



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 11:02 PM GMT

PDB ID : 1W88  
Title : THE CRYSTAL STRUCTURE OF PYRUVATE DEHYDROGENASE  
E1(D180N, E183Q) BOUND TO THE PERIPHERAL SUBUNIT BINDING  
DOMAIN OF E2  
Authors : Frank, R.A.W.; Pratap, J.V.; Pei, X.Y.; Perham, R.N.; Luisi, B.F.  
Deposited on : 2004-09-16  
Resolution : 2.30 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](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

---

The following versions of software and data (see [references ⓘ](#)) 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

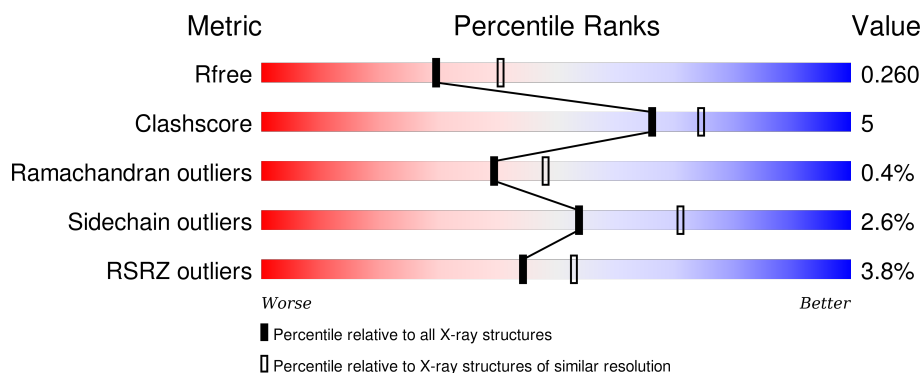
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.30 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	3852 (2.30-2.30)
Clashscore	102246	4452 (2.30-2.30)
Ramachandran outliers	100387	4410 (2.30-2.30)
Sidechain outliers	100360	4409 (2.30-2.30)
RSRZ outliers	91569	3857 (2.30-2.30)

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  $\geq 3$ , 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  $\leq 5\%$ . 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	368	
1	C	368	
1	E	368	
1	G	368	
2	B	324	

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Length	Quality of chain
2	D	324	
2	F	324	
2	H	324	
3	I	49	
3	J	49	

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
5	TDP	E	1370	-	-	-	X
5	TDP	G	1370	-	-	-	X

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 21934 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.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	341	Total	C	N	O	S	0	0	1
			2592	1666	444	475	7			
1	C	343	Total	C	N	O	S	0	0	0
			2659	1705	451	496	7			
1	E	328	Total	C	N	O	S	0	1	0
			2521	1614	431	469	7			
1	G	331	Total	C	N	O	S	0	1	0
			2565	1645	434	479	7			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	180	ASN	ASP	ENGINEERED MUTATION	UNP P21873
A	183	GLN	GLU	ENGINEERED MUTATION	UNP P21873
C	180	ASN	ASP	ENGINEERED MUTATION	UNP P21873
C	183	GLN	GLU	ENGINEERED MUTATION	UNP P21873
E	180	ASN	ASP	ENGINEERED MUTATION	UNP P21873
E	183	GLN	GLU	ENGINEERED MUTATION	UNP P21873
G	180	ASN	ASP	ENGINEERED MUTATION	UNP P21873
G	183	GLN	GLU	ENGINEERED MUTATION	UNP P21873

- Molecule 2 is a protein called PYRUVATE DEHYDROGENASE E1 COMPONENT, BETA SUBUNIT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	324	Total	C	N	O	S	0	1	0
			2428	1546	417	457	8			
2	D	324	Total	C	N	O	S	0	0	0
			2489	1586	424	471	8			
2	F	310	Total	C	N	O	S	0	1	0
			2369	1507	407	447	8			

*Continued on next page...*

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	317	Total	C	N	O	S	0	0	0
			2416	1537	411	460	8			

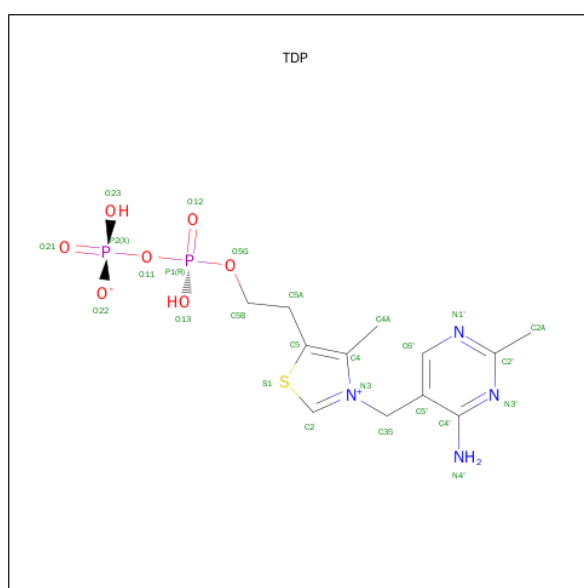
- Molecule 3 is a protein called DIHYDROLIPOYLLYSINE-RESIDUE ACETYLTRANSFERASE COMPONENT OF PYRUVATE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	I	40	Total	C	N	O	S	0	0	0
			303	192	55	55	1			
3	J	43	Total	C	N	O	S	0	0	1
			311	195	59	56	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	1	Total	Mg	0	0
			1	1		
4	C	1	Total	Mg	0	0
			1	1		
4	E	1	Total	Mg	0	0
			1	1		

- Molecule 5 is THIAMIN DIPHOSPHATE (three-letter code: TDP) (formula: C<sub>12</sub>H<sub>18</sub>N<sub>4</sub>O<sub>7</sub>P<sub>2</sub>S).

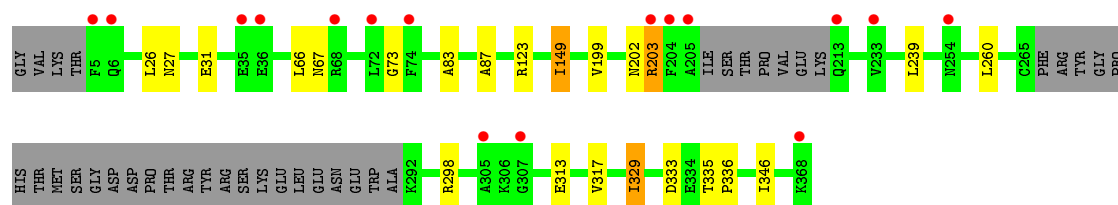


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	N	O	P	S	
			26	12	4	7	2	1	
5	C	1	Total	C	N	O	P	S	
			26	12	4	7	2	1	
5	E	1	Total	C	N	O	P	S	
			26	12	4	7	2	1	
5	G	1	Total	C	N	O	P	S	
			26	12	4	7	2	1	

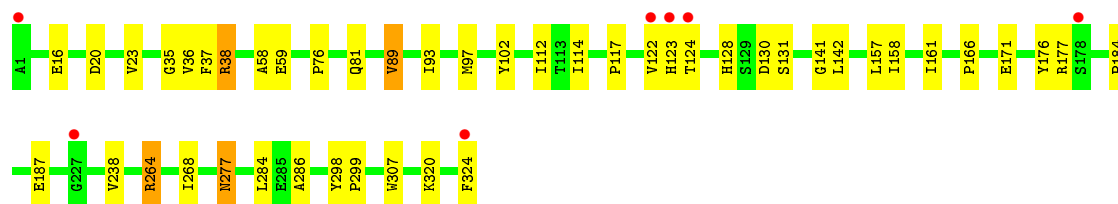
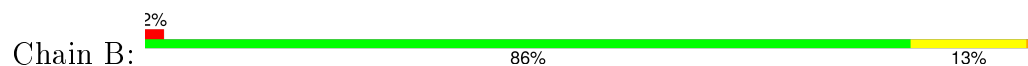
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	96	Total	O		
			96	96	0	0
6	B	124	Total	O		
			124	124	0	0
6	C	168	Total	O		
			168	168	0	0
6	D	209	Total	O		
			209	209	0	0
6	E	78	Total	O		
			78	78	0	0
6	F	194	Total	O		
			194	194	0	0
6	G	88	Total	O		
			88	88	0	0
6	H	161	Total	O		
			161	161	0	0
6	I	24	Total	O		
			24	24	0	0
6	J	31	Total	O		
			31	31	0	0

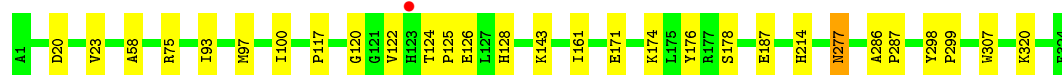




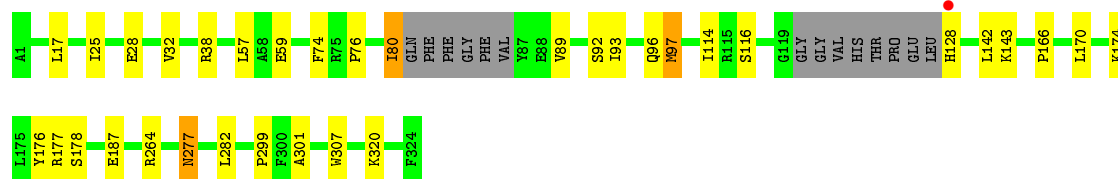
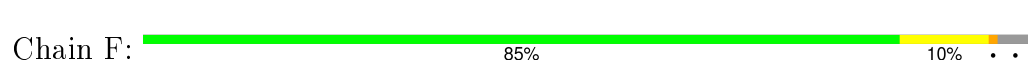
• Molecule 2: PYRUVATE DEHYDROGENASE E1 COMPONENT, BETA SUBUNIT



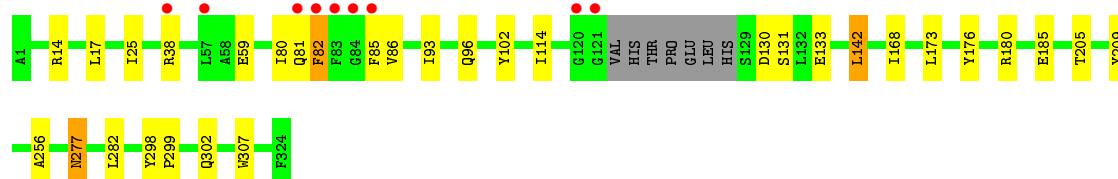
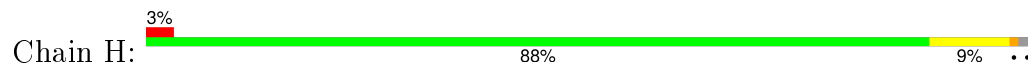
• Molecule 2: PYRUVATE DEHYDROGENASE E1 COMPONENT, BETA SUBUNIT



• Molecule 2: PYRUVATE DEHYDROGENASE E1 COMPONENT, BETA SUBUNIT



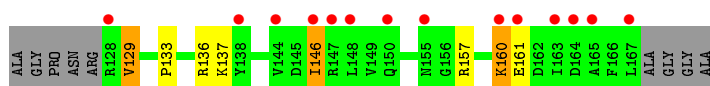
• Molecule 2: PYRUVATE DEHYDROGENASE E1 COMPONENT, BETA SUBUNIT



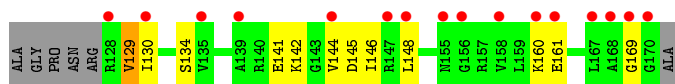
• Molecule 3: DIHYDROLIPOYLLYSINE-RESIDUE ACETYLTRANSFERASE COMPONENT OF PYRUVATE







● Molecule 3: DIHYDROLIPOYLLYSINE-RESIDUE ACETYLTRANSFERASE COMPONENT OF PYRUVATE



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	92.18Å 133.69Å 245.61Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.98 – 2.30 19.99 – 2.10	Depositor EDS
% Data completeness (in resolution range)	100.0 (19.98-2.30) 99.8 (19.99-2.10)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.06 (at 2.09Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, $R_{free}$	0.199 , 0.262 0.200 , 0.260	Depositor DCC
$R_{free}$ test set	6706 reflections (5.23%)	DCC
Wilson B-factor (Å <sup>2</sup> )	33.5	Xtriage
Anisotropy	0.564	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 52.9	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 176406 reflections	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	21934	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.15% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

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

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	0.50	0/2647	0.54	0/3592
1	C	0.52	0/2715	0.56	0/3677
1	E	0.48	0/2571	0.55	1/3482 (0.0%)
1	G	0.46	0/2617	0.56	0/3541
2	B	0.54	0/2476	0.64	1/3369 (0.0%)
2	D	0.55	0/2535	0.63	0/3437
2	F	0.54	0/2411	0.64	0/3267
2	H	0.52	0/2458	0.62	0/3330
3	I	0.46	0/305	0.58	0/408
3	J	0.57	1/313 (0.3%)	0.62	0/420
All	All	0.51	1/21048 (0.0%)	0.59	2/28523 (0.0%)

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	C	0	1
1	E	0	1
All	All	0	2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	J	169	GLY	C-N	-5.12	1.23	1.33

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	294	ASP	CB-CG-OD2	5.18	122.97	118.30
2	B	264	ARG	NE-CZ-NH2	-5.10	117.75	120.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	367	SER	Peptide
1	E	292	LYS	Peptide

## 5.2 Too-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 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	2592	0	2520	25	0
1	C	2659	0	2595	23	0
1	E	2521	0	2455	39	0
1	G	2565	0	2504	15	0
2	B	2428	0	2401	31	0
2	D	2489	0	2515	19	0
2	F	2369	0	2401	23	0
2	H	2416	0	2420	26	0
3	I	303	0	316	10	0
3	J	311	0	318	9	0
4	A	1	0	0	0	0
4	C	1	0	0	0	0
4	E	1	0	0	0	0
4	G	1	0	0	0	0
5	A	26	0	16	1	0
5	C	26	0	16	1	0
5	E	26	0	16	2	0
5	G	26	0	16	1	0
6	A	96	0	0	2	0
6	B	124	0	0	3	0
6	C	168	0	0	0	0
6	D	209	0	0	2	0
6	E	78	0	0	4	0
6	F	194	0	0	3	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	G	88	0	0	2	0
6	H	161	0	0	4	0
6	I	24	0	0	4	0
6	J	31	0	0	3	0
All	All	21934	0	20509	201	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 5.

All (201) 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)
5:C:1370:TDP:H2	5:C:1370:TDP:C2	0.97	1.49
5:A:1370:TDP:H2	5:A:1370:TDP:C2	0.97	1.49
5:G:1370:TDP:H2	5:G:1370:TDP:C2	0.97	1.48
5:E:1370:TDP:H2	5:E:1370:TDP:C2	0.97	1.46
1:E:303:LEU:CD1	1:E:309:TRP:HB2	1.73	1.18
1:E:303:LEU:HD11	1:E:309:TRP:HB2	1.30	1.09
1:E:71:ARG:HH11	1:E:71:ARG:HG2	1.19	1.04
3:J:142:LYS:HB2	6:J:2012:HOH:O	1.71	0.91
6:B:2105:HOH:O	3:I:133:PRO:HB3	1.76	0.85
2:F:143:LYS:HE3	6:F:2095:HOH:O	1.78	0.82
1:E:303:LEU:CD1	1:E:309:TRP:CB	2.59	0.80
1:C:367:SER:N	1:C:368:LYS:HA	1.97	0.79
1:E:303:LEU:HD11	1:E:309:TRP:CB	2.12	0.79
3:I:129:VAL:HG21	3:I:146:ILE:CG2	2.13	0.78
1:C:203:ARG:HA	1:C:210:VAL:HG22	1.64	0.78
2:D:143:LYS:HE2	6:D:2110:HOH:O	1.86	0.75
1:E:93:GLU:HB3	6:E:2022:HOH:O	1.88	0.73
1:A:9:PHE:HZ	1:C:231:ILE:HD11	1.53	0.73
3:J:144:VAL:HG23	6:J:2012:HOH:O	1.88	0.71
2:F:80:ILE:HG13	2:F:114:ILE:HG23	1.73	0.71
1:A:294:ASP:HB3	1:A:297:VAL:HG23	1.73	0.69
1:E:304:GLU:C	1:E:306:LYS:H	1.98	0.67
2:B:157:LEU:O	2:B:161:ILE:HG13	1.95	0.66
2:B:93:ILE:HA	2:B:97:MET:HG2	1.77	0.66
1:E:71:ARG:NH1	1:E:71:ARG:HG2	1.98	0.66
2:H:82:PHE:HB2	2:H:85:PHE:CZ	2.31	0.66
2:B:59:GLU:HB3	2:B:89:VAL:HG22	1.77	0.66
1:E:76:ALA:HB1	1:E:103:ARG:HG2	1.77	0.66
1:E:303:LEU:HD12	1:E:309:TRP:HB2	1.72	0.65

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:129:VAL:HG21	3:I:146:ILE:HG22	1.78	0.65
2:B:142:LEU:HD23	2:B:166:PRO:HB2	1.78	0.64
2:F:277[B]:ASN:HD21	2:H:277:ASN:HB2	1.64	0.63
1:E:71:ARG:CG	1:E:71:ARG:HH11	2.06	0.63
2:B:324:PHE:O	3:I:137:LYS:NZ	2.24	0.63
2:F:277[B]:ASN:ND2	2:H:277:ASN:HB2	2.14	0.62
1:E:83:ALA:O	1:E:87:ALA:HB3	2.00	0.62
1:C:249:ARG:O	1:C:253:ILE:HG23	1.99	0.61
1:E:293:LYS:O	1:E:294:ASP:C	2.38	0.61
2:D:214:HIS:HD2	6:D:2147:HOH:O	1.83	0.61
2:F:80:ILE:HG21	2:F:89:VAL:HG11	1.81	0.60
2:B:277[B]:ASN:ND2	2:D:277:ASN:HB2	2.15	0.60
3:I:161:GLU:HB3	6:I:2018:HOH:O	2.01	0.60
2:B:264:ARG:NH2	6:B:2096:HOH:O	2.34	0.59
1:E:43:ASP:HA	1:E:46:LEU:HD12	1.85	0.58
1:A:344:ILE:HG23	1:A:355:LEU:HD22	1.85	0.58
3:I:160:LYS:HB3	6:I:2017:HOH:O	2.03	0.58
1:A:142:ILE:HG21	2:D:126:GLU:O	2.05	0.57
1:A:228:ILE:HG21	1:A:258:PRO:HG2	1.86	0.56
1:G:83:ALA:O	1:G:87:ALA:HB3	2.05	0.56
1:G:313:GLU:O	1:G:317:VAL:HG23	2.06	0.56
1:G:202:ASN:O	1:G:203:ARG:HB2	2.06	0.56
1:A:249:ARG:O	1:A:253:ILE:HG12	2.06	0.56
1:E:304:GLU:C	1:E:306:LYS:N	2.59	0.55
2:F:299:PRO:HD3	2:F:307:TRP:CD2	2.40	0.55
3:J:129:VAL:HG21	3:J:146:ILE:CG2	2.37	0.55
3:J:145:ASP:HB3	3:J:148:LEU:HD22	1.88	0.55
2:H:93:ILE:HG21	2:H:168:ILE:HD11	1.89	0.55
1:C:367:SER:H	1:C:368:LYS:HA	1.72	0.54
2:D:122:VAL:HG23	2:D:124:THR:HG23	1.89	0.54
2:H:282:LEU:HA	3:J:134:SER:HB3	1.89	0.53
2:F:128:HIS:N	6:F:2072:HOH:O	2.42	0.53
2:H:82:PHE:CZ	2:H:173:LEU:HD11	2.43	0.53
2:F:80:ILE:HG13	2:F:114:ILE:CG2	2.38	0.53
2:D:298:TYR:CG	2:D:299:PRO:HD2	2.44	0.53
3:I:129:VAL:HG21	3:I:146:ILE:HG21	1.90	0.53
1:C:23:PHE:HB3	1:C:233:VAL:HG12	1.89	0.53
1:G:66:LEU:HD13	1:G:329:ILE:HD11	1.92	0.52
1:A:294:ASP:HB3	1:A:297:VAL:CG2	2.38	0.52
1:C:46:LEU:HB3	1:C:303:LEU:HD21	1.90	0.52
2:H:17:LEU:HD11	2:H:25:ILE:HD12	1.92	0.52

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:60:ASP:OD2	1:A:79:ALA:HB2	2.08	0.52
2:H:299:PRO:HD3	2:H:307:TRP:CD2	2.44	0.52
1:A:9:PHE:CZ	1:C:231:ILE:HD11	2.40	0.52
1:E:49:LEU:O	1:E:53:MET:HG3	2.10	0.52
2:F:299:PRO:HA	2:H:102:TYR:OH	2.10	0.52
1:A:183:GLN:OE1	2:B:58:ALA:HB1	2.10	0.52
2:B:284:LEU:HD22	2:B:286:ALA:O	2.10	0.52
2:B:299:PRO:HD3	2:B:307:TRP:CD2	2.45	0.52
1:A:25:ILE:HD12	1:A:240:ALA:HA	1.91	0.52
1:E:304:GLU:O	1:E:307:GLY:N	2.39	0.51
1:A:49:LEU:HD11	1:A:87:ALA:HA	1.93	0.51
1:C:183:GLN:OE1	2:D:58:ALA:HB1	2.10	0.51
2:B:298:TYR:CG	2:B:299:PRO:HD2	2.45	0.51
1:E:23:PHE:HB3	1:E:233:VAL:HG12	1.93	0.51
1:E:78:THR:HG21	1:E:85:GLN:OE1	2.10	0.50
2:D:93:ILE:HA	2:D:97:MET:HG2	1.92	0.50
2:F:28:GLU:HG2	2:F:57:LEU:HD23	1.94	0.50
2:B:35:GLY:HA3	6:B:2014:HOH:O	2.11	0.50
1:G:67:ASN:ND2	1:G:73:GLY:O	2.44	0.50
1:G:66:LEU:HD22	1:G:329:ILE:CD1	2.42	0.49
2:D:75:ARG:HD3	2:D:161:ILE:O	2.11	0.49
1:A:58:ILE:O	1:A:62:ARG:HG2	2.13	0.49
2:D:174:LYS:O	2:D:178:SER:HB3	2.12	0.49
2:H:82:PHE:CB	2:H:85:PHE:CZ	2.96	0.49
1:C:100:PRO:HG3	1:C:108:ILE:HG21	1.94	0.48
1:E:303:LEU:HD12	1:E:309:TRP:CB	2.33	0.48
2:F:174:LYS:O	2:F:178:SER:HB3	2.13	0.48
1:E:36:GLU:HG2	6:E:2005:HOH:O	2.13	0.48
2:B:142:LEU:CD2	2:B:166:PRO:HB2	2.43	0.48
2:D:117:PRO:HA	2:D:171:GLU:O	2.13	0.48
1:E:25:ILE:HD13	1:E:39:PRO:HD3	1.95	0.48
2:H:298:TYR:CG	2:H:299:PRO:HD2	2.48	0.48
2:F:38:ARG:HB2	2:F:177:ARG:HH22	1.79	0.47
1:A:348:PHE:CZ	2:B:141:GLY:HA2	2.49	0.47
1:A:231:ILE:HD11	1:C:9:PHE:HZ	1.79	0.47
3:J:141:GLU:HG3	3:J:142:LYS:HG3	1.96	0.47
1:E:300:ARG:NH2	1:E:314:GLU:OE2	2.44	0.47
1:G:27:ASN:HD21	1:G:31:GLU:HB2	1.80	0.47
2:B:16:GLU:OE2	2:B:158:ILE:HG23	2.14	0.47
2:F:116:SER:HB3	2:F:170:LEU:HD23	1.97	0.47
2:B:102:TYR:OH	2:D:299:PRO:HA	2.15	0.47

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:81:GLN:O	2:B:117:PRO:HG2	2.15	0.47
1:A:88:SER:HB2	1:A:245:VAL:HG21	1.97	0.46
2:B:122:VAL:HG23	2:B:124:THR:HG23	1.96	0.46
2:B:238:VAL:HB	2:B:268:ILE:HG12	1.96	0.46
1:C:83:ALA:O	1:C:87:ALA:HB3	2.16	0.46
1:C:367:SER:N	1:C:368:LYS:CA	2.71	0.46
3:J:129:VAL:HG21	3:J:146:ILE:HG22	1.97	0.46
1:G:149:ILE:HG13	1:G:149:ILE:H	1.41	0.46
1:G:298:ARG:HB3	6:G:2060:HOH:O	2.15	0.46
1:A:9:PHE:CD1	1:C:229:PRO:HB3	2.52	0.46
1:E:294:ASP:C	1:E:294:ASP:OD1	2.54	0.45
2:F:74:PHE:O	2:F:76:PRO:HD3	2.15	0.45
1:A:368:LYS:N	6:A:2095:HOH:O	2.48	0.45
2:H:82:PHE:HZ	2:H:173:LEU:HD11	1.81	0.45
2:H:185:GLU:HG3	6:H:2078:HOH:O	2.15	0.45
6:E:2037:HOH:O	2:F:96:GLN:HG3	2.16	0.45
2:B:20:ASP:HB3	2:B:23:VAL:HG23	1.97	0.45
1:E:38:MET:HE3	1:E:239:LEU:HD13	1.98	0.45
1:E:144:ILE:HD12	5:E:1370:TDP:C2'	2.47	0.45
1:E:60:ASP:OD2	1:E:79:ALA:HB2	2.16	0.45
1:C:51:ARG:HG2	1:C:317:VAL:HG21	1.98	0.45
2:B:128:HIS:HE1	1:C:142:ILE:HD12	1.82	0.44
1:E:42:SER:H	1:E:45[B]:GLN:HE21	1.64	0.44
2:B:36:VAL:HG13	2:B:37:PHE:CD2	2.53	0.44
2:H:133:GLU:OE2	2:H:209:TYR:OH	2.26	0.44
1:A:187:PHE:HE1	2:B:58:ALA:HB3	1.81	0.44
2:B:128:HIS:HE1	1:C:142:ILE:CD1	2.31	0.44
2:H:38:ARG:HG2	6:H:2015:HOH:O	2.16	0.44
1:E:293:LYS:O	1:E:294:ASP:O	2.35	0.44
2:H:114:ILE:HD13	2:H:168:ILE:HD13	1.99	0.44
1:C:203:ARG:NH2	1:C:264:LEU:HD22	2.33	0.43
2:D:299:PRO:HD3	2:D:307:TRP:CD2	2.53	0.43
1:G:26:LEU:HG	1:G:239:LEU:HD12	2.00	0.43
1:A:224:VAL:HG13	1:C:16:VAL:HG11	2.00	0.43
1:A:100:PRO:HG2	1:A:140:PRO:HA	2.00	0.43
2:D:120:GLY:HA3	2:D:298:TYR:OH	2.18	0.43
1:E:326:LYS:O	1:E:329:ILE:HG22	2.18	0.43
2:H:205:THR:O	2:H:256:ALA:HA	2.19	0.43
2:B:59:GLU:HB3	2:B:89:VAL:CG2	2.47	0.43
2:F:264:ARG:NH1	6:F:2156:HOH:O	2.33	0.43
2:H:180:ARG:HD2	6:H:2004:HOH:O	2.19	0.43

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:125:PRO:HG2	2:D:128:HIS:CE1	2.53	0.43
3:I:129:VAL:HG13	6:I:2008:HOH:O	2.19	0.42
2:H:93:ILE:CG2	2:H:168:ILE:HD11	2.49	0.42
1:A:83:ALA:O	1:A:87:ALA:HB3	2.19	0.42
2:B:76:PRO:HD2	2:B:112:ILE:HG12	2.01	0.42
3:J:144:VAL:HG12	6:J:2020:HOH:O	2.19	0.42
1:C:26:LEU:HG	1:C:239:LEU:HD12	2.00	0.42
1:C:203:ARG:O	1:C:209:PRO:HA	2.19	0.42
2:B:284:LEU:O	3:I:136:ARG:HD2	2.19	0.42
2:D:286:ALA:HB1	2:D:287:PRO:HD2	2.00	0.42
1:G:123:ARG:NH2	1:G:333:ASP:OD1	2.46	0.42
6:G:2039:HOH:O	2:H:96:GLN:HG3	2.19	0.42
2:H:14:ARG:HD3	6:H:2018:HOH:O	2.19	0.42
1:E:304:GLU:O	1:E:306:LYS:N	2.53	0.42
2:F:282:LEU:HD13	3:J:130:ILE:HB	2.02	0.42
1:A:298:ARG:HB3	6:A:2071:HOH:O	2.19	0.42
2:F:93:ILE:HA	2:F:97:MET:CG	2.48	0.42
2:H:80:ILE:O	2:H:80:ILE:HG22	2.18	0.42
1:G:66:LEU:HD22	1:G:329:ILE:HD11	2.02	0.42
2:D:20:ASP:HB3	2:D:23:VAL:HG23	2.02	0.42
2:B:117:PRO:HA	2:B:171:GLU:O	2.19	0.42
1:A:105:VAL:N	1:A:106:PRO:CD	2.82	0.41
2:F:17:LEU:HD11	2:F:25:ILE:HD12	2.02	0.41
2:B:299:PRO:HD3	2:B:307:TRP:CE3	2.54	0.41
1:E:78:THR:HG21	1:E:85:GLN:CD	2.40	0.41
2:H:59:GLU:CD	2:H:59:GLU:H	2.24	0.41
2:D:298:TYR:CD2	2:D:299:PRO:HD2	2.56	0.41
2:F:97:MET:SD	2:F:114:ILE:HD11	2.60	0.41
2:F:142:LEU:HD23	2:F:166:PRO:HB2	2.01	0.41
1:E:294:ASP:HA	1:E:295:PRO:HD2	1.91	0.41
1:C:203:ARG:HH21	1:C:264:LEU:HD22	1.85	0.41
1:E:235:GLY:N	1:E:264:LEU:O	2.49	0.41
2:D:97:MET:HA	2:D:100:ILE:HD12	2.02	0.41
1:E:338:GLN:HE21	2:H:302:GLN:HB3	1.85	0.41
1:G:335:THR:HA	1:G:336:PRO:HD3	1.97	0.41
2:F:59:GLU:H	2:F:59:GLU:CD	2.25	0.41
1:E:76:ALA:CB	1:E:103:ARG:HG2	2.47	0.40
1:E:83:ALA:HB3	1:E:235:GLY:O	2.21	0.40
2:F:92:SER:O	2:F:97:MET:HG2	2.22	0.40
2:H:142:LEU:HD22	2:H:168:ILE:HG12	2.03	0.40
1:A:50:MET:O	1:A:54:VAL:HG23	2.21	0.40

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:142:ILE:HG13	6:E:2036:HOH:O	2.22	0.40
2:B:38:ARG:HG3	2:B:177:ARG:NH2	2.36	0.40
3:I:161:GLU:HB2	6:I:2021:HOH:O	2.21	0.40
1:G:346:ILE:HD12	2:H:102:TYR:O	2.21	0.40
1:E:7:PHE:O	1:E:9:PHE:N	2.54	0.40
2:B:97:MET:SD	2:B:114:ILE:HD11	2.61	0.40
1:C:51:ARG:HG2	1:C:317:VAL:CG2	2.52	0.40
1:G:199:VAL:HG23	1:G:260:LEU:HD11	2.02	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all 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	337/368 (92%)	327 (97%)	9 (3%)	1 (0%)	46	57
1	C	339/368 (92%)	329 (97%)	9 (3%)	1 (0%)	46	57
1	E	323/368 (88%)	304 (94%)	16 (5%)	3 (1%)	21	24
1	G	326/368 (89%)	316 (97%)	9 (3%)	1 (0%)	46	57
2	B	323/324 (100%)	309 (96%)	13 (4%)	1 (0%)	46	57
2	D	322/324 (99%)	311 (97%)	11 (3%)	0	100	100
2	F	305/324 (94%)	298 (98%)	6 (2%)	1 (0%)	46	57
2	H	313/324 (97%)	303 (97%)	8 (3%)	2 (1%)	30	36
3	I	38/49 (78%)	38 (100%)	0	0	100	100
3	J	41/49 (84%)	40 (98%)	1 (2%)	0	100	100
All	All	2667/2866 (93%)	2575 (97%)	82 (3%)	10 (0%)	39	48

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	206	ILE
1	C	206	ILE
1	E	305	ALA
1	G	203	ARG
2	H	81	GLN
2	F	301	ALA
1	E	297	VAL
2	B	184	PRO
2	H	86	VAL
1	E	294	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	255/304 (84%)	252 (99%)	3 (1%)	78	89
1	C	267/304 (88%)	260 (97%)	7 (3%)	54	71
1	E	250/304 (82%)	241 (96%)	9 (4%)	42	57
1	G	257/304 (84%)	255 (99%)	2 (1%)	86	94
2	B	247/263 (94%)	237 (96%)	10 (4%)	38	52
2	D	263/263 (100%)	259 (98%)	4 (2%)	72	85
2	F	249/263 (95%)	241 (97%)	8 (3%)	46	62
2	H	251/263 (95%)	245 (98%)	6 (2%)	57	74
3	I	31/36 (86%)	27 (87%)	4 (13%)	5	5
3	J	30/36 (83%)	27 (90%)	3 (10%)	9	11
All	All	2100/2340 (90%)	2044 (97%)	56 (3%)	54	70

All (56) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	43	ASP
1	A	142	ILE
1	A	265	CYS
2	B	38	ARG

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
2	B	89	VAL
2	B	123	HIS
2	B	130	ASP
2	B	131	SER
2	B	176	TYR
2	B	187	GLU
2	B	277[A]	ASN
2	B	277[B]	ASN
2	B	320	LYS
1	C	13	LEU
1	C	142	ILE
1	C	203	ARG
1	C	210	VAL
1	C	211	GLU
1	C	253	ILE
1	C	254	ASN
2	D	176	TYR
2	D	187	GLU
2	D	277	ASN
2	D	320	LYS
1	E	38	MET
1	E	67	ASN
1	E	68	ARG
1	E	71	ARG
1	E	78	THR
1	E	202	ASN
1	E	303	LEU
1	E	329	ILE
1	E	368	LYS
2	F	32	VAL
2	F	80	ILE
2	F	97	MET
2	F	176	TYR
2	F	187	GLU
2	F	277[A]	ASN
2	F	277[B]	ASN
2	F	320	LYS
1	G	149	ILE
1	G	329	ILE
2	H	82	PHE
2	H	130	ASP
2	H	131	SER

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
2	H	142	LEU
2	H	176	TYR
2	H	277	ASN
3	I	129	VAL
3	I	146	ILE
3	I	157	ARG
3	I	160	LYS
3	J	129	VAL
3	J	160	LYS
3	J	161	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	69	GLN
1	E	320	GLN
1	G	67	ASN
1	G	186	ASN
2	H	302	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

### 5.6 Ligand geometry [i](#)

Of 8 ligands modelled in this entry, 4 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
5	TDP	A	1370	4	21,27,27	1.71	4 (19%)	31,40,40	1.94	7 (22%)
5	TDP	C	1370	4	21,27,27	1.38	4 (19%)	31,40,40	2.29	10 (32%)
5	TDP	E	1370	4	21,27,27	1.74	4 (19%)	31,40,40	2.04	9 (29%)
5	TDP	G	1370	4	21,27,27	1.64	4 (19%)	31,40,40	1.75	8 (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	TDP	A	1370	4	-	0/16/17/17	0/2/2/2
5	TDP	C	1370	4	-	0/16/17/17	0/2/2/2
5	TDP	E	1370	4	-	0/16/17/17	0/2/2/2
5	TDP	G	1370	4	-	0/16/17/17	0/2/2/2

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	E	1370	TDP	C4-N3	-4.71	1.35	1.39
5	A	1370	TDP	C4-N3	-4.54	1.35	1.39
5	G	1370	TDP	C4-N3	-4.34	1.35	1.39
5	E	1370	TDP	P2-O11	-4.21	1.51	1.61
5	G	1370	TDP	P2-O11	-3.78	1.52	1.61
5	A	1370	TDP	P2-O11	-3.15	1.53	1.61
5	C	1370	TDP	C4-N3	-2.83	1.37	1.39
5	C	1370	TDP	P2-O11	-2.82	1.54	1.61
5	C	1370	TDP	C4'-N4'	2.59	1.40	1.34
5	G	1370	TDP	C4'-N4'	2.62	1.40	1.34
5	E	1370	TDP	C4'-N4'	2.67	1.40	1.34
5	G	1370	TDP	C5'-C4'	2.83	1.49	1.42
5	E	1370	TDP	C5'-C4'	2.84	1.49	1.42
5	C	1370	TDP	C5'-C4'	2.92	1.49	1.42
5	A	1370	TDP	C4'-N4'	2.96	1.41	1.34
5	A	1370	TDP	C5'-C4'	3.29	1.50	1.42

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	1370	TDP	C5A-C5-S1	-4.71	113.64	120.24
5	E	1370	TDP	C5A-C5-S1	-4.04	114.58	120.24
5	A	1370	TDP	C5A-C5-S1	-3.92	114.75	120.24
5	C	1370	TDP	C4A-C4-C5	-2.62	123.01	128.90
5	E	1370	TDP	C5'-C35-N3	-2.56	109.05	113.33
5	E	1370	TDP	C5'-C6'-N1'	-2.55	119.43	123.86
5	G	1370	TDP	C5'-C6'-N1'	-2.50	119.51	123.86
5	G	1370	TDP	C4A-C4-C5	-2.41	123.49	128.90
5	C	1370	TDP	C5'-C35-N3	-2.32	109.44	113.33
5	G	1370	TDP	C5A-C5-S1	-2.29	117.03	120.24
5	A	1370	TDP	N1'-C2'-N3'	-2.27	121.40	125.60
5	C	1370	TDP	N1'-C2'-N3'	-2.27	121.41	125.60
5	E	1370	TDP	N1'-C2'-N3'	-2.24	121.46	125.60
5	A	1370	TDP	C5'-C6'-N1'	-2.14	120.15	123.86
5	C	1370	TDP	C5'-C6'-N1'	-2.08	120.25	123.86
5	C	1370	TDP	C2A-C2'-N1'	2.08	119.52	117.03
5	G	1370	TDP	N4'-C4'-N3'	2.12	120.02	116.95
5	E	1370	TDP	N4'-C4'-N3'	2.26	120.22	116.95
5	A	1370	TDP	C4A-C4-N3	2.32	125.68	122.59
5	A	1370	TDP	O11-P1-O5G	2.64	109.94	102.94
5	E	1370	TDP	C4A-C4-N3	2.70	126.19	122.59
5	C	1370	TDP	O11-P1-O5G	2.85	110.49	102.94
5	E	1370	TDP	O11-P1-O5G	2.89	110.60	102.94
5	G	1370	TDP	O11-P1-O5G	2.97	110.81	102.94
5	G	1370	TDP	C4A-C4-N3	3.00	126.59	122.59
5	C	1370	TDP	C4A-C4-N3	3.45	127.19	122.59
5	C	1370	TDP	C6'-N1'-C2'	3.54	121.96	115.77
5	G	1370	TDP	C6'-N1'-C2'	3.55	121.97	115.77
5	A	1370	TDP	C6'-N1'-C2'	3.55	121.98	115.77
5	E	1370	TDP	C6'-N1'-C2'	3.78	122.38	115.77
5	G	1370	TDP	C5A-C5-C4	4.55	131.64	127.56
5	E	1370	TDP	C5A-C5-C4	6.30	133.21	127.56
5	A	1370	TDP	C5A-C5-C4	6.31	133.22	127.56
5	C	1370	TDP	C5A-C5-C4	7.83	134.58	127.56

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	1370	TDP	1	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	C	1370	TDP	1	0
5	E	1370	TDP	2	0
5	G	1370	TDP	1	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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	341/368 (92%)	-0.20	6 (1%) 71 78	24, 42, 62, 79	2 (0%)
1	C	343/368 (93%)	-0.25	9 (2%) 59 68	22, 38, 60, 88	2 (0%)
1	E	328/368 (89%)	0.21	24 (7%) 18 25	20, 47, 68, 85	3 (0%)
1	G	331/368 (89%)	-0.00	16 (4%) 34 43	25, 45, 68, 88	1 (0%)
2	B	324/324 (100%)	-0.31	7 (2%) 65 73	20, 37, 53, 67	0
2	D	324/324 (100%)	-0.44	1 (0%) 94 96	20, 30, 45, 61	0
2	F	310/324 (95%)	-0.44	1 (0%) 94 96	17, 30, 47, 67	0
2	H	317/324 (97%)	-0.32	9 (2%) 56 66	18, 33, 54, 93	0
3	I	40/49 (81%)	1.67	14 (35%) 0 0	50, 66, 76, 82	0
3	J	43/49 (87%)	1.79	16 (37%) 0 0	46, 66, 80, 87	0
All	All	2701/2866 (94%)	-0.16	103 (3%) 44 53	17, 38, 65, 93	8 (0%)

All (103) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	204	PHE	10.0
1	E	204	PHE	7.3
1	G	205	ALA	6.8
1	E	205	ALA	6.3
2	H	82	PHE	6.2
1	E	74	PHE	5.9
3	J	168	ALA	5.9
1	A	268	TYR	5.5
3	I	163	ILE	5.4
1	E	6	GLN	4.9
3	J	148	LEU	4.8
1	E	5	PHE	4.5
3	J	169	GLY	4.4

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	A	254	ASN	4.3
1	E	51	ARG	4.3
1	G	5	PHE	4.1
1	C	266	PHE	4.1
3	I	165	ALA	4.1
2	H	120	GLY	4.0
3	I	167	LEU	3.9
3	J	155	ASN	3.8
2	H	57	LEU	3.8
1	E	33	VAL	3.8
2	F	128	HIS	3.7
3	J	167	LEU	3.7
1	E	76	ALA	3.7
1	C	268	TYR	3.5
2	H	84	GLY	3.3
3	J	160	LYS	3.3
1	E	8	PRO	3.3
3	I	150	GLN	3.3
1	G	74	PHE	3.2
1	E	203	ARG	3.2
3	J	128	ARG	3.2
3	I	164	ASP	3.1
3	J	130	ILE	3.0
2	H	121	GLY	2.9
2	B	123	HIS	2.9
3	I	128	ARG	2.9
2	B	1	ALA	2.8
1	C	204	PHE	2.8
1	G	6	GLN	2.8
2	B	178	SER	2.8
1	G	68	ARG	2.8
1	G	254	ASN	2.8
1	E	301	LYS	2.8
1	E	102	TYR	2.8
1	E	368	LYS	2.7
2	H	85	PHE	2.7
2	H	83	PHE	2.7
1	C	267	ARG	2.7
3	I	161	GLU	2.7
3	J	139	ALA	2.7
1	E	305	ALA	2.7
3	I	160	LYS	2.6

*Continued on next page...*

*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
3	I	144	VAL	2.6
1	E	10	ALA	2.6
2	H	81	GLN	2.5
1	E	233	VAL	2.5
2	D	123	HIS	2.5
3	I	147	ARG	2.5
1	E	254	ASN	2.5
1	E	367	SER	2.5
1	G	307	GLY	2.5
3	J	158	VAL	2.5
1	A	266	PHE	2.5
3	I	148	LEU	2.4
1	C	6	GLN	2.4
1	G	213	GLN	2.4
2	B	227	GLY	2.3
3	J	135	VAL	2.3
1	A	204	PHE	2.3
3	I	146	ILE	2.3
3	J	144	VAL	2.3
1	E	308	LEU	2.3
1	E	238	PRO	2.3
1	G	203	ARG	2.3
1	E	202	ASN	2.3
1	G	36	GLU	2.2
3	I	155	ASN	2.2
2	B	324	PHE	2.2
2	B	124	THR	2.2
2	H	38	ARG	2.2
1	A	305	ALA	2.2
1	C	211	GLU	2.2
3	J	170	GLY	2.2
1	C	233	VAL	2.2
1	C	5	PHE	2.2
1	E	28	GLU	2.2
1	G	305	ALA	2.2
2	B	122	VAL	2.1
3	J	156	GLY	2.1
1	C	203	ARG	2.1
3	J	147	ARG	2.1
3	I	138	TYR	2.1
1	G	368	LYS	2.1
3	J	161	GLU	2.1

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	G	233	VAL	2.1
1	G	72	LEU	2.0
1	A	238	PRO	2.0
1	E	77	PRO	2.0
1	E	319	GLU	2.0
1	G	35	GLU	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
5	TDP	E	1370	26/26	0.59	0.54	5.14	172,176,177,178	0
5	TDP	G	1370	26/26	0.57	0.51	4.59	143,149,155,155	0
5	TDP	C	1370	26/26	0.95	0.14	-0.02	34,47,51,53	0
5	TDP	A	1370	26/26	0.96	0.10	-0.79	29,37,40,42	0
4	MG	A	1368	1/1	0.93	0.07	-1.30	28,28,28,28	0
4	MG	C	1368	1/1	0.98	0.05	-1.37	28,28,28,28	0
4	MG	E	1368	1/1	0.45	0.26	-	78,78,78,78	0
4	MG	G	1368	1/1	0.86	0.08	-	66,66,66,66	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.