



Full wwPDB X-ray Structure Validation Report

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)

This is a full wwPDB validation report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

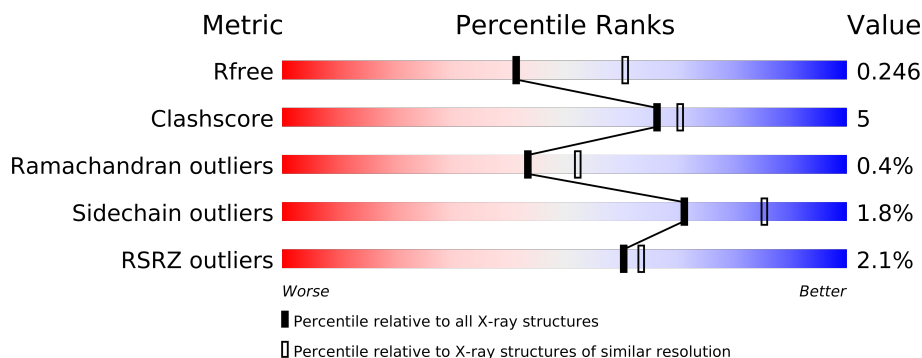
The following versions of software and data (see [references](#)) were used in the production of this report:

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 2.35 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	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	C	N	O	S	0	0	0
			314	195	62	56	1			
3	J	40	Total	C	N	O	S	0	0	0
			294	180	59	54	1			

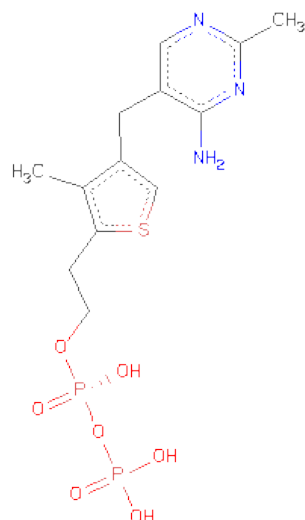
- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

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

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

- Molecule 6 is 2-{4-[(4-AMINO-2-METHYLPYRIMIDIN-5-YL)METHYL]-3-METHYLTHIOPHEN-2-YL}ETHYLTRIHYDROGEN DIPHOSPHATE (three-letter code: TPW) (formula: C₁₃H₁₉N₃O₇P₂S).



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	O	0	0
			5	5		
7	J	4	Total	O	0	0
			4	4		

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: 



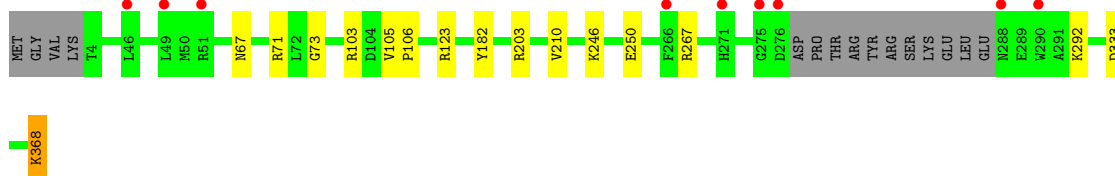
- Molecule 1: Pyruvate dehydrogenase E1 component subunit alpha

Chain C: 



- Molecule 1: Pyruvate dehydrogenase E1 component subunit alpha

Chain E: 



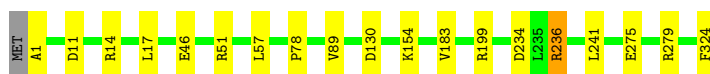
- Molecule 1: Pyruvate dehydrogenase E1 component subunit alpha

Chain G: 



- Molecule 2: Pyruvate dehydrogenase E1 component subunit beta

Chain B: 



- Molecule 2: Pyruvate dehydrogenase E1 component subunit beta

Chain D: 



GLY	ARG	LYS	THR	THR	GLY	THR	ALA	GLU	ALA	VAL
ILE	PRO	LYS	THR	GLY	GLY	GLY	ALA	GLU	ALA	PRO
ALA	ILE	ILE	PHE	LEU	PHE	PRO	GLY	PRO	GLY	THR
LYS	ALA	PRO	PRO	PRO	PRO	PRO	ASN	ASN	VAL	VAL
PRO	LEU	LEU	VAL	VAL	TYR	GLU	ARG	R128	ALA	ALA
ILE	ALA	VAL	VAL	VAL	VAL	THR	ARG	V129	VAL	VAL
ARG	GLN	VAL	LYS	GLU	GLU	LYS	GLU	E141	GLN	GLN
ASP	ILE	ASN	LEU	LEU	MET	MET	THR	THR	THR	THR
GLY	ASN	LEU	VAL	VAL	SER	GLY	VAL	V144	LEU	LEU
GLU	GLU	VAL	SER	SER	GLY	ILE	D145	D145	ILE	ILE
VAL	ALA	ALA	ALA	ALA	ILE	ILE	I146	I146	THR	THR
ALA	GLU	LEU	LEU	ARG	ARG	ARG	R147	R147	LEU	LEU
ALA	LYS	ARG	ARG	ARG	ALA	ALA	L148	L148	ASP	ASP
PRO	ALA	GLU	GLU	ALA	ILE	ILE	V149	V149	ALA	ALA
MET	ARG	TYR	TYR	TYR	ILE	ILE	Q150	Q150	PRO	PRO
LEU	ASP	VAL	VAL	VAL	ALA	ALA	G151	G151	GLY	GLY
ALA	GLY	LYS	VAL	LYS	LYS	LYS	T152	T152	TYR	TYR
SER	LEU	ASN	LEU	LEU	ALA	ALA	G153	G153	GLU	GLU
LEU	LEU	THR	THR	THR	MET	MET	K154	K154	ASN	ASN
SER	THR	THR	THR	THR	VAL	VAL	N155	N155	MET	MET
LEU	PRO	SER	SER	SER	HIS	HIS	G156	G156	THR	THR
PHE	GLY	GLU	ILE	ASP	LYS	LYS	R157	R157	PHE	PHE
ASP	GLU	ASP	ASP	ASP	LYS	LYS	V158	V158	GLY	GLY
HIS	MET	GLY	GLU	GLU	HIS	HIS	L159	L159	GLY	GLY
ARG	GLY	LYS	GLU	THR	THR	THR	K160	K160	GLN	GLN
MET	GLY	THR	THR	THR	ALA	ALA	E161	E161	GLU	GLU
ILE	ALA	GLU	GLU	GLU	PRO	PRO	D162	D162	GLN	GLN
ASP	SER	ILE	ILE	ILE	HIS	HIS	I163	I163	GLU	GLU
GLY	CYS	ILE	ILE	ILE	VAL	VAL	D164	D164	ALA	ALA
ALA	THR	ILE	GLN	LYS	THR	THR	A165	A165	LYS	LYS
THR	ILE	THR	ILE	MET	LEU	LEU	F166	F166	LYS	LYS
ALA	THR	THR	LYS	MET	MET	MET	L167	L167	GLY	GLY
GLN	ASN	ASN	HIS	ASP	ASP	ASP	ALA	ALA	GLU	GLU
LYS	ILE	TYR	TYR	TYR	GLU	GLU	GLY	GLY	GLY	GLY
LEU	GLY	ASN	ASN	ASN	ALA	ALA	ALA	ALA	THR	THR
ASN	ALA	ILE	ILE	ILE	VAL	VAL	LYS	LYS	GLU	GLU
HIS	GLY	GLY	GLY	GLY	THR	THR	PRO	PRO	THR	THR
ILE	GLY	ILE	ILE	ILE	LYS	LYS	VAL	VAL	VAL	VAL
LYS	GLN	ALA	ALA	ALA	LEU	LEU	ALA	ALA	VAL	VAL
ARG	TRP	PHE	ASP	ASP	VAL	VAL	ALA	ALA	LYS	LYS
LEU	LEU	THR	THR	THR	HIS	HIS	ALA	ALA	GLY	GLY
LEU	LEU	THR	THR	THR	ASP	ASP	GLU	GLU	VAL	VAL
SER	SER	ASP	ASP	ASP	ARG	ARG	LYS	LYS	ASP	ASP
PRO	PRO	ILE	ILE	ILE	GLY	GLY	GLU	GLU	VAL	VAL
GLU	GLU	ASN	LEU	LEU	PHE	PHE	ALA	ALA	ALA	ALA
LEU	LEU	HIS	LEU	LEU	LYS	LYS	ALA	ALA	VAL	VAL
LEU	LEU	PRO	VAL	VAL	VAL	VAL	PRO	PRO	ALA	ALA
LEU	LEU	GLU	PRO	PRO	ILE	ILE	ALA	ALA	PRO	PRO
MET	GLU	VAL	VAL	VAL	THR	THR	ALA	ALA	ASN	ASN
GLU	GLU	ALA	ILE	ILE	ALA	ALA	ALA	ALA	ALA	ALA
ALA	ILE	ILE	LYS	LYS	GLU	GLU	LYS	LYS	PRO	PRO
ALA	ALA	LEU	HIS	HIS	THR	THR	PRO	PRO	ALA	ALA
ALA	THR	THR	THR	THR	LYS	LYS	THR	THR	ALA	ALA
ALA	GLY	GLY	GLY	GLY	THR	THR	LYS	LYS	GLY	GLY

4 Data and refinement statistics

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
$\langle I/\sigma(I) \rangle$ 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	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.26$	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.*

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, 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

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
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
2	F	236	ARG	CB-CA-C	-5.61	99.18	110.40
3	I	145	ASP	N-CA-C	-5.16	97.08	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	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.

All (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
3:J:160:LYS:O	3:J:160:LYS:CG	2.30	0.80
3:I:160:LYS:CG	3:I:160:LYS:O	2.29	0.78
3:J:164:ASP:O	3:J:165:ALA:CB	2.30	0.76
1:C:123:ARG:NH1	1:C:333:ASP:OD1	2.20	0.75
3:J:154:LYS:C	3:J:156:GLY:N	2.41	0.72
3:I:166:PHE:C	3:I:168:ALA:N	2.44	0.71
2:D:271:ASN:ND2	7:D:1427:HOH:O	2.25	0.69
3:J:144:VAL:CG1	3:J:145:ASP:N	2.55	0.68
1:A:40:GLU:OE1	1:A:246:LYS:NZ	2.26	0.67
3:J:154:LYS:O	3:J:156:GLY:N	2.29	0.66
3:J:163:ILE:N	3:J:163:ILE:HD13	2.10	0.65
3:I:154:LYS:O	3:I:155:ASN:CB	2.46	0.64
1:E:71:ARG:NH1	7:E:1498:HOH:O	2.29	0.64
3:I:160:LYS:C	3:I:161:GLU:CG	2.67	0.63
2:F:149:THR:N	7:F:1357:HOH:O	2.32	0.62
1:G:7:PHE:N	7:G:1449:HOH:O	2.31	0.62
1:E:267:ARG:NH2	7:E:1518:HOH:O	2.32	0.62
3:J:156:GLY:O	3:J:157:ARG:C	2.36	0.62
1:C:123:ARG:NH2	1:C:333:ASP:OD1	2.32	0.61
1:C:267:ARG:NH1	7:C:1471:HOH:O	2.34	0.60
3:J:156:GLY:C	3:J:157:ARG:O	2.35	0.60
2:B:199:ARG:NH2	7:B:1457:HOH:O	2.37	0.57
1:A:147:GLN:OE1	1:A:147:GLN:N	2.37	0.57
1:E:292:LYS:NZ	7:E:1442:HOH:O	2.37	0.57
1:C:123:ARG:CZ	1:C:333:ASP:OD1	2.53	0.57
3:J:166:PHE:O	3:J:167:LEU:CB	2.54	0.55
3:I:159:LEU:O	3:I:161:GLU:N	2.39	0.55
2:B:324:PHE:O	3:I:157:ARG:NH2	2.40	0.54
3:J:152:THR:OG1	3:J:162:ASP:OD2	2.26	0.53
6:C:1370:TPW:H2	7:C:1455:HOH:O	2.09	0.53
2:F:14:ARG:NH1	2:F:46:GLU:OE1	2.42	0.53
3:I:129:VAL:CG2	3:I:130:ILE:N	2.72	0.53
3:J:157:ARG:CD	7:J:432:HOH:O	2.58	0.52
2:H:143:LYS:NZ	2:H:163:ASP:OD2	2.44	0.51
1:G:271:HIS:CE1	6:G:1370:TPW:H5A2	2.46	0.50
3:J:156:GLY:O	3:J:157:ARG:O	2.29	0.50
3:J:154:LYS:O	3:J:155:ASN:CB	2.59	0.50
3:I:148:LEU:O	3:I:166:PHE:CZ	2.64	0.50

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:I:138:TYR:OH	3:I:164:ASP:OD1	2.30	0.49
2:H:226:GLU:OE1	2:H:319:LYS:NZ	2.45	0.49
1:G:254:ASN:ND2	7:G:1447:HOH:O	2.45	0.49
1:A:123:ARG:NH2	1:A:333:ASP:OD1	2.46	0.49
2:F:17:LEU:O	2:F:51:ARG:NH1	2.45	0.49
2:B:17:LEU:O	2:B:51:ARG:NH1	2.46	0.48
1:C:105:VAL:N	1:C:106:PRO:CD	2.77	0.48
2:D:101:ARG:NH1	7:D:1538:HOH:O	2.47	0.48
1:C:55:TYR:OH	1:C:324:GLU:OE1	2.33	0.47
3:I:162:ASP:N	3:I:162:ASP:OD1	2.44	0.47
2:F:154:LYS:NZ	2:F:186:GLY:O	2.48	0.47
1:G:31:GLU:OE1	1:G:31:GLU:N	2.48	0.47
1:A:292:LYS:N	1:A:292:LYS:CD	2.77	0.47
1:E:246:LYS:NZ	1:E:250:GLU:OE2	2.48	0.47
1:A:278:PRO:O	1:A:279:THR:CG2	2.63	0.46
2:F:162:ARG:NH2	2:F:187:GLU:OE1	2.47	0.46
2:F:143:LYS:NZ	2:F:163:ASP:OD2	2.48	0.46
2:B:1:ALA:N	2:B:183:VAL:O	2.48	0.46
1:C:71:ARG:O	1:C:123:ARG:NE	2.49	0.46
2:B:11:ASP:OD2	2:B:154:LYS:NZ	2.49	0.46
2:H:115:ARG:NE	2:H:171:GLU:OE2	2.48	0.46
1:A:267:ARG:NE	7:A:1415:HOH:O	2.49	0.46
1:G:105:VAL:N	1:G:106:PRO:CD	2.78	0.46
1:C:200:GLN:NE2	7:C:1461:HOH:O	2.49	0.46
2:F:126:GLU:O	2:F:128:HIS:ND1	2.49	0.46
3:I:137:LYS:O	3:I:137:LYS:CG	2.64	0.45
2:H:72:GLN:NE2	7:H:1462:HOH:O	2.49	0.45
1:E:123:ARG:NH2	1:E:333:ASP:OD1	2.49	0.45
1:G:147:GLN:OE1	1:G:147:GLN:N	2.50	0.45
1:A:105:VAL:N	1:A:106:PRO:CD	2.79	0.45
2:B:89:VAL:O	2:B:89:VAL:CG2	2.65	0.45
3:I:166:PHE:O	3:I:168:ALA:N	2.50	0.44
1:E:123:ARG:NH1	1:E:333:ASP:OD1	2.51	0.44
1:E:67:ASN:ND2	1:E:73:GLY:O	2.51	0.44
2:B:275:GLU:OE1	2:B:279:ARG:NE	2.51	0.44
1:A:277:ASP:CB	1:A:278:PRO:CD	2.95	0.44
1:E:105:VAL:N	1:E:106:PRO:CD	2.79	0.44
3:I:151:GLY:CA	3:I:162:ASP:OD2	2.66	0.44
1:E:203:ARG:O	1:E:210:VAL:N	2.50	0.44
3:I:159:LEU:CD1	3:I:161:GLU:OE1	2.66	0.43
3:J:157:ARG:CG	3:J:158:VAL:N	2.80	0.43
2:H:118:PHE:O	2:H:173:LEU:N	2.51	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:F:231:GLU:OE1	2:F:252:LYS:NZ	2.51	0.43
2:H:154:LYS:NZ	2:H:186:GLY:O	2.51	0.43
2:F:298:TYR:OH	2:F:304:GLU:OE2	2.37	0.43
1:G:271:HIS:CE1	6:G:1370:TPW:S1	3.12	0.43
1:A:102:TYR:OH	6:A:1370:TPW:O22	2.36	0.43
1:C:364:GLU:O	1:C:367:SER:OG	2.36	0.43
2:B:14:ARG:NH1	2:B:46:GLU:OE1	2.52	0.42
2:F:31:GLY:N	2:F:54:ASP:OD1	2.53	0.42
1:A:200:GLN:NE2	7:A:1378:HOH:O	2.52	0.42
2:H:168:ILE:N	2:H:168:ILE:CD1	2.82	0.42
3:J:146:ILE:CG2	3:J:147:ARG:N	2.81	0.42
3:J:153:GLY:O	3:J:156:GLY:N	2.52	0.42
1:E:182:TYR:OH	1:G:176:THR:O	2.38	0.42
1:G:116:TYR:OH	7:G:1489:HOH:O	2.21	0.42
2:H:171:GLU:OE1	2:H:176:TYR:OH	2.37	0.42
1:G:129:ASN:O	1:G:131:ILE:CD1	2.67	0.42
1:C:273:MET:CE	7:C:1510:HOH:O	2.68	0.42
1:E:103:ARG:NH2	6:E:1370:TPW:O22	2.53	0.41
1:E:368:LYS:CA	1:E:368:LYS:NZ	2.83	0.41
1:A:182:TYR:OH	1:C:176:THR:O	2.38	0.41
3:J:162:ASP:N	3:J:162:ASP:OD1	2.50	0.41
2:B:57:LEU:CD1	6:C:1370:TPW:H4A3	2.51	0.41
1:A:123:ARG:NH1	1:A:333:ASP:OD1	2.54	0.41
3:J:145:ASP:C	3:J:145:ASP:OD1	2.58	0.41
2:F:99:ARG:O	2:F:103:ARG:N	2.54	0.41
1:A:47:LYS:NZ	1:A:313:GLU:OE1	2.54	0.41
2:F:152:ASP:CB	7:F:1357:HOH:O	2.68	0.40
2:F:110:MET:N	7:F:1349:HOH:O	2.55	0.40
1:G:131:ILE:O	2:H:107:ARG:NE	2.55	0.40

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

All (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
2	D	236	ARG
2	F	236	ARG
3	I	136	ARG
3	I	160	LYS
3	I	155	ASN
3	J	157	ARG
2	F	31	GLY

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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
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

All (41) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	35	GLU
1	A	36	GLU
1	A	173	ASP
1	A	276	ASP
1	A	277	ASP
1	A	280	ARG
1	A	292	LYS
1	A	329	ILE
2	B	78	PRO
2	B	130	ASP
2	B	241	LEU
1	C	173	ASP
1	C	292	LYS
2	D	50	ASP
2	D	130	ASP
2	D	187	GLU
1	E	368	LYS
2	F	50	ASP
2	F	130	ASP
2	F	302	GLN
1	G	36	GLU
1	G	173	ASP
1	G	211	GLU
2	H	130	ASP
3	I	128	ARG
3	I	129	VAL

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Mol	Chain	Res	Type
3	I	137	LYS
3	I	141	GLU
3	I	147	ARG
3	I	148	LEU
3	I	155	ASN
3	I	157	ARG
3	I	159	LEU
3	J	128	ARG
3	J	129	VAL
3	J	146	ILE
3	J	148	LEU
3	J	150	GLN
3	J	155	ASN
3	J	159	LEU
3	J	164	ASP

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

All (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
6	C	1370	TPW	C2-C3	-3.85	1.34	1.37
6	G	1370	TPW	C2-C3	-3.72	1.35	1.37
6	A	1370	TPW	C2-C3	-3.46	1.35	1.37
6	E	1370	TPW	P2-O22	3.14	1.61	1.51
6	G	1370	TPW	P2-O22	3.06	1.61	1.51
6	C	1370	TPW	P2-O22	3.01	1.61	1.51
6	A	1370	TPW	P2-O22	2.99	1.61	1.51
6	C	1370	TPW	C5-C4	2.29	1.39	1.36
6	A	1370	TPW	C5-C4	2.26	1.39	1.36
6	G	1370	TPW	C5-C4	2.24	1.39	1.36
6	E	1370	TPW	P2-O23	2.11	1.62	1.54
6	E	1370	TPW	C5-C4	2.06	1.39	1.36
6	G	1370	TPW	P2-O23	2.04	1.62	1.54

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
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
6	A	1370	TPW	C2-S1-C5	4.28	97.07	91.37
6	G	1370	TPW	C2-S1-C5	4.10	96.83	91.37
6	E	1370	TPW	C2-S1-C5	4.03	96.73	91.37
6	C	1370	TPW	C35-C5'-C6'	-4.00	116.58	121.82
6	C	1370	TPW	C3-C2-S1	-3.88	108.13	112.26
6	G	1370	TPW	P1-O11-P2	-3.79	120.58	131.68
6	A	1370	TPW	C35-C5'-C6'	-3.65	117.04	121.82
6	C	1370	TPW	P1-O11-P2	-3.61	121.10	131.68
6	A	1370	TPW	C3-C2-S1	-3.61	108.42	112.26
6	E	1370	TPW	C3-C2-S1	-3.59	108.44	112.26
6	G	1370	TPW	C35-C5'-C6'	-3.58	117.14	121.82
6	E	1370	TPW	C35-C5'-C6'	-3.43	117.33	121.82
6	E	1370	TPW	P1-O11-P2	-3.42	121.66	131.68
6	C	1370	TPW	C6'-N1'-C2'	3.35	121.56	115.68
6	G	1370	TPW	C3-C2-S1	-3.31	108.73	112.26
6	C	1370	TPW	C35-C5'-C4'	3.28	126.22	122.17
6	E	1370	TPW	C6'-N1'-C2'	3.16	121.22	115.68
6	A	1370	TPW	C6'-N1'-C2'	3.05	121.04	115.68
6	C	1370	TPW	N1'-C2'-N3'	-2.98	120.28	125.65
6	A	1370	TPW	P1-O11-P2	-2.95	123.03	131.68
6	G	1370	TPW	C6'-N1'-C2'	2.93	120.83	115.68
6	E	1370	TPW	N1'-C2'-N3'	-2.90	120.41	125.65
6	A	1370	TPW	N1'-C2'-N3'	-2.84	120.53	125.65
6	A	1370	TPW	C35-C5'-C4'	2.78	125.60	122.17
6	G	1370	TPW	N1'-C2'-N3'	-2.66	120.84	125.65
6	A	1370	TPW	C2A-C2'-N1'	2.59	120.11	117.02
6	E	1370	TPW	C35-C5'-C4'	2.52	125.28	122.17
6	G	1370	TPW	C35-C5'-C4'	2.40	125.13	122.17
6	A	1370	TPW	O21-P2-O11	2.17	115.46	105.14
6	E	1370	TPW	C2A-C2'-N1'	2.10	119.52	117.02
6	E	1370	TPW	O23-P2-O22	-2.09	103.60	110.44

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%)

All (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
3	I	148	LEU	5.5
1	E	290	TRP	5.4
1	A	280	ARG	5.2
1	A	276	ASP	4.7
3	I	155	ASN	4.6
1	A	284	LYS	4.3
1	A	285	GLU	4.1
1	A	287	GLU	4.0

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Mol	Chain	Res	Type	RSRZ
1	A	290	TRP	3.9
3	J	129	VAL	3.8
1	A	282	ARG	3.7
1	A	289	GLU	3.7
1	G	277	ASP	3.6
3	J	149	VAL	3.6
1	E	276	ASP	3.5
3	I	129	VAL	3.4
3	J	163	ILE	3.4
3	J	146	ILE	3.2
1	G	4	THR	3.1
1	C	283	SER	3.1
1	A	292	LYS	3.0
3	J	128	ARG	3.0
3	J	150	GLN	2.9
3	I	146	ILE	2.9
1	E	46	LEU	2.9
3	I	169	GLY	2.8
1	E	51	ARG	2.8
1	C	285	GLU	2.8
3	J	148	LEU	2.8
1	C	279	THR	2.8
1	E	266	PHE	2.7
3	I	144	VAL	2.7
3	J	141	GLU	2.7
3	J	164	ASP	2.7
1	E	271	HIS	2.6
1	A	275	GLY	2.6
3	I	160	LYS	2.6
3	I	147	ARG	2.6
3	I	166	PHE	2.5
1	E	288	ASN	2.5
3	I	156	GLY	2.5
1	G	284	LYS	2.5
1	A	288	ASN	2.4
3	J	151	GLY	2.3
2	F	324	PHE	2.3
1	C	277	ASP	2.3
1	G	31	GLU	2.2
1	E	275	GLY	2.2
2	F	36	VAL	2.2
1	E	49	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
2	H	324	PHE	2.1
1	G	279	THR	2.1
3	J	147	ARG	2.1
3	I	140	ARG	2.0
1	A	279	THR	2.0

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.