



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 02:49 AM GMT

PDB ID : 2IVF
Title : ETHYLBENZENE DEHYDROGENASE FROM AROMATOLEUM AROMATICUM
Authors : Kloer, D.P.; Hagel, C.; Heider, J.; Schulz, G.E.
Deposited on : 2006-06-13
Resolution : 1.88 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

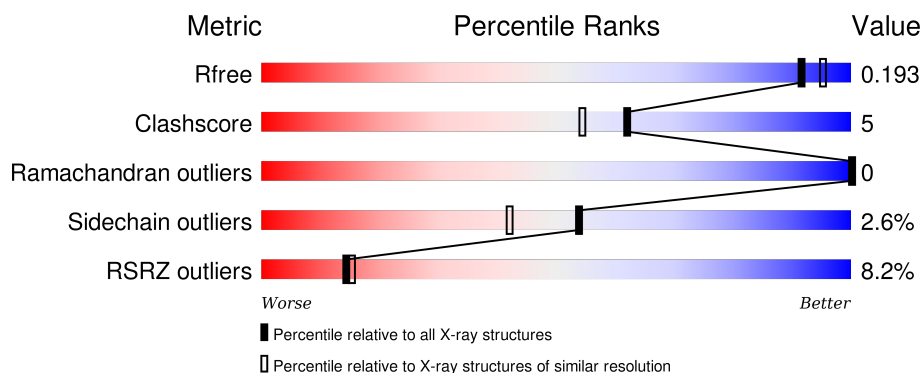
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.88 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	6965 (1.90-1.86)
Clashscore	102246	7778 (1.90-1.86)
Ramachandran outliers	100387	7691 (1.90-1.86)
Sidechain outliers	100360	7692 (1.90-1.86)
RSRZ outliers	91569	6979 (1.90-1.86)

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	976	<div> <div>9%</div> <div>83%</div> <div>10%</div> <div>7%</div> </div>
2	B	352	<div> <div>2%</div> <div>83%</div> <div>13%</div> <div>•</div> </div>
3	C	214	<div> <div>14%</div> <div>78%</div> <div>21%</div> <div>•</div> </div>

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
10	MD1	A	1987	X	-	-	-
11	PO4	B	1354	-	-	-	X
5	ACT	A	1978	-	-	X	-
6	GOL	A	1981	-	-	X	X
6	GOL	B	1353	-	-	-	X
6	GOL	B	1355	-	-	-	X

2 Entry composition [i](#)

There are 14 unique types of molecules in this entry. The entry contains 12639 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 ETHYLBENZENE DEHYDROGENASE ALPHA-SUBUNIT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	912	7285	4651	1254	1331	49	0	0	0

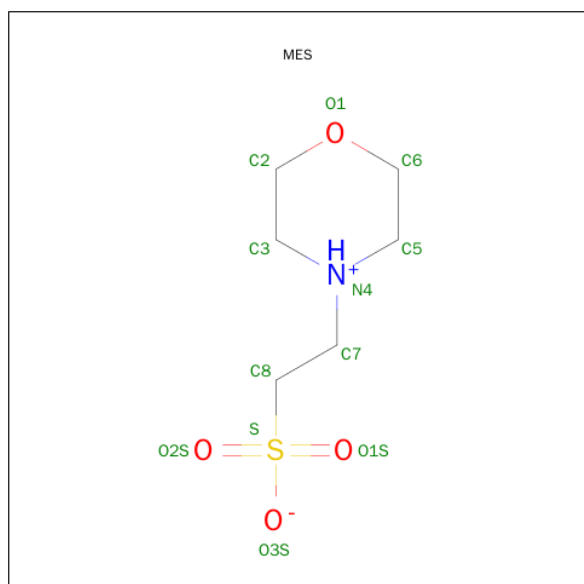
- Molecule 2 is a protein called ETHYLBENZENE DEHYDROGENASE BETA-SUBUNIT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	337	2669	1686	479	484	20	0	0	0

- Molecule 3 is a protein called ETHYLBENZENE DEHYDROGENASE GAMMA-SUBUNIT.

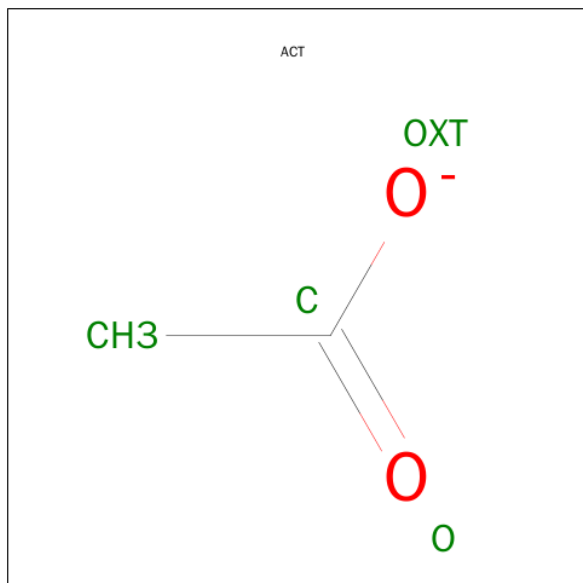
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	C	214	1617	1026	288	293	10	0	0	0

- Molecule 4 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (three-letter code: MES) (formula: C₆H₁₃NO₄S).



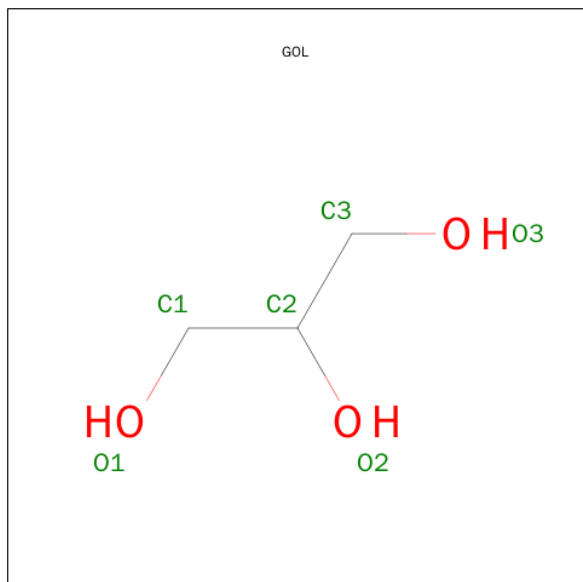
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	S	0	0
			12	6	1	4	1		

- Molecule 5 is ACETATE ION (three-letter code: ACT) (formula: $C_2H_3O_2$).



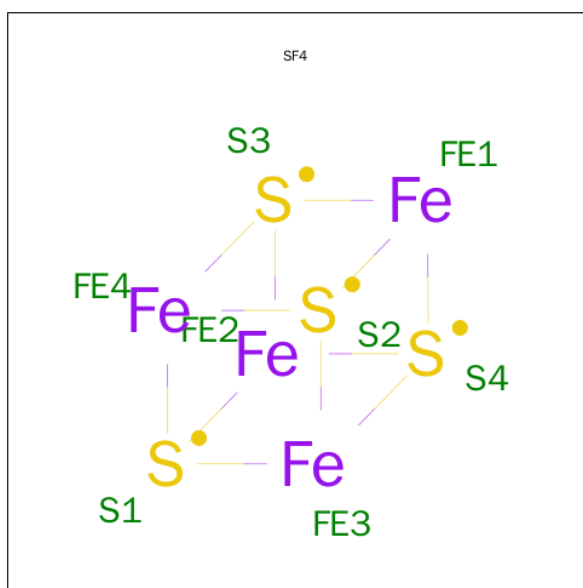
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			4	2	2		
5	A	1	Total	C	O	0	0
			4	2	2		

- Molecule 6 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			6	3	3		
6	A	1	Total	C	O	0	0
			6	3	3		
6	A	1	Total	C	O	0	0
			6	3	3		
6	A	1	Total	C	O	0	0
			6	3	3		
6	B	1	Total	C	O	0	0
			6	3	3		
6	B	1	Total	C	O	0	0
			6	3	3		
6	C	1	Total	C	O	0	0
			6	3	3		
6	C	1	Total	C	O	0	0
			6	3	3		

- Molecule 7 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe₄S₄).

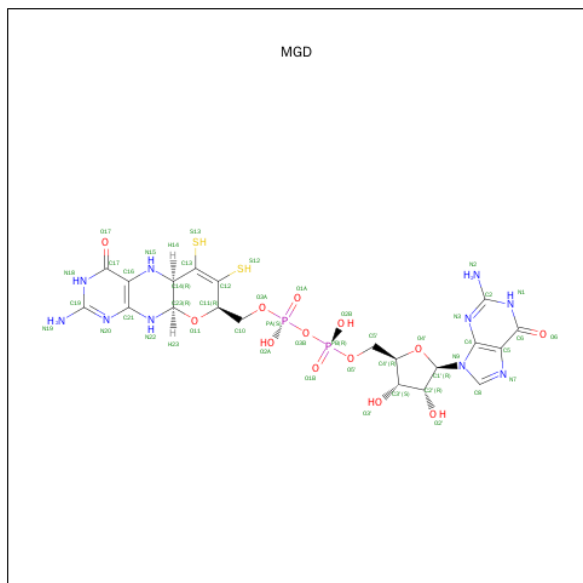


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	Fe	S	0	0
			8	4	4		
7	B	1	Total	Fe	S	0	0
			8	4	4		
7	B	1	Total	Fe	S	0	0
			8	4	4		
7	B	1	Total	Fe	S	0	0
			8	4	4		

- Molecule 8 is MOLYBDENUM ATOM (three-letter code: MO) (formula: Mo).

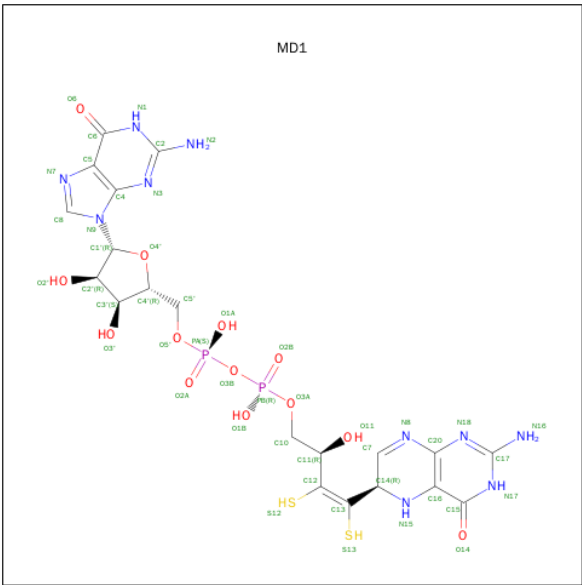
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	1	Total	Mo	0	0
			1	1		

- Molecule 9 is 2-AMINO-5,6-DIMERCAPTO-7-METHYL-3,7,8A,9-TETRAHYDRO-8-OXA-1,3,9,10-TETRAAZA-ANTHRACEN-4-ONE GUANOSINE DINUCLEOTIDE (three-letter code: MGD) (formula: C₂₀H₂₆N₁₀O₁₃P₂S₂).



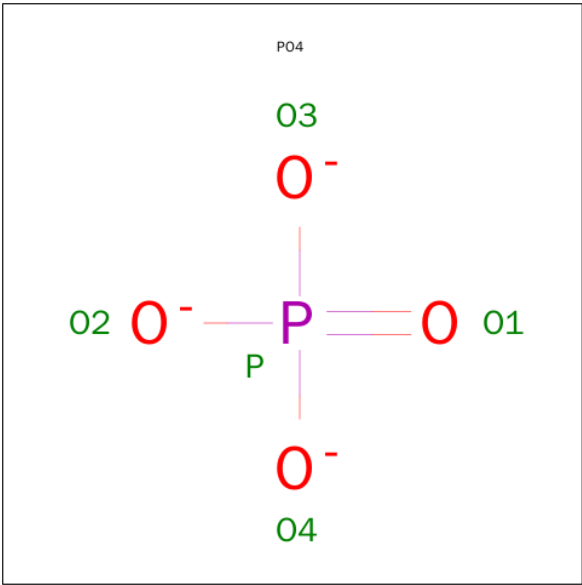
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
9	A	1	Total	C	N	O	P	S	0	0
			47	20	10	13	2	2		

- Molecule 10 is PHOSPHORIC ACID 4-(2-AMINO-4-OXO-3,4,5,6,-TETRAHYDRO-PTE RIDIN-6-YL)-2-HYDROXY-3,4-DIMERCAPTO-BUT-3-EN-YL ESTER GUANYLATE ESTER (three-letter code: MD1) (formula: C₂₀H₂₆N₁₀O₁₃P₂S₂).



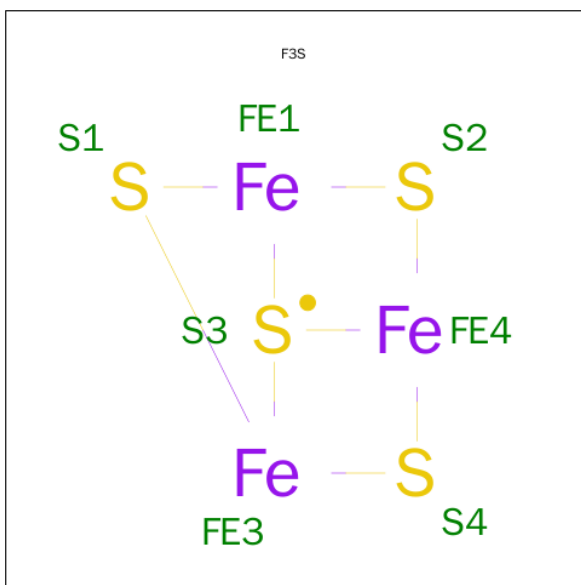
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
10	A	1	Total	C	N	O	P	S	0	0
			47	20	10	13	2	2		

- Molecule 11 is PHOSPHATE ION (three-letter code: PO4) (formula: O₄P).



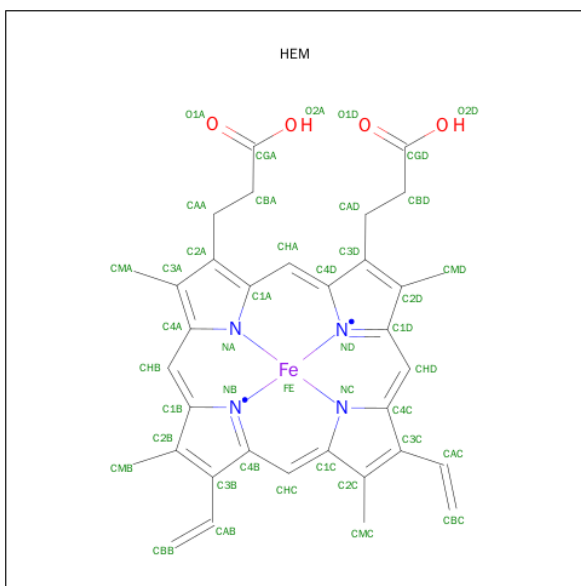
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	B	1	Total	O P	0	0
			5	4 1		

- Molecule 12 is FE3-S4 CLUSTER (three-letter code: F3S) (formula: Fe₃S₄).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
12	B	1	Total	Fe	S		0	0
			7	3	4			

- Molecule 13 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
13	C	1	Total	C	Fe	N	O	
			43	34	1	4	4	

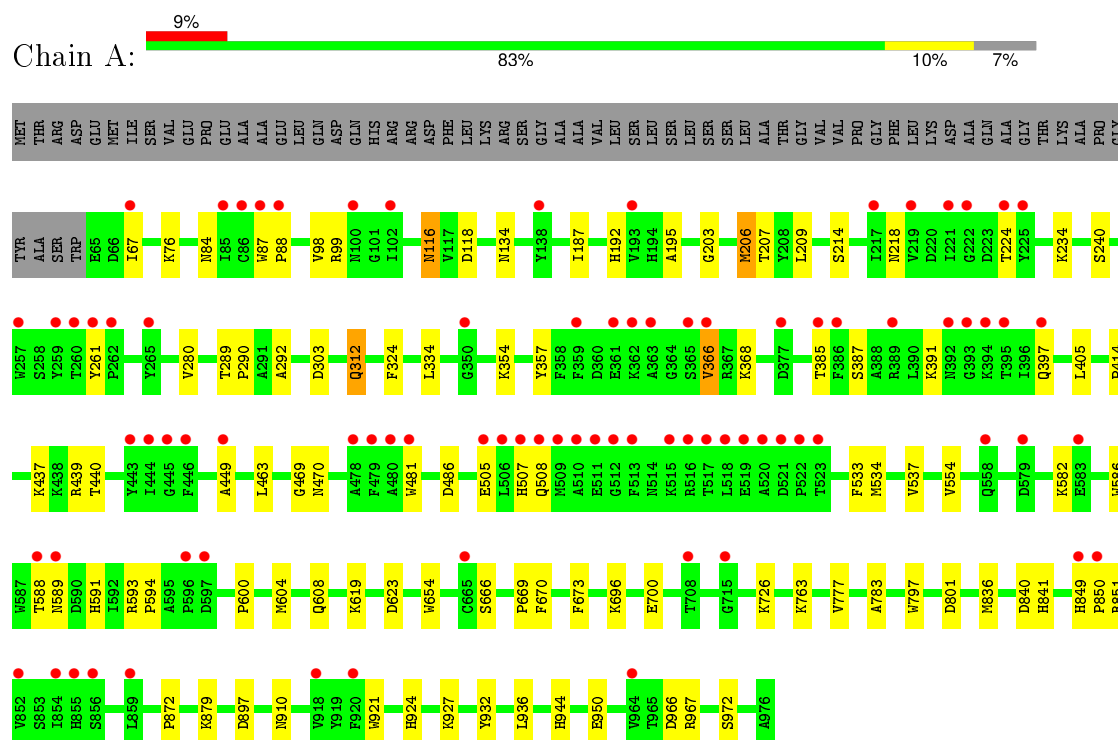
- Molecule 14 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
14	A	492	Total 492	O 492	0	0
14	B	237	Total 237	O 237	0	0
14	C	89	Total 89	O 89	0	0

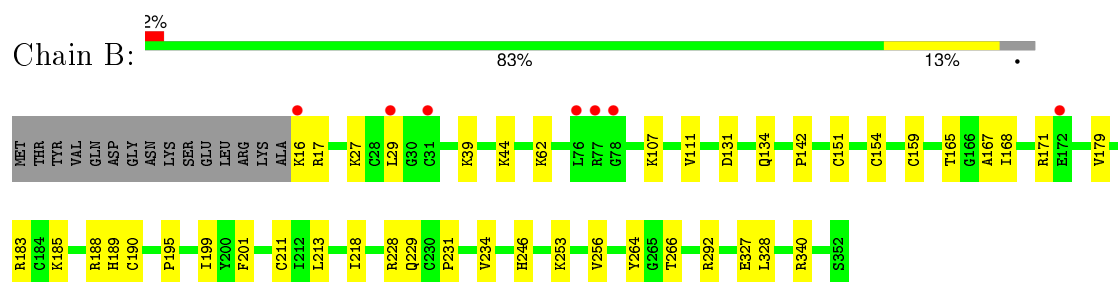
3 Residue-property plots

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.

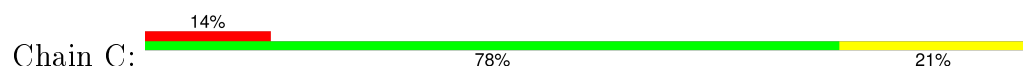
• Molecule 1: ETHYLBENZENE DEHYDROGENASE ALPHA-SUBUNIT

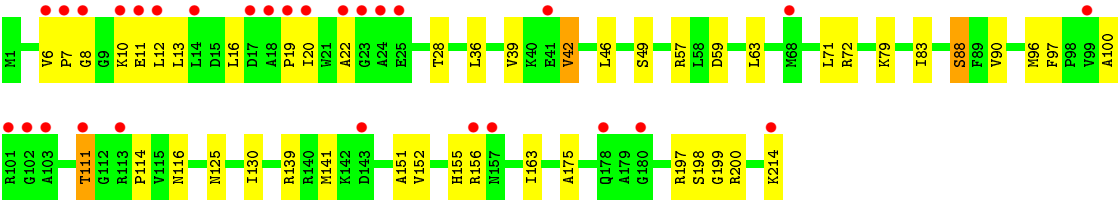


• Molecule 2: ETHYLBENZENE DEHYDROGENASE BETA-SUBUNIT



• Molecule 3: ETHYLBENZENE DEHYDROGENASE GAMMA-SUBUNIT





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	112.53 Å 67.32 Å 114.77 Å 90.00° 111.30° 90.00°	Depositor
Resolution (Å)	46.42 – 1.88 43.36 – 1.88	Depositor EDS
% Data completeness (in resolution range)	98.1 (46.42-1.88) 98.1 (43.36-1.88)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.29 (at 1.88 Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.148 , 0.183 0.161 , 0.193	Depositor DCC
R_{free} test set	6423 reflections (5.29%)	DCC
Wilson B-factor (Å ²)	17.5	Xtriage
Anisotropy	0.063	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.42 , 63.7	EDS
Estimated twinning fraction	0.026 for l,-k,h	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.29$	Xtriage
Outliers	0 of 127861 reflections	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	12639	wwPDB-VP
Average B, all atoms (Å ²)	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.80% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, MGD, MO, PO4, F3S, MES, ACT, HEM, MD1, SF4

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	0.76	0/7494	0.78	2/10140 (0.0%)
2	B	0.81	1/2744 (0.0%)	0.81	0/3715
3	C	0.58	0/1651	0.73	1/2225 (0.0%)
All	All	0.75	1/11889 (0.0%)	0.78	3/16080 (0.0%)

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
3	C	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	292	ARG	CG-CD	-6.22	1.36	1.51

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	96	MET	CG-SD-CE	-7.68	87.92	100.20
1	A	99	ARG	NE-CZ-NH2	-6.43	117.08	120.30
1	A	851	ARG	NE-CZ-NH2	-5.14	117.73	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	C	11	GLU	Peptide

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	7285	0	7052	64	0
2	B	2669	0	2581	30	0
3	C	1617	0	1628	30	0
4	A	12	0	12	0	0
5	A	8	0	6	2	0
6	A	24	0	32	7	0
6	B	12	0	16	3	0
6	C	12	0	16	1	0
7	A	8	0	0	0	0
7	B	24	0	0	0	0
8	A	1	0	0	0	0
9	A	47	0	22	1	0
10	A	47	0	21	4	0
11	B	5	0	0	0	0
12	B	7	0	0	0	0
13	C	43	0	30	3	0
14	A	492	0	0	7	1
14	B	237	0	0	5	1
14	C	89	0	0	1	0
All	All	12639	0	11416	126	1

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 (126) 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)
3:C:116:ASN:HD22	3:C:175:ALA:H	1.21	0.89
3:C:139:ARG:HG2	3:C:141:MET:HE2	1.61	0.82
1:A:944:HIS:HA	6:A:1981:GOL:H12	1.64	0.80
3:C:16:LEU:O	3:C:72:ARG:NH1	2.12	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:8:GLY:HA3	3:C:12:LEU:HD12	1.70	0.74
1:A:67:ILE:HB	14:A:2002:HOH:O	1.87	0.72
1:A:944:HIS:HA	6:A:1981:GOL:C1	2.23	0.68
1:A:206:MET:HE1	1:A:604:MET:SD	2.33	0.67
6:A:1981:GOL:H31	6:A:1982:GOL:O1	1.95	0.66
1:A:134:ASN:HD21	2:B:44:LYS:NZ	1.95	0.65
3:C:6:VAL:HG11	3:C:20:ILE:HG12	1.79	0.64
2:B:165:THR:HG22	13:C:1217:HEM:CGD	2.26	0.64
1:A:505:GLU:HA	1:A:508:GLN:HE21	1.63	0.64
10:A:1987:MD1:C7	10:A:1987:MD1:H11	2.29	0.62
1:A:209:LEU:HD22	1:A:726:LYS:HE3	1.82	0.61
6:B:1355:GOL:H12	14:B:2237:HOH:O	2.00	0.60
3:C:6:VAL:HG13	3:C:7:PRO:HD2	1.83	0.60
1:A:87:TRP:HA	1:A:88:PRO:C	2.22	0.59
1:A:554:VAL:HG12	1:A:554:VAL:O	2.04	0.58
3:C:39:VAL:O	3:C:42:VAL:HG13	2.04	0.57
1:A:841:HIS:HD2	1:A:972:SER:OG	1.87	0.57
1:A:588:THR:H	1:A:591:HIS:HD2	1.52	0.57
1:A:850:PRO:HB3	14:A:2463:HOH:O	2.05	0.57
2:B:340:ARG:CZ	14:B:2225:HOH:O	2.53	0.56
1:A:357:TYR:HB3	1:A:366:VAL:HG22	1.88	0.56
1:A:334:LEU:CD1	1:A:366:VAL:HG23	2.35	0.56
3:C:100:ALA:HB2	3:C:114:PRO:HD2	1.88	0.56
1:A:437:LYS:CE	14:A:2197:HOH:O	2.54	0.55
2:B:27:LYS:HB2	2:B:234:VAL:HG22	1.88	0.55
1:A:593:ARG:HA	1:A:594:PRO:C	2.26	0.55
3:C:116:ASN:ND2	3:C:175:ALA:H	1.99	0.55
3:C:36:LEU:O	3:C:39:VAL:HG22	2.07	0.55
1:A:849:HIS:HD1	9:A:1986:MGD:H15	1.56	0.54
1:A:783:ALA:HA	1:A:797:TRP:CE3	2.43	0.53
1:A:192:HIS:CE1	5:A:1978:ACT:H3	2.44	0.53
2:B:167:ALA:HA	2:B:183:ARG:HE	1.73	0.53
1:A:116:ASN:HD22	1:A:118:ASP:H	1.58	0.52
3:C:6:VAL:CG2	3:C:63:LEU:HD22	2.40	0.52
2:B:107:LYS:HD3	2:B:111:VAL:HG11	1.92	0.52
2:B:165:THR:HG22	13:C:1217:HEM:O1D	2.10	0.52
1:A:385:THR:HG21	1:A:397:GLN:OE1	2.10	0.52
1:A:192:HIS:HE1	5:A:1978:ACT:H3	1.74	0.51
2:B:189:HIS:CE1	3:C:46:LEU:HD13	2.45	0.51
1:A:195:ALA:HA	10:A:1987:MD1:C6	2.41	0.51
1:A:203:GLY:HA2	1:A:206:MET:HE2	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:841:HIS:HE1	1:A:897:ASP:OD1	1.95	0.50
1:A:207:THR:HG21	1:A:214:SER:OG	2.11	0.50
3:C:90:VAL:HG22	6:C:1215:GOL:H11	1.94	0.50
10:A:1987:MD1:H7	10:A:1987:MD1:H11	1.94	0.50
1:A:879:LYS:NZ	14:A:2440:HOH:O	2.44	0.49
1:A:927:LYS:NZ	14:A:2467:HOH:O	2.42	0.49
13:C:1217:HEM:HBB2	13:C:1217:HEM:HHC	1.94	0.49
3:C:79:LYS:HD3	3:C:155:HIS:HB3	1.94	0.49
1:A:936:LEU:HD13	1:A:966:ASP:HB2	1.94	0.49
1:A:696:LYS:NZ	1:A:700:GLU:OE2	2.27	0.49
1:A:586:TRP:O	6:A:1982:GOL:H2	2.13	0.49
1:A:289:THR:N	1:A:290:PRO:CD	2.76	0.48
3:C:198:SER:OG	3:C:199:GLY:N	2.44	0.47
1:A:673:PHE:CZ	1:A:763:LYS:HG2	2.49	0.47
3:C:49:SER:OG	3:C:200:ARG:NH1	2.45	0.47
2:B:218:ILE:C	2:B:218:ILE:HD12	2.35	0.47
1:A:134:ASN:HD21	2:B:44:LYS:HZ2	1.62	0.47
2:B:229:GLN:O	2:B:231:PRO:HD3	2.14	0.47
3:C:152:VAL:HG22	3:C:163:ILE:HB	1.97	0.47
2:B:195:PRO:HB2	2:B:264:TYR:CD2	2.51	0.46
2:B:62:LYS:HE2	14:B:2032:HOH:O	2.15	0.46
3:C:83:ILE:HA	3:C:88:SER:OG	2.15	0.46
1:A:218:ASN:ND2	1:A:481:TRP:HZ2	2.14	0.46
2:B:27:LYS:CB	2:B:234:VAL:HG22	2.46	0.45
1:A:534:MET:HG3	1:A:777:VAL:CG2	2.46	0.45
1:A:669:PRO:HG2	6:A:1979:GOL:H32	1.98	0.45
1:A:440:THR:H	1:A:470:ASN:ND2	2.15	0.45
1:A:836:MET:CE	1:A:840:ASP:HA	2.47	0.45
3:C:139:ARG:CG	3:C:141:MET:HE2	2.40	0.45
1:A:187:ILE:HD11	1:A:600:PRO:HB3	1.98	0.44
1:A:187:ILE:CD1	1:A:600:PRO:HB3	2.46	0.44
1:A:437:LYS:HE2	14:A:2197:HOH:O	2.17	0.44
1:A:589:ASN:OD1	1:A:589:ASN:O	2.34	0.44
6:A:1981:GOL:C3	6:A:1982:GOL:O1	2.63	0.44
1:A:533:PHE:CZ	1:A:537:VAL:HG11	2.53	0.44
1:A:354:LYS:NZ	1:A:950:GLU:OE1	2.50	0.44
1:A:439:ARG:HA	1:A:470:ASN:HD21	1.83	0.44
1:A:224:THR:O	1:A:449:ALA:HB2	2.18	0.44
1:A:872:PRO:HA	1:A:921:TRP:CE2	2.53	0.44
2:B:190:CYS:HB2	2:B:199:ILE:HD12	1.99	0.44
1:A:240:SER:HA	1:A:666:SER:O	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:224:THR:HG22	1:A:449:ALA:HB1	1.99	0.43
3:C:6:VAL:CG1	3:C:7:PRO:HD2	2.48	0.43
2:B:151:CYS:HB3	2:B:211:CYS:HB3	2.01	0.43
2:B:228:ARG:HE	6:B:1353:GOL:H31	1.83	0.43
1:A:218:ASN:ND2	1:A:481:TRP:CZ2	2.87	0.42
2:B:159:CYS:HB2	2:B:199:ILE:HD11	2.00	0.42
3:C:71:LEU:O	3:C:163:ILE:HA	2.19	0.42
3:C:28:THR:HG23	3:C:59:ASP:OD1	2.19	0.42
2:B:131:ASP:HA	2:B:134:GLN:OE1	2.20	0.42
1:A:368:LYS:NZ	14:A:2159:HOH:O	2.45	0.42
3:C:19:PRO:O	3:C:22:ALA:HB3	2.19	0.42
3:C:139:ARG:HG2	3:C:141:MET:CE	2.43	0.42
1:A:619:LYS:NZ	1:A:623:ASP:OD2	2.42	0.42
1:A:534:MET:HG3	1:A:777:VAL:HG22	2.02	0.42
2:B:154:CYS:HB3	2:B:266:THR:O	2.19	0.42
3:C:151:ALA:HA	3:C:163:ILE:O	2.20	0.42
3:C:28:THR:CG2	3:C:57:ARG:HG3	2.50	0.41
2:B:165:THR:HG21	2:B:185:LYS:HD2	2.02	0.41
2:B:340:ARG:NH2	14:B:2225:HOH:O	2.53	0.41
2:B:253:LYS:HZ3	2:B:327:GLU:CD	2.23	0.41
2:B:256:VAL:HG21	2:B:328:LEU:HD11	2.02	0.41
3:C:111:THR:HG23	14:C:2046:HOH:O	2.20	0.41
1:A:324:PHE:CD1	1:A:469:GLY:HA2	2.56	0.41
1:A:967:ARG:HH12	10:A:1987:MD1:H17	1.68	0.41
1:A:76:LYS:HE3	1:A:98:VAL:HG21	2.03	0.41
1:A:312:GLN:NE2	1:A:414:PRO:HD3	2.36	0.41
1:A:797:TRP:O	1:A:801:ASP:HB2	2.20	0.41
1:A:405:LEU:HD21	1:A:463:LEU:HD21	2.03	0.41
2:B:16:LYS:NZ	2:B:17:ARG:O	2.54	0.41
2:B:168:ILE:HG12	2:B:179:VAL:HG22	2.01	0.41
1:A:280:VAL:HG23	1:A:292:ALA:HB2	2.03	0.41
3:C:13:LEU:O	3:C:163:ILE:HD13	2.21	0.41
3:C:97:PHE:HB2	3:C:175:ALA:HB2	2.02	0.40
1:A:944:HIS:O	6:A:1981:GOL:H32	2.21	0.40
3:C:100:ALA:CB	3:C:114:PRO:HD2	2.51	0.40
2:B:188:ARG:HD3	2:B:201:PHE:CG	2.55	0.40
1:A:116:ASN:ND2	1:A:118:ASP:H	2.20	0.40
2:B:171:ARG:HD2	14:B:2118:HOH:O	2.21	0.40
2:B:228:ARG:HE	6:B:1353:GOL:C2	2.34	0.40
1:A:910:ASN:HA	2:B:142:PRO:HG3	2.02	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the sym-

metry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:A:2120:HOH:O	14:B:2149:HOH:O[2_645]	2.09	0.11

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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	910/976 (93%)	887 (98%)	23 (2%)	0	100	100
2	B	335/352 (95%)	323 (96%)	12 (4%)	0	100	100
3	C	212/214 (99%)	204 (96%)	8 (4%)	0	100	100
All	All	1457/1542 (94%)	1414 (97%)	43 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

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	766/816 (94%)	748 (98%)	18 (2%)	58	48
2	B	285/298 (96%)	281 (99%)	4 (1%)	74	69
3	C	163/164 (99%)	154 (94%)	9 (6%)	27	13
All	All	1214/1278 (95%)	1183 (97%)	31 (3%)	54	42

All (31) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	84	ASN
1	A	116	ASN
1	A	206	MET
1	A	234	LYS
1	A	261	TYR
1	A	303	ASP
1	A	312	GLN
1	A	366	VAL
1	A	387	SER
1	A	391	LYS
1	A	486	ASP
1	A	507	HIS
1	A	582	LYS
1	A	608	GLN
1	A	654	TRP
1	A	670	PHE
1	A	924	HIS
1	A	932	TYR
2	B	29	LEU
2	B	39	LYS
2	B	213	LEU
2	B	246	HIS
3	C	10	LYS
3	C	42	VAL
3	C	88	SER
3	C	111	THR
3	C	125	ASN
3	C	130	ILE
3	C	156	ARG
3	C	197	ARG
3	C	214	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	116	ASN
1	A	134	ASN
1	A	312	GLN
1	A	470	ASN
1	A	507	HIS
1	A	508	GLN
1	A	589	ASN
1	A	591	HIS

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Mol	Chain	Res	Type
1	A	747	ASN
1	A	841	HIS
1	A	871	GLN
2	B	55	ASN
2	B	269	ASN
3	C	116	ASN
3	C	161	ASN

5.3.3 RNA ⓘ

There are no RNA molecules 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 21 ligands modelled in this entry, 1 is monoatomic - leaving 20 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
4	MES	A	1977	-	11,12,12	0.81	0	14,16,16	3.41	5 (35%)
5	ACT	A	1978	8	1,3,3	0.36	0	0,3,3	0.00	-
6	GOL	A	1979	-	5,5,5	0.51	0	5,5,5	0.72	0
6	GOL	A	1980	-	5,5,5	0.38	0	5,5,5	0.59	0
6	GOL	A	1981	-	5,5,5	0.37	0	5,5,5	1.58	1 (20%)
6	GOL	A	1982	-	5,5,5	0.26	0	5,5,5	0.65	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	ACT	A	1983	-	1,3,3	1.64	0	0,3,3	0.00	-
7	SF4	A	1984	1	0,12,12	0.00	-	0,24,24	0.00	-
9	MGD	A	1986	8	38,52,52	1.75	10 (26%)	43,81,81	2.72	16 (37%)
10	MD1	A	1987	8	39,51,51	2.71	5 (12%)	37,78,78	2.52	13 (35%)
6	GOL	B	1353	-	5,5,5	0.78	0	5,5,5	2.18	3 (60%)
11	PO4	B	1354	-	4,4,4	0.25	0	6,6,6	0.28	0
6	GOL	B	1355	-	5,5,5	0.46	0	5,5,5	0.41	0
12	F3S	B	1356	2	0,9,9	0.00	-	0,15,15	0.00	-
7	SF4	B	1357	2	0,12,12	0.00	-	0,24,24	0.00	-
7	SF4	B	1358	2	0,12,12	0.00	-	0,24,24	0.00	-
7	SF4	B	1359	2	0,12,12	0.00	-	0,24,24	0.00	-
6	GOL	C	1215	-	5,5,5	0.30	0	5,5,5	0.65	0
6	GOL	C	1216	-	5,5,5	0.30	0	5,5,5	0.28	0
13	HEM	C	1217	3	30,50,50	2.22	6 (20%)	24,82,82	2.59	12 (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
4	MES	A	1977	-	-	0/6/14/14	0/1/1/1
5	ACT	A	1978	8	-	0/0/0/0	0/0/0/0
6	GOL	A	1979	-	-	0/4/4/4	0/0/0/0
6	GOL	A	1980	-	-	0/4/4/4	0/0/0/0
6	GOL	A	1981	-	-	0/4/4/4	0/0/0/0
6	GOL	A	1982	-	-	0/4/4/4	0/0/0/0
5	ACT	A	1983	-	-	0/0/0/0	0/0/0/0
7	SF4	A	1984	1	-	0/0/48/48	0/6/5/5
9	MGD	A	1986	8	-	0/18/66/66	0/6/6/6
10	MD1	A	1987	8	1/1/10/12	0/18/59/59	0/5/5/5
6	GOL	B	1353	-	-	0/4/4/4	0/0/0/0
11	PO4	B	1354	-	-	0/0/0/0	0/0/0/0
6	GOL	B	1355	-	-	0/4/4/4	0/0/0/0
12	F3S	B	1356	2	-	0/0/24/24	0/0/3/3
7	SF4	B	1357	2	-	0/0/48/48	0/6/5/5
7	SF4	B	1358	2	-	0/0/48/48	0/6/5/5
7	SF4	B	1359	2	-	0/0/48/48	0/6/5/5
6	GOL	C	1215	-	-	0/4/4/4	0/0/0/0
6	GOL	C	1216	-	-	0/4/4/4	0/0/0/0
13	HEM	C	1217	3	-	0/10/54/54	0/0/8/8

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	C	1217	HEM	C3B-C4B	-7.59	1.45	1.51
13	C	1217	HEM	C3D-C4D	-5.38	1.44	1.51
9	A	1986	MGD	O11-C11	-4.43	1.37	1.43
10	A	1987	MD1	C14-N15	-4.12	1.42	1.47
13	C	1217	HEM	C2C-C1C	-3.83	1.45	1.52
13	C	1217	HEM	C2D-C1D	-2.20	1.44	1.51
9	A	1986	MGD	PA-O2A	-2.20	1.45	1.54
13	C	1217	HEM	C2B-C1B	-2.13	1.44	1.51
10	A	1987	MD1	C20-N18	-2.02	1.32	1.35
9	A	1986	MGD	C2-N2	2.03	1.38	1.34
9	A	1986	MGD	O4'-C1'	2.27	1.44	1.41
9	A	1986	MGD	C21-N22	2.41	1.39	1.35
10	A	1987	MD1	C6-N1	2.55	1.37	1.33
10	A	1987	MD1	C17-N17	2.60	1.40	1.35
13	C	1217	HEM	C1C-NC	2.82	1.39	1.36
9	A	1986	MGD	C14-N15	2.86	1.49	1.45
9	A	1986	MGD	C2-N1	3.02	1.40	1.35
9	A	1986	MGD	C23-C14	3.13	1.55	1.53
9	A	1986	MGD	C6-N1	3.85	1.40	1.33
9	A	1986	MGD	C17-N18	4.46	1.41	1.33
10	A	1987	MD1	C7-N8	14.91	1.44	1.27

All (50) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	A	1986	MGD	N3-C2-N1	-7.06	116.69	127.44
10	A	1987	MD1	N3-C2-N1	-6.14	118.10	127.44
9	A	1986	MGD	C4'-O4'-C1'	-6.08	103.03	109.72
10	A	1987	MD1	C5-C6-N1	-5.14	116.56	123.59
9	A	1986	MGD	N18-C19-N20	-5.04	117.27	125.53
10	A	1987	MD1	C4'-O4'-C1'	-4.89	104.34	109.72
9	A	1986	MGD	C5-C6-N1	-4.47	117.48	123.59
9	A	1986	MGD	C6-C5-C4	-3.73	116.44	120.90
9	A	1986	MGD	C2'-C1'-N9	-3.41	109.08	114.29
4	A	1977	MES	O1S-S-C8	-3.38	104.02	106.91
10	A	1987	MD1	C2'-C1'-N9	-3.19	109.41	114.29
13	C	1217	HEM	CAA-C2A-C1A	-3.19	123.54	127.01
9	A	1986	MGD	C5'-C4'-C3'	-3.02	103.22	115.21
13	C	1217	HEM	CAA-CBA-CGA	-2.94	107.37	112.75
10	A	1987	MD1	C6-C5-C4	-2.91	117.42	120.90
9	A	1986	MGD	C1'-N9-C4	-2.85	122.64	126.94
10	A	1987	MD1	C1'-N9-C4	-2.53	123.12	126.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	A	1987	MD1	N17-C17-N18	-2.52	121.40	125.53
6	B	1353	GOL	O2-C2-C3	-2.40	97.65	108.65
13	C	1217	HEM	C3C-CAC-CBC	-2.23	121.04	124.46
13	C	1217	HEM	C3B-C4B-NB	-2.14	107.54	111.63
9	A	1986	MGD	C4-C5-N7	-2.03	107.61	109.48
13	C	1217	HEM	CMA-C3A-C4A	-2.00	125.05	128.36
13	C	1217	HEM	C2D-C3D-C4D	2.36	105.50	101.50
9	A	1986	MGD	N22-C21-N20	2.43	120.49	116.62
10	A	1987	MD1	N2-C2-N1	2.44	121.24	117.20
6	B	1353	GOL	C3-C2-C1	2.58	121.23	111.12
6	A	1981	GOL	O1-C1-C2	2.60	122.80	110.18
9	A	1986	MGD	N2-C2-N3	2.67	122.93	117.80
6	B	1353	GOL	O1-C1-C2	2.72	123.38	110.18
4	A	1977	MES	C2-C3-N4	2.77	114.33	110.12
10	A	1987	MD1	C20-N8-C7	2.85	124.95	116.52
10	A	1987	MD1	N16-C17-N18	2.86	121.93	117.20
13	C	1217	HEM	C3B-C4B-CHC	2.87	127.20	123.16
10	A	1987	MD1	O4'-C1'-N9	3.00	114.39	108.10
9	A	1986	MGD	C19-N20-C21	3.28	121.91	114.54
9	A	1986	MGD	C17-C16-C21	3.36	117.60	114.56
13	C	1217	HEM	CMD-C2D-C3D	3.41	129.45	114.35
13	C	1217	HEM	CAD-C3D-C4D	3.45	124.64	112.47
4	A	1977	MES	C7-N4-C5	4.03	121.61	111.27
10	A	1987	MD1	C15-N17-C17	4.35	121.98	115.94
9	A	1986	MGD	N19-C19-N20	4.47	124.60	117.20
13	C	1217	HEM	CMB-C2B-C3B	4.73	128.34	116.53
13	C	1217	HEM	CMC-C2C-C3C	4.76	128.42	116.53
9	A	1986	MGD	C17-N18-C19	5.06	122.97	115.94
13	C	1217	HEM	CAD-C3D-C2D	5.79	129.85	113.22
10	A	1987	MD1	C6-N1-C2	6.27	124.64	115.94
9	A	1986	MGD	C6-N1-C2	6.36	124.77	115.94
4	A	1977	MES	C5-N4-C3	6.46	122.89	108.90
4	A	1977	MES	O2S-S-C8	8.62	114.26	106.91

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
10	A	1987	MD1	C14

There are no torsion outliers.

There are no ring outliers.

10 monomers are involved in 21 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	1978	ACT	2	0
6	A	1979	GOL	1	0
6	A	1981	GOL	5	0
6	A	1982	GOL	3	0
9	A	1986	MGD	1	0
10	A	1987	MD1	4	0
6	B	1353	GOL	2	0
6	B	1355	GOL	1	0
6	C	1215	GOL	1	0
13	C	1217	HEM	3	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	912/976 (93%)	0.47	84 (9%) 11 12	19, 24, 33, 50	0
2	B	337/352 (95%)	0.00	7 (2%) 67 69	18, 24, 31, 46	0
3	C	214/214 (100%)	0.65	29 (13%) 4 4	17, 25, 34, 43	0
All	All	1463/1542 (94%)	0.39	120 (8%) 14 15	17, 24, 33, 50	0

All (120) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	C	101	ARG	7.2
2	B	77	ARG	5.8
1	A	389	ARG	5.7
2	B	76	LEU	5.3
3	C	12	LEU	5.3
1	A	520	ALA	5.1
1	A	392	ASN	4.7
3	C	24	ALA	4.4
1	A	363	ALA	4.3
3	C	11	GLU	4.3
3	C	22	ALA	4.2
1	A	522	PRO	4.1
3	C	14	LEU	4.1
3	C	6	VAL	4.1
1	A	221	ILE	4.0
3	C	7	PRO	3.9
3	C	19	PRO	3.9
3	C	10	LYS	3.9
1	A	393	GLY	3.8
1	A	511	GLU	3.8
1	A	518	LEU	3.7
3	C	8	GLY	3.6
1	A	361	GLU	3.6

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Mol	Chain	Res	Type	RSRZ
1	A	516	ARG	3.5
1	A	85	ILE	3.5
1	A	397	GLN	3.5
1	A	854	ILE	3.4
1	A	519	GLU	3.4
1	A	480	ALA	3.3
1	A	446	PHE	3.3
1	A	138	TYR	3.3
3	C	17	ASP	3.3
1	A	377	ASP	3.2
3	C	111	THR	3.2
3	C	143	ASP	3.1
1	A	597	ASP	3.1
2	B	31	CYS	3.1
1	A	217	ILE	3.1
1	A	385	THR	3.1
1	A	589	ASN	3.1
1	A	193	VAL	3.1
1	A	708	THR	3.0
1	A	67	ILE	3.0
3	C	25	GLU	3.0
3	C	20	ILE	3.0
3	C	102	GLY	3.0
1	A	920	PHE	2.9
1	A	852	VAL	2.9
1	A	225	TYR	2.9
1	A	523	THR	2.8
1	A	859	LEU	2.8
2	B	78	GLY	2.8
3	C	214	LYS	2.8
1	A	386	PHE	2.8
1	A	100	ASN	2.8
3	C	157	ASN	2.8
2	B	172	GLU	2.7
1	A	507	HIS	2.7
1	A	350	GLY	2.7
3	C	18	ALA	2.7
2	B	16	LYS	2.6
3	C	68	MET	2.6
3	C	156	ARG	2.6
1	A	87	TRP	2.6
1	A	481	TRP	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	395	THR	2.6
1	A	261	TYR	2.6
1	A	918	VAL	2.6
1	A	449	ALA	2.6
1	A	362	LYS	2.5
1	A	224	THR	2.5
1	A	445	GLY	2.5
1	A	558	GLN	2.5
1	A	596	PRO	2.5
1	A	515	LYS	2.5
1	A	506	LEU	2.5
1	A	260	THR	2.5
1	A	259	TYR	2.5
1	A	517	THR	2.5
1	A	222	GLY	2.4
3	C	178	GLN	2.4
1	A	443	TYR	2.4
1	A	964	VAL	2.4
1	A	521	ASP	2.4
1	A	444	ILE	2.4
3	C	41	GLU	2.4
1	A	509	MET	2.4
3	C	23	GLY	2.3
1	A	219	VAL	2.3
1	A	855	HIS	2.3
3	C	113	ARG	2.3
1	A	394	LYS	2.3
1	A	257	TRP	2.3
2	B	29	LEU	2.3
1	A	86	CYS	2.3
1	A	365	SER	2.3
1	A	850	PRO	2.3
1	A	856	SER	2.3
1	A	715	GLY	2.3
3	C	99	VAL	2.2
1	A	88	PRO	2.2
1	A	849	HIS	2.2
1	A	513	PHE	2.2
1	A	262	PRO	2.2
1	A	265	TYR	2.2
3	C	180	GLY	2.2
1	A	366	VAL	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	510	ALA	2.2
1	A	505	GLU	2.1
1	A	359	PHE	2.1
1	A	479	PHE	2.1
1	A	579	ASP	2.1
1	A	583	GLU	2.1
1	A	508	GLN	2.1
1	A	478	ALA	2.0
1	A	512	GLY	2.0
1	A	588	THR	2.0
1	A	665	CYS	2.0
3	C	103	ALA	2.0
1	A	102	ILE	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
11	PO4	B	1354	5/5	0.93	0.27	8.83	44,47,47,48	0
6	GOL	B	1353	6/6	0.89	0.16	4.42	24,31,33,37	0
6	GOL	B	1355	6/6	0.89	0.18	3.73	45,46,47,47	0
6	GOL	A	1981	6/6	0.87	0.17	2.44	32,36,38,39	0
5	ACT	A	1983	4/4	0.88	0.19	1.57	34,37,38,38	0
6	GOL	A	1982	6/6	0.93	0.13	0.98	40,41,43,44	0
13	HEM	C	1217	43/43	0.95	0.11	0.11	21,24,27,28	0
6	GOL	C	1216	6/6	0.92	0.10	0.08	33,34,35,36	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
6	GOL	C	1215	6/6	0.92	0.10	-0.10	23,27,30,30	0
6	GOL	A	1980	6/6	0.84	0.16	-0.15	33,36,36,37	0
6	GOL	A	1979	6/6	0.97	0.10	-0.58	16,20,23,24	0
4	MES	A	1977	12/12	0.97	0.10	-0.77	24,27,28,32	0
12	F3S	B	1356	7/7	0.97	0.08	-1.25	20,21,22,22	0
7	SF4	A	1984	8/8	0.98	0.11	-1.41	23,25,26,26	0
7	SF4	B	1359	8/8	0.99	0.08	-1.69	23,24,24,26	0
7	SF4	B	1358	8/8	0.99	0.10	-1.71	24,24,25,25	0
5	ACT	A	1978	4/4	0.91	0.16	-1.82	23,25,26,28	0
10	MD1	A	1987	47/47	0.98	0.06	-2.53	14,16,18,18	0
9	MGD	A	1986	47/47	0.98	0.07	-2.89	10,14,16,17	0
7	SF4	B	1357	8/8	0.99	0.04	-3.86	21,22,23,24	0
8	MO	A	1985	1/1	1.00	0.04	-	19,19,19,19	0

6.5 Other polymers [i](#)

There are no such residues in this entry.