



Full wwPDB X-ray Structure Validation Report

Feb 26, 2014 – 07:30 PM GMT

PDB ID : 2VYN
Title : STRUCTURE OF E.COLI GAPDH RAT SPERM GAPDH HETEROTETRAMER
Authors : Frayne, J.; Taylor, A.; Hall, L.; Hadfield, A.
Deposited on : 2008-07-25
Resolution : 2.20 Å(reported)

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

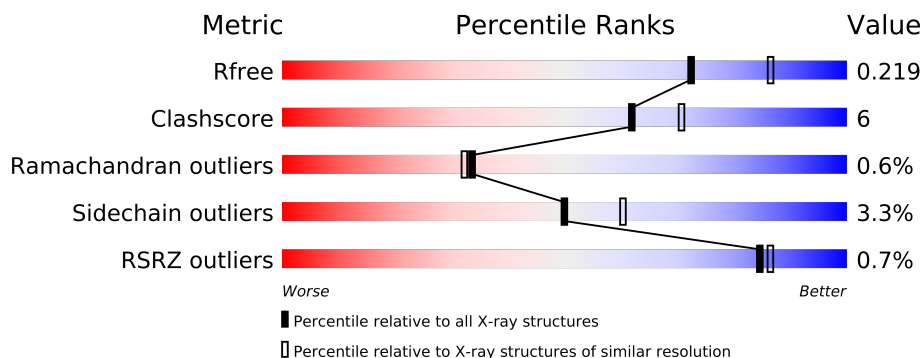
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

The reported resolution of this entry is 2.20 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	66092	2938 (2.20-2.20)
Clashscore	79885	3751 (2.20-2.20)
Ramachandran outliers	78287	3681 (2.20-2.20)
Sidechain outliers	78261	3682 (2.20-2.20)
RSRZ outliers	66119	2939 (2.20-2.20)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	331	
1	B	331	
1	C	331	
2	D	334	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
3	FMT	A	1333	-	X
3	FMT	B	1333	-	X
3	FMT	B	1334	-	X
3	FMT	D	1338	-	X
3	FMT	D	1339	-	X

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 11209 atoms, of which 0 are hydrogen and 0 are deuterium.

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

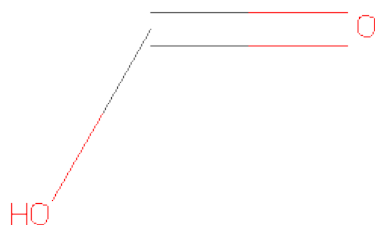
- Molecule 1 is a protein called GLYCERALDEHYDE-3-PHOSPHATEDEHYDROGENASE.

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-PHOSPHATEDEHYDROGENASE.

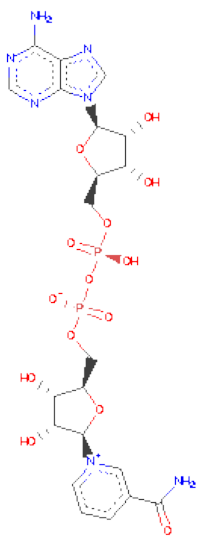
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	334	Total	C	N	O	S	0	4	0
			2579	1629	447	486	17			

- Molecule 3 is FORMIC ACID (three-letter code: FMT) (formula: CH₂O₂).



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: C₂₁H₂₇N₇O₁₄P₂).



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 water.

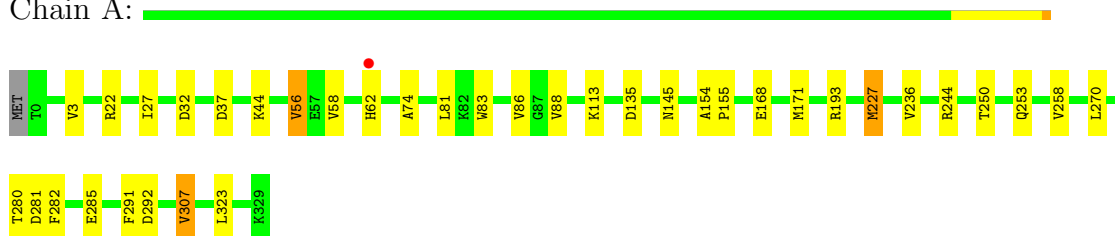
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	217	Total	O	0	0
			217	217		
5	B	211	Total	O	0	0
			211	211		
5	C	189	Total	O	0	0
			189	189		
5	D	227	Total	O	0	0
			227	227		

3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

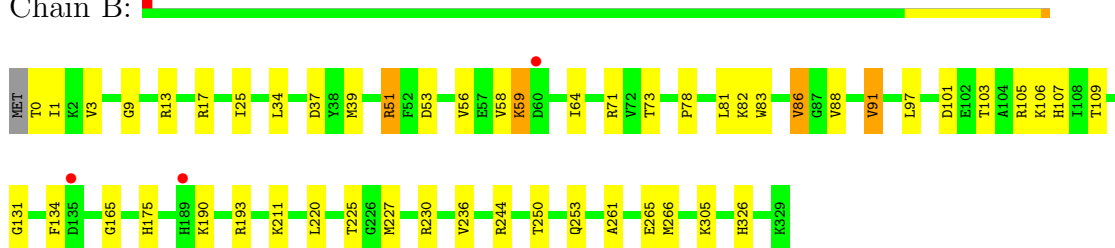
• Molecule 1: GLYCERALDEHYDE-3-PHOSPHATEDEHYDROGENASE

Chain A:



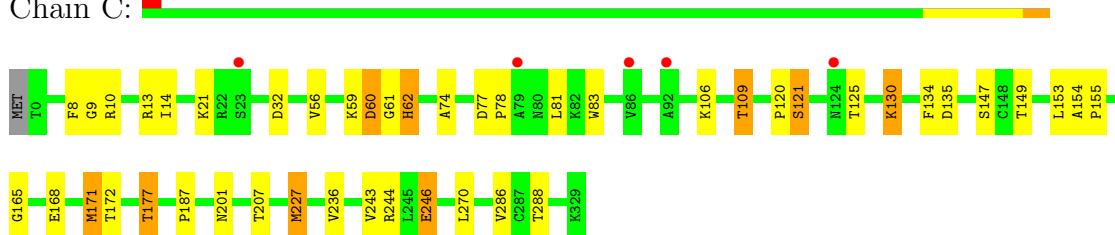
• Molecule 1: GLYCERALDEHYDE-3-PHOSPHATEDEHYDROGENASE

Chain B:



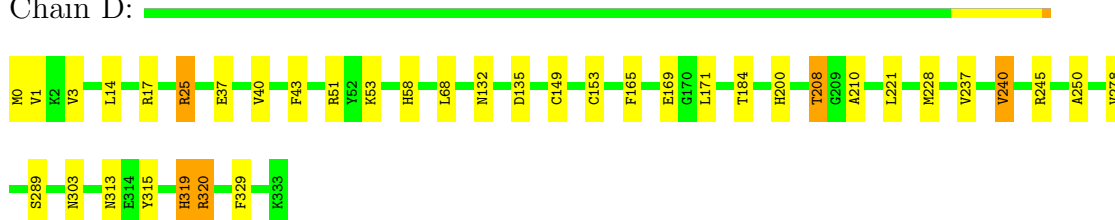
• Molecule 1: GLYCERALDEHYDE-3-PHOSPHATEDEHYDROGENASE

Chain C:



• Molecule 2: GLYCERALDEHYDE-3-PHOSPHATEDEHYDROGENASE

Chain D:



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	68.44Å 103.56Å 177.83Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.20 24.86 – 2.20	Depositor EDS
% Data completeness (in resolution range)	97.7 (30.00-2.20) 97.8 (24.86-2.20)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.11 (at 2.19Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.157 , 0.224 0.158 , 0.219	Depositor DCC
R_{free} test set	3221 reflections (5.34%)	DCC
Wilson B-factor (Å ²)	22.9	Xtriage
Anisotropy	0.047	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 32.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 63545 reflections	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	11209	wwPDB-VP
Average B, all atoms (Å ²)	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.32% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CSD, FMT, CSX, NAD

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	0.46	0/2541	0.58	0/3438
1	B	0.45	0/2557	0.60	0/3461
1	C	0.46	0/2556	0.58	0/3458
2	D	0.49	0/2623	0.62	0/3558
All	All	0.46	0/10277	0.60	0/13915

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

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	60	ASP	Peptide

5.2 Close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the

Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2518	0	2535	27	0
1	B	2528	0	2532	33	0
1	C	2522	0	2545	38	0
2	D	2579	0	2585	28	0
3	A	9	0	3	2	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
4	B	44	0	26	0	0
4	C	44	0	26	1	0
4	D	44	0	26	1	0
5	A	217	0	0	8	0
5	B	211	0	0	6	0
5	C	189	0	0	9	0
5	D	227	0	0	4	0
All	All	11209	0	10315	118	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 6.

All (118) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:153:LEU:HD22	1:C:171:MET:HE3	1.41	1.01
1:B:25:ILE:HG13	5:B:2190:HOH:O	1.73	0.89
1:A:227:MET:HE2	5:C:2157:HOH:O	1.72	0.88
3:A:1334:FMT:C	5:A:2206:HOH:O	2.29	0.80
1:B:244:ARG:HD2	2:D:245:ARG:HD2	1.63	0.79
1:A:244:ARG:HD2	1:C:244:ARG:HD2	1.65	0.78
1:C:246:GLU:HG3	5:C:2129:HOH:O	1.83	0.77
1:B:1:ILE:HB	1:B:25:ILE:HD13	1.66	0.76
1:C:61:GLY:HA3	1:C:62:HIS:HB2	1.67	0.75
1:C:61:GLY:HA2	1:C:62:HIS:ND1	2.03	0.74
1:B:71:ARG:HD3	1:B:73:THR:HG23	1.71	0.72
1:B:34:LEU:HD12	1:B:39[B]:MET:SD	2.30	0.71
3:A:1334:FMT:O2	5:A:2206:HOH:O	2.09	0.69
1:C:59:LYS:O	1:C:61:GLY:HA3	1.91	0.69
1:A:282:PHE:HD1	1:A:285:GLU:HG3	1.59	0.67
1:C:61:GLY:CA	1:C:62:HIS:HB2	2.25	0.66
2:D:37:GLU:HG2	5:D:2016:HOH:O	1.95	0.65
1:C:177:THR:HG21	5:C:2079:HOH:O	1.96	0.65

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:286[A]:VAL:HG12	5:C:2153:HOH:O	1.96	0.64
1:B:244:ARG:CD	2:D:245:ARG:HD2	2.28	0.63
1:C:207:THR:HG23	5:C:2109:HOH:O	1.99	0.63
1:C:81:LEU:HD13	1:C:83:TRP:CZ2	2.33	0.62
1:B:250:THR:H	1:B:253:GLN:HE21	1.47	0.61
2:D:1:VAL:HG23	5:D:2001:HOH:O	2.00	0.61
1:A:37:ASP:HA	1:A:58:VAL:HG21	1.83	0.60
1:C:207:THR:HG22	1:C:227:MET:HA	1.84	0.59
1:A:244:ARG:CD	1:C:244:ARG:HD2	2.32	0.59
1:A:81:LEU:HD13	1:A:83:TRP:CZ2	2.37	0.59
1:C:32:ASP:O	1:C:74:ALA:HA	2.02	0.59
1:B:59:LYS:HB3	1:B:64:ILE:HD11	1.86	0.58
1:A:86:VAL:HG23	1:A:88:VAL:HG23	1.86	0.58
1:C:153:LEU:HD22	1:C:171:MET:CE	2.26	0.57
1:A:292:ASP:HB3	1:A:307:VAL:HG22	1.85	0.57
1:B:261:ALA:HB1	1:B:266:MET:HG3	1.87	0.57
2:D:1:VAL:HG22	2:D:329:PHE:CD2	2.40	0.56
1:A:244:ARG:HD2	1:C:244:ARG:CD	2.33	0.56
1:B:91:VAL:HG11	1:B:107:HIS:HB3	1.88	0.56
2:D:14:LEU:HD23	2:D:17:ARG:HD3	1.87	0.56
2:D:169:GLU:OE2	2:D:245:ARG:HD3	2.06	0.56
1:A:135:ASP:HB2	5:A:2207:HOH:O	2.06	0.55
2:D:208:THR:HG22	2:D:210:ALA:H	1.72	0.55
2:D:17:ARG:HG3	2:D:43:PHE:CE1	2.41	0.55
1:C:135:ASP:HB2	5:C:2064:HOH:O	2.07	0.54
1:C:74:ALA:HB2	5:C:2012:HOH:O	2.07	0.54
2:D:315:TYR:CZ	2:D:319:HIS:HE1	2.25	0.54
1:B:71:ARG:NH2	1:B:82:LYS:O	2.40	0.53
1:C:61:GLY:CA	1:C:62:HIS:CB	2.85	0.53
1:B:17:ARG:HD2	5:B:2003:HOH:O	2.06	0.53
1:A:44:LYS:HG2	1:A:56:VAL:HG13	1.91	0.52
2:D:315:TYR:OH	2:D:319:HIS:HE1	1.93	0.52
2:D:289:SER:OG	2:D:320:ARG:HD2	2.10	0.52
1:A:250:THR:H	1:A:253:GLN:HE21	1.56	0.51
1:B:81:LEU:HD13	1:B:83:TRP:CZ2	2.45	0.51
1:C:59:LYS:O	1:C:62:HIS:HB2	2.10	0.51
2:D:25:ARG:NH2	2:D:68:LEU:HB3	2.26	0.51
1:B:109:THR:HG22	5:B:2045:HOH:O	2.11	0.49
1:C:9:GLY:HA3	4:C:1334:NAD:O5B	2.12	0.49
2:D:51:ARG:HH12	3:D:1337:FMT:H	1.76	0.49
1:B:190:LYS:HB3	5:B:2104:HOH:O	2.12	0.48
1:A:62:HIS:HB3	5:A:2045:HOH:O	2.12	0.48

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:265[A]:GLU:H	1:B:265[A]:GLU:CD	2.16	0.48
1:A:22:ARG:O	5:A:2008:HOH:O	2.20	0.48
1:A:32:ASP:O	1:A:74:ALA:HA	2.14	0.47
1:C:168:GLU:OE2	1:C:244:ARG:HD3	2.13	0.47
1:B:86:VAL:HG23	1:B:88:VAL:HG23	1.97	0.47
1:A:282:PHE:CD1	1:A:285:GLU:HG3	2.47	0.47
1:C:10:ARG:O	1:C:14:ILE:HG12	2.15	0.47
2:D:40:VAL:HG21	2:D:58:HIS:HB3	1.96	0.46
1:C:62:HIS:HA	5:C:2041:HOH:O	2.14	0.46
1:C:130:LYS:HB2	1:C:134:PHE:CZ	2.50	0.46
2:D:153:CYS:SG	2:D:240:VAL:HG13	2.56	0.46
2:D:315:TYR:CZ	2:D:319:HIS:CE1	3.03	0.46
1:C:120:PRO:HG3	1:C:147:SER:HB3	1.97	0.46
1:A:168:GLU:OE2	1:A:244:ARG:HD3	2.16	0.46
3:B:1332:FMT:C	5:B:2201:HOH:O	2.63	0.46
1:C:8:PHE:CZ	1:C:13:ARG:HG3	2.51	0.46
1:C:154:ALA:HB3	1:C:155:PRO:HD3	1.98	0.45
1:B:175:HIS:HB3	1:B:230:ARG:HD3	1.98	0.45
1:A:145:ASN:HD22	1:A:323:LEU:HD22	1.81	0.45
2:D:53:LYS:HE2	5:D:2027:HOH:O	2.17	0.45
1:B:3:VAL:HG13	1:B:25:ILE:HG23	1.98	0.44
1:B:131:GLY:O	1:B:266:MET:HE1	2.17	0.44
2:D:184:THR:HG22	2:D:200:HIS:HE1	1.82	0.44
1:B:305:LYS:HE2	2:D:171:LEU:HB3	2.00	0.44
1:C:21:LYS:HE3	5:C:2008:HOH:O	2.16	0.44
1:B:9:GLY:O	1:B:13:ARG:HG3	2.16	0.44
1:C:171:MET:HG2	1:C:172:THR:N	2.33	0.44
5:A:2123:HOH:O	2:D:200:HIS:HB3	2.17	0.44
1:C:61:GLY:HA2	1:C:62:HIS:CG	2.52	0.43
1:C:149:THR:HG22	1:C:171:MET:HE2	1.99	0.43
1:A:193:ARG:HG3	5:A:2116:HOH:O	2.18	0.43
1:B:250:THR:H	1:B:253:GLN:NE2	2.16	0.43
1:C:121:SER:CB	1:C:125:THR:HB	2.49	0.43
1:B:103:THR:HG21	5:B:2058:HOH:O	2.18	0.43
2:D:132:ASN:O	2:D:135:ASP:HB2	2.19	0.43
1:B:78:PRO:HG2	1:B:106:LYS:HD2	2.00	0.43
2:D:17:ARG:HD2	5:D:2019:HOH:O	2.18	0.42
1:A:280:THR:HG23	1:C:201:ASN:ND2	2.35	0.42
1:A:154:ALA:HB3	1:A:155:PRO:HD3	2.01	0.42
1:B:101:ASP:O	1:B:105:ARG:HB2	2.19	0.42
2:D:149:CSD:OD2	2:D:149:CSD:N	2.49	0.42
1:C:77:ASP:HA	1:C:78:PRO:HD3	1.92	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:D:165:PHE:CD1	2:D:250:ALA:HB2	2.56	0.41
1:A:81:LEU:HD23	1:A:81:LEU:HA	1.87	0.41
1:A:258:VAL:HG11	1:A:291:PHE:CG	2.54	0.41
1:A:281:ASP:O	1:B:51:ARG:HD3	2.21	0.41
1:B:37:ASP:HA	1:B:58:VAL:HG21	2.01	0.41
2:D:245:ARG:HA	2:D:303:ASN:O	2.20	0.41
1:A:307:VAL:HG11	1:C:227:MET:HE1	2.03	0.41
1:B:34:LEU:HD21	1:C:187:PRO:HB3	2.02	0.41
1:B:211:LYS:HE2	1:B:225:THR:HB	2.02	0.41
1:B:193:ARG:HD3	2:D:278:VAL:O	2.20	0.41
1:A:113[B]:LYS:HE3	5:A:2079:HOH:O	2.21	0.41
1:C:106:LYS:HA	1:C:109:THR:CG2	2.50	0.41
1:B:3:VAL:CG1	1:B:25:ILE:HG23	2.51	0.41
1:B:134:PHE:O	1:B:326:HIS:NE2	2.54	0.40
1:A:3:VAL:HB	1:A:27:ILE:HD13	2.04	0.40
2:D:313:ASN:O	4:D:1341:NAD:H4N	2.21	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	329/331 (99%)	313 (95%)	15 (5%)	1 (0%)	50	53
1	B	331/331 (100%)	318 (96%)	11 (3%)	2 (1%)	33	32
1	C	331/331 (100%)	314 (95%)	13 (4%)	4 (1%)	19	14
2	D	333/334 (100%)	320 (96%)	12 (4%)	1 (0%)	50	53
All	All	1324/1327 (100%)	1265 (96%)	51 (4%)	8 (1%)	33	32

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	62	HIS
1	A	236	VAL

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Mol	Chain	Res	Type
1	B	236	VAL
1	C	60	ASP
1	C	236	VAL
2	D	237	VAL
1	B	165	GLY
1	C	165	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%)	261 (98%)	5 (2%)	69	81
1	B	268/264 (102%)	257 (96%)	11 (4%)	41	49
1	C	268/264 (102%)	257 (96%)	11 (4%)	41	49
2	D	278/274 (102%)	268 (96%)	10 (4%)	47	56
All	All	1080/1066 (101%)	1043 (97%)	37 (3%)	50	59

All (37) 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	307	VAL
1	B	0	THR
1	B	51	ARG
1	B	53[A]	ASP
1	B	53[B]	ASP
1	B	56	VAL
1	B	59	LYS
1	B	86	VAL
1	B	91	VAL
1	B	97	LEU
1	B	220	LEU
1	B	227	MET

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Mol	Chain	Res	Type
1	C	56	VAL
1	C	109	THR
1	C	121	SER
1	C	130	LYS
1	C	171	MET
1	C	177	THR
1	C	227	MET
1	C	243	VAL
1	C	246	GLU
1	C	270	LEU
1	C	288	THR
2	D	0[A]	MET
2	D	0[B]	MET
2	D	3	VAL
2	D	25	ARG
2	D	208	THR
2	D	221	LEU
2	D	228	MET
2	D	240	VAL
2	D	319	HIS
2	D	320	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) 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	163	ASN
1	B	253	GLN
1	C	145	ASN
1	C	201	ASN
2	D	146	ASN
2	D	200	HIS
2	D	319	HIS

5.3.3 RNA ⓘ

There are no RNA chains 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	7,7,8	8.42	5 (71%)	6,8,10	3.27	3 (50%)
1	CSD	A	287	1	7,7,8	8.12	4 (57%)	6,8,10	3.72	4 (66%)
1	CSD	B	148	1	7,7,8	8.24	4 (57%)	6,8,10	2.98	4 (66%)
1	CSD	B	287	1	7,7,8	7.97	4 (57%)	6,8,10	3.78	5 (83%)
1	CSD	C	148	1	7,7,8	8.45	5 (71%)	6,8,10	2.95	5 (83%)
1	CSD	C	287	1	7,7,8	8.01	4 (57%)	6,8,10	2.73	4 (66%)
2	CSD	D	149	2	7,7,8	7.85	5 (71%)	6,8,10	3.01	5 (83%)
2	CSX	D	75	2	4,6,7	8.97	1 (25%)	3,6,8	1.55	1 (33%)

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	-	0/3/6/8	0/0/0/0
1	CSD	A	287	1	-	0/3/6/8	0/0/0/0
1	CSD	B	148	1	-	0/3/6/8	0/0/0/0
1	CSD	B	287	1	-	1/3/6/8	0/0/0/0
1	CSD	C	148	1	-	0/3/6/8	0/0/0/0
1	CSD	C	287	1	-	1/3/6/8	0/0/0/0
2	CSD	D	149	2	-	0/3/6/8	0/0/0/0
2	CSX	D	75	2	-	0/2/5/7	0/0/0/0

All (32) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	148	CSD	O-C	18.99	1.24	1.11
1	C	148	CSD	O-C	18.90	1.24	1.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	148	CSD	O-C	18.42	1.24	1.11
2	D	75	CSX	O-C	17.90	1.23	1.11
2	D	149	CSD	O-C	17.53	1.23	1.11
1	A	287	CSD	O-C	17.46	1.23	1.11
1	C	287	CSD	O-C	16.83	1.23	1.11
1	B	287	CSD	O-C	16.71	1.22	1.11
1	C	287	CSD	OD1-SG	12.11	1.64	1.47
1	B	287	CSD	OD1-SG	12.11	1.64	1.47
1	A	287	CSD	OD1-SG	11.77	1.64	1.47
1	C	148	CSD	OD1-SG	11.01	1.63	1.47
1	B	148	CSD	OD1-SG	10.71	1.62	1.47
1	A	148	CSD	OD1-SG	10.70	1.62	1.47
2	D	149	CSD	OD1-SG	10.17	1.62	1.47
1	C	148	CSD	CB-SG	3.51	1.92	1.80
1	B	148	CSD	CB-SG	3.49	1.92	1.80
2	D	149	CSD	CB-SG	3.46	1.91	1.80
1	B	287	CSD	CB-SG	3.40	1.91	1.80
1	A	148	CSD	CB-SG	3.39	1.91	1.80
1	C	287	CSD	CB-SG	3.39	1.91	1.80
1	A	287	CSD	CB-SG	3.29	1.91	1.80
1	A	287	CSD	OD2-SG	2.33	1.72	1.55
1	A	148	CSD	OD2-SG	2.23	1.71	1.55
1	C	148	CSD	OD2-SG	2.23	1.71	1.55
1	C	287	CSD	OD2-SG	2.23	1.71	1.55
1	B	287	CSD	OD2-SG	2.20	1.71	1.55
1	B	148	CSD	OD2-SG	2.15	1.70	1.55
2	D	149	CSD	OD2-SG	2.13	1.70	1.55
1	C	148	CSD	CA-C	2.06	1.52	1.48
1	A	148	CSD	CA-C	2.04	1.52	1.48
2	D	149	CSD	CA-C	2.03	1.52	1.48

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	148	CSD	OD2-SG-OD1	6.45	120.09	109.39
1	A	287	CSD	OD2-SG-OD1	6.01	119.37	109.39
1	B	287	CSD	C-CA-N	-5.91	107.92	113.83
1	A	287	CSD	C-CA-N	-5.55	108.29	113.83
2	D	149	CSD	OD2-SG-OD1	5.21	118.04	109.39
1	C	148	CSD	OD2-SG-OD1	5.15	117.94	109.39
1	B	148	CSD	OD2-SG-OD1	5.09	117.84	109.39
1	C	287	CSD	OD2-SG-OD1	4.54	116.94	109.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	287	CSD	CA-CB-SG	3.85	116.31	110.82
1	B	287	CSD	OD1-SG-CB	-3.54	95.86	105.25
1	C	287	CSD	C-CA-N	-3.49	110.34	113.83
1	B	287	CSD	OD2-SG-CB	3.41	111.13	97.42
1	B	148	CSD	C-CA-N	-3.32	110.51	113.83
1	A	287	CSD	OD1-SG-CB	-3.23	96.69	105.25
1	B	287	CSD	OD2-SG-OD1	3.21	114.72	109.39
1	A	148	CSD	CA-CB-SG	3.15	115.31	110.82
1	C	148	CSD	CA-CB-SG	2.97	115.06	110.82
2	D	149	CSD	C-CA-N	-2.71	111.13	113.83
1	A	148	CSD	OD1-SG-CB	-2.64	98.26	105.25
1	B	148	CSD	CA-CB-SG	2.53	114.43	110.82
2	D	75	CSX	C-CA-N	-2.52	111.32	113.83
2	D	149	CSD	OD1-SG-CB	-2.50	98.62	105.25
1	C	287	CSD	OD2-SG-CB	2.41	107.11	97.42
1	C	148	CSD	C-CA-N	-2.40	111.43	113.83
2	D	149	CSD	CA-CB-SG	2.39	114.23	110.82
1	B	148	CSD	OD1-SG-CB	-2.31	99.12	105.25
2	D	149	CSD	OD2-SG-CB	2.31	106.71	97.42
1	C	148	CSD	OD2-SG-CB	2.29	106.64	97.42
1	C	287	CSD	OD1-SG-CB	-2.25	99.29	105.25
1	C	148	CSD	OD1-SG-CB	-2.19	99.44	105.25
1	A	287	CSD	OD2-SG-CB	2.10	105.88	97.42

There are no chirality outliers.

All (2) torsion outliers are listed below:

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

There are no ring outliers.

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

18 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	1332	-	2,2,2	0.62	0	1,1,1	0.04	0
3	FMT	A	1333	-	2,2,2	0.67	0	1,1,1	0.19	0
3	FMT	A	1334	-	2,2,2	0.60	0	1,1,1	0.30	0
4	NAD	A	1335	-	48,48,48	1.37	4 (8%)	73,73,73	1.81	9 (12%)
3	FMT	B	1332	-	2,2,2	0.62	0	1,1,1	0.11	0
3	FMT	B	1333	-	2,2,2	0.67	0	1,1,1	0.30	0
3	FMT	B	1334	-	2,2,2	0.64	0	1,1,1	0.25	0
3	FMT	B	1335	-	2,2,2	0.65	0	1,1,1	0.30	0
4	NAD	B	1336	-	48,48,48	1.37	4 (8%)	73,73,73	1.66	9 (12%)
3	FMT	C	1332	-	2,2,2	0.63	0	1,1,1	0.06	0
3	FMT	C	1333	-	2,2,2	0.65	0	1,1,1	0.32	0
4	NAD	C	1334	-	48,48,48	1.37	4 (8%)	73,73,73	1.70	11 (15%)
3	FMT	D	1336	-	2,2,2	0.61	0	1,1,1	0.19	0
3	FMT	D	1337	-	2,2,2	0.60	0	1,1,1	0.18	0
3	FMT	D	1338	-	2,2,2	0.64	0	1,1,1	0.33	0
3	FMT	D	1339	-	2,2,2	0.58	0	1,1,1	0.10	0
3	FMT	D	1340	-	2,2,2	0.65	0	1,1,1	0.25	0
4	NAD	D	1341	-	48,48,48	1.36	4 (8%)	73,73,73	1.76	9 (12%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	FMT	A	1332	-	-	0/0/0/0	0/0/0/0
3	FMT	A	1333	-	-	0/0/0/0	0/0/0/0
3	FMT	A	1334	-	-	0/0/0/0	0/0/0/0
4	NAD	A	1335	-	-	0/30/62/62	0/3/5/5
3	FMT	B	1332	-	-	0/0/0/0	0/0/0/0
3	FMT	B	1333	-	-	0/0/0/0	0/0/0/0
3	FMT	B	1334	-	-	0/0/0/0	0/0/0/0
3	FMT	B	1335	-	-	0/0/0/0	0/0/0/0
4	NAD	B	1336	-	-	0/30/62/62	0/3/5/5

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	FMT	C	1332	-	-	0/0/0/0	0/0/0/0
3	FMT	C	1333	-	-	0/0/0/0	0/0/0/0
4	NAD	C	1334	-	-	0/30/62/62	0/3/5/5
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
3	FMT	D	1340	-	-	0/0/0/0	0/0/0/0
4	NAD	D	1341	-	-	0/30/62/62	0/3/5/5

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1335	NAD	O7N-C7N	7.16	1.41	1.24
4	C	1334	NAD	O7N-C7N	6.99	1.40	1.24
4	B	1336	NAD	O7N-C7N	6.83	1.40	1.24
4	D	1341	NAD	O7N-C7N	6.75	1.40	1.24
4	D	1341	NAD	C2A-N3A	3.41	1.38	1.32
4	C	1334	NAD	C2A-N3A	3.37	1.38	1.32
4	B	1336	NAD	C2A-N3A	3.32	1.38	1.32
4	A	1335	NAD	C2A-N3A	2.93	1.38	1.32
4	D	1341	NAD	C2N-N1N	2.65	1.38	1.35
4	B	1336	NAD	C2A-N1A	2.46	1.38	1.33
4	B	1336	NAD	C2N-N1N	2.44	1.38	1.35
4	C	1334	NAD	C2A-N1A	2.40	1.38	1.33
4	A	1335	NAD	C2N-N1N	2.33	1.38	1.35
4	C	1334	NAD	C2N-N1N	2.29	1.38	1.35
4	D	1341	NAD	C2A-N1A	2.17	1.38	1.33
4	A	1335	NAD	C2A-N1A	2.08	1.38	1.33

All (38) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1335	NAD	N3A-C2A-N1A	-11.58	119.03	128.71
4	D	1341	NAD	N3A-C2A-N1A	-11.22	119.33	128.71
4	C	1334	NAD	N3A-C2A-N1A	-10.57	119.87	128.71
4	B	1336	NAD	N3A-C2A-N1A	-10.08	120.28	128.71
4	B	1336	NAD	N3A-C4A-N9A	3.98	132.62	125.43
4	A	1335	NAD	O4D-C1D-N1N	3.63	111.66	107.95
4	C	1334	NAD	N3A-C4A-N9A	3.62	131.97	125.43
4	D	1341	NAD	N3A-C4A-N9A	3.62	131.97	125.43
4	D	1341	NAD	O4D-C1D-N1N	3.30	111.33	107.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	1334	NAD	C3N-C7N-N7N	3.29	121.52	117.77
4	A	1335	NAD	N3A-C4A-N9A	3.27	131.34	125.43
4	D	1341	NAD	C3N-C7N-N7N	3.19	121.40	117.77
4	C	1334	NAD	O4B-C1B-N9A	3.00	111.23	108.44
4	B	1336	NAD	C3N-C7N-N7N	2.74	120.88	117.77
4	A	1335	NAD	C3N-C7N-N7N	2.70	120.84	117.77
4	A	1335	NAD	PN-O3-PA	-2.53	122.06	132.95
4	C	1334	NAD	PN-O3-PA	-2.39	122.67	132.95
4	B	1336	NAD	C5A-C4A-N3A	-2.37	120.54	125.70
4	D	1341	NAD	PN-O3-PA	-2.36	122.81	132.95
4	D	1341	NAD	C2A-N3A-C4A	2.34	120.69	114.01
4	A	1335	NAD	C2A-N3A-C4A	2.28	120.50	114.01
4	D	1341	NAD	C5A-C4A-N3A	-2.26	120.79	125.70
4	A	1335	NAD	C4A-C5A-N7A	-2.24	107.60	109.52
4	C	1334	NAD	N7A-C8A-N9A	-2.24	108.02	114.36
4	B	1336	NAD	N7A-C8A-N9A	-2.22	108.07	114.36
4	B	1336	NAD	O3D-C3D-C4D	-2.18	104.64	111.08
4	B	1336	NAD	O4D-C1D-N1N	2.18	110.18	107.95
4	A	1335	NAD	C5A-C4A-N3A	-2.17	120.97	125.70
4	C	1334	NAD	O4D-C1D-N1N	2.15	110.15	107.95
4	D	1341	NAD	N7A-C8A-N9A	-2.14	108.30	114.36
4	C	1334	NAD	O7N-C7N-C3N	-2.13	117.18	119.58
4	B	1336	NAD	C2A-N3A-C4A	2.12	120.03	114.01
4	A	1335	NAD	N7A-C8A-N9A	-2.11	108.38	114.36
4	C	1334	NAD	C5A-C4A-N3A	-2.10	121.13	125.70
4	D	1341	NAD	O7N-C7N-C3N	-2.03	117.29	119.58
4	C	1334	NAD	C1B-N9A-C4A	-2.03	123.13	126.64
4	C	1334	NAD	C2A-N3A-C4A	2.02	119.77	114.01
4	B	1336	NAD	C4A-C5A-N7A	-2.00	107.81	109.52

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	330/331 (99%)	-0.41	1 (0%) 91 93	11, 22, 38, 54	0
1	B	330/331 (99%)	-0.45	3 (0%) 81 82	11, 23, 41, 52	0
1	C	330/331 (99%)	-0.27	5 (1%) 70 71	13, 27, 45, 51	0
2	D	334/334 (100%)	-0.59	0 100 100	10, 20, 34, 40	0
All	All	1324/1327 (99%)	-0.43	9 (0%) 84 86	10, 22, 40, 54	0

All (9) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	124[A]	ASN	3.5
1	B	189	HIS	3.3
1	A	62	HIS	2.9
1	C	92	ALA	2.5
1	B	135[A]	ASP	2.4
1	C	86	VAL	2.3
1	C	23	SER	2.3
1	C	79	ALA	2.2
1	B	60	ASP	2.1

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å ²)	Q<0.9
1	CSD	B	287	8/9	0.10	1.19	16,19,33,40	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
1	CSD	A	148	8/9	0.10	0.32	14,17,26,28	0
2	CSD	D	149	8/9	0.09	0.28	14,15,18,19	0
1	CSD	A	287	8/9	0.11	0.10	21,26,43,46	0
1	CSD	C	287	8/9	0.10	0.01	22,24,40,41	0
1	CSD	B	148	8/9	0.08	-0.38	16,17,24,25	0
2	CSX	D	75	7/8	0.07	-0.93	21,22,24,26	0
1	CSD	C	148	8/9	0.07	-0.98	17,18,30,34	0

6.3 Carbohydrates

There are no carbohydrates in this entry.

6.4 Ligands

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
3	FMT	B	1334	3/3	0.19	11.64	43,43,46,48	0
3	FMT	D	1339	3/3	0.23	8.78	48,48,49,49	0
3	FMT	A	1333	3/3	0.20	8.68	39,39,43,46	0
3	FMT	B	1333	3/3	0.13	4.31	44,44,44,45	0
3	FMT	D	1338	3/3	0.13	4.23	28,28,29,29	0
3	FMT	D	1340	3/3	0.13	1.59	43,43,44,45	0
3	FMT	A	1332	3/3	0.13	1.05	30,30,31,34	0
3	FMT	C	1332	3/3	0.13	0.92	36,36,37,38	0
3	FMT	D	1336	3/3	0.14	0.54	46,46,47,48	0
3	FMT	D	1337	3/3	0.10	0.11	46,46,47,47	0
3	FMT	A	1334	3/3	0.11	-0.13	35,35,35,36	0
3	FMT	B	1332	3/3	0.09	-0.14	27,27,31,33	0
4	NAD	C	1334	44/44	0.11	-0.33	21,32,39,40	0
3	FMT	B	1335	3/3	0.11	-0.39	34,34,35,37	0
3	FMT	C	1333	3/3	0.08	-0.64	37,37,37,38	0
4	NAD	B	1336	44/44	0.08	-0.88	15,22,24,25	0
4	NAD	A	1335	44/44	0.07	-1.02	15,20,26,27	0
4	NAD	D	1341	44/44	0.06	-1.16	14,18,21,25	0

6.5 Other polymers ⓘ

There are no such residues in this entry.