W O R L D W I D E
wwPDB
PROTEIN DATA BANK

wwPDB X-ray Structure Validation Summary Report (i)

Feb 27, 2014 – 11:32 PM GMT

PDB ID   :   3DVA
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 :   2.35 Å(reported)

1 Overall quality at a glance (i)

The reported resolution of this entry is 2.35 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	Percentile Ranks	Value
Rfree		0.246
Clashscore		5
Ramachandran outliers		0.4%
Sidechain outliers		1.8%
RSRZ outliers		2.1%

■ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution
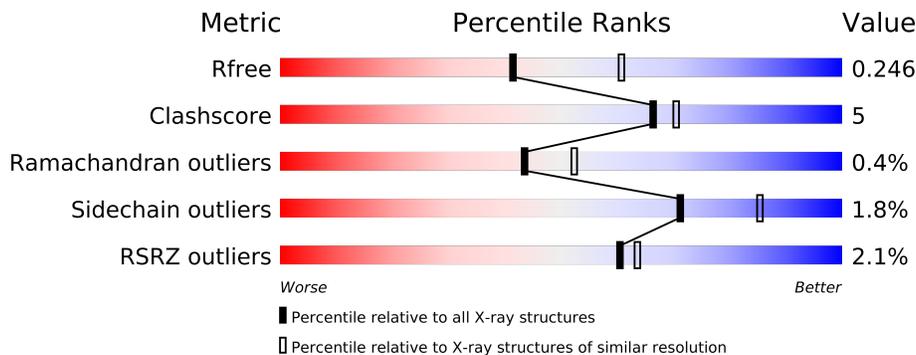
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	66092	3327 (2.40-2.32)
Clashscore	79885	1064 (2.38-2.34)
Ramachandran outliers	78287	1048 (2.38-2.34)
Sidechain outliers	78261	1049 (2.38-2.34)
RSRZ outliers	66119	3330 (2.40-2.32)

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	A	1326	-	X
4	MG	E	369	-	X

2 Entry composition ⓘ

There are 7 unique types of molecules in this entry. The entry contains 23282 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	365	Total	C	N	O	S	0	0	0
			2895	1850	491	546	8			
1	C	365	Total	C	N	O	S	0	0	0
			2895	1850	491	546	8			
1	E	354	Total	C	N	O	S	0	0	0
			2798	1791	473	526	8			
1	G	365	Total	C	N	O	S	0	0	0
			2895	1850	491	546	8			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	206	ALA	ILE	ENGINEERED	UNP P21873
C	206	ALA	ILE	ENGINEERED	UNP P21873
E	206	ALA	ILE	ENGINEERED	UNP P21873
G	206	ALA	ILE	ENGINEERED	UNP P21873

- 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
			2488	1586	424	470	8			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	I	42	Total 314	C 195	N 62	O 56	S 1	0	0	0
3	J	40	Total 294	C 180	N 59	O 54	S 1	0	0	0

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

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

- Molecule 5 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	1	Total 1	K 1	0	0
5	D	1	Total 1	K 1	0	0

- Molecule 6 is 2-{4-[(4-AMINO-2-METHYLPYRIMIDIN-5-YL)METHYL]-3-METHYL THIOPHEN-2-YL}ETHYLTRIHYDROGEN DIPHOSPHATE (three-letter code: TPW) (formula: $C_{13}H_{19}N_3O_7P_2S$).
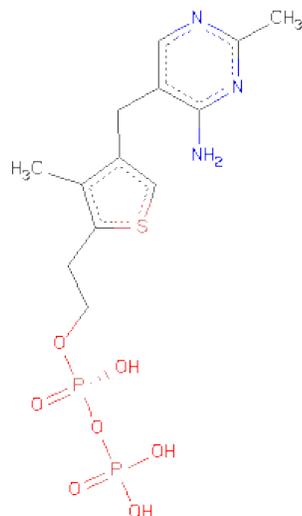
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
6	A	1	Total	C	N	O	P	S	0	0
			26	13	3	7	2	1		
6	C	1	Total	C	N	O	P	S	0	0
			26	13	3	7	2	1		
6	E	1	Total	C	N	O	P	S	0	0
			26	13	3	7	2	1		
6	G	1	Total	C	N	O	P	S	0	0
			26	13	3	7	2	1		

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	150	Total	O	0	0
			150	150		
7	B	139	Total	O	0	0
			139	139		
7	C	148	Total	O	0	0
			148	148		
7	D	161	Total	O	0	0
			161	161		
7	E	100	Total	O	0	0
			100	100		
7	F	126	Total	O	0	0
			126	126		
7	G	139	Total	O	0	0
			139	139		
7	H	155	Total	O	0	0
			155	155		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	I	5	Total 5	O 5	0	0
7	J	4	Total 4	O 4	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
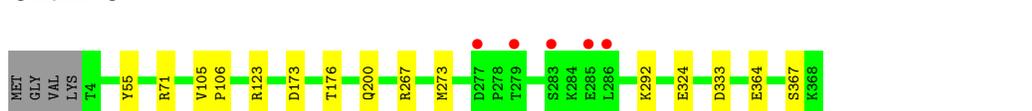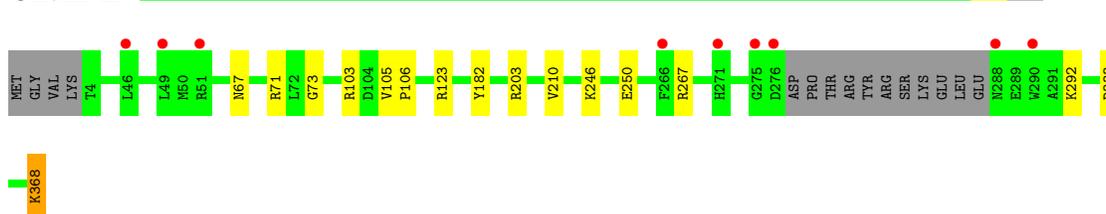
Chain A:

• Molecule 1: Pyruvate dehydrogenase E1 component subunit alpha

Chain C:

• Molecule 1: Pyruvate dehydrogenase E1 component subunit alpha
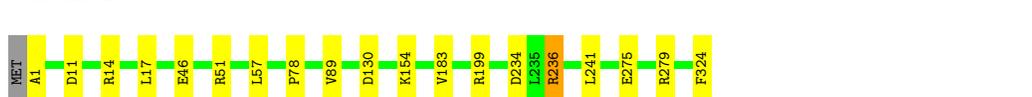
Chain E:

• Molecule 1: Pyruvate dehydrogenase E1 component subunit alpha
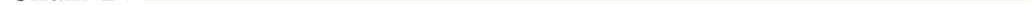
Chain G:

• Molecule 2: Pyruvate dehydrogenase E1 component subunit beta

Chain B:

• Molecule 2: Pyruvate dehydrogenase E1 component subunit beta

Chain D:

MET A1   D50   R101   D130   E187   R236   N271   E285   F324

• Molecule 2: Pyruvate dehydrogenase E1 component subunit beta

Chain F:

MET A1   R14   L17   G31   V36   E46   D50   R51   D54   R99   R103   M110   E126   L127   H128   S129   D130   K143   T149   D152   A153   K154   R162   D163   G186   E187   E231   R236   K252   Y298   A301   Q302   A303   E304   F324

• Molecule 2: Pyruvate dehydrogenase E1 component subunit beta

Chain H:

MET A1   Q72   R107   R115   F118   D130   K143   K154   D163   I168   E171   H172   L173   Y176   G186   E226   K319   F324

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

Chain I:

MET ALA PHE GLU PHE LYS LEU PRO ASP ILE GLY GLU GLY ILE HIS GLU GLY ILE VAL LEU TRP PHE VAL LYS PRO GLY ASP GLU VAL ASN GLU ASP ASP VAL LEU CYS GLU VAL GLN ASN ASP LYS ALA VAL VAL GLU ILE PRO SER PRO VAL LYS GLY LYS VAL LEU GLU ILE LEU

VAL PRO GLU GLY THR VAL ALA THR VAL GLY GLN THR LEU ILE THR LEU ASP ALA PRO GLY TYR GLU ASN MET THR PHE LYS GLY GLN GLU GLU GLU GLU ALA LYS GLU GLU LYS THR GLU VAL SER LYS GLU GLU LYS VAL ASP ALA VAL ALA PRO ASN ALA PRO ALA ALA GLU

ALA GLU ALA GLY PRO ASN ARG R128 V129 I130 R136 K137 Y138 A139 R140 E141 V144 D145 I146 R147 L148 G151 K154 M155 G156 R157 V158 L159 K160 E161 D162 I163 D164 A165 F166 L167 A168 G169 GLY ALA LYS PRO ALA PRO ALA ALA GLU GLU LYS ALA ALA PRO ALA ALA ALA

LYS PRO ALA THR THR GLU GLY GLU PHE PRO GLU THR ARG GLU LYS MET SER GLY ILE ARG ARG ALA ILE ALA LYS ALA MET VAL HIS SER LYS HIS THR ALA PRO HIS VAL THR LEU MET ASP GLU ALA ASP VAL THR LYS LEU VAL ALA HIS ARG LYS LYS PHE LYS ALA ILE ALA ALA

GLU LYS GLY ILE LYS LEU THR PHE LEU PRO TYR VAL VAL LYS ALA LEU VAL SER ALA LEU ARG GLU GLU TYR PRO VAL LEU ASN THR SER ILE ASP ASP GLU THR GLU GLU ILE ILE GLN LYS HIS TYR TYR ASN ILE GLY ILE ALA ALA ASP THR ASP ARG GLY LEU LEU VAL PRO VAL ILE

LYS HIS ALA ASP ARG LYS PRO ILE PHE ALA LEU ALA GLN GLU ILE ASN GLU LEU ALA GLU ARG ASP SER GLY LYS LEU THR PRO GLY GLU MET LYS GLY ALA SER CYS THR ILE THR ASN ILE GLY SER ALA GLY GLY GLN TRP PHE THR PRO VAL ILE ASN HIS PRO GLU VAL ALA

ILE LEU GLY ILE GLY ARG ILE ALA GLU ILE PRO LYS PRO ILE LEU VAL ARG ASP GLY ILE GLU ILE VAL ALA ALA PRO MET LEU ALA LEU SER LEU SER PHE ASP HIS ARG MET ILE ASP GLY ALA THR ALA GLN LYS ALA LEU ASN HIS ILE LYS ARG LEU LEU SER ASP PRO GLU LEU LEU LEU MET GLU

ALA

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

Chain J:

MET ALA PHE GLU PHE LYS LEU PRO ASP ILE GLY GLU GLY ILE HIS GLU GLY ILE VAL LEU TRP PHE VAL LYS PRO GLY ASP GLU VAL ASN GLU ASP ASP VAL LEU CYS GLU VAL GLN ASN ASP LYS ALA VAL VAL GLU ILE PRO SER PRO VAL LYS GLY LYS VAL LEU GLU ILE LEU

VAL PRO GLU GLY THR VAL ALA THR VAL GLY GLN THR LEU ILE THR LEU ASP ALA PRO GLY TYR GLU ASN MET THR PHE LYS GLY GLN GLU GLN GLU GLU ALA LYS GLU GLU LYS THR GLU THR VAL SER LYS GLU GLU LYS VAL ASP VAL ALA PRO ASN ALA PRO ALA ALA GLU

ALA GLU ALA GLY PRO ASN ARG R128 V129 E141 V144 D145 I146 R147 L148 V149 Q150 G151 T152 G153 K154 N155 G156 R157 V158 L159 K160 E161 D162 I163 D164 A165 F166 L167 ALA GLY GLY ALA LYS PRO ALA PRO ALA ALA ALA GLU GLU LYS ALA ALA PRO ALA ALA ALA LYS PRO ALA THR

THR GLU GLY GLU PHE PRO GLU THR ARG GLU LYS MET SER GLY ILE ARG ALA ILE ALA LYS MET VAL HIS SER LYS HIS THR ALA PRO HIS VAL THR LEU MET ASP GLU ALA ASP VAL THR LYS LEU VAL ALA HIS ARG LYS LYS PHE LYS ALA ILE ALA ALA GLU GLU LYS ALA ALA PRO ALA ALA ALA LYS GLY ILE

LYS LEU THR PHE LEU PRO TYR VAL VAL LYS ALA LEU VAL SER ALA LEU ARG GLU ILE ALA LYS MET VAL HIS SER LYS HIS THR ALA PRO VAL LEU ASN THR SER ILE ASP GLU GLU THR GLU GLU GLU ILE ILE GLN LYS HIS TYR TYR ASN ILE GLY ILE ALA ALA ASP THR ALA ARG GLY LEU LEU VAL PRO VAL ILE LYS HIS ALA ASP

ARG LYS PRO ILE PHE ALA LEU LEU GLN GLU ILE ASN GLU LEU ALA GLU GLY LYS ALA LEU ARG GLU ASP GLY LYS LEU THR PRO GLY GLU MET LYS GLY ALA SER CYS THR ILE THR GLN LYS HIS TYR ASN ILE GLY SER ALA GLY GLY GLN TRP PHE THR PRO VAL ILE ASN HIS PRO GLU VAL ALA ILE LYS LEU GLY ILE

GLY ARG ILE ALA GLU LYS PRO ILE VAL ARG ASP GLY GLU ILE VAL ALA ALA PRO MET LEU ALA LEU SER LEU SER PHE ASP HIS ARG MET ILE ASP GLY ALA THR ALA GLN LYS ALA LEU ASN HIS ILE LYS ARG LEU LEU SER ASP PRO GLU GLU LEU LEU MET GLU ALA

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	68.67Å 232.29Å 91.94Å 90.00° 91.20° 90.00°	Depositor
Resolution (Å)	72.17 – 2.35 72.08 – 2.35	Depositor EDS
% Data completeness (in resolution range)	98.9 (72.17-2.35) 98.9 (72.08-2.35)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	0.09	Depositor
$< I/\sigma(I) >$ [1]	5.04 (at 2.34Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.190 , 0.247 0.191 , 0.246	Depositor DCC
R_{free} test set	5906 reflections (5.27%)	DCC
Wilson B-factor (Å^2)	25.7	Xtriage
Anisotropy	0.395	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 22.1	EDS
Estimated twinning fraction	0.049 for h,-k,-l	Xtriage
L-test for twinning	$< |L| > = 0.44, < L^2 > = 0.26$	Xtriage
Outliers	0 of 117882 reflections	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	23282	wwPDB-VP
Average B, all atoms (Å^2)	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.53% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities 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, K, 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	0.38	0/2958	0.53	1/3995 (0.0%)
1	C	0.35	0/2958	0.48	0/3995
1	E	0.33	0/2858	0.45	0/3859
1	G	0.31	0/2958	0.47	0/3995
2	B	0.40	0/2534	0.55	2/3437 (0.1%)
2	D	0.27	0/2534	0.53	1/3437 (0.0%)
2	F	0.26	0/2534	0.52	1/3437 (0.0%)
2	H	0.28	0/2534	0.51	0/3437
3	I	1.44	1/316 (0.3%)	1.17	1/421 (0.2%)
3	J	1.54	0/295	1.16	1/395 (0.3%)
All	All	0.41	1/22479 (0.0%)	0.53	7/30408 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	I	138	TYR	CD2-CE2	-5.70	1.30	1.39

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	277	ASP	CB-CG-OD1	-7.67	111.40	118.30
2	B	234	ASP	CB-CG-OD1	6.80	124.42	118.30
2	B	236	ARG	CB-CA-C	-5.90	98.59	110.40
2	D	236	ARG	CB-CA-C	-5.84	98.72	110.40
3	J	162	ASP	CB-CG-OD1	-5.63	113.23	118.30

There are no chirality outliers.

There are no planarity outliers.

5.2 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 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	2895	0	0	15	0
1	C	2895	0	0	11	0
1	E	2798	0	0	12	0
1	G	2895	0	0	11	0
2	B	2488	0	0	9	0
2	D	2488	0	0	3	0
2	F	2488	0	0	13	0
2	H	2488	0	0	9	0
3	I	314	0	14	17	0
3	J	294	0	30	18	0
4	A	2	0	0	0	0
4	C	1	0	0	0	0
4	E	2	0	0	0	0
4	G	1	0	0	0	0
5	B	1	0	0	0	0
5	D	1	0	0	0	0
6	A	26	0	16	1	0
6	C	26	0	16	2	0
6	E	26	0	16	1	0
6	G	26	0	16	2	0
7	A	150	0	0	2	0
7	B	139	0	0	1	0
7	C	148	0	0	4	0
7	D	161	0	0	2	0
7	E	100	0	0	3	0
7	F	126	0	0	3	0
7	G	139	0	0	3	0
7	H	155	0	0	1	0
7	I	5	0	0	0	0
7	J	4	0	0	1	0
All	All	23282	0	108	114	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 5.

The worst 5 of 114 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:281:TYR:CB	1:A:282:ARG:CA	2.44	0.96
1:A:277:ASP:N	1:A:278:PRO:CD	2.30	0.91
2:D:285:GLU:CG	3:I:140:ARG:NH2	2.41	0.83
3:I:159:LEU:CB	3:I:161:GLU:OE1	2.29	0.80
3:I:160:LYS:O	3:I:161:GLU:CG	2.30	0.80

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	363/369 (98%)	352 (97%)	11 (3%)	0	100	100
1	C	363/369 (98%)	350 (96%)	13 (4%)	0	100	100
1	E	350/369 (95%)	339 (97%)	11 (3%)	0	100	100
1	G	363/369 (98%)	353 (97%)	10 (3%)	0	100	100
2	B	322/325 (99%)	315 (98%)	6 (2%)	1 (0%)	50	62
2	D	322/325 (99%)	312 (97%)	9 (3%)	1 (0%)	50	62
2	F	322/325 (99%)	307 (95%)	12 (4%)	3 (1%)	25	27
2	H	322/325 (99%)	307 (95%)	15 (5%)	0	100	100
3	I	40/428 (9%)	31 (78%)	4 (10%)	5 (12%)	1	0
3	J	38/428 (9%)	30 (79%)	6 (16%)	2 (5%)	3	1
All	All	2805/3632 (77%)	2696 (96%)	97 (4%)	12 (0%)	43	52

5 of 12 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	236	ARG
3	J	165	ALA
2	F	301	ALA
3	I	161	GLU
3	I	167	LEU

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	301/304 (99%)	293 (97%)	8 (3%)	57	74
1	C	301/304 (99%)	299 (99%)	2 (1%)	91	96
1	E	290/304 (95%)	289 (100%)	1 (0%)	96	98
1	G	301/304 (99%)	298 (99%)	3 (1%)	85	93
2	B	263/264 (100%)	260 (99%)	3 (1%)	84	93
2	D	263/264 (100%)	260 (99%)	3 (1%)	84	93
2	F	263/264 (100%)	260 (99%)	3 (1%)	84	93
2	H	263/264 (100%)	262 (100%)	1 (0%)	95	98
3	I	30/341 (9%)	21 (70%)	9 (30%)	0	0
3	J	28/341 (8%)	20 (71%)	8 (29%)	0	0
All	All	2303/2954 (78%)	2262 (98%)	41 (2%)	71	85

5 of 41 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	F	130	ASP
1	G	211	GLU
3	J	150	GLN
2	F	302	GLN
1	G	36	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 12 ligands modelled in this entry, 8 are monoatomic - leaving 4 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	#$|Z| > 2$
6	TPW	A	1370	4	27,27,27	2.01	4 (14%)	40,40,40	1.92	10 (25%)
6	TPW	C	1370	4	27,27,27	1.91	4 (14%)	40,40,40	2.06	8 (20%)
6	TPW	E	1370	4	27,27,27	1.93	5 (18%)	40,40,40	1.93	10 (25%)
6	TPW	G	1370	4	27,27,27	1.92	5 (18%)	40,40,40	1.90	8 (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
6	TPW	A	1370	4	-	0/17/17/17	0/2/2/2
6	TPW	C	1370	4	-	0/17/17/17	0/2/2/2
6	TPW	E	1370	4	-	0/17/17/17	0/2/2/2
6	TPW	G	1370	4	-	0/17/17/17	0/2/2/2

The worst 5 of 18 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	1370	TPW	C5-S1	-7.95	1.67	1.73
6	E	1370	TPW	C5-S1	-7.12	1.68	1.73
6	G	1370	TPW	C5-S1	-6.82	1.68	1.73
6	C	1370	TPW	C5-S1	-6.78	1.68	1.73
6	E	1370	TPW	C2-C3	-4.00	1.34	1.37

The worst 5 of 36 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	C	1370	TPW	C4-C5-S1	-5.74	105.89	110.91
6	G	1370	TPW	C4-C5-S1	-5.25	106.32	110.91
6	A	1370	TPW	C4-C5-S1	-4.99	106.55	110.91
6	E	1370	TPW	C4-C5-S1	-4.95	106.58	110.91
6	C	1370	TPW	C2-S1-C5	4.62	97.52	91.37

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	365/369 (98%)	0.10	15 (4%)	35	39	15, 25, 44, 58	2 (0%)
1	C	365/369 (98%)	-0.04	5 (1%)	72	76	14, 24, 45, 58	2 (0%)
1	E	354/369 (95%)	0.14	9 (2%)	54	58	21, 32, 48, 60	2 (0%)
1	G	365/369 (98%)	-0.02	5 (1%)	72	76	20, 29, 48, 55	2 (0%)
2	B	324/325 (99%)	-0.19	0	100	100	16, 24, 34, 38	0
2	D	324/325 (99%)	-0.17	0	100	100	15, 20, 27, 30	0
2	F	324/325 (99%)	-0.12	2 (0%)	86	89	21, 27, 34, 36	0
2	H	324/325 (99%)	-0.14	1 (0%)	91	94	21, 25, 31, 32	0
3	I	42/428 (9%)	1.63	12 (28%)	1	1	22, 62, 70, 74	0
3	J	40/428 (9%)	1.40	11 (27%)	1	1	20, 53, 75, 78	0
All	All	2827/3632 (77%)	-0.00	60 (2%)	60	63	14, 26, 47, 78	8 (0%)

The worst 5 of 60 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	283	SER	7.8
1	A	286	LEU	7.4
1	C	286	LEU	6.1
1	A	281	TYR	6.0
3	I	128	ARG	5.7

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
4	MG	E	369	1/1	0.31	9.00	45,45,45,45	0
4	MG	A	1326	1/1	0.17	3.68	30,30,30,30	0
4	MG	A	1368	1/1	0.12	-0.07	3,3,3,3	0
6	TPW	A	1370	26/26	0.12	-0.34	13,13,15,15	0
4	MG	C	1368	1/1	0.11	-0.44	7,7,7,7	0
6	TPW	E	1370	26/26	0.10	-0.61	19,20,20,20	0
4	MG	G	369	1/1	0.11	-0.69	16,16,16,16	0
6	TPW	C	1370	26/26	0.10	-0.80	12,12,13,13	0
6	TPW	G	1370	26/26	0.10	-0.85	23,23,24,24	0
4	MG	E	370	1/1	0.09	-2.32	33,33,33,33	0
5	K	D	1325	1/1	0.07	-3.33	10,10,10,10	0
5	K	B	1325	1/1	0.05	-3.71	16,16,16,16	0

6.5 Other polymers ⓘ

There are no such residues in this entry.