



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 09:41 PM UTC

PDB ID : 1B4E / pdb_00001b4e
Title : X-ray structure of 5-aminolevulinic acid dehydratase complexed with the inhibitor levulinic acid
Authors : Erskine, P.T.; Cooper, J.B.; Lewis, G.; Spencer, P.; Wood, S.P.; Shoolingin-Jordan, P.M.
Deposited on : 1998-12-19
Resolution : 2.00 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

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtrriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

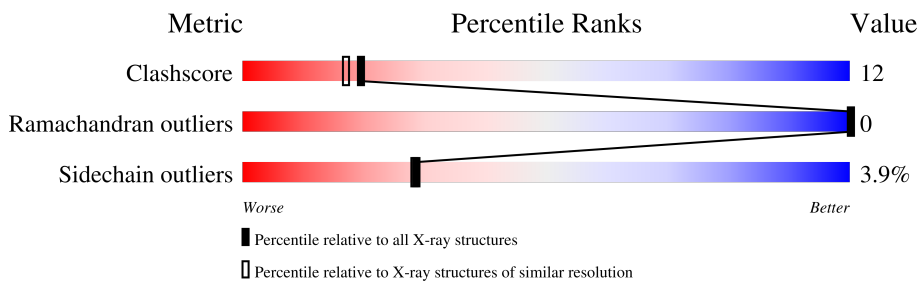
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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))
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)

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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. 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 $\leq 5\%$

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	323	

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
5	GOL	A	408	-	X	-	-

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 2893 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 PROTEIN (5-AMINOLEVULINIC ACID DEHYDRATASE).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	323	2479	1550	433	478	18	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	5	SER	ILE	conflict	UNP P0ACB2
A	134	LYS	CYS	conflict	UNP P0ACB2

- Molecule 2 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



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

Continued on next page...

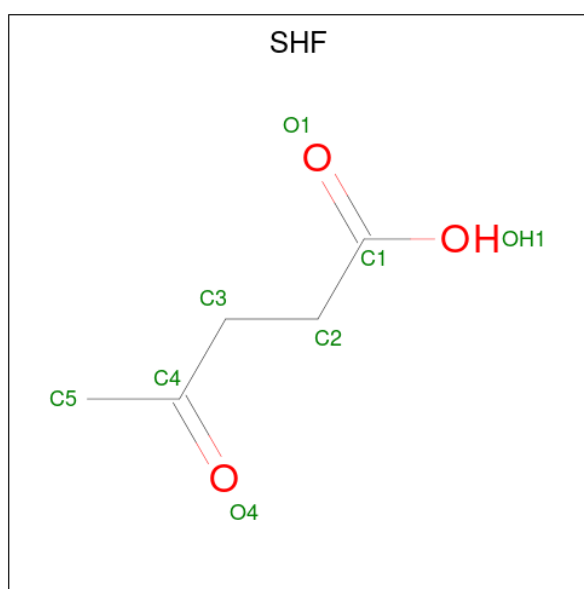
Continued from previous page...

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

- Molecule 3 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	3	Total	Zn	0	0
			3	3		

- Molecule 4 is LAEVULINIC ACID (CCD ID: SHF) (formula: C₅H₈O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			7	5	2		

- Molecule 5 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



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

- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	371	Total O 371 371	0	0

3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. 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. 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.

Note EDS was not executed.

- Molecule 1: PROTEIN (5-AMINOLEVULINIC ACID DEHYDRATASE)



4 Data and refinement statistics

Xtrriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	I 4 2 2	Depositor
Cell constants a, b, c, α , β , γ	126.70Å 126.70Å 141.60Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	8.00 – 2.00	Depositor
% Data completeness (in resolution range)	(Not available) (8.00-2.00)	Depositor
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	RESTRAIN	Depositor
R, R_{free}	0.188 , 0.255	Depositor
Estimated twinning fraction	No twinning to report.	Xtrriage
Total number of atoms	2893	wwPDB-VP
Average B, all atoms (Å ²)	23.0	wwPDB-VP

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: ZN, SHF, SO4, GOL

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	0.98	2/2518 (0.1%)	1.81	42/3392 (1.2%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	225	ASN	CA-C	-5.67	1.46	1.53
1	A	20	MET	SD-CE	-5.31	1.66	1.79

All (42) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	265	LEU	CA-C-N	-7.95	112.16	120.03
1	A	265	LEU	C-N-CA	-7.95	112.16	120.03
1	A	310	PHE	CA-CB-CG	-7.18	106.62	113.80
1	A	161	PHE	CA-C-N	-7.05	113.88	122.90
1	A	161	PHE	C-N-CA	-7.05	113.88	122.90
1	A	33	LEU	CA-C-N	-6.88	112.88	119.76
1	A	33	LEU	C-N-CA	-6.88	112.88	119.76
1	A	192	TYR	N-CA-C	-6.73	101.33	110.68
1	A	225	ASN	N-CA-C	6.67	120.17	108.56
1	A	240	GLY	N-CA-C	6.55	124.67	115.43
1	A	46	ALA	CA-C-N	-6.19	114.75	122.48
1	A	46	ALA	C-N-CA	-6.19	114.75	122.48
1	A	242	ASP	CA-CB-CG	-6.01	106.58	112.60
1	A	309	ILE	CA-C-N	-5.94	114.87	122.77
1	A	309	ILE	C-N-CA	-5.94	114.87	122.77
1	A	153	VAL	CA-CB-CG2	5.85	120.34	110.40
1	A	141	ASP	N-CA-C	5.83	117.64	111.28
1	A	60	HIS	CA-CB-CG	-5.81	107.99	113.80
1	A	76	VAL	O-C-N	5.71	129.47	123.02

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	121	PHE	CA-CB-CG	-5.70	108.10	113.80
1	A	139	ASP	CA-CB-CG	-5.69	106.91	112.60
1	A	42	ASP	CA-C-N	-5.58	113.89	122.87
1	A	42	ASP	C-N-CA	-5.58	113.89	122.87
1	A	116	MET	CA-C-N	-5.56	115.38	122.77
1	A	116	MET	C-N-CA	-5.56	115.38	122.77
1	A	212	LEU	N-CA-C	5.55	118.22	109.96
1	A	118	ASP	O-C-N	5.53	129.73	122.93
1	A	191	SER	CA-C-N	-5.51	113.81	122.08
1	A	191	SER	C-N-CA	-5.51	113.81	122.08
1	A	270	TYR	N-CA-C	5.50	117.61	108.20
1	A	44	TYR	CA-C-N	-5.50	114.96	122.93
1	A	44	TYR	C-N-CA	-5.50	114.96	122.93
1	A	66	GLU	CA-CB-CG	5.41	124.92	114.10
1	A	12	ARG	CA-C-N	5.35	127.71	120.38
1	A	12	ARG	C-N-CA	5.35	127.71	120.38
1	A	216	ARG	CA-CB-CG	-5.20	103.70	114.10
1	A	6	GLN	OE1-CD-NE2	5.18	127.78	122.60
1	A	65	ILE	CA-C-O	5.06	126.21	120.95
1	A	51	PRO	CA-CB-CG	-5.03	94.94	104.50
1	A	12	ARG	CG-CD-NE	-5.02	100.95	112.00
1	A	79	PHE	CA-C-N	-5.01	116.97	122.38
1	A	79	PHE	C-N-CA	-5.01	116.97	122.38

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [\(i\)](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2479	0	2460	57	1
2	A	15	0	0	0	0
3	A	3	0	0	0	0
4	A	7	0	7	3	0
5	A	18	0	23	2	0
6	A	371	0	0	5	1

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	2893	0	2490	58	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 12.

All (58) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:42:ASP:HA	1:A:59:LYS:HE2	1.39	1.03
1:A:42:ASP:HA	1:A:59:LYS:CE	2.09	0.80
1:A:134:LYS:HD2	1:A:136:HIS:HB2	1.62	0.79
1:A:75:SER:HB2	1:A:114:ILE:HB	1.66	0.76
1:A:134:LYS:HD2	1:A:136:HIS:CB	2.14	0.76
1:A:173:GLN:O	1:A:177:GLN:HG3	1.88	0.74
1:A:205:ARG:HD3	6:A:721:HOH:O	1.88	0.72
1:A:227:ARG:HD3	6:A:795:HOH:O	1.88	0.72
1:A:97:GLY:O	1:A:101:ARG:HG3	1.93	0.68
1:A:134:LYS:HD2	1:A:136:HIS:H	1.60	0.66
1:A:165:SER:HB3	1:A:192:TYR:CE1	2.30	0.66
1:A:254:ASP:O	1:A:258:GLU:HG3	1.94	0.66
1:A:211:ALA:O	1:A:213:LYS:HE3	1.97	0.64
1:A:135:GLU:HG3	1:A:136:HIS:CD2	2.34	0.63
1:A:134:LYS:HD2	1:A:136:HIS:CG	2.34	0.62
1:A:135:GLU:HG3	1:A:136:HIS:HD2	1.65	0.61
1:A:134:LYS:HD2	1:A:136:HIS:CD2	2.36	0.60
1:A:130:CYS:HB2	1:A:219:TYR:CE2	2.36	0.60
1:A:134:LYS:CD	1:A:136:HIS:H	2.16	0.58
1:A:247:LYS:CE	4:A:407:SHF:H21	2.34	0.58
1:A:57:PRO:HG2	1:A:60:HIS:HD2	1.70	0.57
1:A:193:SER:HB2	1:A:233:SER:HA	1.86	0.57
1:A:197:ALA:HA	1:A:220:GLN:HE21	1.68	0.57
1:A:104:ARG:O	1:A:108:GLN:HG3	2.04	0.56
1:A:276:TYR:CD2	1:A:312:TYR:HB2	2.40	0.56
1:A:20:MET:HG2	6:A:546:HOH:O	2.07	0.55
1:A:134:LYS:CD	1:A:136:HIS:CD2	2.91	0.53
1:A:2:THR:HG22	1:A:3:ASP:N	2.24	0.52
1:A:79:PHE:CE1	4:A:407:SHF:H52	2.43	0.52
1:A:134:LYS:HD2	1:A:136:HIS:N	2.26	0.51
1:A:247:LYS:HG3	1:A:270:TYR:HB3	1.93	0.50
1:A:247:LYS:HE3	4:A:407:SHF:H21	1.93	0.50
1:A:296:GLU:HA	5:A:409:GOL:H31	1.93	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:271:GLN:HG3	1:A:275:GLU:OE1	2.11	0.49
1:A:50:MET:HE2	1:A:53:VAL:HG21	1.95	0.48
1:A:134:LYS:HG2	1:A:139:ASP:HB2	1.96	0.47
1:A:302:LYS:HB3	1:A:302:LYS:HE3	1.57	0.47
1:A:2:THR:CG2	1:A:3:ASP:N	2.77	0.47
1:A:245:MET:HG2	1:A:246:VAL:N	2.29	0.46
1:A:196:PHE:CD1	1:A:223:PRO:HA	2.50	0.45
1:A:14:SER:HB2	1:A:15:PRO:HD2	1.98	0.45
1:A:203:PRO:HB2	1:A:273:SER:HB2	1.99	0.44
5:A:408:GOL:H2	6:A:864:HOH:O	2.18	0.44
1:A:165:SER:HB3	1:A:192:TYR:CZ	2.54	0.43
1:A:201:TYR:O	1:A:202:GLY:C	2.61	0.43
1:A:165:SER:HB3	1:A:192:TYR:CD1	2.54	0.43
1:A:44:TYR:HB3	1:A:54:MET:HE3	2.00	0.42
1:A:65:ILE:HD12	1:A:65:ILE:HA	1.73	0.42
1:A:221:MET:HB2	1:A:221:MET:HE3	1.69	0.42
1:A:41:ILE:HG13	1:A:57:PRO:HB3	2.02	0.42
1:A:245:MET:HA	1:A:268:GLY:O	2.20	0.41
1:A:65:ILE:CG2	1:A:66:GLU:N	2.83	0.41
1:A:144:LEU:HD22	1:A:171:GLN:HA	2.02	0.41
1:A:90:SER:HA	1:A:93:TRP:CZ3	2.56	0.41
1:A:107:LYS:HE2	6:A:670:HOH:O	2.20	0.41
1:A:123:GLU:HG2	1:A:208:ALA:HB1	2.03	0.41
1:A:107:LYS:HA	1:A:107:LYS:HD2	1.89	0.40
1:A:165:SER:HB2	1:A:195:LYS:NZ	2.36	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:94:ARG:NH2	6:A:591:HOH:O[16_445]	2.13	0.07

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	321/323 (99%)	312 (97%)	9 (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	257/258 (100%)	247 (96%)	10 (4%)	28	28

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	SER
1	A	45	LYS
1	A	51	PRO
1	A	107	LYS
1	A	134	LYS
1	A	135	GLU
1	A	205	ARG
1	A	213	LYS
1	A	223	PRO
1	A	321	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	108	GLN
1	A	136	HIS
1	A	171	GLN
1	A	220	GLN
1	A	271	GLN

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 10 ligands modelled in this entry, 3 are monoatomic - leaving 7 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	SHF	A	407	1	6,6,7	1.04	1 (16%)	6,6,8	0.80	0
5	GOL	A	409	-	5,5,5	1.60	1 (20%)	5,5,5	1.50	1 (20%)
2	SO4	A	401	-	4,4,4	0.31	0	6,6,6	0.25	0
5	GOL	A	408	-	5,5,5	1.66	1 (20%)	5,5,5	1.92	2 (40%)
2	SO4	A	403	-	4,4,4	0.27	0	6,6,6	0.35	0
5	GOL	A	410	-	5,5,5	1.88	1 (20%)	5,5,5	1.49	2 (40%)
2	SO4	A	402	-	4,4,4	0.22	0	6,6,6	0.22	0

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	GOL	A	410	-	-	2/4/4/4	-
5	GOL	A	408	-	-	4/4/4/4	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	SHF	A	407	1	-	1/4/4/5	-
5	GOL	A	409	-	-	3/4/4/4	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	410	GOL	O2-C2	3.90	1.54	1.43
5	A	409	GOL	O1-C1	3.01	1.55	1.42
5	A	408	GOL	O3-C3	2.87	1.54	1.42
4	A	407	SHF	OH1-C1	-2.05	1.24	1.30

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	408	GOL	O1-C1-C2	3.35	125.48	110.38
5	A	409	GOL	C3-C2-C1	2.61	121.36	111.80
5	A	410	GOL	O2-C2-C3	-2.29	99.71	109.18
5	A	408	GOL	O3-C3-C2	-2.04	101.20	110.38
5	A	410	GOL	O1-C1-C2	2.01	119.42	110.38

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	408	GOL	O1-C1-C2-C3
5	A	409	GOL	O1-C1-C2-C3
5	A	409	GOL	C1-C2-C3-O3
5	A	410	GOL	C1-C2-C3-O3
5	A	408	GOL	O1-C1-C2-O2
5	A	408	GOL	O2-C2-C3-O3
5	A	409	GOL	O2-C2-C3-O3
5	A	408	GOL	C1-C2-C3-O3
5	A	410	GOL	O2-C2-C3-O3
4	A	407	SHF	C2-C3-C4-C5

There are no ring outliers.

3 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	407	SHF	3	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	409	GOL	1	0
5	A	408	GOL	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

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.