	C	2776	0	2745	60	0
1	E	2698	0	2664	126	0
1	G	2758	0	2714	117	0
2	B	2488	0	2515	51	0
2	D	2488	0	2515	48	0
2	F	2488	0	2515	102	0
2	H	2489	0	2515	82	0
3	I	299	0	294	19	0
3	J	269	0	232	14	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	E	1	0	0	0	0
4	G	2	0	0	0	0
5	A	26	0	16	3	0
5	C	26	0	16	8	0
5	E	26	0	16	9	0
5	G	26	0	16	3	0
6	B	1	0	0	0	0
6	D	1	0	0	0	0
6	F	1	0	0	0	0
6	H	1	0	0	0	0
7	B	6	0	3	2	0
7	D	6	0	3	1	0
8	A	125	0	0	11	0
8	B	143	0	0	9	0
8	C	146	0	0	11	0
8	D	151	0	0	6	0
8	E	76	0	0	5	0
8	F	87	0	0	6	0
8	G	101	0	0	11	0
8	H	127	0	0	10	0
8	I	19	0	0	1	0
8	J	15	0	0	0	0
All	All	22633	0	21515	645	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 15.

The worst 5 of 645 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
7:B:502:PYR:H32	8:C:1401:HOH:O	1.62	0.98
2:H:76:PRO:HG2	2:H:112:ILE:HG12	1.48	0.95
2:F:122:VAL:HG23	2:F:124:THR:HG23	1.51	0.91
1:A:292:LYS:HD2	1:A:292:LYS:H	1.35	0.91
1:G:27:ASN:HD21	1:G:31:GLU:HB2	1.38	0.86

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	A	345/369 (94%)	329 (95%)	13 (4%)	3 (1%)	25	42
1	C	347/369 (94%)	330 (95%)	15 (4%)	2 (1%)	33	55
1	E	340/369 (92%)	320 (94%)	17 (5%)	3 (1%)	25	42
1	G	346/369 (94%)	320 (92%)	23 (7%)	3 (1%)	25	42
2	B	322/325 (99%)	308 (96%)	14 (4%)	0	100	100
2	D	322/325 (99%)	307 (95%)	13 (4%)	2 (1%)	33	55
2	F	322/325 (99%)	303 (94%)	15 (5%)	4 (1%)	19	32
2	H	322/325 (99%)	307 (95%)	15 (5%)	0	100	100
3	I	39/428 (9%)	34 (87%)	4 (10%)	1 (3%)	8	11
3	J	39/428 (9%)	26 (67%)	9 (23%)	4 (10%)	1	0
All	All	2744/3632 (76%)	2584 (94%)	138 (5%)	22 (1%)	27	46

5 of 22 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	290	TRP
3	J	150	GLN
2	F	81	GLN
1	G	270	PRO

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Mol	Chain	Res	Type
3	J	154	LYS

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	286/305 (94%)	279 (98%)	7 (2%)	61	86
1	C	287/305 (94%)	284 (99%)	3 (1%)	85	97
1	E	277/305 (91%)	272 (98%)	5 (2%)	71	91
1	G	283/305 (93%)	280 (99%)	3 (1%)	84	96
2	B	263/264 (100%)	258 (98%)	5 (2%)	69	90
2	D	263/264 (100%)	261 (99%)	2 (1%)	89	98
2	F	263/264 (100%)	256 (97%)	7 (3%)	57	83
2	H	263/264 (100%)	256 (97%)	7 (3%)	57	83
3	I	27/341 (8%)	23 (85%)	4 (15%)	4	8
3	J	19/341 (6%)	19 (100%)	0	100	100
All	All	2231/2958 (75%)	2188 (98%)	43 (2%)	69	90

5 of 43 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	142	ILE
2	F	109	HIS
3	I	130	ILE
1	E	329	ILE
1	E	335	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 26 such sidechains are listed below:

Mol	Chain	Res	Type
1	E	24	GLN
1	E	150	GLN
2	H	310	ASN

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Mol	Chain	Res	Type
1	E	81	GLN
1	E	129	ASN

5.3.3 RNA ⓘ

There are no RNA chains 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 carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 16 ligands modelled in this entry, 10 are monoatomic - leaving 6 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$
5	TPW	A	1370	-	27,27,27	1.58	3 (11%)	40,40,40	1.77	9 (22%)
7	PYR	B	502	-	5,5,5	2.88	1 (20%)	6,6,6	0.92	0
5	TPW	C	1370	-	27,27,27	1.56	3 (11%)	40,40,40	1.83	9 (22%)
7	PYR	D	502	-	5,5,5	2.87	1 (20%)	6,6,6	0.87	0
5	TPW	E	1370	-	27,27,27	1.57	3 (11%)	40,40,40	1.87	9 (22%)
5	TPW	G	1370	-	27,27,27	1.56	3 (11%)	40,40,40	1.84	10 (25%)

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
5	TPW	A	1370	-	-	0/17/17/17	0/2/2/2
7	PYR	B	502	-	-	0/4/4/4	0/0/0/0
5	TPW	C	1370	-	-	0/17/17/17	0/2/2/2
7	PYR	D	502	-	-	0/4/4/4	0/0/0/0
5	TPW	E	1370	-	-	0/17/17/17	0/2/2/2
5	TPW	G	1370	-	-	0/17/17/17	0/2/2/2

The worst 5 of 14 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	B	502	PYR	O3-C2	6.01	1.36	1.23
7	D	502	PYR	O3-C2	6.00	1.36	1.23
5	A	1370	TPW	C2-C3	-5.65	1.33	1.37
5	E	1370	TPW	C2-C3	-5.62	1.33	1.37
5	G	1370	TPW	C2-C3	-5.55	1.33	1.37

The worst 5 of 37 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	E	1370	TPW	C4-C5-S1	-6.05	105.62	110.91
5	G	1370	TPW	C4-C5-S1	-5.72	105.91	110.91
5	C	1370	TPW	C4-C5-S1	-5.62	106.00	110.91
5	A	1370	TPW	C4-C5-S1	-5.46	106.14	110.91
5	C	1370	TPW	P1-O11-P2	-3.73	120.74	131.68

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

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	349/369 (94%)	-0.51	3 (0%) 81 82	11, 26, 61, 99	2 (0%)
1	C	351/369 (95%)	-0.58	3 (0%) 81 82	8, 24, 60, 100	2 (0%)
1	E	344/369 (93%)	-0.11	2 (0%) 86 88	27, 52, 80, 94	2 (0%)
1	G	352/369 (95%)	-0.30	9 (2%) 53 55	21, 40, 73, 100	2 (0%)
2	B	324/325 (99%)	-0.71	0 100 100	8, 24, 43, 58	0
2	D	324/325 (99%)	-0.67	0 100 100	8, 19, 35, 47	0
2	F	324/325 (99%)	-0.37	0 100 100	21, 40, 61, 81	0
2	H	324/325 (99%)	-0.63	0 100 100	14, 27, 42, 56	0
3	I	43/428 (10%)	0.36	2 (4%) 30 31	39, 61, 73, 82	0
3	J	41/428 (9%)	0.55	5 (12%) 5 4	43, 65, 81, 86	0
All	All	2776/3632 (76%)	-0.45	24 (0%) 81 82	8, 32, 68, 100	8 (0%)

The worst 5 of 24 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	270	PRO	8.2
1	G	269	GLY	6.4
1	A	290	TRP	5.7
1	G	277	ASP	5.1
1	G	279	THR	4.7

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	RSR	LLDF	B-factors(Å ²)	Q<0.9
7	PYR	D	502	6/6	0.75	25.87	44,49,53,61	6
4	MG	G	1326	1/1	0.19	7.82	45,45,45,45	0
4	MG	C	1368	1/1	0.33	6.04	59,59,59,59	0
7	PYR	B	502	6/6	0.40	5.02	37,41,44,57	6
4	MG	B	1326	1/1	0.16	4.28	48,48,48,48	0
4	MG	E	1368	1/1	0.15	1.45	54,54,54,54	0
4	MG	A	1368	1/1	0.17	1.00	12,12,12,12	0
6	K	H	1325	1/1	0.12	0.39	26,26,26,26	0
5	TPW	E	1370	26/26	0.12	0.19	19,37,59,72	0
5	TPW	A	1370	26/26	0.12	0.02	2,16,28,31	0
5	TPW	C	1370	26/26	0.11	-0.16	13,20,27,42	0
4	MG	G	1367	1/1	0.10	-0.69	36,36,36,36	0
5	TPW	G	1370	26/26	0.09	-0.72	21,39,46,52	0
6	K	B	1325	1/1	0.08	-1.49	32,32,32,32	0
6	K	F	1325	1/1	0.08	-1.54	46,46,46,46	0
6	K	D	1325	1/1	0.09	-2.25	15,15,15,15	0

6.5 Other polymers ⓘ

There are no such residues in this entry.