



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 07:37 PM 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 X-ray Structure 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/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

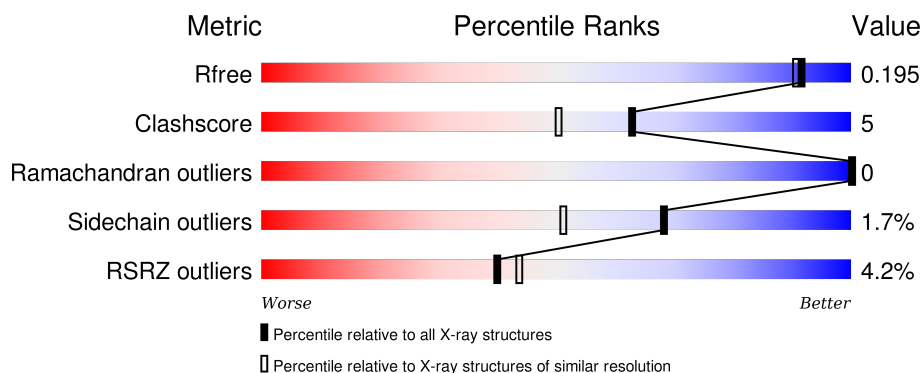
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	91344	3190 (1.70-1.70)
Clashscore	102246	3585 (1.70-1.70)
Ramachandran outliers	100387	3527 (1.70-1.70)
Sidechain outliers	100360	3527 (1.70-1.70)
RSRZ outliers	91569	3200 (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. 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	256	<div> <div>5%</div> <div>84%</div> <div>15%</div> </div>
1	B	256	<div> <div>5%</div> <div>86%</div> <div>13%</div> </div>
1	C	256	<div> <div>7%</div> <div>84%</div> <div>15%</div> </div>
1	D	256	<div> <div>3%</div> <div>88%</div> <div>11%</div> </div>
1	E	256	<div> <div>7%</div> <div>84%</div> <div>15%</div> </div>

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	F	256	
1	G	256	
1	H	256	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	GLC	F	307	-	-	-	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

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 16227 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 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).

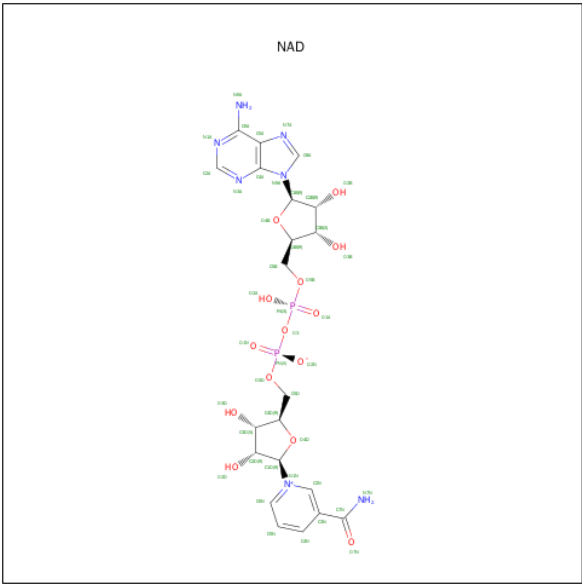


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			12	6	6		
2	B	1	Total	C	O	0	0
			12	6	6		
2	C	1	Total	C	O	0	0
			12	6	6		
2	D	1	Total	C	O	0	0
			12	6	6		
2	E	1	Total	C	O	0	0
			12	6	6		
2	F	1	Total	C	O	0	0
			12	6	6		
2	G	1	Total	C	O	0	0
			12	6	6		
2	H	1	Total	C	O	0	0
			12	6	6		

- 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: 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		
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: C₂H₆OS).



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		

Continued on next page...

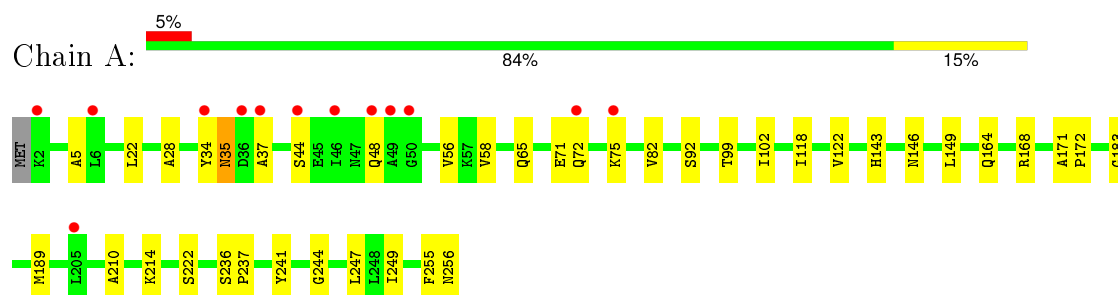
Continued from previous page...

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

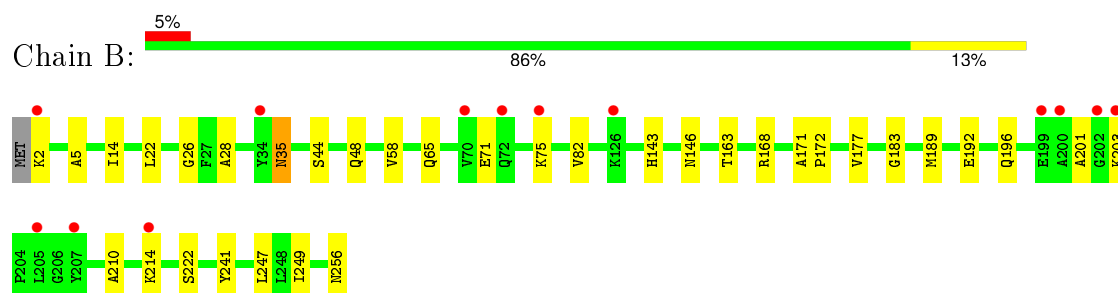
3 Residue-property plots [i](#)

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

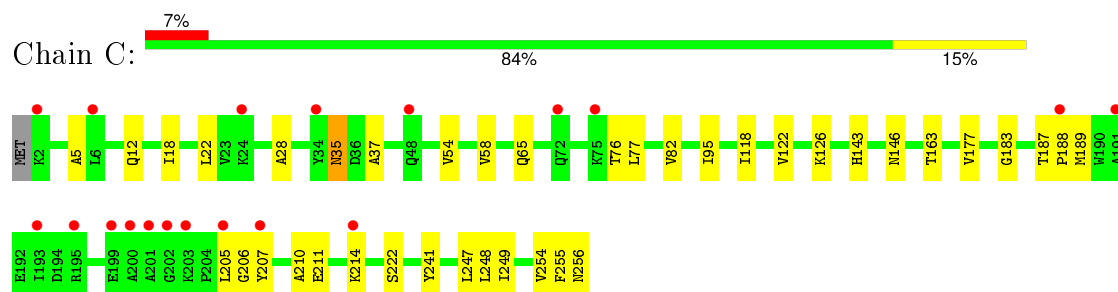
• Molecule 1: ACETOIN REDUCTASE



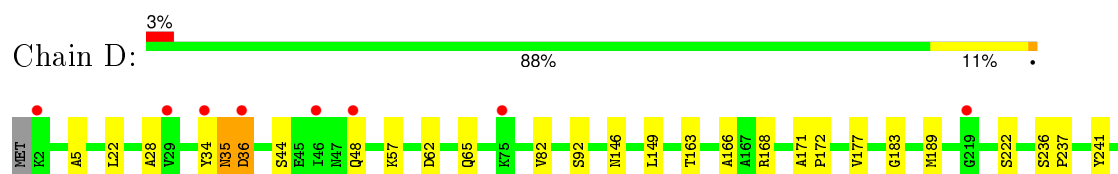
• Molecule 1: ACETOIN REDUCTASE



• Molecule 1: ACETOIN REDUCTASE

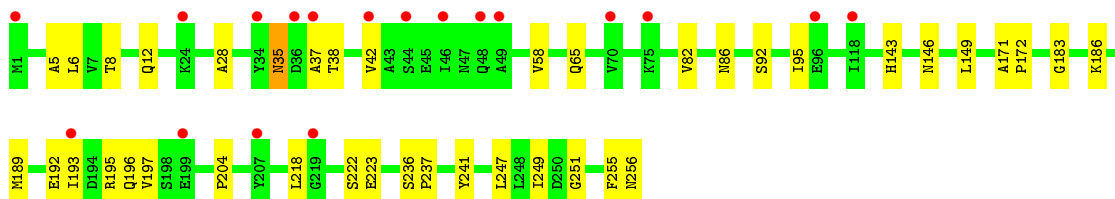
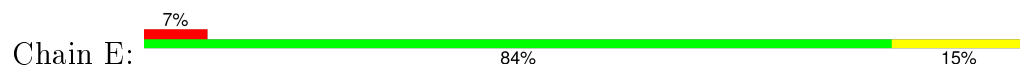


• Molecule 1: ACETOIN REDUCTASE

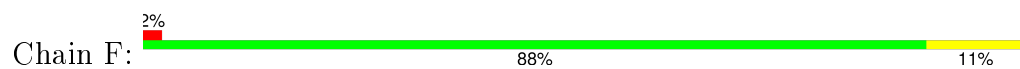




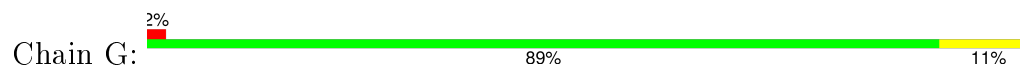
● Molecule 1: ACETOIN REDUCTASE



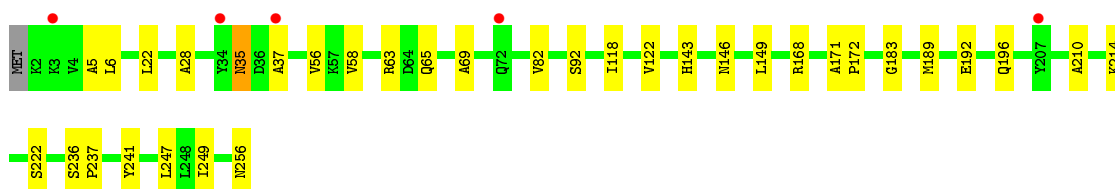
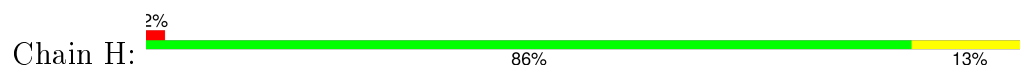
● Molecule 1: ACETOIN REDUCTASE



● Molecule 1: ACETOIN REDUCTASE



● Molecule 1: ACETOIN REDUCTASE



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 , 51.7	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	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.

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

5 Model quality

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 Too-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 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	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
5	H	4	0	5	1	0
6	A	118	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

All (162) 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: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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:192:GLU:O	1:H:196:GLN:HG3	2.15	0.47
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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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%)	61	42
1	B	190/191 (100%)	187 (98%)	3 (2%)	70	54
1	C	190/191 (100%)	188 (99%)	2 (1%)	80	69
1	D	190/191 (100%)	185 (97%)	5 (3%)	54	32
1	E	191/191 (100%)	189 (99%)	2 (1%)	82	72
1	F	190/191 (100%)	186 (98%)	4 (2%)	61	42
1	G	190/191 (100%)	187 (98%)	3 (2%)	70	54
1	H	190/191 (100%)	187 (98%)	3 (2%)	70	54
All	All	1521/1528 (100%)	1495 (98%)	26 (2%)	68	51

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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	F	22	LEU
1	F	34	TYR
1	F	35	ASN
1	F	146	ASN
1	G	22	LEU
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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	G	35	ASN
1	G	52	HIS
1	G	72	GLN
1	G	143	HIS
1	H	12	GLN
1	H	35	ASN
1	H	72	GLN
1	H	143	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 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	1.87	1 (33%)	2,2,2	1.72	1 (50%)
4	NAD	A	2001	-	38,48,48	2.05	6 (15%)	47,73,73	1.62	5 (10%)
2	GLC	A	302	-	12,12,12	0.32	0	17,17,17	0.36	0
4	NAD	B	2002	-	38,48,48	2.09	6 (15%)	47,73,73	1.64	6 (12%)
5	BME	B	2462	-	3,3,3	1.89	1 (33%)	2,2,2	1.66	1 (50%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	GLC	B	303	-	12,12,12	0.38	0	17,17,17	0.44	0
2	GLC	C	304	-	12,12,12	0.41	0	17,17,17	0.43	0
4	NAD	C	305	-	38,48,48	2.09	6 (15%)	47,73,73	1.61	6 (12%)
5	BME	C	3462	-	3,3,3	1.92	1 (33%)	2,2,2	1.68	1 (50%)
2	GLC	D	305	-	12,12,12	0.36	0	17,17,17	0.44	0
4	NAD	D	306	-	38,48,48	2.06	6 (15%)	47,73,73	1.66	6 (12%)
5	BME	D	4462	-	3,3,3	1.85	1 (33%)	2,2,2	1.74	1 (50%)
2	GLC	E	306	-	12,12,12	0.38	0	17,17,17	0.47	0
4	NAD	E	307	-	38,48,48	2.08	6 (15%)	47,73,73	1.63	6 (12%)
5	BME	E	5462	-	3,3,3	1.85	1 (33%)	2,2,2	1.74	1 (50%)
2	GLC	F	307	-	12,12,12	0.45	0	17,17,17	0.53	0
4	NAD	F	308	-	38,48,48	2.08	6 (15%)	47,73,73	1.62	5 (10%)
5	BME	F	6462	-	3,3,3	1.88	1 (33%)	2,2,2	1.70	1 (50%)
4	NAD	G	2003	-	38,48,48	2.08	6 (15%)	47,73,73	1.63	5 (10%)
2	GLC	G	308	-	12,12,12	0.37	0	17,17,17	0.44	0
5	BME	G	7462	-	3,3,3	1.89	1 (33%)	2,2,2	1.70	1 (50%)
4	NAD	H	2004	-	38,48,48	2.08	6 (15%)	47,73,73	1.66	7 (14%)
2	GLC	H	309	-	12,12,12	0.39	0	17,17,17	0.48	0
5	BME	H	8462	-	3,3,3	1.87	1 (33%)	2,2,2	1.70	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	-	-	0/22/62/62	0/5/5/5
2	GLC	A	302	-	-	0/2/22/22	0/1/1/1
4	NAD	B	2002	-	-	0/22/62/62	0/5/5/5
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	-	-	0/22/62/62	0/5/5/5
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	-	-	0/22/62/62	0/5/5/5
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	-	-	0/22/62/62	0/5/5/5

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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	-	-	0/22/62/62	0/5/5/5
5	BME	F	6462	-	-	0/1/1/1	0/0/0/0
4	NAD	G	2003	-	-	0/22/62/62	0/5/5/5
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	-	-	0/22/62/62	0/5/5/5
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 (56) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	306	NAD	C6N-C5N	-3.30	1.31	1.38
5	C	3462	BME	O1-C1	-3.30	1.24	1.42
5	G	7462	BME	O1-C1	-3.25	1.24	1.42
4	B	2002	NAD	C6N-C5N	-3.25	1.31	1.38
5	B	2462	BME	O1-C1	-3.25	1.24	1.42
5	F	6462	BME	O1-C1	-3.23	1.24	1.42
5	A	1462	BME	O1-C1	-3.22	1.24	1.42
5	H	8462	BME	O1-C1	-3.22	1.24	1.42
4	G	2003	NAD	C6N-C5N	-3.21	1.31	1.38
5	D	4462	BME	O1-C1	-3.18	1.24	1.42
5	E	5462	BME	O1-C1	-3.17	1.24	1.42
4	E	307	NAD	C6N-C5N	-3.16	1.31	1.38
4	A	2001	NAD	C6N-C5N	-3.14	1.31	1.38
4	H	2004	NAD	C6N-C5N	-3.12	1.31	1.38
4	C	305	NAD	C6N-C5N	-3.03	1.31	1.38
4	F	308	NAD	C6N-C5N	-2.84	1.32	1.38
4	D	306	NAD	C2A-N1A	2.02	1.37	1.33
4	F	308	NAD	C2A-N1A	2.13	1.38	1.33
4	G	2003	NAD	C2A-N1A	2.16	1.38	1.33
4	C	305	NAD	C2A-N1A	2.19	1.38	1.33
4	A	2001	NAD	C2A-N1A	2.21	1.38	1.33
4	E	307	NAD	C2A-N1A	2.26	1.38	1.33
4	H	2004	NAD	C2A-N1A	2.29	1.38	1.33
4	B	2002	NAD	C2A-N1A	2.36	1.38	1.33
4	D	306	NAD	C6N-N1N	2.58	1.42	1.35
4	B	2002	NAD	C6N-N1N	2.63	1.42	1.35
4	A	2001	NAD	C6N-N1N	2.63	1.42	1.35
4	H	2004	NAD	C6N-N1N	2.65	1.42	1.35

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	G	2003	NAD	C6N-N1N	2.66	1.42	1.35
4	F	308	NAD	C6N-N1N	2.71	1.42	1.35
4	C	305	NAD	C6N-N1N	2.72	1.42	1.35
4	E	307	NAD	C6N-N1N	2.79	1.42	1.35
4	A	2001	NAD	C5N-C4N	4.80	1.48	1.38
4	B	2002	NAD	C5N-C4N	4.85	1.48	1.38
4	D	306	NAD	C5N-C4N	4.95	1.49	1.38
4	G	2003	NAD	C5N-C4N	4.96	1.49	1.38
4	E	307	NAD	C5N-C4N	4.99	1.49	1.38
4	H	2004	NAD	C5N-C4N	5.00	1.49	1.38
4	C	305	NAD	C5N-C4N	5.03	1.49	1.38
4	F	308	NAD	C5N-C4N	5.13	1.49	1.38
4	D	306	NAD	C2N-C3N	6.70	1.49	1.39
4	A	2001	NAD	C2N-C3N	6.75	1.49	1.39
4	H	2004	NAD	C2N-C3N	6.83	1.49	1.39
4	E	307	NAD	C2N-C3N	6.86	1.49	1.39
4	F	308	NAD	C2N-C3N	6.88	1.49	1.39
4	G	2003	NAD	C2N-C3N	6.91	1.49	1.39
4	C	305	NAD	C2N-C3N	6.99	1.49	1.39
4	B	2002	NAD	C2N-C3N	7.06	1.49	1.39
4	D	306	NAD	C4N-C3N	7.28	1.51	1.39
4	E	307	NAD	C4N-C3N	7.36	1.51	1.39
4	G	2003	NAD	C4N-C3N	7.38	1.51	1.39
4	A	2001	NAD	C4N-C3N	7.39	1.52	1.39
4	C	305	NAD	C4N-C3N	7.44	1.52	1.39
4	H	2004	NAD	C4N-C3N	7.44	1.52	1.39
4	B	2002	NAD	C4N-C3N	7.48	1.52	1.39
4	F	308	NAD	C4N-C3N	7.53	1.52	1.39

All (54) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	2002	NAD	C5N-C4N-C3N	-5.82	113.02	120.33
4	A	2001	NAD	C5N-C4N-C3N	-5.76	113.09	120.33
4	H	2004	NAD	C5N-C4N-C3N	-5.75	113.11	120.33
4	F	308	NAD	C5N-C4N-C3N	-5.73	113.13	120.33
4	C	305	NAD	C5N-C4N-C3N	-5.72	113.14	120.33
4	E	307	NAD	C5N-C4N-C3N	-5.71	113.16	120.33
4	D	306	NAD	C5N-C4N-C3N	-5.70	113.17	120.33
4	G	2003	NAD	C5N-C4N-C3N	-5.64	113.24	120.33
4	D	306	NAD	O7N-C7N-C3N	-3.04	116.27	119.59
4	H	2004	NAD	O7N-C7N-C3N	-2.94	116.38	119.59

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	G	2003	NAD	O7N-C7N-C3N	-2.90	116.42	119.59
4	E	307	NAD	O7N-C7N-C3N	-2.75	116.58	119.59
4	B	2002	NAD	O7N-C7N-C3N	-2.75	116.59	119.59
4	F	308	NAD	O7N-C7N-C3N	-2.72	116.61	119.59
4	A	2001	NAD	O7N-C7N-C3N	-2.70	116.64	119.59
4	C	305	NAD	O7N-C7N-C3N	-2.58	116.77	119.59
4	D	306	NAD	O3-PN-O5D	-2.27	96.91	102.94
4	B	2002	NAD	O3-PN-O5D	-2.23	97.01	102.94
4	E	307	NAD	O3-PN-O5D	-2.18	97.15	102.94
4	D	306	NAD	O4B-C4B-C5B	-2.12	101.73	109.32
4	C	305	NAD	O3-PN-O5D	-2.09	97.40	102.94
4	H	2004	NAD	O3-PN-O5D	-2.08	97.42	102.94
4	A	2001	NAD	O3-PN-O5D	-2.08	97.42	102.94
4	B	2002	NAD	O7N-C7N-N7N	-2.06	119.70	122.59
4	H	2004	NAD	O4B-C4B-C5B	-2.04	102.03	109.32
4	H	2004	NAD	O7N-C7N-N7N	-2.03	119.73	122.59
4	G	2003	NAD	O4B-C4B-C5B	-2.03	102.06	109.32
4	E	307	NAD	O7N-C7N-N7N	-2.02	119.75	122.59
4	F	308	NAD	O7N-C7N-N7N	-2.01	119.76	122.59
4	C	305	NAD	O4D-C1D-N1N	2.20	110.55	108.13
5	B	2462	BME	O1-C1-C2	2.31	120.96	110.83
5	C	3462	BME	O1-C1-C2	2.34	121.09	110.83
5	H	8462	BME	O1-C1-C2	2.35	121.15	110.83
5	G	7462	BME	O1-C1-C2	2.36	121.18	110.83
5	F	6462	BME	O1-C1-C2	2.37	121.19	110.83
5	A	1462	BME	O1-C1-C2	2.39	121.31	110.83
5	E	5462	BME	O1-C1-C2	2.42	121.41	110.83
5	D	4462	BME	O1-C1-C2	2.42	121.45	110.83
4	G	2003	NAD	C6N-C5N-C4N	4.06	125.57	119.44
4	A	2001	NAD	C6N-C5N-C4N	4.11	125.65	119.44
4	F	308	NAD	C6N-C5N-C4N	4.12	125.67	119.44
4	D	306	NAD	C6N-C5N-C4N	4.14	125.69	119.44
4	C	305	NAD	C6N-C5N-C4N	4.14	125.69	119.44
4	H	2004	NAD	C6N-C5N-C4N	4.14	125.70	119.44
4	E	307	NAD	C6N-C5N-C4N	4.17	125.74	119.44
4	B	2002	NAD	C6N-C5N-C4N	4.24	125.85	119.44
4	C	305	NAD	C3N-C7N-N7N	5.05	123.34	117.82
4	A	2001	NAD	C3N-C7N-N7N	5.23	123.54	117.82
4	F	308	NAD	C3N-C7N-N7N	5.30	123.62	117.82
4	E	307	NAD	C3N-C7N-N7N	5.35	123.67	117.82
4	B	2002	NAD	C3N-C7N-N7N	5.39	123.72	117.82
4	G	2003	NAD	C3N-C7N-N7N	5.45	123.78	117.82

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	306	NAD	C3N-C7N-N7N	5.49	123.83	117.82
4	H	2004	NAD	C3N-C7N-N7N	5.54	123.88	117.82

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

18 monomers are involved in 30 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	1462	BME	1	0
4	A	2001	NAD	3	0
4	B	2002	NAD	4	0
5	B	2462	BME	1	0
4	C	305	NAD	4	0
5	C	3462	BME	1	0
4	D	306	NAD	3	0
5	D	4462	BME	1	0
4	E	307	NAD	4	0
5	E	5462	BME	1	0
2	F	307	GLC	1	0
4	F	308	NAD	3	0
5	F	6462	BME	1	0
4	G	2003	NAD	3	0
5	G	7462	BME	1	0
4	H	2004	NAD	3	0
2	H	309	GLC	2	0
5	H	8462	BME	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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%)	0.34	13 (5%) 32 34	8, 13, 22, 26	0
1	B	255/256 (99%)	0.36	13 (5%) 32 34	8, 13, 22, 29	0
1	C	255/256 (99%)	0.39	19 (7%) 17 19	7, 13, 24, 31	0
1	D	255/256 (99%)	0.20	8 (3%) 52 57	7, 11, 18, 23	0
1	E	256/256 (100%)	0.43	18 (7%) 19 21	7, 14, 23, 26	0
1	F	255/256 (99%)	0.19	4 (1%) 74 79	6, 11, 18, 23	0
1	G	255/256 (99%)	0.20	6 (2%) 62 66	6, 11, 20, 21	0
1	H	255/256 (99%)	0.24	5 (1%) 68 73	6, 12, 19, 23	0
All	All	2041/2048 (99%)	0.29	86 (4%) 40 44	6, 12, 21, 31	0

All (86) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	34	TYR	7.9
1	F	34	TYR	7.2
1	G	34	TYR	6.3
1	D	34	TYR	6.1
1	D	2	LYS	6.0
1	C	199	GLU	5.6
1	H	34	TYR	5.5
1	C	202	GLY	5.3
1	E	1	MET	4.7
1	B	203	LYS	4.7
1	B	34	TYR	4.4
1	D	48	GLN	4.3
1	A	49	ALA	4.1
1	B	2	LYS	3.9
1	H	37	ALA	3.8
1	E	48	GLN	3.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	34	TYR	3.7
1	E	49	ALA	3.5
1	B	202	GLY	3.5
1	A	48	GLN	3.4
1	F	48	GLN	3.4
1	E	219	GLY	3.4
1	C	2	LYS	3.4
1	C	205	LEU	3.3
1	B	205	LEU	3.3
1	G	202	GLY	3.2
1	D	75	LYS	3.2
1	F	49	ALA	3.2
1	A	75	LYS	3.1
1	C	214	LYS	3.1
1	C	188	PRO	3.0
1	E	34	TYR	2.9
1	E	207	TYR	2.9
1	C	24	LYS	2.9
1	A	36	ASP	2.7
1	E	75	LYS	2.7
1	A	2	LYS	2.7
1	C	48	GLN	2.6
1	A	44	SER	2.6
1	C	75	LYS	2.5
1	E	118	ILE	2.5
1	G	75	LYS	2.5
1	B	200	ALA	2.5
1	D	36	ASP	2.5
1	B	199	GLU	2.5
1	E	37	ALA	2.5
1	E	96	GLU	2.5
1	B	126	LYS	2.5
1	E	193	ILE	2.5
1	C	72	GLN	2.5
1	E	199	GLU	2.4
1	C	203	LYS	2.4
1	B	207	TYR	2.4
1	E	70	VAL	2.4
1	C	193	ILE	2.4
1	G	48	GLN	2.4
1	A	205	LEU	2.3
1	C	6	LEU	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	E	46	ILE	2.3
1	A	37	ALA	2.3
1	G	2	LYS	2.3
1	D	219	GLY	2.3
1	E	36	ASP	2.3
1	C	201	ALA	2.3
1	H	3	LYS	2.3
1	B	75	LYS	2.2
1	C	191	ALA	2.2
1	C	195	ARG	2.2
1	A	72	GLN	2.2
1	A	6	LEU	2.2
1	B	214	LYS	2.2
1	F	2	LYS	2.2
1	D	46	ILE	2.2
1	B	72	GLN	2.1
1	A	50	GLY	2.1
1	B	70	VAL	2.1
1	H	72	GLN	2.1
1	A	46	ILE	2.1
1	D	29	VAL	2.0
1	C	207	TYR	2.0
1	H	207	TYR	2.0
1	G	199	GLU	2.0
1	E	42	VAL	2.0
1	C	200	ALA	2.0
1	E	44	SER	2.0
1	E	24	LYS	2.0

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron

density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 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	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
2	GLC	F	307	12/12	0.66	0.30	8.88	32,32,32,32	0
5	BME	E	5462	4/4	0.86	0.21	3.53	19,20,20,20	0
5	BME	B	2462	4/4	0.89	0.14	3.45	14,14,15,16	0
5	BME	A	1462	4/4	0.87	0.17	3.42	14,15,15,16	0
5	BME	F	6462	4/4	0.91	0.14	2.77	14,15,15,15	0
5	BME	D	4462	4/4	0.94	0.13	2.05	11,11,12,12	0
5	BME	G	7462	4/4	0.93	0.14	1.97	12,13,13,14	0
5	BME	H	8462	4/4	0.93	0.12	1.44	14,14,14,15	0
5	BME	C	3462	4/4	0.90	0.14	1.13	20,20,20,20	0
4	NAD	C	305	44/44	0.90	0.13	0.66	15,18,19,19	0
4	NAD	E	307	44/44	0.92	0.11	0.40	13,15,17,17	0
4	NAD	A	2001	44/44	0.93	0.10	0.01	11,13,14,14	0
4	NAD	G	2003	44/44	0.95	0.10	-0.06	10,11,12,13	0
4	NAD	H	2004	44/44	0.96	0.09	-0.22	9,10,10,10	0
4	NAD	F	308	44/44	0.96	0.08	-0.26	9,10,11,11	0
4	NAD	D	306	44/44	0.96	0.08	-0.29	8,10,11,11	0
4	NAD	B	2002	44/44	0.96	0.08	-0.43	10,11,12,12	0
3	MG	A	2000	1/1	0.97	0.14	-	27,27,27,27	0
2	GLC	G	308	12/12	0.66	0.36	-	36,36,36,36	0
2	GLC	A	302	12/12	0.77	0.27	-	31,31,31,31	0
2	GLC	E	306	12/12	0.75	0.28	-	34,35,35,35	0
3	MG	B	2001	1/1	0.93	0.08	-	31,31,31,31	0
2	GLC	D	305	12/12	0.72	0.21	-	37,37,37,37	0
3	MG	G	2002	1/1	0.89	0.09	-	36,36,36,36	0
2	GLC	H	309	12/12	0.49	0.51	-	40,40,40,40	0
2	GLC	C	304	12/12	0.70	0.29	-	41,41,41,41	0
3	MG	H	2003	1/1	0.94	0.07	-	29,29,29,29	0
2	GLC	B	303	12/12	0.80	0.26	-	37,37,37,37	0

6.5 Other polymers [i](#)

There are no such residues in this entry.