



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2017 – 12:13 am GMT

PDB ID : 1UMC  
Title : branched-chain 2-oxo acid dehydrogenase (E1) from *Thermus thermophilus* HB8 with 4-methylpentanoate  
Authors : Nakai, T.; Nakagawa, N.; Maoka, N.; Masui, R.; Kuramitsu, S.; Kamiya, N.; RIKEN Structural Genomics/Proteomics Initiative (RSGI)  
Deposited on : 2003-09-25  
Resolution : 2.40 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	:	1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix)	:	1.9-1692
EDS	:	trunk28620
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
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)	:	recalc28949

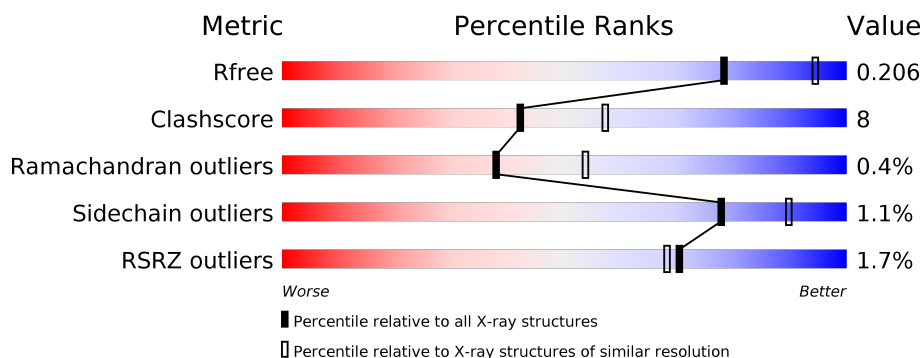
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.40 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))
$R_{free}$	100719	3166 (2.40-2.40)
Clashscore	112137	3674 (2.40-2.40)
Ramachandran outliers	110173	3616 (2.40-2.40)
Sidechain outliers	110143	3617 (2.40-2.40)
RSRZ outliers	101464	3195 (2.40-2.40)

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	367	<div> <div>3%</div> <div>79%</div> <div>19%</div> <div>.</div> </div>
1	C	367	<div> <div>3%</div> <div>80%</div> <div>19%</div> <div>.</div> </div>
2	B	324	<div> <div>82%</div> <div>18%</div> </div>
2	D	324	<div> <div>82%</div> <div>17%</div> </div>

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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	4MV	D	1403	-	-	X	X

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 11472 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 2-oxo acid dehydrogenase alpha subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	362	Total	C	N	O	S	0	0	0
			2879	1844	504	523	8			
1	C	361	Total	C	N	O	S	0	0	0
			2870	1838	503	521	8			

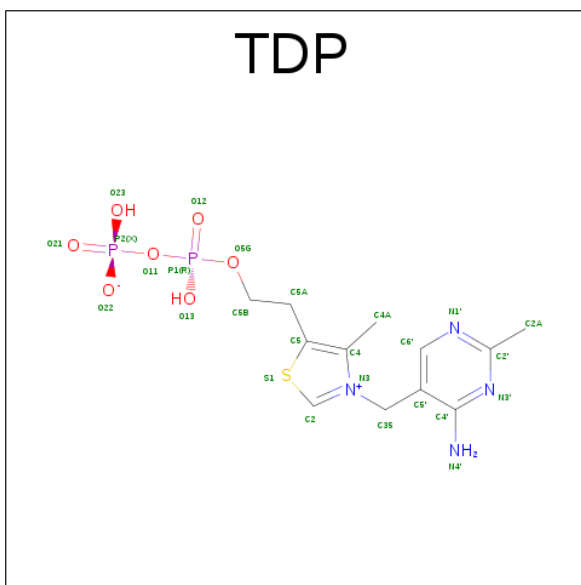
- Molecule 2 is a protein called 2-oxo acid dehydrogenase beta subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	323	Total	C	N	O	S	0	0	0
			2463	1570	425	457	11			
2	D	323	Total	C	N	O	S	0	0	0
			2463	1570	425	457	11			

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

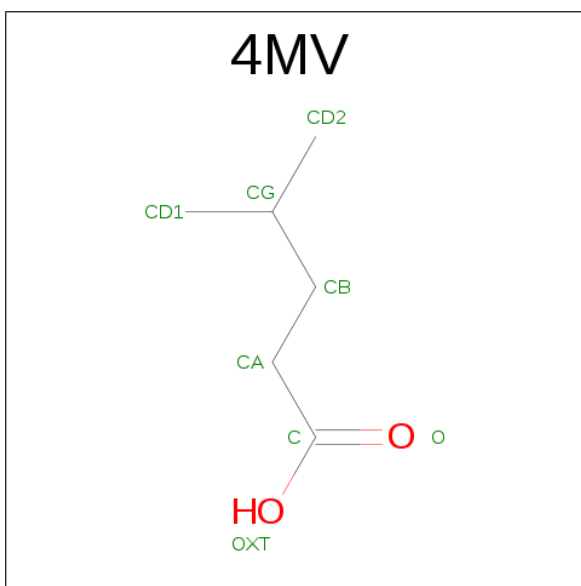
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Mg	0	0
			1	1		
3	C	1	Total	Mg	0	0
			1	1		

- Molecule 4 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
4	A	1	Total	C	N	O	P	S	0	0
			26	12	4	7	2	1		
4	C	1	Total	C	N	O	P	S	0	0
			26	12	4	7	2	1		

- Molecule 5 is 4-METHYL VALERIC ACID (three-letter code: 4MV) (formula:  $C_6H_{12}O_2$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	D	1	Total	C	O	0	0
			8	6	2		

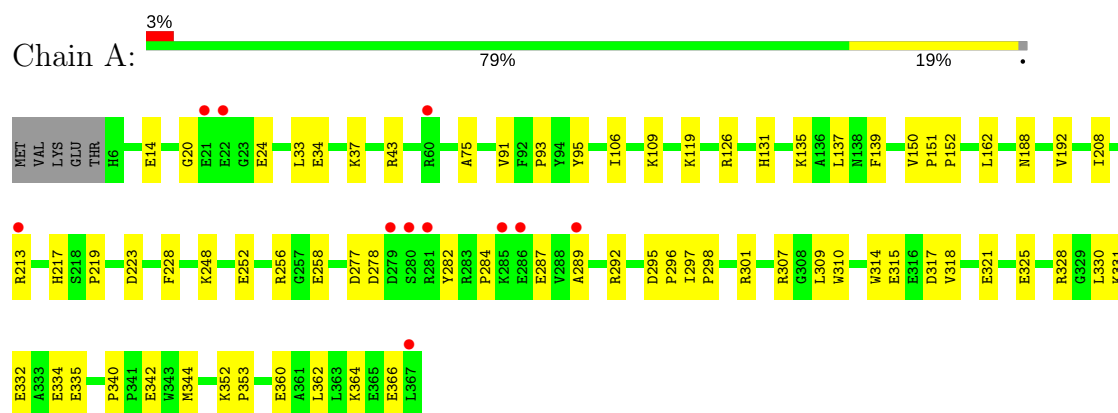
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	186	Total 186	O 186	0	0
6	B	165	Total 165	O 165	0	0
6	C	225	Total 225	O 225	0	0
6	D	159	Total 159	O 159	0	0

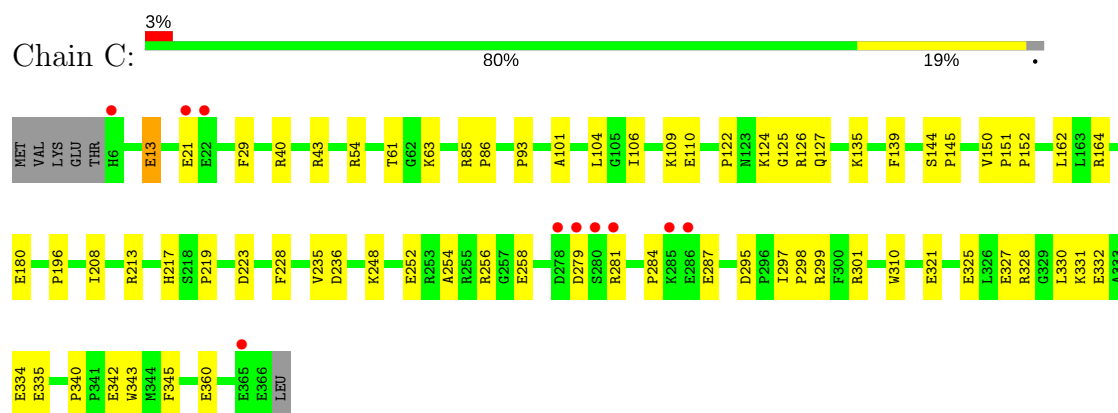
### 3 Residue-property plots [i](#)

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

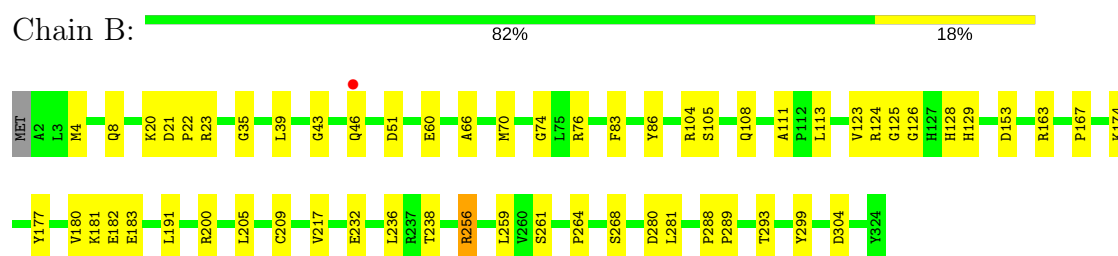
#### • Molecule 1: 2-oxo acid dehydrogenase alpha subunit



#### • Molecule 1: 2-oxo acid dehydrogenase alpha subunit



#### • Molecule 2: 2-oxo acid dehydrogenase beta subunit

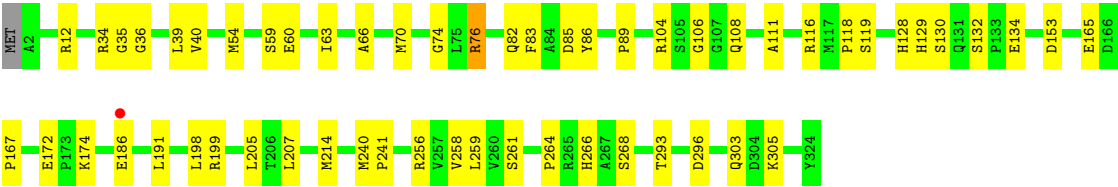


#### • Molecule 2: 2-oxo acid dehydrogenase beta subunit

Chain D: 

82%

17%





## 4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	127.20Å 247.22Å 137.56Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.95 – 2.40 19.95 – 2.40	Depositor EDS
% Data completeness (in resolution range)	99.5 (19.95-2.40) 99.6 (19.95-2.40)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.12 (at 2.41Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, $R_{free}$	0.172 , 0.206 0.172 , 0.206	Depositor DCC
$R_{free}$ test set	4205 reflections (4.99%)	DCC
Wilson B-factor (Å <sup>2</sup> )	25.1	Xtriage
Anisotropy	0.289	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 47.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	11472	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.63% 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, 0.333 respectively for untwinned datasets, and 0.375, 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, 4MV

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	0.32	0/2960	0.54	0/4015
1	C	0.33	0/2951	0.55	0/4004
2	B	0.31	0/2513	0.61	0/3415
2	D	0.31	0/2513	0.60	0/3415
All	All	0.32	0/10937	0.57	0/14849

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 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	2879	0	2793	58	0
1	C	2870	0	2782	47	0
2	B	2463	0	2505	36	0
2	D	2463	0	2505	35	0
3	A	1	0	0	0	0
3	C	1	0	0	0	0
4	A	26	0	16	3	0
4	C	26	0	16	2	0
5	D	8	0	11	6	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	A	186	0	0	4	0
6	B	165	0	0	1	0
6	C	225	0	0	3	0
6	D	159	0	0	3	0
All	All	11472	0	10628	169	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 8.

All (169) 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)
4:A:1402:TDP:C2	4:A:1402:TDP:H2	0.97	1.49
4:C:2402:TDP:H2	4:C:2402:TDP:C2	0.97	1.48
1:A:213:ARG:HH22	1:A:217:HIS:HA	1.16	1.06
6:A:1575:HOH:O	5:D:1403:4MV:HA2	1.71	0.89
2:D:85:ASP:OD2	2:D:130:SER:HA	1.77	0.84
1:A:256:ARG:HD2	1:A:258:GLU:OE2	1.78	0.83
1:A:131:HIS:HE1	5:D:1403:4MV:HD21	1.45	0.81
1:A:321:GLU:O	1:A:325:GLU:HG3	1.83	0.79
2:D:132:SER:HB3	2:D:134:GLU:OE1	1.86	0.76
2:B:60:GLU:HG2	2:B:86:TYR:O	1.88	0.74
1:A:317:ASP:O	1:A:321:GLU:HG3	1.89	0.72
2:D:60:GLU:HG2	2:D:86:TYR:O	1.89	0.71
1:C:331:LYS:O	1:C:335:GLU:HG3	1.92	0.70
2:B:128:HIS:O	2:B:129:HIS:HD2	1.76	0.68
1:A:297:ILE:HB	1:A:298:PRO:HD3	1.74	0.67
1:C:297:ILE:HB	1:C:298:PRO:HD3	1.76	0.67
1:A:292:ARG:HG3	1:A:292:ARG:HH11	1.61	0.64
1:A:331:LYS:O	1:A:335:GLU:HG2	1.98	0.63
1:C:13:GLU:CD	1:C:13:GLU:H	2.01	0.63
1:C:213:ARG:HG2	1:C:213:ARG:HH11	1.64	0.62
1:A:24:GLU:HG3	6:A:1534:HOH:O	2.00	0.61
1:C:328:ARG:O	1:C:332:GLU:HG3	2.01	0.61
1:C:21:GLU:CD	1:C:21:GLU:H	2.02	0.61
1:A:328:ARG:O	1:A:332:GLU:HG3	2.01	0.60
1:A:33:LEU:HD22	1:A:37:LYS:HD3	1.84	0.59
2:D:305:LYS:HG3	6:D:1456:HOH:O	2.01	0.59
2:B:264:PRO:O	2:B:268:SER:HB3	2.03	0.59
1:C:109:LYS:HE3	6:C:2473:HOH:O	2.02	0.59
1:A:151:PRO:HB2	1:A:152:PRO:HD3	1.85	0.58

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:219:PRO:HG2	1:A:223:ASP:OD2	2.02	0.58
1:C:151:PRO:HB2	1:C:152:PRO:HD3	1.85	0.58
1:A:91:VAL:HG12	1:A:93:PRO:HD3	1.86	0.58
2:B:4:MET:HB2	2:B:8:GLN:HB2	1.86	0.57
1:A:301:ARG:HH11	1:A:301:ARG:HG2	1.69	0.57
2:D:76:ARG:HH22	2:D:165:GLU:CD	2.08	0.57
2:B:66:ALA:O	2:B:70:MET:HG3	2.05	0.57
1:A:213:ARG:NH2	1:A:217:HIS:HA	2.02	0.57
1:C:248:LYS:O	1:C:252:GLU:HG3	2.04	0.57
1:C:150:VAL:HB	1:C:151:PRO:HD3	1.88	0.56
1:C:256:ARG:HD2	1:C:258:GLU:OE2	2.05	0.56
2:D:264:PRO:O	2:D:268:SER:HB3	2.05	0.56
2:B:200:ARG:O	2:B:232:GLU:HG3	2.06	0.56
2:D:128:HIS:HB2	5:D:1403:4MV:O	2.06	0.56
1:C:93:PRO:HG3	1:C:139:PHE:CZ	2.42	0.55
1:C:135:LYS:HB2	2:D:108:GLN:HB3	1.89	0.55
1:C:164:ARG:HG2	1:C:164:ARG:HH11	1.71	0.55
1:A:93:PRO:HG3	1:A:139:PHE:CZ	2.42	0.55
2:B:111:ALA:HB3	2:B:167:PRO:HG3	1.88	0.55
2:D:118:PRO:HA	2:D:172:GLU:O	2.06	0.54
2:D:12:ARG:HD3	2:D:186:GLU:OE1	2.08	0.54
1:C:321:GLU:O	1:C:325:GLU:HG3	2.07	0.54
2:D:66:ALA:O	2:D:70:MET:HG3	2.08	0.54
1:A:330:LEU:O	1:A:334:GLU:HG3	2.07	0.54
2:B:182:GLU:HG2	2:B:183:GLU:N	2.23	0.53
1:A:188:ASN:O	1:A:192:VAL:HG23	2.07	0.53
2:B:180:VAL:HG22	2:B:181:LYS:N	2.23	0.53
1:A:95:TYR:CD2	5:D:1403:4MV:HD13	2.44	0.53
1:A:150:VAL:HB	1:A:151:PRO:HD3	1.89	0.53
2:D:153:ASP:OD2	2:D:199:ARG:NH2	2.40	0.53
2:B:43:GLY:O	2:B:46:GLN:HG2	2.09	0.53
2:B:123:VAL:HG21	2:B:174:LYS:HD2	1.91	0.53
2:B:280:ASP:O	2:B:281:LEU:HD23	2.08	0.52
1:C:54:ARG:HH22	1:C:327:GLU:CD	2.13	0.52
1:C:284:PRO:HG2	1:C:287:GLU:HB2	1.92	0.52
1:C:40:ARG:NH2	1:C:43:ARG:HD2	2.24	0.52
2:D:261:SER:O	2:D:293:THR:HA	2.10	0.52
1:A:228:PHE:O	1:C:217:HIS:HB3	2.10	0.52
1:A:307:ARG:HG3	1:A:307:ARG:HH11	1.75	0.51
2:B:23:ARG:CZ	2:B:76:ARG:HD2	2.40	0.51
1:A:162:LEU:HD22	2:B:51:ASP:HB3	1.93	0.51

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:217:HIS:HB3	1:C:228:PHE:O	2.10	0.51
2:B:261:SER:O	2:B:293:THR:HA	2.11	0.50
1:A:248:LYS:O	1:A:252:GLU:HG3	2.10	0.50
2:D:129:HIS:HD2	2:D:174:LYS:NZ	2.10	0.50
2:D:83:PHE:HB2	2:D:86:TYR:CD2	2.46	0.50
2:B:20:LYS:NZ	2:B:163:ARG:NH2	2.60	0.50
1:A:43:ARG:HG2	1:A:318:VAL:CG1	2.42	0.50
1:A:292:ARG:NH1	1:A:292:ARG:HG3	2.26	0.49
2:B:128:HIS:O	2:B:129:HIS:CD2	2.61	0.49
2:B:125:GLY:O	2:B:129:HIS:HB2	2.12	0.49
2:B:259:LEU:N	2:B:259:LEU:HD12	2.27	0.49
1:C:330:LEU:O	1:C:334:GLU:HG3	2.12	0.49
1:C:61:THR:OG1	1:C:63:LYS:HG2	2.11	0.49
1:A:131:HIS:CE1	5:D:1403:4MV:HD21	2.35	0.49
1:C:219:PRO:HG2	1:C:223:ASP:OD2	2.12	0.49
1:A:126:ARG:HH11	1:A:126:ARG:HG3	1.78	0.49
2:B:113:LEU:HD12	2:B:113:LEU:C	2.33	0.48
2:D:111:ALA:HB3	2:D:167:PRO:HG3	1.94	0.48
1:A:109:LYS:NZ	1:A:109:LYS:HB3	2.28	0.48
2:D:36:GLY:HA3	6:D:1427:HOH:O	2.14	0.48
1:C:63:LYS:HE2	1:C:334:GLU:OE2	2.14	0.47
1:A:20:GLY:HA3	1:A:24:GLU:HG2	1.95	0.47
2:B:209:CYS:SG	2:B:217:VAL:HG11	2.54	0.47
2:B:23:ARG:NH2	2:B:76:ARG:HD2	2.30	0.47
2:B:124:ARG:HA	2:B:304:ASP:OD2	2.15	0.46
2:D:86:TYR:O	2:D:89:PRO:HD2	2.16	0.46
1:A:344:MET:HE2	2:D:303:GLN:HB3	1.96	0.46
2:D:35:GLY:O	2:D:39:LEU:HA	2.14	0.46
1:A:342:GLU:H	1:A:342:GLU:CD	2.18	0.46
2:B:83:PHE:HB2	2:B:86:TYR:CD2	2.51	0.46
1:C:124:LYS:HE3	2:D:106:GLY:O	2.15	0.46
1:A:307:ARG:O	1:A:309:LEU:HD13	2.15	0.45
1:A:34:GLU:H	1:A:34:GLU:CD	2.20	0.45
1:A:301:ARG:HD2	1:A:310:TRP:CZ2	2.51	0.45
1:C:110:GLU:HG2	1:C:122:PRO:HD3	1.97	0.45
1:A:119:LYS:HD3	1:A:340:PRO:HD3	1.98	0.45
2:D:259:LEU:N	2:D:259:LEU:HD12	2.32	0.45
1:A:109:LYS:HE2	6:A:1568:HOH:O	2.16	0.45
2:D:266:HIS:HD1	2:D:296:ASP:CG	2.20	0.45
2:B:126:GLY:O	2:B:299:TYR:HB3	2.17	0.45
1:C:86:PRO:HB3	1:C:104:LEU:HD12	1.99	0.45

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:284:PRO:HG2	1:C:287:GLU:CB	2.47	0.45
4:A:1402:TDP:H2	5:D:1403:4MV:HB1	1.98	0.44
1:C:144:SER:N	1:C:145:PRO:HD2	2.32	0.44
2:B:128:HIS:HB2	1:C:144:SER:HB2	1.99	0.44
2:D:119:SER:HA	2:D:130:SER:HB3	1.98	0.44
1:C:162:LEU:HD11	2:D:54:MET:CE	2.47	0.44
1:A:295:ASP:HB3	1:A:298:PRO:HD2	2.00	0.44
2:B:35:GLY:O	2:B:39:LEU:HA	2.17	0.44
1:C:29:PHE:HD1	1:C:29:PHE:H	1.66	0.44
1:C:301:ARG:HD2	1:C:310:TRP:CZ2	2.52	0.43
1:C:299:ARG:HD2	6:C:2476:HOH:O	2.17	0.43
2:D:59:SER:O	2:D:63:ILE:HG13	2.18	0.43
1:A:284:PRO:HG2	1:A:287:GLU:HB2	2.00	0.43
1:A:307:ARG:NH1	1:A:307:ARG:HG3	2.34	0.43
2:D:12:ARG:HD3	2:D:186:GLU:OE2	2.18	0.43
1:C:126:ARG:HH11	1:C:126:ARG:HG3	1.82	0.43
2:D:153:ASP:HA	2:D:191:LEU:CD1	2.48	0.43
1:A:135:LYS:HB2	2:B:108:GLN:HB3	2.00	0.43
1:A:344:MET:HE2	2:D:303:GLN:CB	2.49	0.43
2:B:104:ARG:HD3	6:B:380:HOH:O	2.19	0.43
1:C:127:GLN:NE2	2:D:104:ARG:HD2	2.34	0.43
1:A:75:ALA:HB2	1:A:296:PRO:HB2	2.01	0.42
1:A:256:ARG:HH11	1:A:258:GLU:CD	2.21	0.42
2:B:205:LEU:HD12	2:B:256:ARG:O	2.19	0.42
1:C:101:ALA:HB1	1:C:106:ILE:HD12	2.00	0.42
1:C:196:PRO:HA	1:C:254:ALA:HB1	2.00	0.42
1:A:362:LEU:HD21	6:D:1521:HOH:O	2.18	0.42
1:C:54:ARG:NH2	1:C:327:GLU:CD	2.73	0.42
1:A:314:TRP:O	1:A:318:VAL:HG23	2.19	0.42
1:C:279:ASP:C	1:C:281:ARG:H	2.23	0.42
2:D:12:ARG:HD3	2:D:186:GLU:CD	2.40	0.42
2:B:21:ASP:HA	2:B:22:PRO:HD3	1.87	0.42
2:B:236:LEU:O	2:B:238:THR:N	2.52	0.42
1:C:345:PHE:CE2	1:C:360:GLU:HA	2.55	0.42
1:A:256:ARG:NH1	1:A:258:GLU:OE1	2.53	0.41
2:D:40:VAL:HG11	2:D:116:ARG:NH2	2.34	0.41
1:A:106:ILE:HG12	1:A:137:LEU:HD12	2.03	0.41
2:B:105:SER:O	2:B:108:GLN:HG3	2.21	0.41
1:C:295:ASP:HB3	1:C:298:PRO:HD2	2.02	0.41
1:C:340:PRO:HD2	1:C:343:TRP:CD2	2.56	0.41
1:A:43:ARG:HG2	1:A:318:VAL:HG11	2.03	0.41

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:364:LYS:C	1:A:366:GLU:N	2.74	0.41
2:B:180:VAL:CG2	2:B:181:LYS:N	2.82	0.41
2:D:207:LEU:HD23	2:D:258:VAL:HB	2.03	0.41
1:C:180:GLU:OE2	4:C:2402:TDP:H2A3	2.20	0.41
1:A:277:ASP:CG	1:A:278:ASP:N	2.74	0.41
1:A:289:ALA:O	1:A:292:ARG:HB2	2.20	0.41
1:C:85:ARG:HA	1:C:86:PRO:HD2	1.97	0.41
4:A:1402:TDP:H351	2:D:82:GLN:OE1	2.20	0.41
1:A:352:LYS:HA	1:A:353:PRO:HD3	1.91	0.41
1:C:125:GLY:HA2	6:C:2512:HOH:O	2.20	0.41
1:A:20:GLY:HA3	1:A:24:GLU:CD	2.41	0.40
1:A:360:GLU:HG2	1:A:364:LYS:HE3	2.02	0.40
2:D:240:MET:HA	2:D:241:PRO:HA	1.89	0.40
1:A:252:GLU:HG2	6:A:1550:HOH:O	2.21	0.40
2:B:288:PRO:HA	2:B:289:PRO:HD3	1.97	0.40
1:C:235:VAL:HG12	1:C:236:ASP:N	2.37	0.40
2:B:153:ASP:HA	2:B:191:LEU:CD1	2.51	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	360/367 (98%)	346 (96%)	12 (3%)	2 (1%)	28	41
1	C	359/367 (98%)	347 (97%)	11 (3%)	1 (0%)	44	60
2	B	321/324 (99%)	305 (95%)	15 (5%)	1 (0%)	44	60
2	D	321/324 (99%)	303 (94%)	17 (5%)	1 (0%)	44	60
All	All	1361/1382 (98%)	1301 (96%)	55 (4%)	5 (0%)	38	54

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	208	ILE
1	C	208	ILE
2	D	74	GLY
1	A	282	TYR
2	B	74	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	286/295 (97%)	284 (99%)	2 (1%)	87	94
1	C	285/295 (97%)	283 (99%)	2 (1%)	87	94
2	B	258/259 (100%)	256 (99%)	2 (1%)	85	93
2	D	258/259 (100%)	252 (98%)	6 (2%)	56	75
All	All	1087/1108 (98%)	1075 (99%)	12 (1%)	78	90

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	14	GLU
1	A	315	GLU
2	B	177	TYR
2	B	256	ARG
1	C	13	GLU
1	C	342	GLU
2	D	34	ARG
2	D	76	ARG
2	D	198	LEU
2	D	205	LEU
2	D	214	MET
2	D	256	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:



Mol	Chain	Res	Type
1	A	193	GLN
2	B	249	ASN
2	B	316	ASN
1	C	193	GLN
1	C	226	HIS
2	D	46	GLN
2	D	129	HIS

### 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 5 ligands modelled in this entry, 2 are monoatomic - leaving 3 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	$\# Z  > 2$
4	TDP	A	1402	3	21,27,27	1.43	4 (19%)	25,40,40	1.72	7 (28%)
4	TDP	C	2402	3	21,27,27	1.40	4 (19%)	25,40,40	1.76	7 (28%)
5	4MV	D	1403	-	4,7,7	0.21	0	4,8,8	0.34	0

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
4	TDP	A	1402	3	-	0/16/17/17	0/2/2/2
4	TDP	C	2402	3	-	0/16/17/17	0/2/2/2
5	4MV	D	1403	-	-	0/3/5/5	0/0/0/0

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	2402	TDP	P2-O22	-2.33	1.45	1.54
4	A	1402	TDP	P2-O22	-2.15	1.46	1.54
4	C	2402	TDP	C35-N3	2.47	1.53	1.48
4	A	1402	TDP	C35-N3	2.66	1.53	1.48
4	C	2402	TDP	C2'-N1'	2.90	1.39	1.34
4	A	1402	TDP	C2'-N1'	2.96	1.39	1.34
4	C	2402	TDP	C4'-N3'	3.15	1.39	1.35
4	A	1402	TDP	C4'-N3'	3.49	1.40	1.35

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	2402	TDP	N1'-C2'-N3'	-2.60	121.09	125.59
4	A	1402	TDP	N1'-C2'-N3'	-2.52	121.23	125.59
4	C	2402	TDP	C5'-C35-N3	-2.50	109.15	113.33
4	A	1402	TDP	C5'-C35-N3	-2.40	109.32	113.33
4	C	2402	TDP	C5-C4-N3	2.06	111.69	107.57
4	A	1402	TDP	C5-C4-N3	2.12	111.81	107.57
4	A	1402	TDP	P1-O5G-C5B	2.22	133.22	121.60
4	C	2402	TDP	P1-O5G-C5B	2.28	133.53	121.60
4	A	1402	TDP	O22-P2-O21	2.40	119.89	110.50
4	C	2402	TDP	O22-P2-O21	2.42	119.97	110.50
4	A	1402	TDP	C2A-C2'-N1'	3.32	120.81	117.06
4	C	2402	TDP	C2A-C2'-N1'	3.75	121.29	117.06
4	C	2402	TDP	C5A-C5-C4	4.47	131.02	127.43
4	A	1402	TDP	C5A-C5-C4	4.69	131.20	127.43

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1402	TDP	3	0
4	C	2402	TDP	2	0
5	D	1403	4MV	6	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	362/367 (98%)	-0.50	11 (3%) 51 49	12, 23, 52, 75	0
1	C	361/367 (98%)	-0.62	10 (2%) 53 51	11, 21, 49, 78	0
2	B	323/324 (99%)	-0.68	1 (0%) 93 93	12, 26, 45, 55	0
2	D	323/324 (99%)	-0.81	1 (0%) 93 93	12, 24, 42, 58	0
All	All	1369/1382 (99%)	-0.65	23 (1%) 70 68	11, 23, 48, 78	0

All (23) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	280	SER	5.7
1	A	281	ARG	5.0
1	C	279	ASP	4.3
1	C	6	HIS	4.0
1	A	280	SER	3.9
1	A	60	ARG	3.9
1	A	286	GLU	3.7
1	C	281	ARG	3.7
1	C	286	GLU	3.7
1	A	279	ASP	3.3
1	A	285	LYS	3.1
1	A	367	LEU	2.8
1	C	21	GLU	2.8
1	A	21	GLU	2.6
1	C	285	LYS	2.5
1	C	22	GLU	2.4
1	A	289	ALA	2.3
1	C	278	ASP	2.3
1	A	22	GLU	2.3
1	C	365	GLU	2.1
1	A	213	ARG	2.1

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
2	D	186	GLU	2.1
2	B	46	GLN	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	4MV	D	1403	8/8	0.92	0.23	10.59	48,52,56,57	0
4	TDP	C	2402	26/26	0.99	0.07	-0.46	13,16,17,19	0
4	TDP	A	1402	26/26	0.99	0.07	-0.75	15,18,19,20	0
3	MG	A	1401	1/1	0.99	0.04	-2.16	17,17,17,17	0
3	MG	C	2401	1/1	0.99	0.03	-2.46	22,22,22,22	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.