



Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 07:42 AM GMT

PDB ID : 1GEG
Title : CRYATAL STRUCTURE ANALYSIS OF MESO-2,3-BUTANEDIOL DEHYDROGENASE
Authors : Otagiri, M.; Kurisu, G.; Ui, S.; Kusunoki, M.
Deposited on : 2000-11-10
Resolution : 1.70 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>

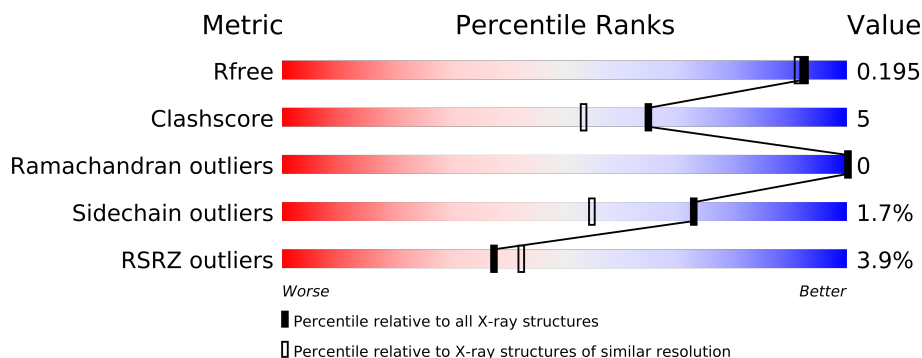
The following versions of software and data (see [references](#)) were used in the production of this report:

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 1.70 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	2456 (1.70-1.70)
Clashscore	79885	2929 (1.70-1.70)
Ramachandran outliers	78287	2878 (1.70-1.70)
Sidechain outliers	78261	2878 (1.70-1.70)
RSRZ outliers	66119	2456 (1.70-1.70)

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	256	
1	B	256	
1	C	256	
1	D	256	
1	E	256	
1	F	256	
1	G	256	
1	H	256	

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

Mol	Type	Chain	Res	Geometry	Electron density
2	GLC	A	302	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
2	GLC	B	303	-	X
2	GLC	C	304	-	X
2	GLC	D	305	-	X
2	GLC	F	307	-	X
2	GLC	G	308	-	X
2	GLC	H	309	-	X
5	BME	A	1462	-	X
5	BME	B	2462	-	X
5	BME	D	4462	-	X
5	BME	E	5462	-	X
5	BME	F	6462	-	X
5	BME	G	7462	-	X

2 Entry composition

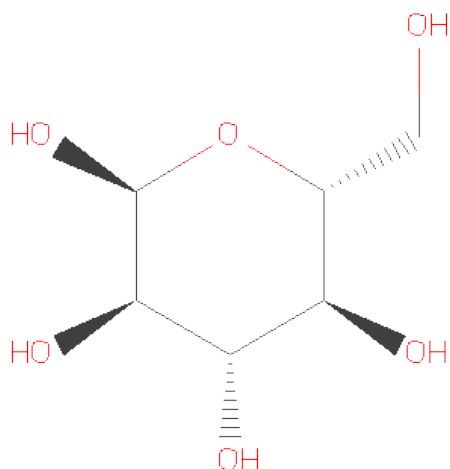
There are 6 unique types of molecules in this entry. The entry contains 16227 atoms, of which 0 are hydrogen and 0 are deuterium.

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 ACETOIN REDUCTASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	255	Total	C	N	O	S	0	0	0
			1862	1174	322	360	6			
1	B	255	Total	C	N	O	S	0	0	0
			1862	1174	322	360	6			
1	C	255	Total	C	N	O	S	0	0	0
			1862	1174	322	360	6			
1	D	255	Total	C	N	O	S	0	0	0
			1862	1174	322	360	6			
1	E	256	Total	C	N	O	S	0	0	0
			1870	1179	323	361	7			
1	F	255	Total	C	N	O	S	0	0	0
			1862	1174	322	360	6			
1	G	255	Total	C	N	O	S	0	0	0
			1862	1174	322	360	6			
1	H	255	Total	C	N	O	S	0	0	0
			1862	1174	322	360	6			

- Molecule 2 is GLUCOSE (three-letter code: GLC) (formula: C₆H₁₂O₆).

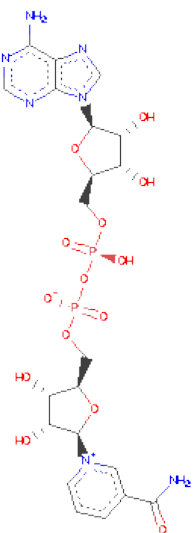


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			12	6	6		
2	B	1	Total	C	O	0	0
			12	6	6		
2	C	1	Total	C	O	0	0
			12	6	6		
2	D	1	Total	C	O	0	0
			12	6	6		
2	E	1	Total	C	O	0	0
			12	6	6		
2	F	1	Total	C	O	0	0
			12	6	6		
2	G	1	Total	C	O	0	0
			12	6	6		
2	H	1	Total	C	O	0	0
			12	6	6		

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

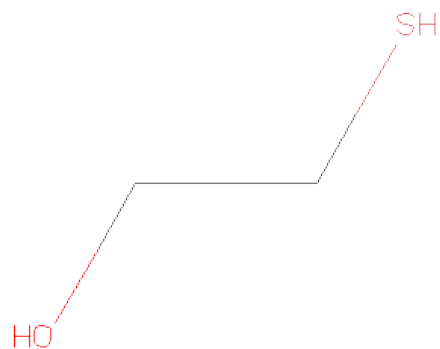
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	H	1	Total	Mg	0	0
			1	1		
3	G	1	Total	Mg	0	0
			1	1		
3	B	1	Total	Mg	0	0
			1	1		
3	A	1	Total	Mg	0	0
			1	1		

- 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		
4	E	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
4	F	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
4	G	1	Total	C	N	O	P	0	0
			44	21	7	14	2		
4	H	1	Total	C	N	O	P	0	0
			44	21	7	14	2		

- Molecule 5 is BETA-MERCAPTOETHANOL (three-letter code: BME) (formula: C_2H_6OS).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	O	S	0	0
			4	2	1	1		
5	B	1	Total	C	O	S	0	0
			4	2	1	1		
5	C	1	Total	C	O	S	0	0
			4	2	1	1		
5	D	1	Total	C	O	S	0	0
			4	2	1	1		
5	E	1	Total	C	O	S	0	0
			4	2	1	1		
5	F	1	Total	C	O	S	0	0
			4	2	1	1		
5	G	1	Total	C	O	S	0	0
			4	2	1	1		
5	H	1	Total	C	O	S	0	0
			4	2	1	1		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	118	Total	O	0	0
			118	118		
6	B	107	Total	O	0	0
			107	107		
6	C	93	Total	O	0	0
			93	93		
6	D	111	Total	O	0	0
			111	111		

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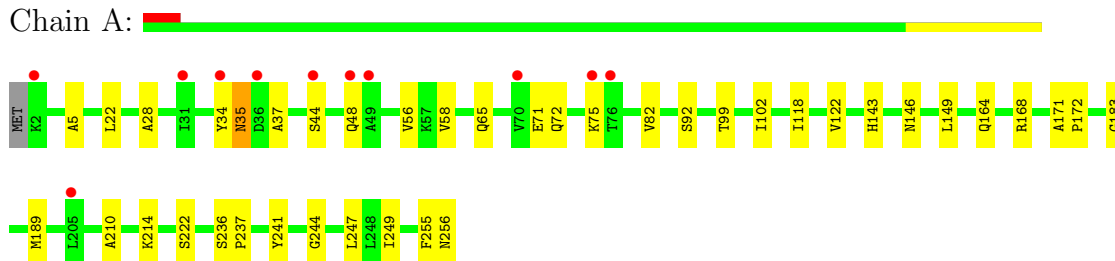
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	E	87	Total 87	O 87	0	0
6	F	115	Total 115	O 115	0	0
6	G	112	Total 112	O 112	0	0
6	H	96	Total 96	O 96	0	0

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.

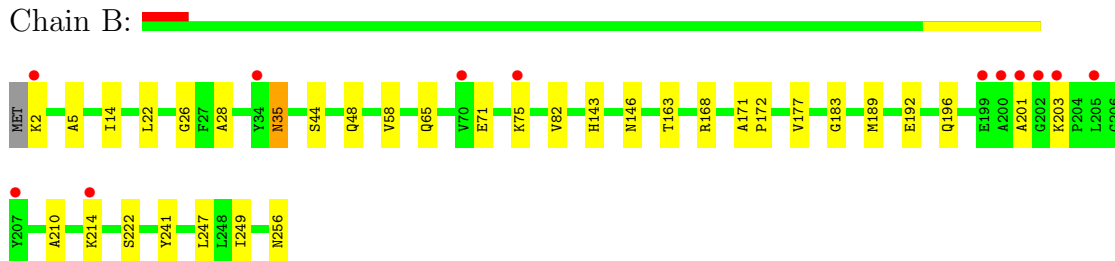
• Molecule 1: ACETOIN REDUCTASE

Chain A:



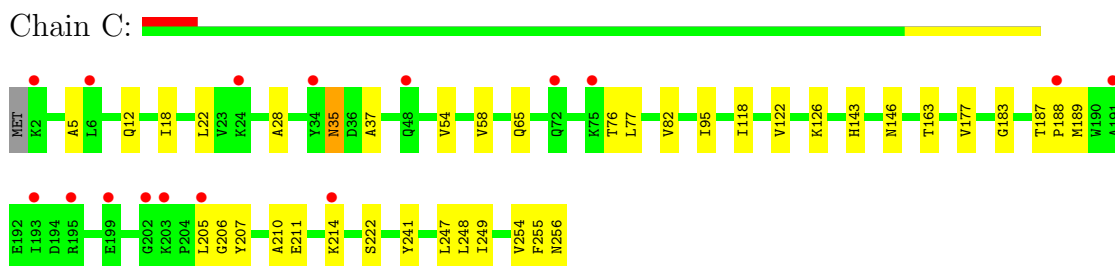
• Molecule 1: ACETOIN REDUCTASE

Chain B:



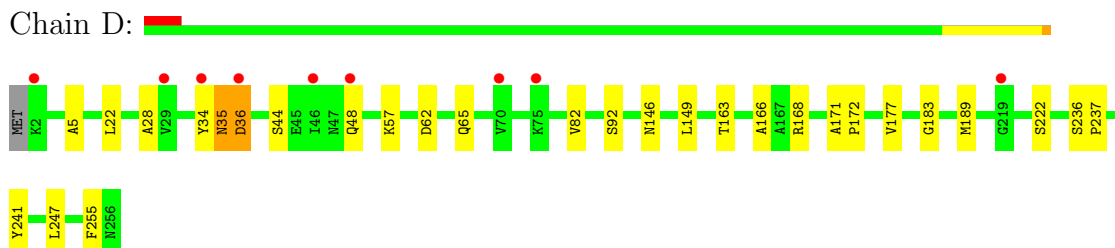
• Molecule 1: ACETOIN REDUCTASE

Chain C:

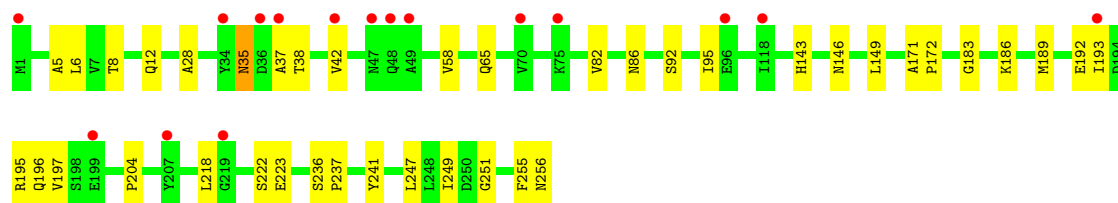


• Molecule 1: ACETOIN REDUCTASE

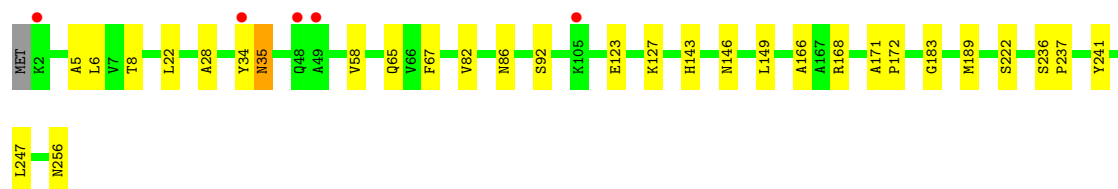
Chain D:



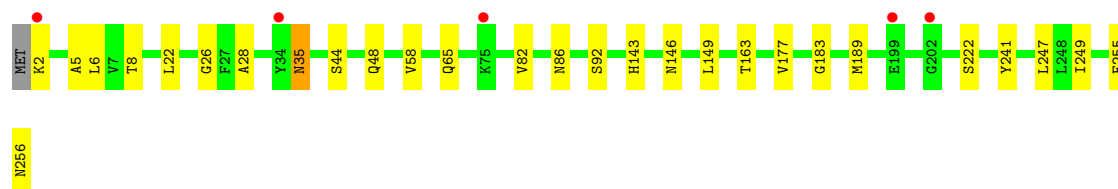
- Molecule 1: ACETOIN REDUCTASE

Chain E: 

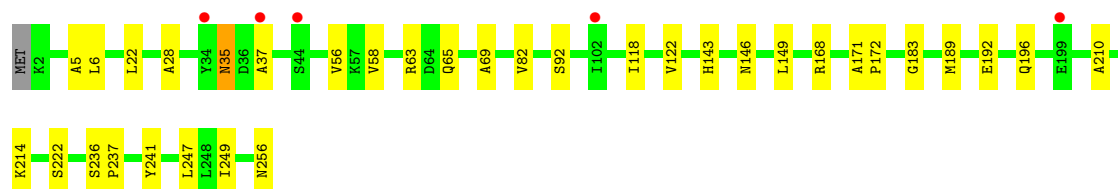
- Molecule 1: ACETOIN REDUCTASE

Chain F: 

- Molecule 1: ACETOIN REDUCTASE

Chain G: 

- Molecule 1: ACETOIN REDUCTASE

Chain H: 

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	69.16Å 109.78Å 127.28Å 90.00° 102.29° 90.00°	Depositor
Resolution (Å)	40.00 – 1.70 18.30 – 1.70	Depositor EDS
% Data completeness (in resolution range)	(Not available) (40.00-1.70) 100.0 (18.30-1.70)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	6.05 (at 1.70Å)	Xtriage
Refinement program	CNS 0.9	Depositor
R, R_{free}	0.193 , 0.209 0.193 , 0.195	Depositor DCC
R_{free} test set	10229 reflections (5.30%)	DCC
Wilson B-factor (Å ²)	11.9	Xtriage
Anisotropy	0.314	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.49 , 39.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	2 of 203386 reflections (0.001%)	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	16227	wwPDB-VP
Average B, all atoms (Å ²)	13.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 19.53% 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: MG, GLC, NAD, BME

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	0.27	0/1892	0.57	1/2567 (0.0%)
1	B	0.27	0/1892	0.58	1/2567 (0.0%)
1	C	0.27	0/1892	0.58	1/2567 (0.0%)
1	D	0.28	0/1892	0.59	1/2567 (0.0%)
1	E	0.27	0/1900	0.58	1/2577 (0.0%)
1	F	0.28	0/1892	0.59	1/2567 (0.0%)
1	G	0.28	0/1892	0.59	1/2567 (0.0%)
1	H	0.28	0/1892	0.59	1/2567 (0.0%)
All	All	0.28	0/15144	0.59	8/20546 (0.0%)

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	28	ALA	N-CA-C	-6.12	94.47	111.00
1	E	28	ALA	N-CA-C	-6.09	94.56	111.00
1	D	28	ALA	N-CA-C	-6.09	94.56	111.00
1	B	28	ALA	N-CA-C	-6.03	94.72	111.00
1	G	28	ALA	N-CA-C	-5.94	94.95	111.00
1	C	28	ALA	N-CA-C	-5.81	95.32	111.00
1	A	28	ALA	N-CA-C	-5.78	95.40	111.00
1	F	28	ALA	N-CA-C	-5.69	95.64	111.00

There are no chirality outliers.

There are no planarity outliers.

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	1862	0	1877	25	0
1	B	1862	0	1877	20	0
1	C	1862	0	1877	28	0
1	D	1862	0	1877	19	0
1	E	1870	0	1889	27	0
1	F	1862	0	1877	18	0
1	G	1862	0	1877	17	0
1	H	1862	0	1877	21	0
2	A	12	0	12	0	0
2	B	12	0	12	0	0
2	C	12	0	12	0	0
2	D	12	0	12	0	0
2	E	12	0	12	0	0
2	F	12	0	12	1	0
2	G	12	0	12	0	0
2	H	12	0	12	2	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	G	1	0	0	0	0
3	H	1	0	0	0	0
4	A	44	0	26	3	0
4	B	44	0	26	4	0
4	C	44	0	26	4	0
4	D	44	0	26	3	0
4	E	44	0	26	4	0
4	F	44	0	26	3	0
4	G	44	0	26	3	0
4	H	44	0	26	3	0
5	A	4	0	5	1	0
5	B	4	0	5	1	0
5	C	4	0	5	1	0
5	D	4	0	5	1	0
5	E	4	0	5	1	0
5	F	4	0	5	1	0
5	G	4	0	5	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	H	4	0	5	1	0
6	A	118	0	0	0	0
6	B	107	0	0	0	0
6	C	93	0	0	0	0
6	D	111	0	0	0	0
6	E	87	0	0	0	0
6	F	115	0	0	0	0
6	G	112	0	0	0	0
6	H	96	0	0	0	0
All	All	16227	0	15372	162	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 5.

All (162) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:F:247:LEU:HD22	1:G:247:LEU:HD22	1.49	0.93
1:B:247:LEU:HD22	1:C:247:LEU:HD22	1.56	0.88
1:A:247:LEU:HD22	1:D:247:LEU:HD22	1.60	0.82
1:E:247:LEU:HD22	1:H:247:LEU:HD22	1.64	0.78
1:C:18:ILE:O	1:C:22:LEU:HD13	1.95	0.66
1:C:205:LEU:HD23	1:C:206:GLY:N	2.10	0.65
1:C:210:ALA:O	1:C:214:LYS:HG3	1.98	0.63
1:A:35:ASN:HD22	1:A:35:ASN:C	2.02	0.62
1:E:186:LYS:HE3	1:E:223:GLU:OE2	2.00	0.60
1:C:54:VAL:HG11	1:C:76:THR:CG2	2.32	0.60
1:C:54:VAL:HG11	1:C:76:THR:HG21	1.83	0.60
1:B:192:GLU:O	1:B:196:GLN:HG3	2.03	0.59
1:D:35:ASN:HD22	1:D:35:ASN:C	2.06	0.58
1:D:36:ASP:OD2	1:D:57:LYS:HD2	2.04	0.58
1:F:35:ASN:HD22	1:F:35:ASN:C	2.07	0.57
1:B:35:ASN:C	1:B:35:ASN:HD22	2.08	0.57
1:A:99:THR:OG1	1:A:102:ILE:HG12	2.05	0.56
1:E:241:TYR:CE2	1:H:222:SER:HB2	2.40	0.56
4:F:308:NAD:C4N	5:F:6462:BME:S2	2.93	0.56
4:D:306:NAD:C4N	5:D:4462:BME:S2	2.94	0.56
1:E:35:ASN:HD22	1:E:35:ASN:C	2.09	0.56
1:H:183:GLY:O	4:H:2004:NAD:H4N	2.06	0.56
1:C:35:ASN:C	1:C:35:ASN:HD22	2.08	0.56
1:B:58:VAL:HG23	1:B:65:GLN:HB3	1.88	0.55
1:B:2:LYS:HD2	1:B:26:GLY:O	2.07	0.55
1:D:44:SER:O	1:D:48:GLN:HG3	2.06	0.54

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:187:THR:HB	1:C:188:PRO:HD2	1.90	0.54
4:G:2003:NAD:C4N	5:G:7462:BME:S2	2.95	0.54
1:B:183:GLY:O	4:B:2002:NAD:H4N	2.07	0.54
1:E:236:SER:HB2	1:E:237:PRO:HD2	1.90	0.53
1:C:122:VAL:O	1:C:126:LYS:HG3	2.08	0.53
1:C:54:VAL:HG13	1:C:77:LEU:HD21	1.90	0.53
1:E:183:GLY:O	4:E:307:NAD:H4N	2.08	0.53
1:A:183:GLY:O	4:A:2001:NAD:H4N	2.09	0.53
1:H:35:ASN:HD22	1:H:35:ASN:C	2.12	0.53
1:C:205:LEU:HD12	1:E:223:GLU:HG3	1.90	0.52
1:B:168:ARG:HD2	1:C:255:PHE:HE1	1.74	0.52
1:G:143:HIS:CD2	1:G:256:ASN:HD21	2.27	0.52
1:E:255:PHE:HE1	1:H:168:ARG:HD2	1.74	0.52
4:H:2004:NAD:C4N	5:H:8462:BME:S2	2.98	0.51
1:A:222:SER:HB2	1:D:241:TYR:CE2	2.45	0.51
1:B:171:ALA:N	1:B:172:PRO:HD2	2.26	0.51
1:B:71:GLU:O	1:B:75:LYS:HE2	2.11	0.51
1:H:58:VAL:HG23	1:H:65:GLN:HB3	1.92	0.50
4:A:2001:NAD:C4N	5:A:1462:BME:S2	2.99	0.50
1:F:222:SER:HB2	1:G:241:TYR:CE2	2.47	0.50
1:F:123:GLU:HG2	1:F:127:LYS:HE3	1.93	0.50
1:C:37:ALA:HB1	1:E:204:PRO:HB3	1.93	0.50
1:A:171:ALA:HB3	1:A:172:PRO:HD3	1.92	0.50
1:H:171:ALA:N	1:H:172:PRO:HD2	2.27	0.50
1:G:183:GLY:O	4:G:2003:NAD:H4N	2.12	0.50
1:H:143:HIS:CD2	1:H:256:ASN:HD21	2.29	0.50
1:F:236:SER:HB2	1:F:237:PRO:HD2	1.93	0.50
1:B:44:SER:O	1:B:48:GLN:HG3	2.12	0.49
1:F:183:GLY:O	4:F:308:NAD:H4N	2.12	0.49
1:E:192:GLU:O	1:E:196:GLN:HG3	2.11	0.49
1:H:63:ARG:CZ	2:H:309:GLC:H61	2.42	0.49
4:B:2002:NAD:C4N	5:B:2462:BME:S2	3.00	0.49
1:F:92:SER:HA	1:F:149:LEU:HD23	1.94	0.49
1:A:44:SER:O	1:A:48:GLN:HG3	2.14	0.48
1:G:35:ASN:HD22	1:G:35:ASN:C	2.15	0.48
1:H:118:ILE:O	1:H:122:VAL:HG23	2.13	0.48
1:C:183:GLY:O	4:C:305:NAD:H4N	2.13	0.48
1:D:183:GLY:O	4:D:306:NAD:H4N	2.13	0.48
1:B:201:ALA:O	1:B:203:LYS:HG3	2.14	0.47
1:A:58:VAL:HG23	1:A:65:GLN:HB3	1.96	0.47
1:B:222:SER:HB2	1:C:241:TYR:CE2	2.49	0.47
1:H:192:GLU:O	1:H:196:GLN:HG3	2.15	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:143:HIS:CD2	1:A:256:ASN:HD21	2.32	0.47
1:E:143:HIS:CD2	1:E:256:ASN:HD21	2.32	0.47
1:B:249:ILE:O	1:B:249:ILE:HG23	2.15	0.47
1:A:56:VAL:HG13	1:A:72:GLN:NE2	2.30	0.47
1:D:189:MET:SD	4:D:306:NAD:H2D	2.56	0.46
4:E:307:NAD:C4N	5:E:5462:BME:S2	3.04	0.46
1:H:249:ILE:HG23	1:H:249:ILE:O	2.16	0.46
1:C:12:GLN:HG2	4:C:305:NAD:O3B	2.16	0.46
1:H:236:SER:HB2	1:H:237:PRO:HD2	1.98	0.46
1:A:92:SER:HA	1:A:149:LEU:HD23	1.96	0.46
1:B:210:ALA:O	1:B:214:LYS:HG3	2.15	0.46
1:E:92:SER:HA	1:E:149:LEU:HD23	1.97	0.46
1:H:6:LEU:HD23	1:H:6:LEU:C	2.36	0.46
1:D:92:SER:HA	1:D:149:LEU:HD23	1.98	0.46
1:G:5:ALA:HA	1:G:82:VAL:O	2.16	0.45
1:C:95:ILE:CD1	1:D:166:ALA:HA	2.46	0.45
1:H:5:ALA:HA	1:H:82:VAL:O	2.17	0.45
1:B:241:TYR:CE2	1:C:222:SER:HB2	2.52	0.45
1:A:118:ILE:O	1:A:122:VAL:HG23	2.17	0.45
1:A:241:TYR:CE2	1:D:222:SER:HB2	2.51	0.45
1:E:5:ALA:HA	1:E:82:VAL:O	2.15	0.45
1:F:189:MET:SD	4:F:308:NAD:H2D	2.57	0.45
1:D:62:ASP:OD2	1:D:65:GLN:HG3	2.17	0.45
1:A:210:ALA:O	1:A:214:LYS:HG3	2.16	0.44
1:A:236:SER:HB2	1:A:237:PRO:HD2	1.99	0.44
1:C:143:HIS:CD2	1:C:256:ASN:HD21	2.35	0.44
1:C:249:ILE:HG23	1:C:249:ILE:O	2.17	0.44
4:C:305:NAD:C4N	5:C:3462:BME:S2	3.06	0.44
1:G:44:SER:O	1:G:48:GLN:HG3	2.18	0.44
1:E:218:LEU:HD12	1:E:251:GLY:HA2	2.00	0.44
1:G:2:LYS:HD2	1:G:26:GLY:O	2.18	0.44
1:F:6:LEU:HD23	1:F:6:LEU:C	2.38	0.44
1:A:255:PHE:HE1	1:D:168:ARG:HD2	1.82	0.43
1:B:5:ALA:HA	1:B:82:VAL:O	2.17	0.43
1:C:207:TYR:O	1:C:211:GLU:HG2	2.18	0.43
1:E:195:ARG:HH21	1:E:195:ARG:HG2	1.83	0.43
1:E:222:SER:HB2	1:H:241:TYR:CE2	2.53	0.43
1:A:44:SER:OG	1:A:48:GLN:NE2	2.52	0.43
1:F:143:HIS:CD2	1:F:256:ASN:HD21	2.36	0.43
1:E:95:ILE:HD11	1:F:166:ALA:HA	1.99	0.43
1:E:12:GLN:HG2	4:E:307:NAD:O3B	2.18	0.43
1:A:164:GLN:O	1:A:168:ARG:HG3	2.19	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:5:ALA:HA	1:A:82:VAL:O	2.18	0.43
1:B:189:MET:SD	4:B:2002:NAD:H2D	2.58	0.43
1:H:92:SER:HA	1:H:149:LEU:HD23	2.00	0.43
1:C:5:ALA:HA	1:C:82:VAL:O	2.18	0.43
1:G:92:SER:HA	1:G:149:LEU:HD23	2.00	0.43
1:F:168:ARG:HD2	1:G:255:PHE:HE1	1.84	0.43
1:E:193:ILE:O	1:E:197:VAL:HG22	2.18	0.43
1:C:95:ILE:HD11	1:D:166:ALA:HA	2.01	0.43
1:F:58:VAL:HG23	1:F:65:GLN:HB3	2.00	0.43
1:F:67:PHE:HB3	2:F:307:GLC:O4	2.19	0.43
1:C:58:VAL:HG23	1:C:65:GLN:HB3	2.00	0.42
1:F:171:ALA:N	1:F:172:PRO:CD	2.83	0.42
1:E:38:THR:O	1:E:42:VAL:HG23	2.19	0.42
1:H:35:ASN:HD21	1:H:37:ALA:HB3	1.84	0.42
1:A:244:GLY:HA3	1:D:255:PHE:CD2	2.54	0.42
1:E:249:ILE:O	1:E:249:ILE:HG23	2.19	0.42
1:A:35:ASN:HD21	1:A:37:ALA:HB3	1.83	0.42
1:E:35:ASN:HD21	1:E:37:ALA:HB3	1.85	0.42
1:A:71:GLU:O	1:A:75:LYS:HE2	2.19	0.42
1:G:8:THR:O	1:G:86:ASN:HB3	2.19	0.42
1:D:5:ALA:HA	1:D:82:VAL:O	2.19	0.42
1:E:189:MET:SD	4:E:307:NAD:H2D	2.59	0.42
1:A:189:MET:SD	4:A:2001:NAD:H2D	2.59	0.42
1:F:5:ALA:HA	1:F:82:VAL:O	2.19	0.42
1:E:171:ALA:N	1:E:172:PRO:CD	2.82	0.42
1:B:163:THR:HG23	1:B:177:VAL:HG12	2.02	0.42
1:F:8:THR:O	1:F:86:ASN:HB3	2.20	0.42
1:C:118:ILE:O	1:C:122:VAL:HG23	2.20	0.42
1:G:249:ILE:O	1:G:249:ILE:HG23	2.20	0.42
1:G:189:MET:SD	4:G:2003:NAD:H2D	2.60	0.42
1:D:163:THR:HG23	1:D:177:VAL:HG12	2.02	0.42
1:G:58:VAL:HG23	1:G:65:GLN:HB3	2.02	0.41
1:E:58:VAL:HG23	1:E:65:GLN:HB3	2.01	0.41
1:C:248:LEU:HD13	1:C:254:VAL:O	2.20	0.41
1:G:163:THR:HG23	1:G:177:VAL:HG12	2.02	0.41
1:G:6:LEU:HD23	1:G:6:LEU:C	2.40	0.41
1:H:56:VAL:HG11	1:H:69:ALA:HA	2.01	0.41
1:A:171:ALA:N	1:A:172:PRO:CD	2.84	0.41
2:H:309:GLC:H62	2:H:309:GLC:H1	1.91	0.41
1:A:249:ILE:HG23	1:A:249:ILE:O	2.20	0.41
1:B:143:HIS:CD2	1:B:256:ASN:HD21	2.39	0.41
1:D:236:SER:HB2	1:D:237:PRO:HD2	2.03	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:E:6:LEU:C	1:E:6:LEU:HD23	2.41	0.41
1:H:189:MET:SD	4:H:2004:NAD:H2D	2.61	0.41
1:D:171:ALA:N	1:D:172:PRO:CD	2.84	0.41
1:H:210:ALA:O	1:H:214:LYS:HG3	2.20	0.40
1:C:189:MET:SD	4:C:305:NAD:H2D	2.60	0.40
1:B:14:ILE:HB	4:B:2002:NAD:H51N	2.02	0.40
1:D:171:ALA:HB3	1:D:172:PRO:HD3	2.02	0.40
1:C:163:THR:HG23	1:C:177:VAL:HG12	2.04	0.40
1:F:241:TYR:CE2	1:G:222:SER:HB2	2.56	0.40
1:E:8:THR:O	1:E:86:ASN:HB3	2.20	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	253/256 (99%)	247 (98%)	6 (2%)	0	100	100
1	B	253/256 (99%)	247 (98%)	6 (2%)	0	100	100
1	C	253/256 (99%)	250 (99%)	3 (1%)	0	100	100
1	D	253/256 (99%)	249 (98%)	4 (2%)	0	100	100
1	E	254/256 (99%)	249 (98%)	5 (2%)	0	100	100
1	F	253/256 (99%)	248 (98%)	5 (2%)	0	100	100
1	G	253/256 (99%)	248 (98%)	5 (2%)	0	100	100
1	H	253/256 (99%)	248 (98%)	5 (2%)	0	100	100
All	All	2025/2048 (99%)	1986 (98%)	39 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	190/191 (100%)	186 (98%)	4 (2%)	66	45
1	B	190/191 (100%)	187 (98%)	3 (2%)	75	58
1	C	190/191 (100%)	188 (99%)	2 (1%)	84	72
1	D	190/191 (100%)	185 (97%)	5 (3%)	59	35
1	E	191/191 (100%)	189 (99%)	2 (1%)	85	76
1	F	190/191 (100%)	186 (98%)	4 (2%)	66	45
1	G	190/191 (100%)	187 (98%)	3 (2%)	75	58
1	H	190/191 (100%)	187 (98%)	3 (2%)	75	58
All	All	1521/1528 (100%)	1495 (98%)	26 (2%)	73	55

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	22	LEU
1	A	34	TYR
1	A	35	ASN
1	A	146	ASN
1	B	22	LEU
1	B	35	ASN
1	B	146	ASN
1	C	35	ASN
1	C	146	ASN
1	D	22	LEU
1	D	34	TYR
1	D	35	ASN
1	D	36	ASP
1	D	146	ASN
1	E	35	ASN
1	E	146	ASN
1	F	22	LEU
1	F	34	TYR
1	F	35	ASN
1	F	146	ASN
1	G	22	LEU

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Mol	Chain	Res	Type
1	G	35	ASN
1	G	146	ASN
1	H	22	LEU
1	H	35	ASN
1	H	146	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (36) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	12	GLN
1	A	35	ASN
1	A	48	GLN
1	A	52	HIS
1	A	72	GLN
1	A	143	HIS
1	B	12	GLN
1	B	35	ASN
1	B	52	HIS
1	B	72	GLN
1	B	143	HIS
1	C	12	GLN
1	C	35	ASN
1	C	72	GLN
1	C	143	HIS
1	D	12	GLN
1	D	35	ASN
1	D	48	GLN
1	D	72	GLN
1	D	143	HIS
1	E	35	ASN
1	E	72	GLN
1	E	143	HIS
1	F	12	GLN
1	F	35	ASN
1	F	72	GLN
1	F	143	HIS
1	G	12	GLN
1	G	35	ASN
1	G	52	HIS
1	G	72	GLN
1	G	143	HIS
1	H	12	GLN

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Mol	Chain	Res	Type
1	H	35	ASN
1	H	72	GLN
1	H	143	HIS

5.3.3 RNA ⓘ

There are no RNA chains in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 28 ligands modelled in this entry, 4 are monoatomic - leaving 24 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	BME	A	1462	-	3,3,3	1.89	1 (33%)	2,2,2	1.89	1 (50%)
4	NAD	A	2001	-	48,48,48	2.02	9 (18%)	73,73,73	1.46	8 (10%)
2	GLC	A	302	-	12,12,12	0.31	0	17,17,17	0.35	0
4	NAD	B	2002	-	48,48,48	2.06	8 (16%)	73,73,73	1.45	9 (12%)
5	BME	B	2462	-	3,3,3	1.90	1 (33%)	2,2,2	1.78	1 (50%)
2	GLC	B	303	-	12,12,12	0.37	0	17,17,17	0.43	0
2	GLC	C	304	-	12,12,12	0.40	0	17,17,17	0.42	0
4	NAD	C	305	-	48,48,48	2.05	9 (18%)	73,73,73	1.47	9 (12%)
5	BME	C	3462	-	3,3,3	1.93	1 (33%)	2,2,2	1.83	1 (50%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	GLC	D	305	-	12,12,12	0.36	0	17,17,17	0.43	0
4	NAD	D	306	-	48,48,48	2.02	7 (14%)	73,73,73	1.48	10 (13%)
5	BME	D	4462	-	3,3,3	1.87	1 (33%)	2,2,2	1.87	1 (50%)
2	GLC	E	306	-	12,12,12	0.37	0	17,17,17	0.47	0
4	NAD	E	307	-	48,48,48	2.04	9 (18%)	73,73,73	1.46	7 (9%)
5	BME	E	5462	-	3,3,3	1.87	1 (33%)	2,2,2	1.94	1 (50%)
2	GLC	F	307	-	12,12,12	0.44	0	17,17,17	0.54	0
4	NAD	F	308	-	48,48,48	2.03	8 (16%)	73,73,73	1.45	8 (10%)
5	BME	F	6462	-	3,3,3	1.90	1 (33%)	2,2,2	1.85	1 (50%)
4	NAD	G	2003	-	48,48,48	2.04	8 (16%)	73,73,73	1.46	8 (10%)
2	GLC	G	308	-	12,12,12	0.36	0	17,17,17	0.44	0
5	BME	G	7462	-	3,3,3	1.90	1 (33%)	2,2,2	1.86	1 (50%)
4	NAD	H	2004	-	48,48,48	2.03	9 (18%)	73,73,73	1.47	9 (12%)
2	GLC	H	309	-	12,12,12	0.38	0	17,17,17	0.47	0
5	BME	H	8462	-	3,3,3	1.89	1 (33%)	2,2,2	1.88	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
5	BME	A	1462	-	-	0/1/1/1	0/0/0/0
4	NAD	A	2001	-	-	0/30/62/62	0/3/5/5
2	GLC	A	302	-	-	0/2/22/22	0/1/1/1
4	NAD	B	2002	-	-	0/30/62/62	0/3/5/5
5	BME	B	2462	-	-	0/1/1/1	0/0/0/0
2	GLC	B	303	-	-	0/2/22/22	0/1/1/1
2	GLC	C	304	-	-	0/2/22/22	0/1/1/1
4	NAD	C	305	-	-	0/30/62/62	0/3/5/5
5	BME	C	3462	-	-	0/1/1/1	0/0/0/0
2	GLC	D	305	-	-	0/2/22/22	0/1/1/1
4	NAD	D	306	-	-	0/30/62/62	0/3/5/5
5	BME	D	4462	-	-	0/1/1/1	0/0/0/0
2	GLC	E	306	-	-	0/2/22/22	0/1/1/1
4	NAD	E	307	-	-	0/30/62/62	0/3/5/5
5	BME	E	5462	-	-	0/1/1/1	0/0/0/0
2	GLC	F	307	-	-	0/2/22/22	0/1/1/1
4	NAD	F	308	-	-	0/30/62/62	0/3/5/5
5	BME	F	6462	-	-	0/1/1/1	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAD	G	2003	-	-	0/30/62/62	0/3/5/5
2	GLC	G	308	-	-	0/2/22/22	0/1/1/1
5	BME	G	7462	-	-	0/1/1/1	0/0/0/0
4	NAD	H	2004	-	-	0/30/62/62	0/3/5/5
2	GLC	H	309	-	-	0/2/22/22	0/1/1/1
5	BME	H	8462	-	-	0/1/1/1	0/0/0/0

All (75) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	2002	NAD	C2N-C3N	7.66	1.49	1.38
4	C	305	NAD	C2N-C3N	7.58	1.49	1.38
4	G	2003	NAD	C2N-C3N	7.50	1.49	1.38
4	F	308	NAD	C2N-C3N	7.47	1.49	1.38
4	E	307	NAD	C2N-C3N	7.45	1.49	1.38
4	F	308	NAD	C4N-C3N	7.44	1.52	1.39
4	H	2004	NAD	C2N-C3N	7.42	1.49	1.38
4	B	2002	NAD	C4N-C3N	7.39	1.52	1.39
4	C	305	NAD	C4N-C3N	7.35	1.52	1.39
4	H	2004	NAD	C4N-C3N	7.35	1.52	1.39
4	A	2001	NAD	C2N-C3N	7.33	1.49	1.38
4	A	2001	NAD	C4N-C3N	7.30	1.52	1.39
4	G	2003	NAD	C4N-C3N	7.29	1.51	1.39
4	D	306	NAD	C2N-C3N	7.28	1.49	1.38
4	E	307	NAD	C4N-C3N	7.26	1.51	1.39
4	D	306	NAD	C4N-C3N	7.19	1.51	1.39
4	B	2002	NAD	C2N-N1N	4.90	1.41	1.35
4	F	308	NAD	C2N-N1N	4.88	1.41	1.35
4	D	306	NAD	C2N-N1N	4.83	1.41	1.35
4	E	307	NAD	C2N-N1N	4.82	1.41	1.35
4	C	305	NAD	C2N-N1N	4.81	1.41	1.35
4	G	2003	NAD	C2N-N1N	4.79	1.41	1.35
4	H	2004	NAD	C2N-N1N	4.76	1.41	1.35
4	A	2001	NAD	C2N-N1N	4.62	1.41	1.35
4	F	308	NAD	C5N-C4N	4.51	1.49	1.39
4	C	305	NAD	C5N-C4N	4.42	1.49	1.39
4	H	2004	NAD	C5N-C4N	4.40	1.49	1.39
4	E	307	NAD	C5N-C4N	4.39	1.49	1.39
4	G	2003	NAD	C5N-C4N	4.36	1.49	1.39
4	D	306	NAD	C5N-C4N	4.35	1.49	1.39
4	B	2002	NAD	C5N-C4N	4.26	1.48	1.39
4	A	2001	NAD	C5N-C4N	4.22	1.48	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	C	3462	BME	O1-C1	-3.31	1.24	1.42
5	G	7462	BME	O1-C1	-3.26	1.24	1.42
5	B	2462	BME	O1-C1	-3.26	1.24	1.42
5	F	6462	BME	O1-C1	-3.25	1.24	1.42
5	A	1462	BME	O1-C1	-3.23	1.24	1.42
5	H	8462	BME	O1-C1	-3.23	1.24	1.42
5	D	4462	BME	O1-C1	-3.20	1.24	1.42
5	E	5462	BME	O1-C1	-3.18	1.24	1.42
4	D	306	NAD	C6N-C5N	-3.16	1.31	1.38
4	B	2002	NAD	C6N-C5N	-3.11	1.31	1.38
4	G	2003	NAD	C6N-C5N	-3.07	1.31	1.38
4	E	307	NAD	C6N-C5N	-3.02	1.31	1.38
4	A	2001	NAD	C6N-C5N	-3.00	1.31	1.38
4	H	2004	NAD	C6N-C5N	-2.98	1.31	1.38
4	C	305	NAD	C6N-C5N	-2.89	1.31	1.38
4	A	2001	NAD	C2D-C1D	-2.77	1.49	1.53
4	F	308	NAD	C6N-C5N	-2.71	1.32	1.38
4	E	307	NAD	C6N-N1N	2.63	1.42	1.35
4	C	305	NAD	C6N-N1N	2.57	1.42	1.35
4	F	308	NAD	C6N-N1N	2.55	1.42	1.35
4	G	2003	NAD	C6N-N1N	2.51	1.42	1.35
4	H	2004	NAD	C6N-N1N	2.50	1.42	1.35
4	A	2001	NAD	C6N-N1N	2.48	1.42	1.35
4	B	2002	NAD	C6N-N1N	2.47	1.42	1.35
4	D	306	NAD	C2D-C1D	-2.45	1.50	1.53
4	B	2002	NAD	C2D-C1D	-2.44	1.50	1.53
4	D	306	NAD	C6N-N1N	2.43	1.42	1.35
4	C	305	NAD	C2D-C1D	-2.42	1.50	1.53
4	H	2004	NAD	C2D-C1D	-2.37	1.50	1.53
4	F	308	NAD	C2D-C1D	-2.35	1.50	1.53
4	G	2003	NAD	C2D-C1D	-2.29	1.50	1.53
4	B	2002	NAD	C2A-N1A	2.27	1.38	1.33
4	E	307	NAD	C2D-C1D	-2.23	1.50	1.53
4	E	307	NAD	PN-O3	2.23	1.64	1.60
4	H	2004	NAD	C2A-N1A	2.20	1.38	1.33
4	H	2004	NAD	PN-O3	2.18	1.64	1.60
4	E	307	NAD	C2A-N1A	2.17	1.38	1.33
4	C	305	NAD	PA-O3	-2.16	1.56	1.59
4	A	2001	NAD	C2A-N1A	2.13	1.38	1.33
4	C	305	NAD	C2A-N1A	2.10	1.38	1.33
4	A	2001	NAD	PN-O3	2.09	1.64	1.60
4	G	2003	NAD	C2A-N1A	2.08	1.38	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	F	308	NAD	C2A-N1A	2.05	1.38	1.33

All (76) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	2002	NAD	C5N-C4N-C3N	-5.62	113.02	120.32
4	A	2001	NAD	C5N-C4N-C3N	-5.57	113.09	120.32
4	H	2004	NAD	C5N-C4N-C3N	-5.55	113.11	120.32
4	F	308	NAD	C5N-C4N-C3N	-5.54	113.13	120.32
4	C	305	NAD	C5N-C4N-C3N	-5.53	113.14	120.32
4	E	307	NAD	C5N-C4N-C3N	-5.51	113.16	120.32
4	D	306	NAD	C5N-C4N-C3N	-5.51	113.17	120.32
4	G	2003	NAD	C5N-C4N-C3N	-5.45	113.24	120.32
4	H	2004	NAD	C3N-C7N-N7N	5.37	123.88	117.77
4	D	306	NAD	C3N-C7N-N7N	5.32	123.83	117.77
4	G	2003	NAD	C3N-C7N-N7N	5.28	123.78	117.77
4	B	2002	NAD	C3N-C7N-N7N	5.22	123.72	117.77
4	E	307	NAD	C3N-C7N-N7N	5.19	123.67	117.77
4	F	308	NAD	C3N-C7N-N7N	5.14	123.62	117.77
4	A	2001	NAD	C3N-C7N-N7N	5.07	123.54	117.77
4	C	305	NAD	C3N-C7N-N7N	4.90	123.34	117.77
4	B	2002	NAD	C6N-C5N-C4N	4.04	125.85	119.44
4	E	307	NAD	C6N-C5N-C4N	3.97	125.74	119.44
4	H	2004	NAD	C6N-C5N-C4N	3.94	125.70	119.44
4	C	305	NAD	C6N-C5N-C4N	3.94	125.69	119.44
4	D	306	NAD	C6N-C5N-C4N	3.94	125.69	119.44
4	F	308	NAD	C6N-C5N-C4N	3.92	125.67	119.44
4	A	2001	NAD	C6N-C5N-C4N	3.91	125.65	119.44
4	G	2003	NAD	C6N-C5N-C4N	3.86	125.57	119.44
4	D	306	NAD	O7N-C7N-C3N	-2.93	116.27	119.58
4	H	2004	NAD	O7N-C7N-C3N	-2.84	116.38	119.58
4	G	2003	NAD	O7N-C7N-C3N	-2.80	116.42	119.58
4	E	307	NAD	O7N-C7N-C3N	-2.66	116.58	119.58
4	B	2002	NAD	O7N-C7N-C3N	-2.65	116.59	119.58
4	C	305	NAD	C6N-N1N-C2N	-2.65	119.05	122.04
4	F	308	NAD	O7N-C7N-C3N	-2.63	116.61	119.58
4	A	2001	NAD	O7N-C7N-C3N	-2.61	116.64	119.58
4	B	2002	NAD	C6N-N1N-C2N	-2.61	119.09	122.04
4	E	307	NAD	C6N-N1N-C2N	-2.57	119.14	122.04
4	A	2001	NAD	C6N-N1N-C2N	-2.55	119.16	122.04
4	C	305	NAD	O4D-C1D-N1N	2.54	110.55	107.95
4	F	308	NAD	C6N-N1N-C2N	-2.50	119.22	122.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	305	NAD	O7N-C7N-C3N	-2.49	116.77	119.58
4	G	2003	NAD	C6N-N1N-C2N	-2.47	119.24	122.04
4	D	306	NAD	C6N-N1N-C2N	-2.46	119.27	122.04
4	H	2004	NAD	C6N-N1N-C2N	-2.45	119.28	122.04
4	H	2004	NAD	C5A-C6A-N6A	2.43	126.22	120.72
5	D	4462	BME	O1-C1-C2	2.43	121.45	110.86
5	E	5462	BME	O1-C1-C2	2.42	121.41	110.86
4	C	305	NAD	C5A-C6A-N6A	2.42	126.19	120.72
5	A	1462	BME	O1-C1-C2	2.40	121.31	110.86
4	G	2003	NAD	C5A-C6A-N6A	2.38	126.09	120.72
5	F	6462	BME	O1-C1-C2	2.37	121.19	110.86
5	G	7462	BME	O1-C1-C2	2.37	121.18	110.86
4	A	2001	NAD	C5A-C6A-N6A	2.37	126.07	120.72
5	H	8462	BME	O1-C1-C2	2.36	121.15	110.86
4	D	306	NAD	C5A-C6A-N6A	2.36	126.05	120.72
4	C	305	NAD	O4B-C1B-N9A	-2.36	106.25	108.44
4	F	308	NAD	C5A-C6A-N6A	2.35	126.03	120.72
5	C	3462	BME	O1-C1-C2	2.35	121.09	110.86
5	B	2462	BME	O1-C1-C2	2.32	120.96	110.86
4	E	307	NAD	O4B-C1B-C2B	-2.31	103.24	106.77
4	D	306	NAD	O4B-C1B-N9A	-2.30	106.30	108.44
4	E	307	NAD	C5A-C6A-N6A	2.30	125.93	120.72
4	B	2002	NAD	C5A-C6A-N6A	2.27	125.86	120.72
4	G	2003	NAD	O4B-C1B-N9A	-2.22	106.37	108.44
4	F	308	NAD	O4B-C1B-C2B	-2.20	103.40	106.77
4	A	2001	NAD	O4B-C1B-C2B	-2.17	103.45	106.77
4	B	2002	NAD	O4B-C1B-C2B	-2.15	103.47	106.77
4	D	306	NAD	O4B-C4B-C5B	-2.14	101.73	109.36
4	D	306	NAD	O4B-C1B-C2B	-2.10	103.55	106.77
4	H	2004	NAD	O4B-C1B-C2B	-2.10	103.56	106.77
4	D	306	NAD	C4A-C5A-N7A	2.08	111.30	109.52
4	F	308	NAD	C4A-C5A-N7A	2.07	111.29	109.52
4	C	305	NAD	O4B-C1B-C2B	-2.06	103.62	106.77
4	H	2004	NAD	O4B-C4B-C5B	-2.05	102.03	109.36
4	G	2003	NAD	O4B-C4B-C5B	-2.04	102.06	109.36
4	B	2002	NAD	C4A-C5A-N7A	2.02	111.25	109.52
4	H	2004	NAD	C4A-C5A-N7A	2.00	111.24	109.52
4	B	2002	NAD	O7N-C7N-N7N	-2.00	119.70	122.59
4	A	2001	NAD	O4B-C4B-C5B	-2.00	102.21	109.36

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	255/256 (99%)	0.32	11 (4%) 34 38	8, 13, 22, 26	0
1	B	255/256 (99%)	0.34	12 (4%) 30 34	8, 13, 22, 29	0
1	C	255/256 (99%)	0.39	16 (6%) 19 24	7, 13, 24, 31	0
1	D	255/256 (99%)	0.21	9 (3%) 42 47	7, 11, 18, 23	0
1	E	256/256 (100%)	0.40	16 (6%) 19 24	7, 14, 23, 26	0
1	F	255/256 (99%)	0.19	5 (1%) 62 67	6, 11, 18, 23	0
1	G	255/256 (99%)	0.19	5 (1%) 62 67	6, 11, 20, 21	0
1	H	255/256 (99%)	0.24	5 (1%) 62 67	6, 12, 19, 23	0
All	All	2041/2048 (99%)	0.29	79 (3%) 37 42	6, 12, 21, 31	0

All (79) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	34	TYR	7.1
1	G	34	TYR	6.5
1	A	34	TYR	6.5
1	D	2	LYS	6.1
1	D	34	TYR	6.0
1	C	199	GLU	5.2
1	C	202	GLY	4.9
1	H	34	TYR	4.9
1	B	34	TYR	4.7
1	E	1	MET	4.7
1	B	203	LYS	4.6
1	E	48	GLN	4.4
1	C	34	TYR	4.2
1	E	49	ALA	3.9
1	G	202	GLY	3.7
1	D	48	GLN	3.7

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Mol	Chain	Res	Type	RSRZ
1	B	205	LEU	3.7
1	B	2	LYS	3.7
1	E	219	GLY	3.4
1	D	75	LYS	3.4
1	H	37	ALA	3.4
1	G	2	LYS	3.3
1	C	205	LEU	3.3
1	A	2	LYS	3.2
1	E	34	TYR	3.2
1	A	205	LEU	3.1
1	A	48	GLN	3.0
1	A	49	ALA	3.0
1	A	70	VAL	2.9
1	A	44	SER	2.9
1	A	75	LYS	2.9
1	C	24	LYS	2.9
1	C	2	LYS	2.8
1	C	214	LYS	2.8
1	C	75	LYS	2.8
1	C	48	GLN	2.7
1	E	75	LYS	2.7
1	C	72	GLN	2.6
1	F	48	GLN	2.6
1	B	201	ALA	2.6
1	H	44	SER	2.6
1	D	36	ASP	2.6
1	B	200	ALA	2.6
1	F	2	LYS	2.5
1	B	199	GLU	2.5
1	B	207	TYR	2.5
1	E	70	VAL	2.5
1	E	96	GLU	2.5
1	B	214	LYS	2.5
1	G	199	GLU	2.4
1	C	191	ALA	2.3
1	A	36	ASP	2.3
1	D	29	VAL	2.3
1	H	199	GLU	2.3
1	D	219	GLY	2.3
1	B	202	GLY	2.3
1	E	199	GLU	2.2
1	E	47	ASN	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	188	PRO	2.2
1	C	193	ILE	2.2
1	B	75	LYS	2.2
1	E	207	TYR	2.2
1	C	195	ARG	2.2
1	E	42	VAL	2.2
1	A	31	ILE	2.2
1	F	105	LYS	2.2
1	D	70	VAL	2.1
1	E	118	ILE	2.1
1	E	193	ILE	2.1
1	F	49	ALA	2.1
1	G	75	LYS	2.1
1	D	46	ILE	2.1
1	A	76	THR	2.1
1	B	70	VAL	2.0
1	E	37	ALA	2.0
1	C	6	LEU	2.0
1	H	102	ILE	2.0
1	C	203	LYS	2.0
1	E	36	ASP	2.0

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

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

6.3 Carbohydrates ⓘ

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(Å ²)	Q<0.9
2	GLC	H	309	12/12	0.61	14.32	40,40,40,40	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
2	GLC	F	307	12/12	0.27	6.88	32,32,32,32	0
2	GLC	G	308	12/12	0.33	5.41	36,36,36,36	0
2	GLC	B	303	12/12	0.26	4.19	37,37,37,37	0
5	BME	E	5462	4/4	0.21	3.92	19,20,20,20	0
5	BME	F	6462	4/4	0.15	3.78	14,15,15,15	0
5	BME	A	1462	4/4	0.17	3.48	14,15,15,16	0
5	BME	B	2462	4/4	0.14	3.14	14,14,15,16	0
2	GLC	D	305	12/12	0.20	2.64	37,37,37,37	0
5	BME	G	7462	4/4	0.14	2.37	12,13,13,14	0
5	BME	D	4462	4/4	0.14	2.33	11,11,12,12	0
2	GLC	C	304	12/12	0.23	2.28	41,41,41,41	0
2	GLC	A	302	12/12	0.24	2.14	31,31,31,31	0
2	GLC	E	306	12/12	0.24	1.83	34,35,35,35	0
5	BME	C	3462	4/4	0.15	1.24	20,20,20,20	0
4	NAD	C	305	44/44	0.14	1.00	15,18,19,19	0
5	BME	H	8462	4/4	0.11	0.81	14,14,14,15	0
4	NAD	E	307	44/44	0.11	0.55	13,15,17,17	0
3	MG	A	2000	1/1	0.13	0.43	27,27,27,27	0
4	NAD	G	2003	44/44	0.10	0.05	10,11,12,13	0
4	NAD	A	2001	44/44	0.10	-0.04	11,13,14,14	0
4	NAD	F	308	44/44	0.09	-0.20	9,10,11,11	0
4	NAD	D	306	44/44	0.09	-0.22	8,10,11,11	0
4	NAD	H	2004	44/44	0.08	-0.24	9,10,10,10	0
4	NAD	B	2002	44/44	0.09	-0.29	10,11,12,12	0
3	MG	G	2002	1/1	0.08	-1.01	36,36,36,36	0
3	MG	B	2001	1/1	0.08	-1.69	31,31,31,31	0
3	MG	H	2003	1/1	0.06	-3.86	29,29,29,29	0

6.5 Other polymers ⓘ

There are no such residues in this entry.