Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 04:59 AM GMT

PDB ID	:	2OZL
Title	:	Human pyruvate dehydrogenase S264E variant
Authors	:	Ciszak, E.M.; Dominiak, P.M.; Patel, M.S.; Korotchkina, L.G.
Deposited on	:	2007-02-26
Resolution	:	1.90 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

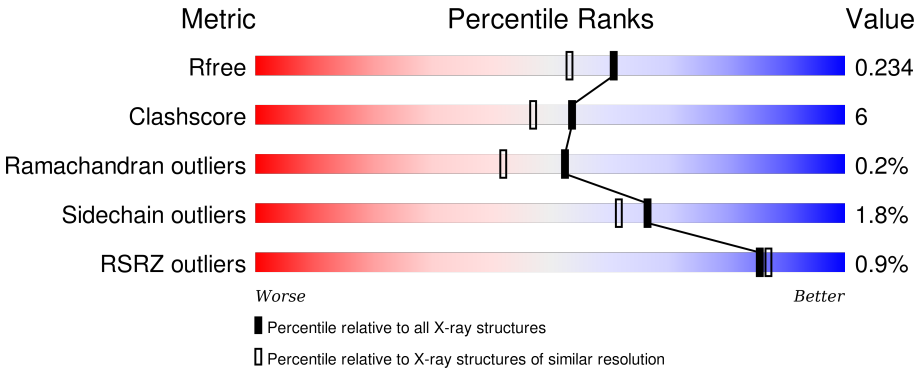
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 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}	91344	4755 (1.90-1.90)
Clashscore	102246	5398 (1.90-1.90)
Ramachandran outliers	100387	5338 (1.90-1.90)
Sidechain outliers	100360	5339 (1.90-1.90)
RSRZ outliers	91569	4766 (1.90-1.90)

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. 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% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	365	87% 12%
1	C	365	84% 15%
2	B	341	84% 12%
2	D	341	83% 13%

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
3	MG	A	2331	-	-	-	X
3	MG	C	1331	-	-	-	X

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 11517 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Pyruvate dehydrogenase E1 component alpha subunit, somatic form.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	362	Total	C	N	O	S	0	0	0
			2827	1774	496	533	24			
1	C	362	Total	C	N	O	S	0	0	0
			2827	1774	496	533	24			

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-3	MET	-	CLONING ARTIFACT	UNP P08559
A	-2	ARG	-	CLONING ARTIFACT	UNP P08559
A	-1	GLY	-	CLONING ARTIFACT	UNP P08559
A	0	SER	-	CLONING ARTIFACT	UNP P08559
A	264	GLU	SER	ENGINEERED	UNP P08559
C	-3	MET	-	CLONING ARTIFACT	UNP P08559
C	-2	ARG	-	CLONING ARTIFACT	UNP P08559
C	-1	GLY	-	CLONING ARTIFACT	UNP P08559
C	0	SER	-	CLONING ARTIFACT	UNP P08559
C	264	GLU	SER	ENGINEERED	UNP P08559

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	330	Total	C	N	O	S	0	0	0
			2525	1607	428	471	19			
2	D	330	Total	C	N	O	S	0	0	0
			2525	1607	428	471	19			

There are 26 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-11	MET	-	EXPRESSION TAG	UNP P11177

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-10	ARG	-	EXPRESSION TAG	UNP P11177
B	-9	GLY	-	EXPRESSION TAG	UNP P11177
B	-8	SER	-	EXPRESSION TAG	UNP P11177
B	-7	HIS	-	EXPRESSION TAG	UNP P11177
B	-6	HIS	-	EXPRESSION TAG	UNP P11177
B	-5	HIS	-	EXPRESSION TAG	UNP P11177
B	-4	HIS	-	EXPRESSION TAG	UNP P11177
B	-3	HIS	-	EXPRESSION TAG	UNP P11177
B	-2	HIS	-	EXPRESSION TAG	UNP P11177
B	-1	GLY	-	EXPRESSION TAG	UNP P11177
B	0	SER	-	EXPRESSION TAG	UNP P11177
B	1	LEU	-	EXPRESSION TAG	UNP P11177
D	-11	MET	-	EXPRESSION TAG	UNP P11177
D	-10	ARG	-	EXPRESSION TAG	UNP P11177
D	-9	GLY	-	EXPRESSION TAG	UNP P11177
D	-8	SER	-	EXPRESSION TAG	UNP P11177
D	-7	HIS	-	EXPRESSION TAG	UNP P11177
D	-6	HIS	-	EXPRESSION TAG	UNP P11177
D	-5	HIS	-	EXPRESSION TAG	UNP P11177
D	-4	HIS	-	EXPRESSION TAG	UNP P11177
D	-3	HIS	-	EXPRESSION TAG	UNP P11177
D	-2	HIS	-	EXPRESSION TAG	UNP P11177
D	-1	GLY	-	EXPRESSION TAG	UNP P11177
D	0	SER	-	EXPRESSION TAG	UNP P11177
D	1	LEU	-	EXPRESSION TAG	UNP P11177

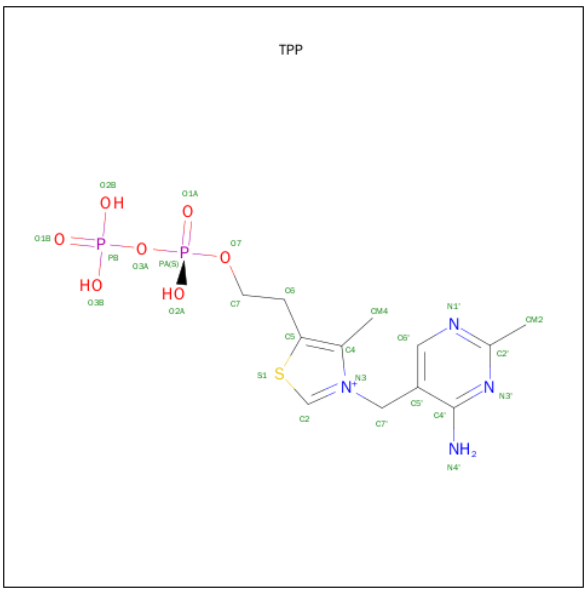
- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Mg 1 1	0	0
3	C	1	Total Mg 1 1	0	0

- Molecule 4 is POTASSIUM ION (three-letter code: K) (formula: K).

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

- Molecule 5 is THIAMINE DIPHOSPHATE (three-letter code: TPP) (formula: $C_{12}H_{19}N_4O_7P_2S$).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
5	C	1	Total	C	N	O	P	S	0	0
			26	12	4	7	2	1		
5	A	1	Total	C	N	O	P	S	0	0
			26	12	4	7	2	1		

- Molecule 6 is water.

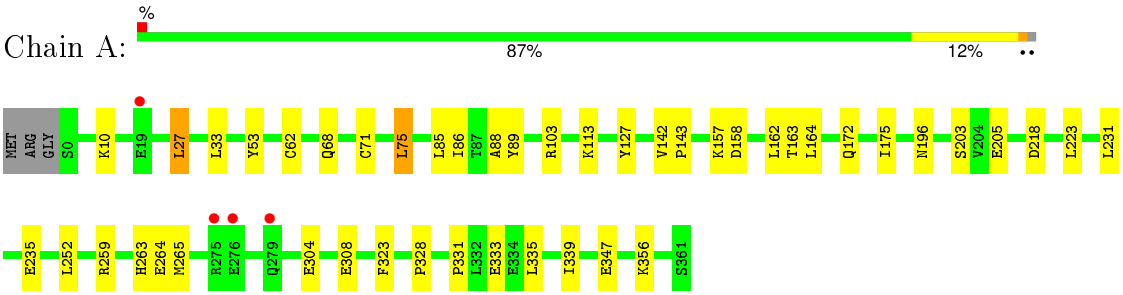
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	202	Total	O	0	0
			202	202		
6	B	188	Total	O	0	0
			188	188		
6	C	186	Total	O	0	0
			186	186		
6	D	181	Total	O	0	0
			181	181		

3 Residue-property plots (i)

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.

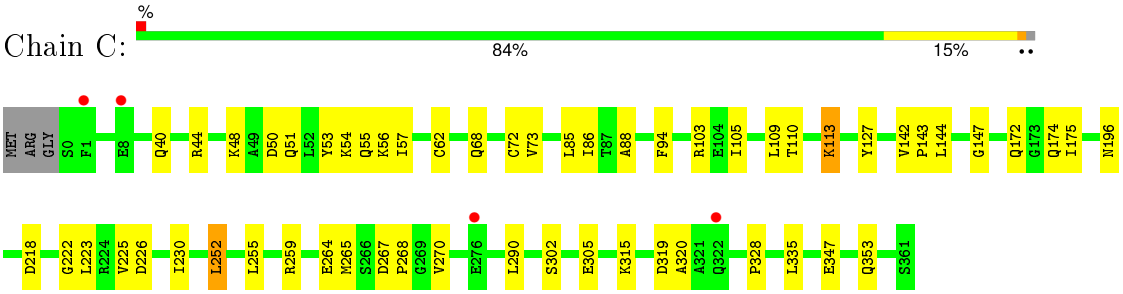
• Molecule 1: Pyruvate dehydrogenase E1 component alpha subunit, somatic form

Chain A:



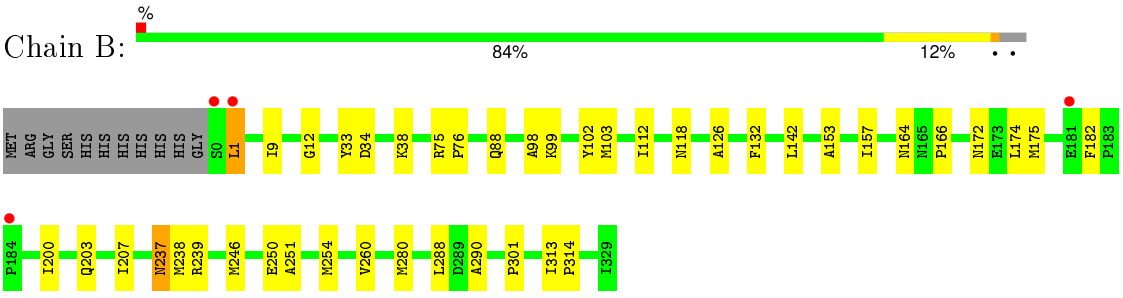
• Molecule 1: Pyruvate dehydrogenase E1 component alpha subunit, somatic form

Chain C:



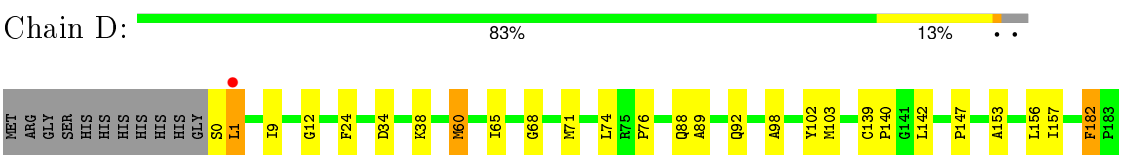
• Molecule 2: Pyruvate dehydrogenase E1 component subunit beta

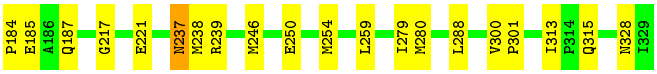
Chain B:



• Molecule 2: Pyruvate dehydrogenase E1 component subunit beta

Chain D:




P184
E185
A186
Q187
G217
E221
N237
M238
R239
M246
E250
M254
L259
I279
M280
L288
V300
P301
I313
P314
Q315
N328
I329

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	64.90Å 126.40Å 190.40Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 1.90 45.38 – 1.90	Depositor EDS
% Data completeness (in resolution range)	85.9 (50.00-1.90) 85.9 (45.38-1.90)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	0.08	Depositor
$< I/\sigma(I) >$ [1]	4.38 (at 1.89Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.186 , 0.221 0.205 , 0.234	Depositor DCC
R_{free} test set	10709 reflections (10.01%)	DCC
Wilson B-factor (Å^2)	10.5	Xtriage
Anisotropy	0.725	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 41.7	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Outliers	1 of 111238 reflections (0.001%)	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	11517	wwPDB-VP
Average B, all atoms (Å^2)	14.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.38% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

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	0.31	0/2883	0.57	0/3882
1	C	0.31	0/2883	0.56	0/3882
2	B	0.32	0/2580	0.61	0/3496
2	D	0.31	0/2580	0.61	0/3496
All	All	0.32	0/10926	0.59	0/14756

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	89	TYR	Sidechain

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	2827	0	2781	34	0
1	C	2827	0	2781	38	0
2	B	2525	0	2522	34	0
2	D	2525	0	2522	43	0
3	A	1	0	0	0	0
3	C	1	0	0	0	0
4	B	1	0	0	0	0
4	D	1	0	0	0	0
5	A	26	0	16	2	0
5	C	26	0	16	0	0
6	A	202	0	0	3	0
6	B	188	0	0	1	0
6	C	186	0	0	2	0
6	D	181	0	0	2	0
All	All	11517	0	10638	138	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 6.

All (138) 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)
2:D:60:MET:HE3	2:D:89:ALA:HA	1.23	1.08
2:B:118:ASN:HD21	2:B:132:PHE:H	1.15	0.94
2:D:12:GLY:HA3	2:D:157:ILE:HD11	1.62	0.82
2:D:60:MET:HE3	2:D:89:ALA:CA	2.09	0.81
2:B:12:GLY:HA3	2:B:157:ILE:HD11	1.67	0.75
2:D:98:ALA:HB2	2:D:142:LEU:HD13	1.67	0.74
2:B:301:PRO:HG2	2:D:102:TYR:CD2	2.23	0.73
1:A:172:GLN:HE22	2:D:88:GLN:HE22	1.39	0.69
1:C:113:LYS:HD3	1:C:328:PRO:HG2	1.75	0.67
1:A:68:GLN:HE22	1:A:196:ASN:HD22	1.42	0.66
1:C:268:PRO:HG2	6:C:1508:HOH:O	1.95	0.66
1:A:235:GLU:HG2	6:A:2408:HOH:O	1.96	0.64
2:B:118:ASN:HD21	2:B:132:PHE:N	1.91	0.64
1:A:10:LYS:HG2	6:A:2461:HOH:O	1.97	0.64
2:B:102:TYR:CD2	2:D:301:PRO:HG2	2.33	0.63
2:D:60:MET:CE	2:D:92:GLN:HG2	2.28	0.63
2:B:9:ILE:HA	2:B:157:ILE:HD13	1.81	0.63
2:D:139:CYS:HB3	6:D:1494:HOH:O	1.98	0.62
2:D:0:SER:HB3	2:D:187:GLN:HE22	1.65	0.62
2:B:118:ASN:ND2	2:B:132:PHE:H	1.93	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:207:ILE:HD11	2:B:260:VAL:HG23	1.84	0.59
1:A:113:LYS:HG2	1:A:328:PRO:O	2.03	0.59
2:D:1:LEU:HD12	2:D:182:PHE:HB3	1.85	0.58
1:A:85:LEU:HD23	1:A:86:ILE:N	2.19	0.57
2:B:200:ILE:HG21	2:B:203:GLN:NE2	2.19	0.57
2:D:9:ILE:HA	2:D:157:ILE:HD13	1.86	0.57
2:B:88:GLN:HE22	1:C:172:GLN:HE22	1.52	0.57
1:A:142:VAL:HB	1:A:143:PRO:HD3	1.86	0.57
2:D:0:SER:HB3	2:D:187:GLN:NE2	2.20	0.56
1:A:157:LYS:O	1:A:158:ASP:HB3	2.07	0.55
2:B:75:ARG:HH22	2:B:164:ASN:ND2	2.05	0.55
1:C:53:TYR:CG	1:C:265:MET:HG3	2.41	0.54
1:C:62:CYS:HB3	1:C:265:MET:HG2	1.89	0.54
2:D:1:LEU:CD1	2:D:182:PHE:HB3	2.38	0.54
1:C:113:LYS:NZ	1:C:113:LYS:HB2	2.23	0.54
1:C:142:VAL:HB	1:C:143:PRO:HD3	1.90	0.54
2:D:60:MET:HE1	2:D:92:GLN:HG2	1.89	0.53
1:C:85:LEU:HD23	1:C:86:ILE:N	2.24	0.53
2:D:0:SER:HB2	2:D:184:PRO:HD3	1.91	0.53
1:A:142:VAL:HG21	1:A:175:ILE:HG12	1.91	0.52
2:B:12:GLY:HA3	2:B:157:ILE:CD1	2.38	0.52
2:B:126:ALA:HB3	2:D:103:MET:SD	2.49	0.52
2:B:33:TYR:O	2:B:34:ASP:HB2	2.10	0.52
2:D:185:GLU:HB2	6:D:1511:HOH:O	2.08	0.52
2:B:75:ARG:HH22	2:B:164:ASN:HD22	1.59	0.51
2:B:102:TYR:CG	2:D:301:PRO:HG2	2.45	0.51
1:C:302:SER:OG	1:C:305:GLU:HB2	2.09	0.51
1:C:223:LEU:HD23	1:C:223:LEU:N	2.25	0.51
1:A:203:SER:HB2	1:A:205:GLU:OE2	2.11	0.51
2:B:250:GLU:O	2:B:254:MET:HG3	2.11	0.51
2:D:313:ILE:HG23	2:D:315:GLN:NE2	2.25	0.51
1:C:103:ARG:HG2	1:C:320:ALA:HA	1.93	0.50
1:A:331:PRO:HB2	1:A:333:GLU:HG2	1.93	0.50
1:A:68:GLN:NE2	1:A:196:ASN:HD22	2.08	0.50
1:C:73:VAL:HG12	1:C:230:ILE:HD11	1.93	0.50
2:D:250:GLU:O	2:D:254:MET:HG3	2.11	0.50
2:B:251:ALA:HA	2:B:254:MET:HE3	1.94	0.50
2:B:246:MET:O	2:B:250:GLU:HG3	2.12	0.49
2:D:147:PRO:HB3	2:D:156:LEU:HD12	1.94	0.49
2:B:301:PRO:HG2	2:D:102:TYR:CG	2.48	0.49
1:A:205:GLU:CD	1:A:205:GLU:H	2.15	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:172:ASN:HD21	2:B:174:LEU:HB2	1.78	0.49
1:A:335:LEU:C	1:A:335:LEU:HD23	2.32	0.48
2:D:34:ASP:O	2:D:38:LYS:HA	2.13	0.48
1:A:103:ARG:HG3	1:A:323:PHE:CD2	2.49	0.48
1:C:50:ASP:OD2	1:C:54:LYS:HE3	2.14	0.48
2:D:60:MET:HE2	2:D:92:GLN:CG	2.44	0.48
6:B:2371:HOH:O	1:C:353:GLN:HG2	2.13	0.47
1:A:71:CYS:O	1:A:75:LEU:HB2	2.14	0.47
1:A:113:LYS:HD3	1:A:328:PRO:HG2	1.97	0.47
1:C:335:LEU:C	1:C:335:LEU:HD23	2.35	0.47
2:B:98:ALA:HB2	2:B:142:LEU:HG	1.96	0.47
1:A:75:LEU:HG	1:A:162:LEU:HD23	1.96	0.47
1:A:304:GLU:O	1:A:308:GLU:HG3	2.15	0.47
2:B:142:LEU:HD23	2:B:166:PRO:HB2	1.96	0.47
2:B:99:LYS:O	2:B:103:MET:HG3	2.15	0.47
1:C:270:VAL:HG22	1:C:270:VAL:O	2.15	0.47
1:A:53:TYR:CG	1:A:265:MET:HG3	2.49	0.46
2:D:238:MET:O	2:D:239:ARG:HB2	2.14	0.46
1:C:174:GLN:HB3	2:D:60:MET:HG2	1.95	0.46
1:A:127:TYR:N	1:A:127:TYR:CD1	2.84	0.46
2:D:153:ALA:O	2:D:157:ILE:HG23	2.16	0.46
1:C:88:ALA:HB3	6:C:1356:HOH:O	2.14	0.46
2:D:139:CYS:HA	2:D:140:PRO:HD3	1.78	0.46
2:B:238:MET:O	2:B:239:ARG:HB2	2.16	0.45
2:B:172:ASN:HD22	2:B:175:MET:H	1.64	0.45
2:D:12:GLY:HA3	2:D:157:ILE:CD1	2.40	0.45
1:A:223:LEU:N	1:A:223:LEU:HD23	2.30	0.45
1:A:223:LEU:HD23	1:A:252:LEU:O	2.16	0.45
2:B:34:ASP:O	2:B:38:LYS:HA	2.16	0.45
2:B:313:ILE:CG2	2:B:314:PRO:HD2	2.46	0.45
1:A:263:HIS:CE1	5:A:2330:TPP:H62	2.52	0.45
1:A:339:ILE:HD11	2:D:300:VAL:HG12	1.98	0.45
1:C:68:GLN:HE21	1:C:259:ARG:HB3	1.82	0.44
1:C:57:ILE:HG22	1:C:110:THR:HG22	1.99	0.44
1:A:347:GLU:OE2	1:A:356:LYS:HD3	2.17	0.44
1:C:222:GLY:HA2	1:C:252:LEU:O	2.16	0.44
1:C:53:TYR:CD2	1:C:265:MET:HG3	2.53	0.44
2:B:251:ALA:HA	2:B:254:MET:CE	2.47	0.44
1:C:113:LYS:HG2	1:C:328:PRO:O	2.18	0.44
1:C:85:LEU:C	1:C:85:LEU:HD23	2.38	0.44
2:B:280:MET:SD	2:D:280:MET:HE3	2.58	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:60:MET:HE2	2:D:92:GLN:HG2	1.99	0.44
1:A:88:ALA:HB3	6:A:2352:HOH:O	2.17	0.44
2:D:24:PHE:CZ	2:D:76:PRO:HB3	2.52	0.44
1:A:164:LEU:HD12	1:A:164:LEU:N	2.34	0.43
1:C:72:CYS:HA	1:C:94:PHE:CE1	2.53	0.43
2:D:68:GLY:HA2	2:D:71:MET:HE2	2.01	0.43
2:B:237:ASN:HD22	2:B:237:ASN:C	2.22	0.43
2:D:60:MET:CE	2:D:92:GLN:CG	2.97	0.43
1:C:142:VAL:HG21	1:C:175:ILE:HG12	1.99	0.43
5:A:2330:TPP:HN42	5:A:2330:TPP:H2	1.84	0.43
2:D:237:ASN:HD22	2:D:237:ASN:C	2.22	0.43
1:A:27:LEU:HG	1:A:231:LEU:HD21	2.01	0.42
1:A:62:CYS:HB3	1:A:265:MET:HG2	2.02	0.42
1:C:267:ASP:HA	1:C:268:PRO:HD2	1.95	0.42
1:A:103:ARG:HE	1:A:103:ARG:HB2	1.69	0.42
2:B:76:PRO:HG2	2:B:112:ILE:HG13	2.01	0.41
1:C:48:LYS:NZ	1:C:51:GLN:HE22	2.18	0.41
1:C:55:GLN:O	1:C:56:LYS:HB2	2.20	0.41
2:D:217:GLY:O	2:D:221:GLU:HG3	2.19	0.41
2:B:288:LEU:HG	2:B:290:ALA:O	2.20	0.41
1:C:315:LYS:HE2	1:C:319:ASP:OD2	2.20	0.41
2:B:153:ALA:O	2:B:157:ILE:HG23	2.20	0.41
1:C:113:LYS:HZ2	1:C:113:LYS:HB2	1.84	0.41
1:A:142:VAL:HA	1:A:163:THR:CG2	2.51	0.41
1:C:40:GLN:O	1:C:44:ARG:HG2	2.21	0.41
1:A:68:GLN:HE21	1:A:259:ARG:HB3	1.85	0.41
1:A:335:LEU:HD23	1:A:335:LEU:O	2.21	0.41
1:C:68:GLN:HE22	1:C:196:ASN:HD22	1.69	0.41
1:C:144:LEU:HD22	2:D:71:MET:HE2	2.03	0.40
2:D:60:MET:HE1	2:D:92:GLN:H	1.85	0.40
1:C:147:GLY:HA2	2:D:65:ILE:HG23	2.02	0.40
1:C:127:TYR:CD1	1:C:127:TYR:N	2.89	0.40
1:C:105:ILE:O	1:C:109:LEU:HG	2.21	0.40
2:D:246:MET:O	2:D:250:GLU:HG3	2.20	0.40
1:C:225:VAL:HG12	1:C:226:ASP:N	2.37	0.40
2:D:259:LEU:CD2	2:D:279:ILE:HG13	2.52	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	360/365 (99%)	348 (97%)	11 (3%)	1 (0%)	46	35
1	C	360/365 (99%)	348 (97%)	11 (3%)	1 (0%)	46	35
2	B	328/341 (96%)	316 (96%)	11 (3%)	1 (0%)	46	35
2	D	328/341 (96%)	316 (96%)	12 (4%)	0	100	100
All	All	1376/1412 (98%)	1328 (96%)	45 (3%)	3 (0%)	52	42

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	218	ASP
2	B	1	LEU
1	C	218	ASP

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	295/297 (99%)	291 (99%)	4 (1%)	74	71
1	C	295/297 (99%)	289 (98%)	6 (2%)	63	57
2	B	269/278 (97%)	266 (99%)	3 (1%)	80	79
2	D	269/278 (97%)	262 (97%)	7 (3%)	54	45
All	All	1128/1150 (98%)	1108 (98%)	20 (2%)	66	61

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	27	LEU
1	A	33	LEU
1	A	75	LEU
1	A	264	GLU
2	B	1	LEU
2	B	182	PHE
2	B	237	ASN
1	C	113	LYS
1	C	252	LEU
1	C	255	LEU
1	C	264	GLU
1	C	290	LEU
1	C	347	GLU
2	D	1	LEU
2	D	60	MET
2	D	74	LEU
2	D	182	PHE
2	D	237	ASN
2	D	288	LEU
2	D	328	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	3	ASN
1	A	40	GLN
1	A	55	GLN
1	A	68	GLN
1	A	80	ASN
1	A	130	ASN
1	A	297	ASN
2	B	32	GLN
2	B	88	GLN
2	B	118	ASN
2	B	164	ASN
2	B	172	ASN
2	B	203	GLN
2	B	218	HIS
2	B	237	ASN
1	C	3	ASN
1	C	51	GLN
1	C	55	GLN
1	C	68	GLN

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Mol	Chain	Res	Type
1	C	80	ASN
1	C	299	ASN
2	D	88	GLN
2	D	187	GLN
2	D	237	ASN
2	D	328	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

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	$\#\|Z\| > 2$
5	TPP	A	2330	3	20,27,27	2.56	2 (10%)	31,40,40	1.67	5 (16%)
5	TPP	C	1330	3	20,27,27	2.80	2 (10%)	31,40,40	1.67	4 (12%)

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	TPP	A	2330	3	-	0/16/17/17	0/2/2/2
5	TPP	C	1330	3	-	0/16/17/17	0/2/2/2

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	C	1330	TPP	CM4-C4	2.20	1.54	1.49
5	A	2330	TPP	CM4-C4	2.27	1.54	1.49
5	A	2330	TPP	C4-N3	10.21	1.48	1.39
5	C	1330	TPP	C4-N3	11.43	1.49	1.39

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	A	2330	TPP	C6-C5-S1	-4.55	113.87	120.24
5	C	1330	TPP	C6-C5-S1	-4.53	113.90	120.24
5	A	2330	TPP	C5'-C7'-N3	-2.24	109.58	113.33
5	A	2330	TPP	C6'-N1'-C2'	2.92	120.87	115.77
5	C	1330	TPP	C6'-N1'-C2'	2.96	120.94	115.77
5	C	1330	TPP	O3A-PA-O7	3.24	111.52	102.94
5	A	2330	TPP	O3A-PA-O7	3.46	112.12	102.94
5	A	2330	TPP	C6-C5-C4	3.55	130.75	127.56
5	C	1330	TPP	C6-C5-C4	3.76	130.94	127.56

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	2330	TPP	2	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} 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	362/365 (99%)	0.20	4 (1%)	82	84	5, 12, 25, 37	0
1	C	362/365 (99%)	0.36	4 (1%)	82	84	5, 14, 30, 44	0
2	B	330/341 (96%)	0.09	4 (1%)	81	83	5, 10, 21, 49	0
2	D	330/341 (96%)	0.05	1 (0%)	94	94	5, 10, 21, 36	0
All	All	1384/1412 (98%)	0.18	13 (0%)	85	87	5, 11, 26, 49	0

All (13) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	0	SER	5.7
2	D	1	LEU	4.3
1	C	276	GLU	3.6
2	B	1	LEU	3.5
1	A	276	GLU	3.1
1	A	275	ARG	3.1
1	C	1	PHE	2.7
1	A	19	GLU	2.5
1	A	279	GLN	2.4
2	B	184	PRO	2.1
1	C	8	GLU	2.0
2	B	181	GLU	2.0
1	C	322	GLN	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 (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. 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, 95^{th} 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	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
3	MG	A	2331	1/1	0.98	0.18	3.09	5,5,5,5	0
3	MG	C	1331	1/1	0.96	0.16	2.07	5,5,5,5	0
5	TPP	C	1330	26/26	0.95	0.13	0.43	5,10,15,16	0
5	TPP	A	2330	26/26	0.96	0.10	-0.52	5,8,12,12	0
4	K	B	2332	1/1	0.98	0.08	-2.32	10,10,10,10	0
4	K	D	1332	1/1	0.99	0.06	-2.51	11,11,11,11	0

6.5 Other polymers (i)

There are no such residues in this entry.