



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 14, 2017 – 11:03 pm GMT

PDB ID : 2VYV  
Title : STRUCTURE OF E.COLI GAPDH RAT SPERM GAPDH HETEROTETRAMER  
Authors : Frayne, J.; Taylor, A.; Hall, L.; Hadfield, A.  
Deposited on : 2008-07-29  
Resolution : 2.38 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 : trunk28683  
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

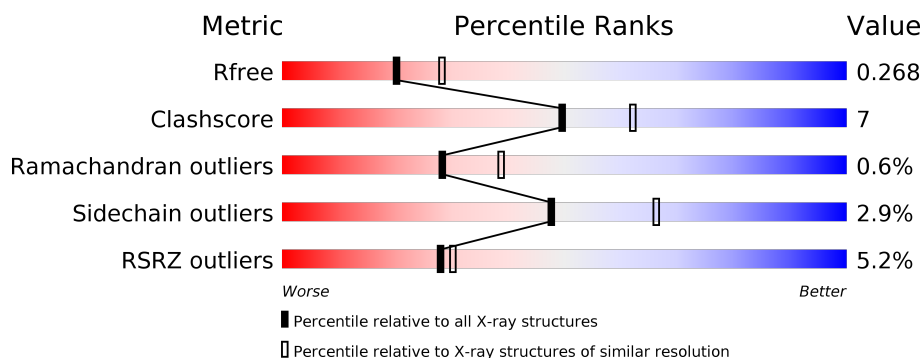
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.38 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	4388 (2.40-2.36)
Clashscore	112137	4984 (2.40-2.36)
Ramachandran outliers	110173	4907 (2.40-2.36)
Sidechain outliers	110143	4909 (2.40-2.36)
RSRZ outliers	101464	4423 (2.40-2.36)

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	331	<div> <div>5%</div> <div> <div></div> <div>83%</div> <div>15%</div> <div>.</div> </div> </div>
1	B	331	<div> <div>5%</div> <div> <div></div> <div>84%</div> <div>15%</div> <div>.</div> </div> </div>
1	C	331	<div> <div>7%</div> <div> <div></div> <div>82%</div> <div>16%</div> <div>.</div> </div> </div>
2	D	334	<div> <div>4%</div> <div> <div></div> <div>86%</div> <div>13%</div> <div>.</div> </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
3	FMT	A	1331	-	-	-	X
3	FMT	B	1331	-	-	-	X
3	FMT	D	1336	-	-	-	X
3	FMT	D	1337	-	-	-	X
3	FMT	D	1338	-	-	-	X
5	1GP	D	1334	-	-	-	X

## 2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 11215 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.

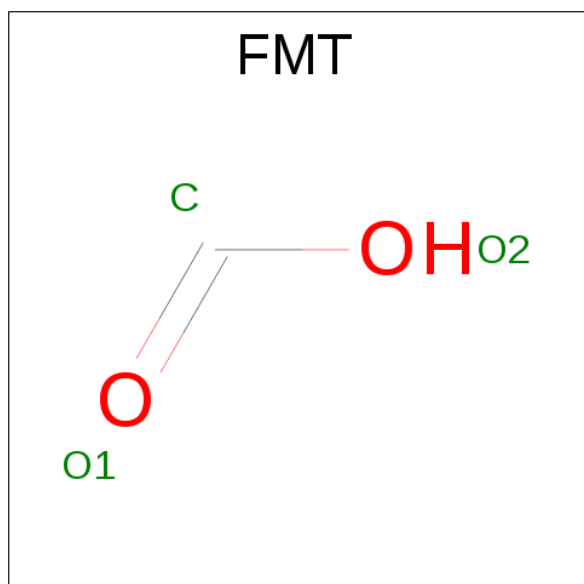
- Molecule 1 is a protein called GLYCERALDEHYDE-3-PHOSPHATE DEHYDROGENASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	330	Total	C	N	O	S	0	3	0
			2518	1579	437	492	10			
1	B	330	Total	C	N	O	S	0	5	0
			2528	1584	434	499	11			
1	C	330	Total	C	N	O	S	0	5	0
			2522	1584	434	494	10			

- Molecule 2 is a protein called GLYCERALDEHYDE-3-PHOSPHATE DEHYDROGENASE.

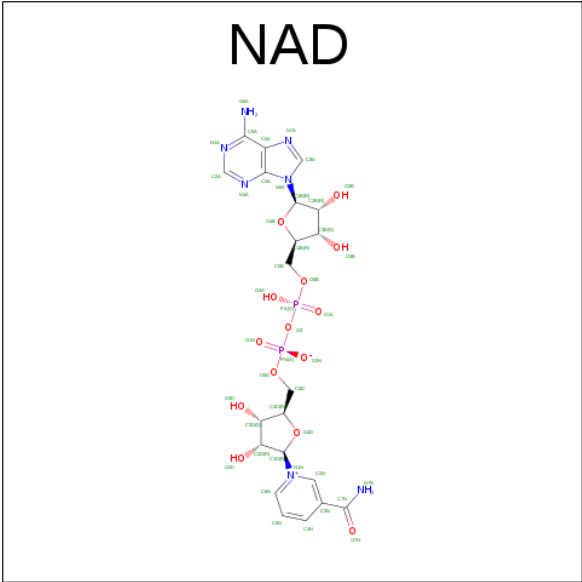
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	334	Total	C	N	O	S	0	4	0
			2579	1629	447	486	17			

- Molecule 3 is FORMIC ACID (three-letter code: FMT) (formula: CH<sub>2</sub>O<sub>2</sub>).



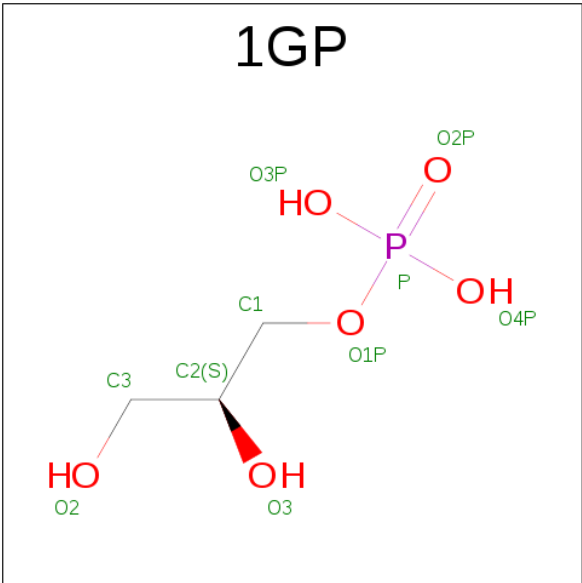
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 3 1 2	0	0
3	A	1	Total C O 3 1 2	0	0
3	A	1	Total C O 3 1 2	0	0
3	B	1	Total C O 3 1 2	0	0
3	B	1	Total C O 3 1 2	0	0
3	B	1	Total C O 3 1 2	0	0
3	B	1	Total C O 3 1 2	0	0
3	C	1	Total C O 3 1 2	0	0
3	C	1	Total C O 3 1 2	0	0
3	D	1	Total C O 3 1 2	0	0
3	D	1	Total C O 3 1 2	0	0
3	D	1	Total C O 3 1 2	0	0
3	D	1	Total C O 3 1 2	0	0
3	D	1	Total C O 3 1 2	0	0

- Molecule 4 is NICOTINAMIDE-ADENINE-DINUCLEOTIDE (three-letter code: NAD) (formula:  $C_{21}H_{27}N_7O_{14}P_2$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
4	B	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
4	C	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
4	D	1	Total	C	N	O	P	0	0
			44	21	7	14	2		

- Molecule 5 is SN-GLYCEROL-1-PHOSPHATE (three-letter code: 1GP) (formula: C<sub>3</sub>H<sub>9</sub>O<sub>6</sub>P).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	D	1	Total	C	O	P	0	0
			10	3	6	1		

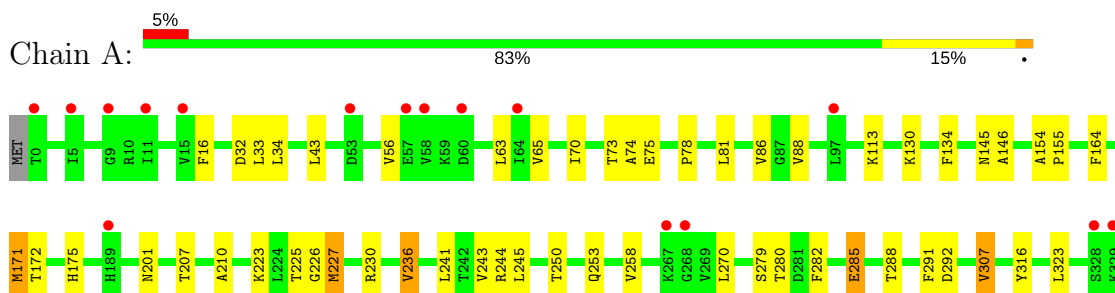
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	219	Total	O	0	0
			219	219		
6	B	208	Total	O	0	0
			208	208		
6	C	191	Total	O	0	0
			191	191		
6	D	222	Total	O	0	0
			222	222		

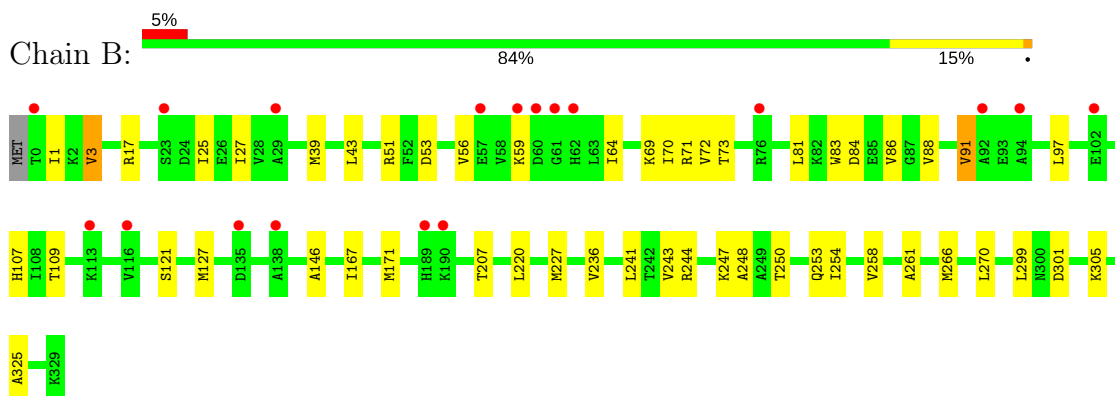
### 3 Residue-property plots [i](#)

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.

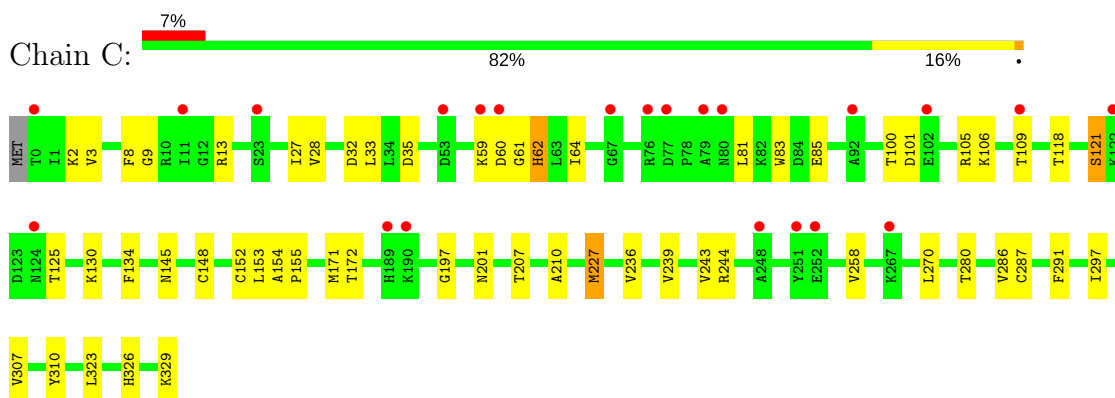
#### • Molecule 1: GLYCERALDEHYDE-3-PHOSPHATE DEHYDROGENASE



#### • Molecule 1: GLYCERALDEHYDE-3-PHOSPHATE DEHYDROGENASE

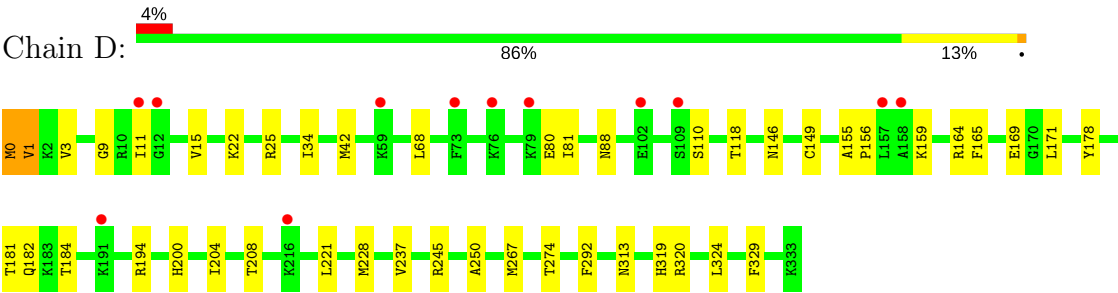


#### • Molecule 1: GLYCERALDEHYDE-3-PHOSPHATE DEHYDROGENASE



#### • Molecule 2: GLYCERALDEHYDE-3-PHOSPHATE DEHYDROGENASE





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	68.44Å 103.56Å 177.83Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	28.62 – 2.38 28.19 – 2.36	Depositor EDS
% Data completeness (in resolution range)	94.6 (28.62-2.38) 93.0 (28.19-2.36)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.49 (at 2.36Å)	Xtriage
Refinement program	REFMAC 5	Depositor
R, $R_{free}$	0.180 , 0.251 0.208 , 0.268	Depositor DCC
$R_{free}$ test set	2421 reflections (4.98%)	DCC
Wilson B-factor (Å <sup>2</sup> )	43.1	Xtriage
Anisotropy	0.068	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 44.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.52$ , $\langle L^2 \rangle = 0.36$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	11215	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.99% 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: CSD, FMT, CSX, NAD, 1GP

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	0.49	0/2541	0.62	0/3438
1	B	0.48	0/2557	0.63	0/3461
1	C	0.48	0/2556	0.59	0/3458
2	D	0.51	0/2623	0.65	0/3558
All	All	0.49	0/10277	0.62	0/13915

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	2518	0	2535	35	0
1	B	2528	0	2532	38	1
1	C	2522	0	2545	43	0
2	D	2579	0	2585	26	1
3	A	9	0	3	1	0
3	B	12	0	4	1	0
3	C	6	0	2	0	0
3	D	15	0	5	1	0
4	A	44	0	26	0	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	44	0	26	0	0
4	C	44	0	26	2	0
4	D	44	0	26	3	0
5	D	10	0	7	3	0
6	A	219	0	0	4	0
6	B	208	0	0	11	1
6	C	191	0	0	8	0
6	D	222	0	0	4	1
All	All	11215	0	10322	138	2

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 7.

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)
1:A:227:MET:HE3	6:C:2167:HOH:O	1.72	0.88
1:C:207:THR:HG23	6:C:2117:HOH:O	1.82	0.79
1:B:86:VAL:HG23	1:B:88:VAL:HG23	1.64	0.78
1:A:145:ASN:HD22	1:A:323:LEU:HD22	1.47	0.78
1:C:61:GLY:HA2	1:C:62:HIS:HB2	1.66	0.77
1:C:61:GLY:CA	1:C:62:HIS:HB2	2.16	0.76
2:D:149:CSD:OD2	5:D:1334:1GP:H2	1.92	0.70
1:B:250:THR:H	1:B:253:GLN:HE21	1.38	0.70
1:A:241:LEU:HG	1:A:243:VAL:HG13	1.74	0.69
1:C:286[A]:VAL:HG12	6:C:2158:HOH:O	1.97	0.64
1:A:244:ARG:HD2	1:C:244:ARG:HD2	1.82	0.62
1:B:39[B]:MET:HE2	1:B:72:VAL:HG13	1.81	0.62
1:C:227:MET:SD	6:C:2127:HOH:O	2.57	0.60
3:D:1337:FMT:O2	6:D:2213:HOH:O	2.16	0.60
1:A:154:ALA:HB3	1:A:155:PRO:HD3	1.83	0.60
1:B:3:VAL:HG22	1:B:27:ILE:HD12	1.83	0.60
1:A:250:THR:H	1:A:253:GLN:HE21	1.48	0.59
1:B:241:LEU:HG	1:B:243:VAL:HG13	1.85	0.59
2:D:146:ASN:HD22	2:D:324:LEU:HD22	1.67	0.58
1:A:292:ASP:HB3	1:A:307:VAL:HG22	1.86	0.57
1:B:3:VAL:CG1	1:B:25:ILE:HG23	2.34	0.57
1:C:153:LEU:HD22	1:C:171:MET:HE3	1.87	0.57
1:C:145:ASN:HD22	1:C:323:LEU:HD22	1.70	0.56
1:B:325:ALA:HB2	6:B:2192:HOH:O	2.05	0.56
1:C:3:VAL:HB	1:C:27:ILE:HD13	1.88	0.56

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:75:GLU:HB2	1:A:81:LEU:HD21	1.86	0.56
2:D:34:ILE:HD13	2:D:42:MET:SD	2.45	0.55
1:C:81:LEU:HD13	1:C:83:TRP:CZ2	2.41	0.55
2:D:1:VAL:HG13	2:D:329:PHE:CD1	2.41	0.55
1:A:164:PHE:HB2	1:A:245:LEU:HD22	1.89	0.54
1:B:109:THR:HG22	6:B:2040:HOH:O	2.07	0.54
1:C:154:ALA:HB3	1:C:155:PRO:HD3	1.88	0.54
1:A:32:ASP:O	1:A:74:ALA:HA	2.06	0.54
1:C:153:LEU:HD22	1:C:171:MET:CE	2.38	0.54
1:A:33:LEU:O	1:A:34:LEU:HD23	2.09	0.53
1:C:297:ILE:HG22	6:C:2167:HOH:O	2.08	0.53
1:B:250:THR:H	1:B:253:GLN:NE2	2.04	0.53
1:C:258:VAL:HG11	1:C:291:PHE:CG	2.44	0.53
1:B:59:LYS:HB3	1:B:64:ILE:HD11	1.92	0.52
1:A:75:GLU:HB2	1:A:81:LEU:CD2	2.39	0.52
1:B:121:SER:H	1:B:127:MET:HE2	1.75	0.52
1:C:207:THR:HG22	1:C:227:MET:HA	1.91	0.52
1:B:261:ALA:HB1	1:B:266:MET:HG3	1.91	0.51
1:A:16:PHE:CD1	1:A:43:LEU:HD11	2.45	0.51
1:C:2:LYS:HD2	1:C:28:VAL:HG11	1.93	0.51
2:D:81:ILE:O	2:D:110:SER:HB2	2.11	0.51
2:D:165:PHE:CD1	2:D:250:ALA:HB2	2.46	0.51
1:C:32:ASP:OD1	1:C:33:LEU:N	2.36	0.50
2:D:80[B]:GLU:OE1	6:D:2055:HOH:O	2.18	0.50
1:A:130:LYS:HB2	1:A:134:PHE:CZ	2.46	0.50
1:B:17:ARG:HD2	6:B:2002:HOH:O	2.10	0.50
1:C:62:HIS:HA	6:C:2047:HOH:O	2.12	0.50
1:A:201:ASN:ND2	1:C:280:THR:HG23	2.27	0.49
1:A:113[B]:LYS:NZ	6:A:2085:HOH:O	2.39	0.49
1:C:118:THR:O	4:C:1332:NAD:H1D	2.13	0.49
1:B:248:ALA:HB1	1:B:301:ASP:HB3	1.94	0.49
1:C:121:SER:CB	1:C:125:THR:HB	2.42	0.49
2:D:181:THR:HG23	5:D:1334:1GP:O2P	2.14	0.48
2:D:178:TYR:HA	2:D:182:GLN:OE1	2.13	0.48
1:A:207:THR:HG22	1:A:227:MET:HA	1.95	0.48
1:B:1:ILE:HB	1:B:25:ILE:HD13	1.94	0.48
1:A:78:PRO:HA	1:A:81:LEU:CD1	2.44	0.47
2:D:9:GLY:HA3	4:D:1340:NAD:O5B	2.14	0.47
1:B:254:ILE:O	1:B:258:VAL:HG23	2.13	0.47
1:C:59:LYS:O	1:C:62:HIS:HB2	2.13	0.47
2:D:22:LYS:NZ	6:D:2012:HOH:O	2.27	0.47

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:86:VAL:HG23	1:A:88:VAL:HG23	1.97	0.47
1:B:27:ILE:O	1:B:70:ILE:HD12	2.14	0.47
3:B:1330:FMT:C	6:B:2197:HOH:O	2.62	0.47
1:A:73:THR:HG23	6:A:2050:HOH:O	2.15	0.46
2:D:11:ILE:O	2:D:15:VAL:HG23	2.16	0.46
1:B:69:LYS:O	1:B:70:ILE:HD13	2.16	0.46
1:B:25:ILE:HG13	6:B:2192:HOH:O	2.15	0.46
1:B:3:VAL:HG22	1:B:27:ILE:CD1	2.46	0.46
2:D:155:ALA:HB3	2:D:156:PRO:HD3	1.98	0.46
1:B:71:ARG:HD3	1:B:73:THR:HG23	1.98	0.45
1:C:153:LEU:CD2	1:C:171:MET:HE3	2.46	0.45
1:C:134:PHE:CE1	1:C:323:LEU:HD13	2.52	0.45
1:C:106:LYS:HA	1:C:109:THR:HG22	1.99	0.45
2:D:194:ARG:HB3	2:D:204:ILE:HG23	1.99	0.45
1:A:258:VAL:HG11	1:A:291:PHE:CB	2.47	0.45
1:C:121:SER:HB2	1:C:125:THR:HB	1.98	0.45
1:B:207:THR:HG23	6:B:2122:HOH:O	2.17	0.44
1:B:84:ASP:HB2	6:B:2044:HOH:O	2.17	0.44
1:C:286[A]:VAL:HG13	1:C:287:CSD:OD2	2.18	0.44
1:C:326:HIS:HA	1:C:329:LYS:HE2	1.99	0.44
1:A:282:PHE:HD1	1:A:285:GLU:HG3	1.82	0.44
1:C:148:CSD:OD2	1:C:148:CSD:N	2.51	0.44
1:A:146:ALA:O	1:A:316:TYR:OH	2.30	0.44
2:D:184:THR:HG22	2:D:200:HIS:HE1	1.83	0.44
1:B:43:LEU:HD12	6:B:2002:HOH:O	2.17	0.44
1:A:223:LYS:NZ	6:A:2144:HOH:O	2.51	0.44
1:A:63:LEU:HB2	1:A:70:ILE:HB	2.00	0.44
1:C:106:LYS:HA	1:C:109:THR:CG2	2.48	0.44
1:B:121:SER:N	1:B:127:MET:HE2	2.32	0.43
2:D:25:ARG:NH2	2:D:68:LEU:HB3	2.32	0.43
1:B:59:LYS:CB	1:B:64:ILE:HD11	2.49	0.43
1:B:258:VAL:HG13	1:B:270:LEU:HD21	2.01	0.43
1:A:236:VAL:HG11	1:A:279:SER:O	2.18	0.42
3:A:1332:FMT:O2	6:A:2209:HOH:O	2.22	0.42
2:D:313:ASN:O	4:D:1340:NAD:H4N	2.18	0.42
1:C:171:MET:HE3	1:C:210:ALA:HB2	2.01	0.42
1:B:81:LEU:HD13	1:B:83:TRP:CZ2	2.54	0.42
1:B:91:VAL:HG11	1:B:107:HIS:HB3	2.00	0.42
2:D:274:THR:HG22	2:D:292:PHE:O	2.19	0.42
1:A:201:ASN:ND2	1:C:280:THR:H	2.18	0.42
1:C:100:THR:HG23	6:C:2060:HOH:O	2.19	0.42

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:172:THR:HA	1:C:227:MET:O	2.18	0.42
1:A:210:ALA:HB3	1:A:225:THR:HA	2.02	0.42
1:A:175:HIS:HB3	1:A:230:ARG:HD3	2.02	0.42
1:B:247:LYS:NZ	6:B:2142:HOH:O	2.53	0.42
2:D:149:CSD:SG	5:D:1334:1GP:H2	2.59	0.42
2:D:1:VAL:HG13	2:D:329:PHE:CG	2.55	0.42
1:A:171:MET:HE2	1:A:226:GLY:HA3	2.00	0.42
1:A:280:THR:H	1:C:201:ASN:ND2	2.18	0.42
1:B:167:ILE:HG21	1:B:244:ARG:NH1	2.35	0.41
1:B:244:ARG:HD2	2:D:245:ARG:HD2	2.02	0.41
1:A:16:PHE:CE1	1:A:65:VAL:HG11	2.55	0.41
1:C:101:ASP:O	1:C:105:ARG:HB2	2.20	0.41
1:B:305:LYS:HE2	2:D:171:LEU:HB3	2.01	0.41
2:D:118:THR:O	4:D:1340:NAD:H1D	2.20	0.41
1:B:84:ASP:HA	6:B:2046:HOH:O	2.19	0.41
1:C:9:GLY:HA3	4:C:1332:NAD:O5B	2.20	0.41
1:A:258:VAL:HG11	1:A:291:PHE:HB2	2.03	0.41
2:D:159:LYS:HD3	2:D:267:MET:CE	2.51	0.41
1:A:171:MET:HG2	1:A:172:THR:N	2.36	0.41
1:C:152:CYS:HG	1:C:310:TYR:HD1	1.65	0.41
1:C:64:ILE:HG22	6:C:2044:HOH:O	2.20	0.41
1:B:83:TRP:CE3	1:B:88:VAL:HG21	2.56	0.41
1:C:8:PHE:CZ	1:C:13:ARG:HG3	2.56	0.41
1:C:258:VAL:HG11	1:C:291:PHE:CB	2.51	0.41
1:C:59:LYS:C	1:C:61:GLY:HA3	2.41	0.41
1:B:146:ALA:HB1	6:B:2081:HOH:O	2.20	0.40
1:B:299:LEU:HD23	2:D:169:GLU:HB2	2.03	0.40
1:A:227:MET:HE2	1:C:307:VAL:HG21	2.04	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:B:2178:HOH:O	6:D:2080:HOH:O[4_545]	2.11	0.09
1:B:301:ASP:OD2	2:D:88:ASN:ND2[4_545]	2.15	0.05

## 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	329/331 (99%)	308 (94%)	20 (6%)	1 (0%)	44	59
1	B	331/331 (100%)	313 (95%)	17 (5%)	1 (0%)	44	59
1	C	331/331 (100%)	307 (93%)	19 (6%)	5 (2%)	12	15
2	D	333/334 (100%)	320 (96%)	12 (4%)	1 (0%)	44	59
All	All	1324/1327 (100%)	1248 (94%)	68 (5%)	8 (1%)	28	39

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	60	ASP
1	A	236	VAL
1	B	236	VAL
1	C	62	HIS
1	C	236	VAL
2	D	237	VAL
1	C	35	ASP
1	C	197	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	266/264 (101%)	259 (97%)	7 (3%)	51	70
1	B	268/264 (102%)	260 (97%)	8 (3%)	46	65

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	268/264 (102%)	261 (97%)	7 (3%)	51	70
2	D	278/274 (102%)	268 (96%)	10 (4%)	40	58
All	All	1080/1066 (101%)	1048 (97%)	32 (3%)	48	65

All (32) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	56	VAL
1	A	171	MET
1	A	227	MET
1	A	270	LEU
1	A	285	GLU
1	A	288	THR
1	A	307	VAL
1	B	3	VAL
1	B	51	ARG
1	B	56	VAL
1	B	91	VAL
1	B	97	LEU
1	B	171	MET
1	B	220	LEU
1	B	227	MET
1	C	85	GLU
1	C	121	SER
1	C	130	LYS
1	C	227	MET
1	C	239	VAL
1	C	243	VAL
1	C	270	LEU
2	D	0[A]	MET
2	D	0[B]	MET
2	D	1	VAL
2	D	3	VAL
2	D	164	ARG
2	D	208	THR
2	D	221	LEU
2	D	228	MET
2	D	319	HIS
2	D	320	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	145	ASN
1	A	201	ASN
1	A	253	GLN
1	B	145	ASN
1	B	253	GLN
1	B	302	ASN
1	C	145	ASN
1	C	201	ASN
2	D	146	ASN
2	D	200	HIS
2	D	277	GLN
2	D	303	ASN
2	D	319	HIS

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

8 non-standard protein/DNA/RNA residues are modelled in this entry.

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	$\# Z  > 2$
1	CSD	A	148	1	4,7,8	1.36	1 (25%)	2,8,10	1.75	0
1	CSD	A	287	1	4,7,8	1.23	1 (25%)	2,8,10	1.97	1 (50%)
1	CSD	B	148	1	4,7,8	1.41	1 (25%)	2,8,10	1.79	1 (50%)
1	CSD	B	287	1	4,7,8	1.13	1 (25%)	2,8,10	2.47	1 (50%)
1	CSD	C	148	1	4,7,8	1.37	1 (25%)	2,8,10	1.55	0
1	CSD	C	287	1	4,7,8	1.29	1 (25%)	2,8,10	1.62	0
2	CSD	D	149	2	4,7,8	1.37	1 (25%)	2,8,10	1.82	1 (50%)
2	CSX	D	75	2	4,6,7	0.52	0	2,6,8	1.90	1 (50%)

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
1	CSD	A	148	1	-	0/2/6/8	0/0/0/0
1	CSD	A	287	1	-	0/2/6/8	0/0/0/0
1	CSD	B	148	1	-	0/2/6/8	0/0/0/0
1	CSD	B	287	1	-	1/2/6/8	0/0/0/0
1	CSD	C	148	1	-	0/2/6/8	0/0/0/0
1	CSD	C	287	1	-	1/2/6/8	0/0/0/0
2	CSD	D	149	2	-	0/2/6/8	0/0/0/0
2	CSX	D	75	2	-	0/1/5/7	0/0/0/0

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	287	CSD	CB-SG	2.17	1.91	1.79
1	A	287	CSD	CB-SG	2.27	1.91	1.79
1	C	287	CSD	CB-SG	2.36	1.92	1.79
1	C	148	CSD	CB-SG	2.43	1.92	1.79
1	A	148	CSD	CB-SG	2.51	1.93	1.79
2	D	149	CSD	CB-SG	2.55	1.93	1.79
1	B	148	CSD	CB-SG	2.63	1.93	1.79

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	287	CSD	OD1-SG-CB	-3.03	99.92	105.61
1	A	287	CSD	OD1-SG-CB	-2.35	101.20	105.61
1	B	148	CSD	OD1-SG-CB	-2.10	101.67	105.61
2	D	75	CSX	CA-CB-SG	-2.06	108.84	113.47
2	D	149	CSD	OD1-SG-CB	-2.04	101.79	105.61

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	B	287	CSD	CA-CB-SG-OD1
1	C	287	CSD	CA-CB-SG-OD1

There are no ring outliers.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	C	148	CSD	1	0
1	C	287	CSD	1	0
2	D	149	CSD	2	0

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

19 ligands are modelled in this entry.

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	$\# Z  > 2$
3	FMT	A	1330	-	0,2,2	0.00	-	0,1,1	0.00	-
3	FMT	A	1331	-	0,2,2	0.00	-	0,1,1	0.00	-
3	FMT	A	1332	-	0,2,2	0.00	-	0,1,1	0.00	-
4	NAD	A	1333	-	41,48,48	1.68	3 (7%)	43,73,73	1.65	3 (6%)
3	FMT	B	1330	-	0,2,2	0.00	-	0,1,1	0.00	-
3	FMT	B	1331	-	0,2,2	0.00	-	0,1,1	0.00	-
3	FMT	B	1332	-	0,2,2	0.00	-	0,1,1	0.00	-
3	FMT	B	1333	-	0,2,2	0.00	-	0,1,1	0.00	-
4	NAD	B	1334	-	41,48,48	1.63	3 (7%)	43,73,73	1.76	1 (2%)
3	FMT	C	1330	-	0,2,2	0.00	-	0,1,1	0.00	-
3	FMT	C	1331	-	0,2,2	0.00	-	0,1,1	0.00	-
4	NAD	C	1332	-	41,48,48	1.64	3 (7%)	43,73,73	1.70	1 (2%)
5	1GP	D	1334	-	9,9,9	0.54	0	11,12,12	0.71	0
3	FMT	D	1335	-	0,2,2	0.00	-	0,1,1	0.00	-
3	FMT	D	1336	-	0,2,2	0.00	-	0,1,1	0.00	-
3	FMT	D	1337	-	0,2,2	0.00	-	0,1,1	0.00	-
3	FMT	D	1338	-	0,2,2	0.00	-	0,1,1	0.00	-
3	FMT	D	1339	-	0,2,2	0.00	-	0,1,1	0.00	-
4	NAD	D	1340	-	41,48,48	1.67	3 (7%)	43,73,73	1.86	1 (2%)

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
3	FMT	A	1330	-	-	0/0/0/0	0/0/0/0
3	FMT	A	1331	-	-	0/0/0/0	0/0/0/0
3	FMT	A	1332	-	-	0/0/0/0	0/0/0/0
4	NAD	A	1333	-	-	0/22/62/62	0/5/5/5
3	FMT	B	1330	-	-	0/0/0/0	0/0/0/0
3	FMT	B	1331	-	-	0/0/0/0	0/0/0/0
3	FMT	B	1332	-	-	0/0/0/0	0/0/0/0
3	FMT	B	1333	-	-	0/0/0/0	0/0/0/0
4	NAD	B	1334	-	-	0/22/62/62	0/5/5/5
3	FMT	C	1330	-	-	0/0/0/0	0/0/0/0
3	FMT	C	1331	-	-	0/0/0/0	0/0/0/0
4	NAD	C	1332	-	-	0/22/62/62	0/5/5/5
5	1GP	D	1334	-	-	0/8/8/8	0/0/0/0
3	FMT	D	1335	-	-	0/0/0/0	0/0/0/0
3	FMT	D	1336	-	-	0/0/0/0	0/0/0/0
3	FMT	D	1337	-	-	0/0/0/0	0/0/0/0
3	FMT	D	1338	-	-	0/0/0/0	0/0/0/0
3	FMT	D	1339	-	-	0/0/0/0	0/0/0/0
4	NAD	D	1340	-	-	0/22/62/62	0/5/5/5

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	1332	NAD	C2A-N1A	2.57	1.38	1.33
4	D	1340	NAD	C2A-N1A	2.60	1.38	1.33
4	B	1334	NAD	C2A-N1A	2.63	1.38	1.33
4	A	1333	NAD	C2A-N1A	2.64	1.38	1.33
4	B	1334	NAD	C2A-N3A	3.76	1.38	1.32
4	A	1333	NAD	C2A-N3A	3.81	1.38	1.32
4	D	1340	NAD	C2A-N3A	3.93	1.38	1.32
4	C	1332	NAD	C2A-N3A	3.95	1.38	1.32
4	B	1334	NAD	O7N-C7N	8.29	1.41	1.24
4	C	1332	NAD	O7N-C7N	8.37	1.41	1.24
4	D	1340	NAD	O7N-C7N	8.52	1.41	1.24
4	A	1333	NAD	O7N-C7N	8.63	1.42	1.24

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	1340	NAD	N3A-C2A-N1A	-11.13	119.17	128.86
4	B	1334	NAD	N3A-C2A-N1A	-10.33	119.86	128.86
4	C	1332	NAD	N3A-C2A-N1A	-9.98	120.16	128.86
4	A	1333	NAD	N3A-C2A-N1A	-9.32	120.74	128.86
4	A	1333	NAD	C4A-C5A-N7A	-2.41	107.08	109.41
4	A	1333	NAD	O7N-C7N-N7N	-2.01	119.73	122.58

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

6 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1332	FMT	1	0
3	B	1330	FMT	1	0
4	C	1332	NAD	2	0
5	D	1334	1GP	3	0
3	D	1337	FMT	1	0
4	D	1340	NAD	3	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	328/331 (99%)	0.38	16 (4%)	30 33	29, 43, 58, 75	0
1	B	328/331 (99%)	0.33	18 (5%)	26 28	26, 41, 63, 73	0
1	C	328/331 (99%)	0.55	22 (6%)	19 19	29, 48, 65, 72	0
2	D	332/334 (99%)	0.27	12 (3%)	43 46	25, 39, 51, 56	0
All	All	1316/1327 (99%)	0.38	68 (5%)	28 30	25, 42, 62, 75	0

All (68) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	60	ASP	4.4
1	C	60	ASP	4.1
1	B	0	THR	4.0
1	C	189	HIS	4.0
1	C	79	ALA	3.9
1	A	60	ASP	3.9
1	B	135[A]	ASP	3.8
1	A	58	VAL	3.7
1	C	23	SER	3.7
1	C	124[A]	ASN	3.6
1	C	102[A]	GLU	3.6
1	A	5	ILE	3.5
1	B	189	HIS	3.5
1	C	92	ALA	3.4
1	C	190	LYS	3.3
1	A	268	GLY	3.2
1	C	122	LYS	3.2
1	A	0	THR	3.1
1	B	138	ALA	3.0
2	D	79	LYS	3.0
1	C	109	THR	2.9

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	A	97	LEU	2.7
1	B	190	LYS	2.7
1	B	62	HIS	2.7
1	C	77	ASP	2.6
2	D	216	LYS	2.6
1	B	57	GLU	2.6
1	B	116	VAL	2.6
1	A	11	ILE	2.6
2	D	11	ILE	2.6
1	C	80	ASN	2.6
2	D	12	GLY	2.5
1	B	94	ALA	2.5
1	C	251	TYR	2.5
1	B	113	LYS	2.5
1	C	267	LYS	2.5
2	D	59	LYS	2.4
1	A	189	HIS	2.4
1	C	0	THR	2.4
1	C	53	ASP	2.4
1	B	61	GLY	2.3
1	C	252[A]	GLU	2.3
1	A	329	LYS	2.3
2	D	157	LEU	2.3
2	D	102	GLU	2.3
1	C	67	GLY	2.2
2	D	76	LYS	2.2
1	A	53	ASP	2.2
1	B	59	LYS	2.2
2	D	73	PHE	2.2
1	C	11	ILE	2.2
1	A	64	ILE	2.1
1	B	76	ARG	2.1
1	C	248	ALA	2.1
2	D	191	LYS	2.1
1	C	76	ARG	2.1
1	A	15	VAL	2.1
1	B	92	ALA	2.1
2	D	109	SER	2.1
1	A	267	LYS	2.1
1	B	23	SER	2.1
1	B	102[A]	GLU	2.1
1	C	59	LYS	2.1

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	A	57	GLU	2.0
1	A	9	GLY	2.0
1	B	29	ALA	2.0
1	A	328	SER	2.0
2	D	158	ALA	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains [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
2	CSD	D	149	8/9	0.98	0.14	-	32,33,35,38	0
1	CSD	C	148	8/9	0.94	0.14	-	39,42,50,59	0
2	CSX	D	75	7/8	0.88	0.15	-	43,45,49,50	0
1	CSD	A	148	8/9	0.94	0.16	-	34,35,48,48	0
1	CSD	B	148	8/9	0.96	0.16	-	34,36,55,57	0
1	CSD	C	287	8/9	0.91	0.14	-	42,43,52,61	0
1	CSD	A	287	8/9	0.91	0.14	-	42,44,58,59	0
1	CSD	B	287	8/9	0.94	0.12	-	34,36,43,45	0

## 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
3	FMT	D	1338	3/3	0.62	0.41	9.36	83,83,83,83	0
3	FMT	B	1331	3/3	0.84	0.32	8.79	73,73,73,74	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
3	FMT	D	1337	3/3	0.92	0.26	7.24	47,47,48,48	0
5	1GP	D	1334	10/10	0.79	0.34	5.51	73,76,80,85	0
3	FMT	A	1331	3/3	0.86	0.21	4.80	58,58,61,64	0
3	FMT	D	1336	3/3	0.70	0.21	3.99	66,66,66,66	0
3	FMT	C	1330	3/3	0.77	0.27	1.45	65,65,66,66	0
4	NAD	C	1332	44/44	0.82	0.23	0.90	64,72,80,81	0
3	FMT	B	1333	3/3	0.94	0.25	0.49	50,50,52,54	0
3	FMT	A	1332	3/3	0.91	0.16	0.31	49,49,49,51	0
4	NAD	B	1334	44/44	0.88	0.18	0.16	45,63,70,71	0
4	NAD	A	1333	44/44	0.90	0.16	-0.21	45,54,61,64	0
3	FMT	D	1335	3/3	0.81	0.14	-0.38	70,70,70,71	0
3	FMT	B	1330	3/3	0.93	0.12	-0.49	56,56,57,57	0
4	NAD	D	1340	44/44	0.92	0.15	-0.59	41,51,56,58	0
3	FMT	A	1330	3/3	0.86	0.11	-0.74	43,43,45,46	0
3	FMT	C	1331	3/3	0.94	0.14	-1.79	53,53,53,54	0
3	FMT	D	1339	3/3	0.83	0.23	-	72,72,73,73	0
3	FMT	B	1332	3/3	0.73	0.27	-	86,86,87,88	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.