



# Full wwPDB X-ray Structure Validation Report i

Jun 23, 2024 – 11:44 PM EDT

PDB ID : 6QAO  
Title : Structure of human aldehyde dehydrogenase 9A1 in P21 space group  
Authors : Morera, S.; Vigouroux, A.  
Deposited on : 2018-12-19  
Resolution : 2.89 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](mailto: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 i symbol.

The types of validation reports are described at  
<http://www.wwpdb.org/validation/2017/FAQs#types>.

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The following versions of software and data (see [references](#) ①) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 2022.3.0, CSD as543be (2022)  
Xtriage (Phenix) : 1.20.1  
EDS : 2.37.1  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.37.1

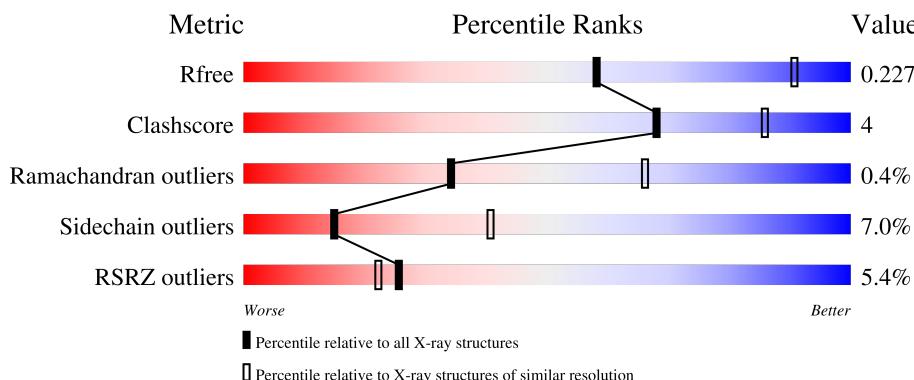
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## X-RAY DIFFRACTION

The reported resolution of this entry is 2.89 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))
$R_{free}$	130704	1957 (2.90-2.90)
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)
RSRZ outliers	127900	1906 (2.90-2.90)

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  $\geq 3$ , 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  $\leq 5\%$ . 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.



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Mol	Chain	Length	Quality of chain			
1	F	508	3%	79%	12%	• 7%
1	G	508	7%	78%	13%	• 8%
1	H	508	5%	79%	12%	• 8%

## 2 Entry composition [\(i\)](#)

There are 3 unique types of molecules in this entry. The entry contains 28772 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 4-trimethylaminobutyraldehyde dehydrogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	470	Total	C 3600	N 2279	O 615	S 678	28	0	0
1	B	469	Total	C 3596	N 2277	O 614	S 677	28	0	0
1	C	470	Total	C 3600	N 2279	O 615	S 678	28	0	0
1	D	468	Total	C 3594	N 2277	O 613	S 675	29	0	1
1	E	465	Total	C 3567	N 2258	O 610	S 671	28	0	0
1	F	470	Total	C 3597	N 2277	O 615	S 677	28	0	0
1	G	469	Total	C 3596	N 2277	O 614	S 677	28	0	0
1	H	468	Total	C 3589	N 2273	O 613	S 675	28	0	0

There are 112 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-13	MET	-	initiating methionine	UNP P49189
A	-12	GLY	-	expression tag	UNP P49189
A	-11	SER	-	expression tag	UNP P49189
A	-10	SER	-	expression tag	UNP P49189
A	-9	HIS	-	expression tag	UNP P49189
A	-8	HIS	-	expression tag	UNP P49189
A	-7	HIS	-	expression tag	UNP P49189
A	-6	HIS	-	expression tag	UNP P49189
A	-5	HIS	-	expression tag	UNP P49189
A	-4	HIS	-	expression tag	UNP P49189
A	-3	SER	-	expression tag	UNP P49189
A	-2	GLN	-	expression tag	UNP P49189
A	-1	ASP	-	expression tag	UNP P49189

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Chain	Residue	Modelled	Actual	Comment	Reference
A	0	PRO	-	expression tag	UNP P49189
B	-13	MET	-	initiating methionine	UNP P49189
B	-12	GLY	-	expression tag	UNP P49189
B	-11	SER	-	expression tag	UNP P49189
B	-10	SER	-	expression tag	UNP P49189
B	-9	HIS	-	expression tag	UNP P49189
B	-8	HIS	-	expression tag	UNP P49189
B	-7	HIS	-	expression tag	UNP P49189
B	-6	HIS	-	expression tag	UNP P49189
B	-5	HIS	-	expression tag	UNP P49189
B	-4	HIS	-	expression tag	UNP P49189
B	-3	SER	-	expression tag	UNP P49189
B	-2	GLN	-	expression tag	UNP P49189
B	-1	ASP	-	expression tag	UNP P49189
B	0	PRO	-	expression tag	UNP P49189
C	-13	MET	-	initiating methionine	UNP P49189
C	-12	GLY	-	expression tag	UNP P49189
C	-11	SER	-	expression tag	UNP P49189
C	-10	SER	-	expression tag	UNP P49189
C	-9	HIS	-	expression tag	UNP P49189
C	-8	HIS	-	expression tag	UNP P49189
C	-7	HIS	-	expression tag	UNP P49189
C	-6	HIS	-	expression tag	UNP P49189
C	-5	HIS	-	expression tag	UNP P49189
C	-4	HIS	-	expression tag	UNP P49189
C	-3	SER	-	expression tag	UNP P49189
C	-2	GLN	-	expression tag	UNP P49189
C	-1	ASP	-	expression tag	UNP P49189
C	0	PRO	-	expression tag	UNP P49189
D	-13	MET	-	initiating methionine	UNP P49189
D	-12	GLY	-	expression tag	UNP P49189
D	-11	SER	-	expression tag	UNP P49189
D	-10	SER	-	expression tag	UNP P49189
D	-9	HIS	-	expression tag	UNP P49189
D	-8	HIS	-	expression tag	UNP P49189
D	-7	HIS	-	expression tag	UNP P49189
D	-6	HIS	-	expression tag	UNP P49189
D	-5	HIS	-	expression tag	UNP P49189
D	-4	HIS	-	expression tag	UNP P49189
D	-3	SER	-	expression tag	UNP P49189
D	-2	GLN	-	expression tag	UNP P49189
D	-1	ASP	-	expression tag	UNP P49189

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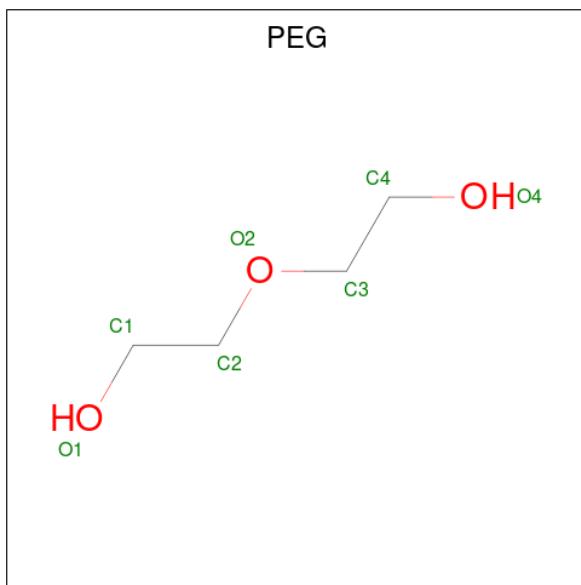
Chain	Residue	Modelled	Actual	Comment	Reference
D	0	PRO	-	expression tag	UNP P49189
E	-13	MET	-	initiating methionine	UNP P49189
E	-12	GLY	-	expression tag	UNP P49189
E	-11	SER	-	expression tag	UNP P49189
E	-10	SER	-	expression tag	UNP P49189
E	-9	HIS	-	expression tag	UNP P49189
E	-8	HIS	-	expression tag	UNP P49189
E	-7	HIS	-	expression tag	UNP P49189
E	-6	HIS	-	expression tag	UNP P49189
E	-5	HIS	-	expression tag	UNP P49189
E	-4	HIS	-	expression tag	UNP P49189
E	-3	SER	-	expression tag	UNP P49189
E	-2	GLN	-	expression tag	UNP P49189
E	-1	ASP	-	expression tag	UNP P49189
E	0	PRO	-	expression tag	UNP P49189
F	-13	MET	-	initiating methionine	UNP P49189
F	-12	GLY	-	expression tag	UNP P49189
F	-11	SER	-	expression tag	UNP P49189
F	-10	SER	-	expression tag	UNP P49189
F	-9	HIS	-	expression tag	UNP P49189
F	-8	HIS	-	expression tag	UNP P49189
F	-7	HIS	-	expression tag	UNP P49189
F	-6	HIS	-	expression tag	UNP P49189
F	-5	HIS	-	expression tag	UNP P49189
F	-4	HIS	-	expression tag	UNP P49189
F	-3	SER	-	expression tag	UNP P49189
F	-2	GLN	-	expression tag	UNP P49189
F	-1	ASP	-	expression tag	UNP P49189
F	0	PRO	-	expression tag	UNP P49189
G	-13	MET	-	initiating methionine	UNP P49189
G	-12	GLY	-	expression tag	UNP P49189
G	-11	SER	-	expression tag	UNP P49189
G	-10	SER	-	expression tag	UNP P49189
G	-9	HIS	-	expression tag	UNP P49189
G	-8	HIS	-	expression tag	UNP P49189
G	-7	HIS	-	expression tag	UNP P49189
G	-6	HIS	-	expression tag	UNP P49189
G	-5	HIS	-	expression tag	UNP P49189
G	-4	HIS	-	expression tag	UNP P49189
G	-3	SER	-	expression tag	UNP P49189
G	-2	GLN	-	expression tag	UNP P49189
G	-1	ASP	-	expression tag	UNP P49189

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Chain	Residue	Modelled	Actual	Comment	Reference
G	0	PRO	-	expression tag	UNP P49189
H	-13	MET	-	initiating methionine	UNP P49189
H	-12	GLY	-	expression tag	UNP P49189
H	-11	SER	-	expression tag	UNP P49189
H	-10	SER	-	expression tag	UNP P49189
H	-9	HIS	-	expression tag	UNP P49189
H	-8	HIS	-	expression tag	UNP P49189
H	-7	HIS	-	expression tag	UNP P49189
H	-6	HIS	-	expression tag	UNP P49189
H	-5	HIS	-	expression tag	UNP P49189
H	-4	HIS	-	expression tag	UNP P49189
H	-3	SER	-	expression tag	UNP P49189
H	-2	GLN	-	expression tag	UNP P49189
H	-1	ASP	-	expression tag	UNP P49189
H	0	PRO	-	expression tag	UNP P49189

- Molecule 2 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: C<sub>4</sub>H<sub>10</sub>O<sub>3</sub>) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	B	1	Total    C    O 7    4    3	0	0

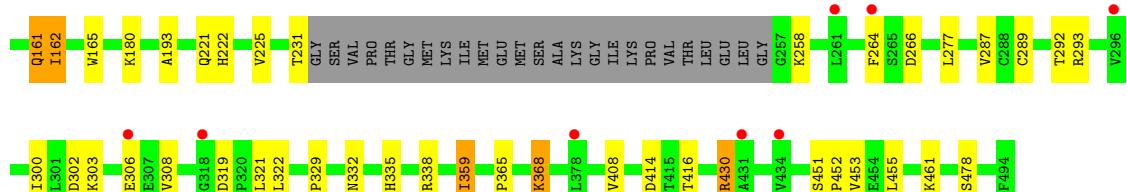
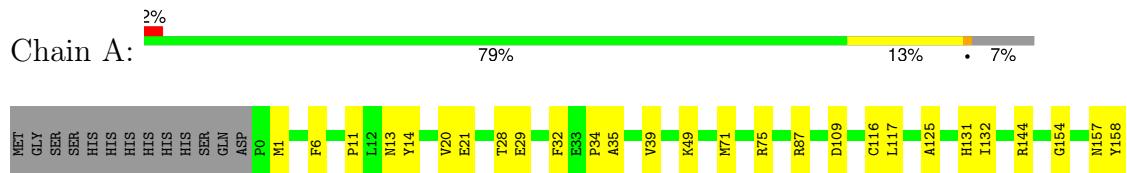
- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total O 1 1	0	0
3	B	4	Total O 4 4	0	0
3	C	5	Total O 5 5	0	0
3	D	7	Total O 7 7	0	0
3	E	3	Total O 3 3	0	0
3	F	4	Total O 4 4	0	0
3	H	2	Total O 2 2	0	0

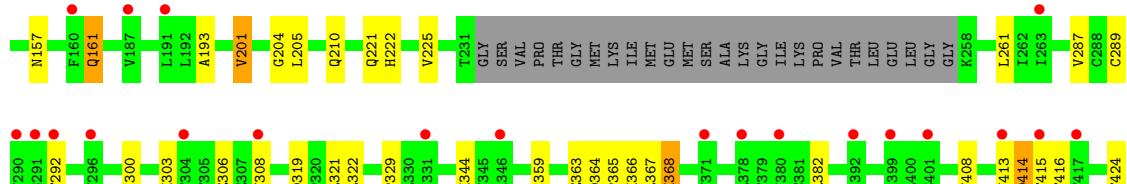
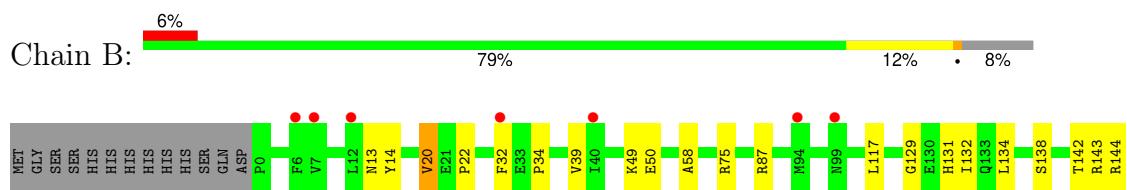
### 3 Residue-property plots

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 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.

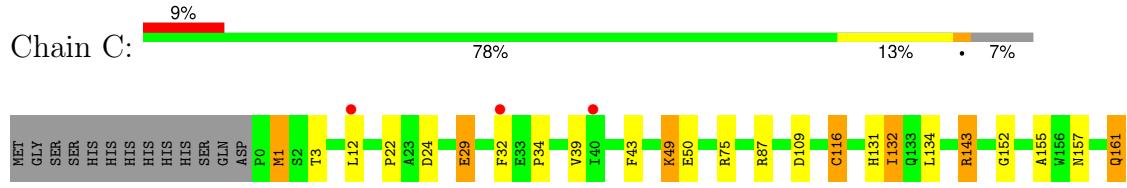
- Molecule 1: 4-trimethylaminobutyraldehyde dehydrogenase

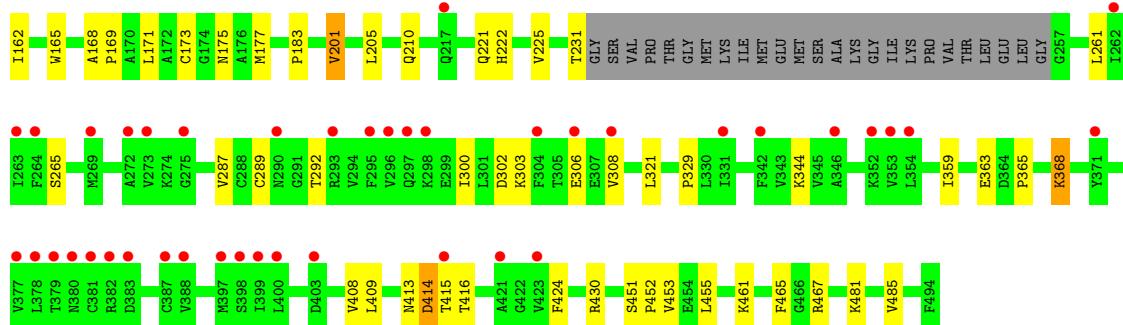


- Molecule 1: 4-trimethylaminobutyraldehyde dehydrogenase

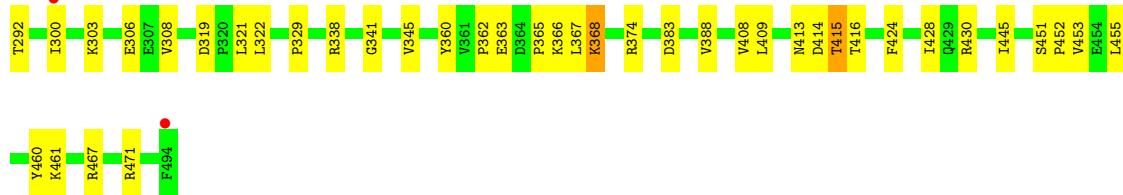
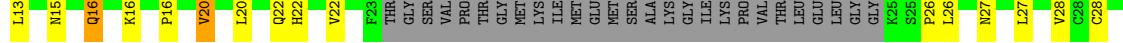
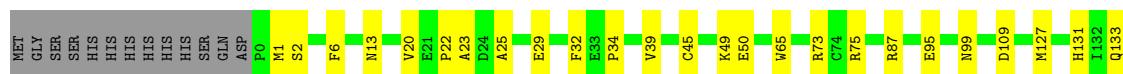
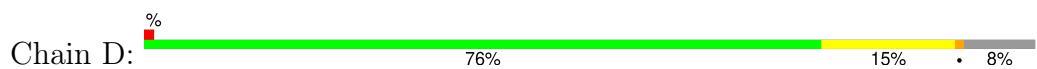


- Molecule 1: 4-trimethylaminobutyraldehyde dehydrogenase

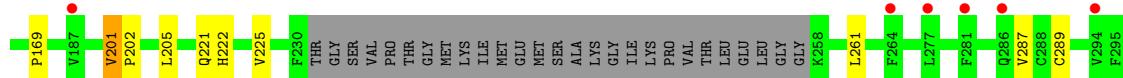
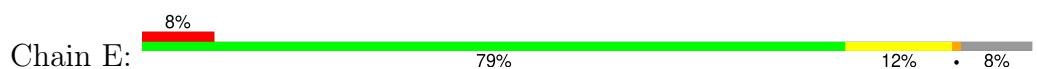




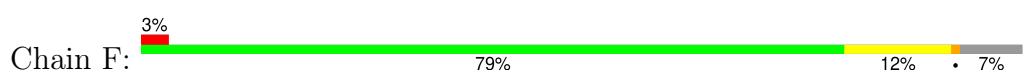
- Molecule 1: 4-trimethylaminobutyraldehyde dehydrogenase

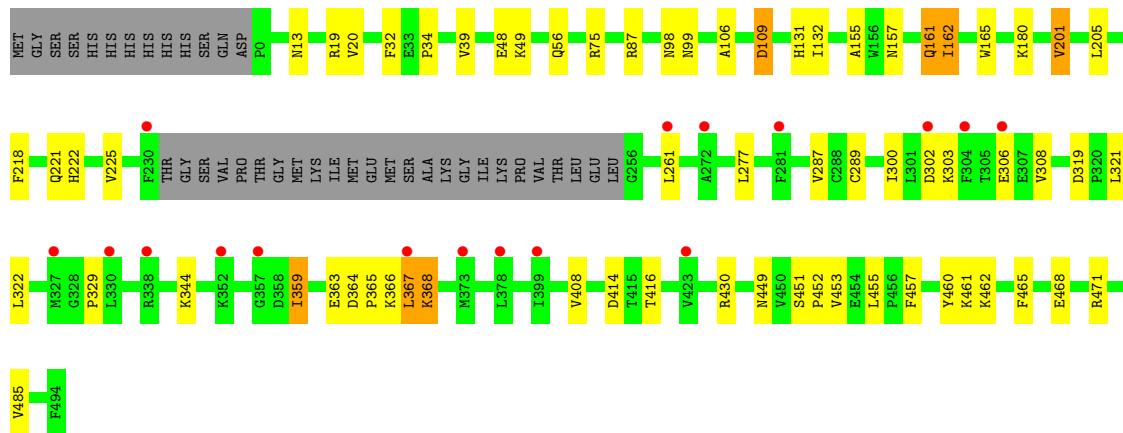


- Molecule 1: 4-trimethylaminobutyraldehyde dehydrogenase

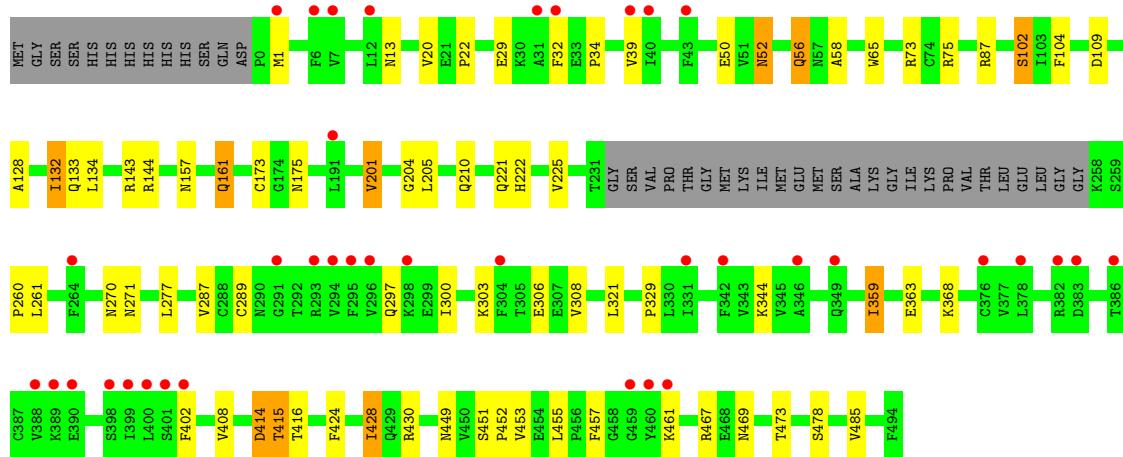
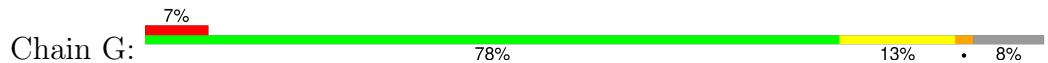


- Molecule 1: 4-trimethylaminobutyraldehyde dehydrogenase

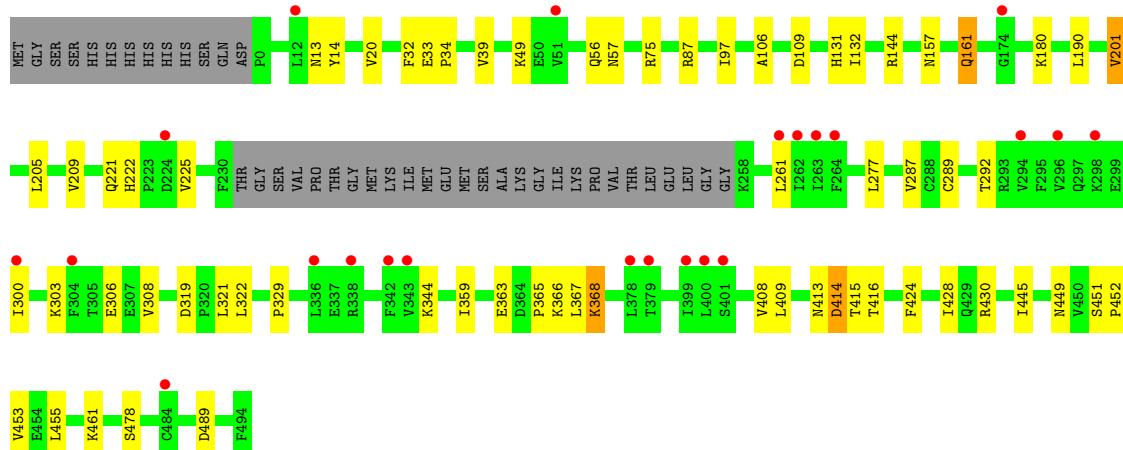
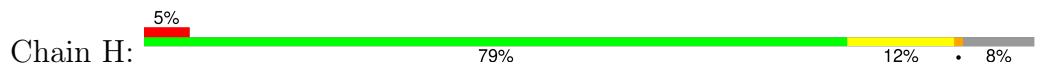




- Molecule 1: 4-trimethylaminobutyraldehyde dehydrogenase



- Molecule 1: 4-trimethylaminobutyraldehyde dehydrogenase



## 4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	113.73Å    167.45Å    116.14Å 90.00°    90.94°    90.00°	Depositor
Resolution (Å)	49.71 – 2.89 49.71 – 2.89	Depositor EDS
% Data completeness (in resolution range)	99.5 (49.71-2.89) 99.5 (49.71-2.89)	Depositor EDS
$R_{merge}$	0.20	Depositor
$R_{sym}$	0.19	Depositor
$< I/\sigma(I) >$ <sup>1</sup>	1.61 (at 2.91Å)	Xtriage
Refinement program	BUSTER 2.10.3	Depositor
$R$ , $R_{free}$	0.179 , 0.213 0.193 , 0.227	Depositor DCC
$R_{free}$ test set	4819 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	79.7	Xtriage
Anisotropy	0.246	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 69.8	EDS
L-test for twinning <sup>2</sup>	$<  L  > = 0.49$ , $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.000 for l,k,-h 0.016 for h,-k,-l 0.014 for l,-k,h	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	28772	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	89.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.21% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $< |L| >$ ,  $< L^2 >$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 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:  
PEG

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	0.54	0/3672	0.73	0/4966
1	B	0.51	0/3668	0.71	0/4961
1	C	0.50	0/3672	0.71	0/4966
1	D	0.55	0/3669	0.73	0/4961
1	E	0.52	0/3637	0.72	0/4917
1	F	0.52	0/3669	0.71	0/4961
1	G	0.52	0/3668	0.72	0/4961
1	H	0.52	0/3661	0.71	0/4951
All	All	0.52	0/29316	0.72	0/39644

There are no bond length outliers.

There are no bond angle outliers.

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	3600	0	3574	28	0
1	B	3596	0	3571	27	0
1	C	3600	0	3574	34	0
1	D	3594	0	3573	34	0
1	E	3567	0	3544	31	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	F	3597	0	3570	27	0
1	G	3596	0	3571	31	0
1	H	3589	0	3564	26	0
2	B	7	0	10	0	0
3	A	1	0	0	0	0
3	B	4	0	0	0	0
3	C	5	0	0	0	0
3	D	7	0	0	0	0
3	E	3	0	0	0	0
3	F	4	0	0	0	0
3	H	2	0	0	0	0
All	All	28772	0	28551	220	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 4.

All (220) 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:154:GLY:HA2	1:A:162:ILE:HD11	1.36	1.05
1:E:132:ILE:HD13	1:F:457:PHE:CZ	2.12	0.84
1:A:258:LYS:HD2	1:A:293:ARG:HG3	1.61	0.81
1:E:201:VAL:HG13	1:E:205:LEU:HB3	1.62	0.79
1:G:457:PHE:CZ	1:H:132:ILE:HD13	2.20	0.77
1:F:201:VAL:HG13	1:F:205:LEU:HB3	1.75	0.69
1:D:260:PRO:HD3	1:D:415:THR:HG21	1.75	0.68
1:G:260:PRO:HD3	1:G:415:THR:HG21	1.74	0.68
1:B:201:VAL:HG13	1:B:205:LEU:HB3	1.77	0.66
1:G:428:ILE:HD13	1:G:428:ILE:H	1.61	0.66
1:C:201:VAL:HG13	1:C:205:LEU:HB3	1.76	0.66
1:F:300:ILE:HA	1:F:303:LYS:HE2	1.79	0.65
1:B:300:ILE:HA	1:B:303:LYS:HE2	1.80	0.64
1:G:300:ILE:HA	1:G:303:LYS:HE2	1.80	0.64
1:D:201:VAL:HG13	1:D:205:LEU:HB3	1.78	0.64
1:A:300:ILE:HA	1:A:303:LYS:HE2	1.80	0.63
1:C:300:ILE:HA	1:C:303:LYS:HE2	1.80	0.63
1:G:102:SER:HB2	1:G:104:PHE:HB3	1.81	0.62
1:E:300:ILE:HA	1:E:303:LYS:HE2	1.80	0.62
1:D:300:ILE:HA	1:D:303:LYS:HE2	1.81	0.62
1:F:161:GLN:OE1	1:F:452:PRO:HG2	1.99	0.62
1:C:29:GLU:HG2	1:C:183:PRO:HB2	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:143:ARG:HD3	1:D:133:GLN:HG3	1.82	0.62
1:H:300:ILE:HA	1:H:303:LYS:HE2	1.82	0.61
1:C:143:ARG:HH21	1:C:481:LYS:HD2	1.65	0.61
1:B:13:ASN:HB2	1:B:20:VAL:O	2.02	0.59
1:A:332:ASN:OD1	1:A:335:HIS:HB2	2.02	0.59
1:G:201:VAL:HG13	1:G:205:LEU:HB3	1.84	0.59
1:G:32:PHE:CE1	1:G:39:VAL:HG22	2.37	0.59
1:F:131:HIS:HB2	1:H:131:HIS:HB2	1.86	0.58
1:G:58:ALA:HA	1:G:204:GLY:O	2.04	0.57
1:D:34:PRO:HB2	1:D:329:PRO:HG2	1.87	0.56
1:D:362:PRO:HG2	1:D:367:LEU:HB3	1.86	0.56
1:A:14:TYR:CD2	1:A:193:ALA:HB1	2.41	0.56
1:F:366:LYS:HG3	1:F:367:LEU:HD13	1.87	0.56
1:F:165:TRP:HH2	1:F:465:PHE:HE2	1.53	0.56
1:E:8:VAL:HG11	1:E:12:LEU:HD21	1.89	0.55
1:H:201:VAL:HG13	1:H:205:LEU:HB3	1.88	0.55
1:E:34:PRO:HB2	1:E:329:PRO:HG2	1.88	0.55
1:A:264:PHE:HB3	1:A:430:ARG:HH21	1.71	0.55
1:A:34:PRO:HB2	1:A:329:PRO:HG2	1.89	0.55
1:B:131:HIS:HB2	1:D:131:HIS:HB2	1.88	0.54
1:A:359:ILE:H	1:A:359:ILE:HD12	1.72	0.54
1:G:297:GLN:HG3	1:G:402:PHE:CE1	2.43	0.54
1:B:364:ASP:HB3	1:B:367:LEU:HD22	1.90	0.54
1:D:161:GLN:OE1	1:D:452:PRO:HG2	2.08	0.54
1:F:365:PRO:O	1:F:368:LYS:HB2	2.08	0.54
1:C:152:GLY:HA3	1:C:177:MET:CE	2.38	0.54
1:H:409:LEU:O	1:H:413:ASN:HB2	2.08	0.53
1:H:34:PRO:HB2	1:H:329:PRO:HG2	1.89	0.53
1:B:451:SER:HB2	1:B:455:LEU:HD12	1.91	0.53
1:E:359:ILE:HD12	1:E:359:ILE:H	1.73	0.53
1:F:165:TRP:CH2	1:F:465:PHE:HE2	2.26	0.53
1:G:132:ILE:HG22	1:G:134:LEU:CD1	2.39	0.53
1:F:34:PRO:HB2	1:F:329:PRO:HG2	1.90	0.53
1:G:359:ILE:HD12	1:G:359:ILE:H	1.74	0.53
1:A:365:PRO:O	1:A:368:LYS:HB2	2.10	0.52
1:E:161:GLN:OE1	1:E:452:PRO:HG2	2.09	0.52
1:E:132:ILE:HD11	1:G:128:ALA:HB2	1.90	0.52
1:E:451:SER:HB2	1:E:455:LEU:HD12	1.92	0.52
1:E:132:ILE:HG22	1:E:134:LEU:CD1	2.40	0.52
1:A:158:TYR:HB2	1:A:162:ILE:HG23	1.92	0.51
1:H:365:PRO:O	1:H:368:LYS:HB2	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:132:ILE:HG22	1:C:134:LEU:CD1	2.39	0.51
1:C:451:SER:HB2	1:C:455:LEU:HD12	1.92	0.51
1:H:106:ALA:O	1:H:109:ASP:HB2	2.11	0.51
1:B:34:PRO:HB2	1:B:329:PRO:HG2	1.92	0.51
1:C:152:GLY:HA3	1:C:177:MET:HE1	1.92	0.51
1:H:161:GLN:OE1	1:H:452:PRO:HG2	2.11	0.51
1:B:161:GLN:OE1	1:B:452:PRO:HG2	2.11	0.51
1:C:34:PRO:HB2	1:C:329:PRO:HG2	1.92	0.51
1:D:366:LYS:HG3	1:D:367:LEU:HD13	1.92	0.51
1:C:161:GLN:OE1	1:C:452:PRO:HG2	2.11	0.51
1:G:34:PRO:HB2	1:G:329:PRO:HG2	1.92	0.51
1:C:162:ILE:HD11	1:C:231:THR:OG1	2.10	0.51
1:F:165:TRP:HH2	1:F:465:PHE:CE2	2.30	0.50
1:F:451:SER:HB2	1:F:455:LEU:HD12	1.93	0.50
1:B:359:ILE:HD12	1:B:359:ILE:H	1.76	0.50
1:B:428:ILE:HD12	1:D:428:ILE:HD12	1.93	0.50
1:F:359:ILE:H	1:F:359:ILE:HD12	1.75	0.50
1:E:332:ASN:OD1	1:E:335:HIS:HB2	2.12	0.50
1:H:451:SER:HB2	1:H:455:LEU:HD12	1.94	0.49
1:B:366:LYS:HG3	1:B:367:LEU:HD13	1.94	0.49
1:D:166:LYS:O	1:D:169:PRO:HD2	2.13	0.49
1:C:24:ASP:HB2	1:C:49:LYS:HB2	1.94	0.49
1:C:409:LEU:O	1:C:413:ASN:HB2	2.13	0.49
1:C:365:PRO:O	1:C:368:LYS:HB2	2.12	0.49
1:A:365:PRO:HD2	1:E:23:ALA:HB1	1.95	0.49
1:B:58:ALA:HA	1:B:204:GLY:O	2.11	0.49
1:G:161:GLN:OE1	1:G:452:PRO:HG2	2.12	0.49
1:G:451:SER:HB2	1:G:455:LEU:HD12	1.94	0.49
1:E:201:VAL:HG22	1:E:205:LEU:HD23	1.93	0.49
1:H:359:ILE:HD12	1:H:359:ILE:H	1.76	0.48
1:G:22:PRO:HB3	1:G:50:GLU:HG2	1.93	0.48
1:H:366:LYS:HG3	1:H:367:LEU:HD13	1.95	0.48
1:B:365:PRO:O	1:B:368:LYS:HB2	2.14	0.48
1:C:359:ILE:HD12	1:C:359:ILE:H	1.77	0.48
1:E:365:PRO:O	1:E:368:LYS:HB2	2.13	0.48
1:E:143:ARG:HD3	1:G:133:GLN:HG3	1.95	0.48
1:A:131:HIS:HB2	1:C:131:HIS:HB2	1.96	0.48
1:E:222:HIS:HB3	1:E:225:VAL:HG23	1.96	0.48
1:D:451:SER:HB2	1:D:455:LEU:HD12	1.95	0.47
1:F:13:ASN:HB2	1:F:20:VAL:O	2.14	0.47
1:D:365:PRO:O	1:D:368:LYS:HB2	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:116:CYS:HB2	1:C:165:TRP:CZ3	2.49	0.47
1:B:210:GLN:HA	1:B:210:GLN:NE2	2.30	0.47
1:D:409:LEU:O	1:D:413:ASN:HB2	2.14	0.47
1:D:360:TYR:HB2	1:D:374:ARG:HG3	1.96	0.47
1:E:65:TRP:CE2	1:E:73:ARG:HD2	2.50	0.47
1:A:32:PHE:CE2	1:A:39:VAL:HG22	2.50	0.47
1:A:1:MET:SD	1:A:6:PHE:HB2	2.56	0.46
1:E:13:ASN:HB2	1:E:20:VAL:O	2.15	0.46
1:E:201:VAL:CG1	1:E:205:LEU:HB3	2.41	0.46
1:A:158:TYR:O	1:A:162:ILE:HG23	2.15	0.46
1:A:71:MET:CE	1:A:125:ALA:HB1	2.46	0.46
1:D:23:ALA:HB1	1:H:365:PRO:HD2	1.97	0.46
1:E:133:GLN:HG3	1:G:143:ARG:HD3	1.97	0.46
1:H:13:ASN:HB2	1:H:20:VAL:O	2.16	0.46
1:F:364:ASP:HB3	1:F:367:LEU:HD22	1.97	0.46
1:G:210:GLN:OE1	1:G:210:GLN:HA	2.16	0.46
1:B:222:HIS:HB3	1:B:225:VAL:HG23	1.97	0.45
1:C:168:ALA:HB3	1:C:169:PRO:HD3	1.98	0.45
1:D:1[B]:MET:HE3	1:D:2:SER:H	1.81	0.45
1:G:428:ILE:H	1:G:428:ILE:CD1	2.28	0.45
1:B:14:TYR:CD2	1:B:193:ALA:HB1	2.51	0.45
1:D:65:TRP:CE2	1:D:73:ARG:HD2	2.52	0.45
1:F:32:PHE:CE2	1:F:39:VAL:HG22	2.50	0.45
1:E:445:ILE:HD12	1:F:485:VAL:HG22	1.98	0.45
1:D:287:VAL:HG12	1:D:289:CYS:H	1.82	0.45
1:F:13:ASN:O	1:F:19:ARG:HA	2.17	0.45
1:C:287:VAL:HG12	1:C:289:CYS:H	1.82	0.45
1:F:201:VAL:CG1	1:F:205:LEU:HB3	2.46	0.45
1:C:261:LEU:HD11	1:C:424:PHE:HE1	1.81	0.45
1:D:95:GLU:O	1:D:99:ASN:HB3	2.17	0.45
1:F:222:HIS:HB3	1:F:225:VAL:HG23	1.98	0.45
1:G:287:VAL:HG12	1:G:289:CYS:H	1.82	0.45
1:A:451:SER:HB2	1:A:455:LEU:HD22	1.98	0.45
1:C:222:HIS:HB3	1:C:225:VAL:HG23	1.99	0.45
1:E:287:VAL:HG12	1:E:289:CYS:H	1.81	0.45
1:C:485:VAL:HG22	1:D:445:ILE:HD12	1.99	0.45
1:G:261:LEU:HD11	1:G:424:PHE:HE1	1.82	0.45
1:C:210:GLN:HA	1:C:210:GLN:NE2	2.32	0.44
1:F:468:GLU:HG3	1:F:471:ARG:HH22	1.83	0.44
1:B:287:VAL:HG12	1:B:289:CYS:H	1.82	0.44
1:G:222:HIS:HB3	1:G:225:VAL:HG23	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:261:LEU:HD11	1:D:424:PHE:HE1	1.83	0.44
1:G:144:ARG:HD3	1:G:478:SER:OG	2.18	0.44
1:B:261:LEU:HD11	1:B:424:PHE:HE1	1.83	0.44
1:G:13:ASN:HB2	1:G:20:VAL:O	2.18	0.44
1:D:1[B]:MET:CE	1:D:6:PHE:HB2	2.47	0.44
1:G:485:VAL:HG22	1:H:445:ILE:HD12	2.00	0.44
1:H:222:HIS:HB3	1:H:225:VAL:HG23	2.00	0.44
1:B:22:PRO:HB3	1:B:50:GLU:HG2	2.00	0.43
1:A:158:TYR:HB3	1:A:161:GLN:HB3	2.00	0.43
1:G:52:ASN:O	1:G:56:GLN:HB2	2.19	0.43
1:A:116:CYS:HB2	1:A:165:TRP:CZ3	2.53	0.43
1:E:6:PHE:O	1:E:40:ILE:HG22	2.18	0.43
1:A:161:GLN:OE1	1:A:452:PRO:HG2	2.18	0.43
1:E:144:ARG:HD3	1:E:478:SER:OG	2.19	0.43
1:A:287:VAL:HG12	1:A:289:CYS:H	1.82	0.43
1:B:134:LEU:HB2	1:B:138:SER:O	2.19	0.43
1:D:32:PHE:CE2	1:D:39:VAL:HG22	2.53	0.43
1:H:32:PHE:CE2	1:H:39:VAL:HG22	2.53	0.43
1:E:32:PHE:CE2	1:E:39:VAL:HG22	2.53	0.43
1:H:413:ASN:C	1:H:415:THR:H	2.22	0.43
1:A:13:ASN:HB2	1:A:20:VAL:O	2.18	0.43
1:B:32:PHE:CE2	1:B:39:VAL:HG22	2.54	0.43
1:C:32:PHE:CE2	1:C:39:VAL:HG22	2.53	0.43
1:C:173:CYS:HB2	1:C:175:ASN:ND2	2.33	0.43
1:F:287:VAL:HG12	1:F:289:CYS:H	1.83	0.43
1:B:144:ARG:HD3	1:B:478:SER:OG	2.19	0.42
1:D:383:ASP:HA	1:D:388:VAL:HG11	2.01	0.42
1:F:106:ALA:O	1:F:109:ASP:HB2	2.18	0.42
1:D:22:PRO:HB3	1:D:50:GLU:HG2	2.01	0.42
1:H:287:VAL:HG12	1:H:289:CYS:H	1.84	0.42
1:C:1:MET:H	1:C:1:MET:HG3	1.74	0.42
1:G:173:CYS:HB2	1:G:175:ASN:ND2	2.34	0.42
1:G:469:ASN:O	1:G:473:THR:HG23	2.19	0.42
1:H:261:LEU:HD11	1:H:424:PHE:HE1	1.83	0.42
1:B:413:ASN:C	1:B:415:THR:H	2.23	0.42
1:D:25:ALA:HA	1:D:45:CYS:O	2.19	0.42
1:E:353:VAL:HG22	1:E:378:LEU:HD21	2.01	0.42
1:A:222:HIS:HB3	1:A:225:VAL:HG23	2.02	0.42
1:B:364:ASP:HA	1:B:365:PRO:HD3	1.97	0.42
1:D:319:ASP:HB3	1:D:322:LEU:HD22	2.02	0.42
1:C:134:LEU:HD23	1:D:460:TYR:CD2	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:202:PRO:HD2	1:E:205:LEU:HD22	2.02	0.41
1:E:402:PHE:CG	1:E:408:VAL:HG13	2.55	0.41
1:A:144:ARG:HD3	1:A:478:SER:OG	2.20	0.41
1:E:261:LEU:HD11	1:E:424:PHE:HE1	1.85	0.41
1:H:33:GLU:HA	1:H:97:ILE:O	2.19	0.41
1:B:129:GLY:HA3	1:B:142:THR:O	2.20	0.41
1:D:222:HIS:HB3	1:D:225:VAL:HG23	2.01	0.41
1:F:155:ALA:H	1:F:162:ILE:HG21	1.85	0.41
1:G:271:ASN:OD1	1:H:489:ASP:HA	2.21	0.41
1:C:155:ALA:H	1:C:162:ILE:HG21	1.86	0.41
1:G:65:TRP:CE2	1:G:73:ARG:HD2	2.55	0.41
1:H:180:LYS:HA	1:H:209:VAL:O	2.21	0.41
1:H:319:ASP:HB3	1:H:322:LEU:HD22	2.01	0.41
1:A:71:MET:HE2	1:A:125:ALA:HB1	2.01	0.41
1:D:341:GLY:O	1:D:345:VAL:HG23	2.20	0.41
1:A:11:PRO:HB3	1:A:21:GLU:HG2	2.02	0.41
1:D:467:ARG:HG2	1:D:471:ARG:HH21	1.85	0.41
1:A:35:ALA:HA	1:A:329:PRO:HG3	2.03	0.41
1:A:319:ASP:HB3	1:A:322:LEU:HD22	2.03	0.41
1:B:319:ASP:HB3	1:B:322:LEU:HD22	2.03	0.41
1:C:12:LEU:HD12	1:C:43:PHE:HB3	2.03	0.41
1:E:169:PRO:HB2	1:E:477:TYR:CD2	2.56	0.41
1:H:14:TYR:HB2	1:H:190:LEU:HD23	2.03	0.41
1:C:22:PRO:HB3	1:C:50:GLU:HG2	2.03	0.41
1:E:134:LEU:HD23	1:F:460:TYR:CD2	2.56	0.41
1:F:319:ASP:HB3	1:F:322:LEU:HD22	2.03	0.41
1:C:165:TRP:HH2	1:C:465:PHE:CE1	2.39	0.40
1:D:1[B]:MET:HE2	1:D:6:PHE:HB2	2.02	0.40
1:C:132:ILE:HG22	1:C:134:LEU:HD11	2.03	0.40
1:C:413:ASN:C	1:C:415:THR:H	2.25	0.40
1:F:48:GLU:HB3	1:F:218:PHE:CD1	2.57	0.40
1:C:265:SER:HA	1:C:300:ILE:HG12	2.03	0.40
1:D:13:ASN:HB2	1:D:20:VAL:O	2.20	0.40
1:H:144:ARG:HD3	1:H:478:SER:OG	2.21	0.40

There are no symmetry-related clashes.

## 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	466/508 (92%)	452 (97%)	13 (3%)	1 (0%)	47 78
1	B	465/508 (92%)	452 (97%)	11 (2%)	2 (0%)	34 66
1	C	466/508 (92%)	452 (97%)	13 (3%)	1 (0%)	47 78
1	D	465/508 (92%)	452 (97%)	11 (2%)	2 (0%)	34 66
1	E	459/508 (90%)	445 (97%)	12 (3%)	2 (0%)	34 66
1	F	466/508 (92%)	454 (97%)	10 (2%)	2 (0%)	34 66
1	G	465/508 (92%)	451 (97%)	11 (2%)	3 (1%)	25 58
1	H	464/508 (91%)	452 (97%)	10 (2%)	2 (0%)	34 66
All	All	3716/4064 (91%)	3610 (97%)	91 (2%)	15 (0%)	34 66

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	461	LYS
1	F	461	LYS
1	G	368	LYS
1	A	461	LYS
1	D	414	ASP
1	G	414	ASP
1	G	461	LYS
1	H	461	LYS
1	B	461	LYS
1	D	461	LYS
1	F	414	ASP
1	C	414	ASP
1	E	414	ASP
1	B	414	ASP
1	H	414	ASP

### 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	384/416 (92%)	355 (92%)	29 (8%)	13 36
1	B	384/416 (92%)	359 (94%)	25 (6%)	17 45
1	C	384/416 (92%)	354 (92%)	30 (8%)	12 34
1	D	384/416 (92%)	359 (94%)	25 (6%)	17 45
1	E	381/416 (92%)	360 (94%)	21 (6%)	21 53
1	F	383/416 (92%)	352 (92%)	31 (8%)	11 33
1	G	384/416 (92%)	354 (92%)	30 (8%)	12 34
1	H	383/416 (92%)	359 (94%)	24 (6%)	18 46
All	All	3067/3328 (92%)	2852 (93%)	215 (7%)	15 41

All (215) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	28	THR
1	A	29	GLU
1	A	49	LYS
1	A	75	ARG
1	A	87	ARG
1	A	109	ASP
1	A	117	LEU
1	A	132	ILE
1	A	157	ASN
1	A	161	GLN
1	A	162	ILE
1	A	180	LYS
1	A	221	GLN
1	A	231	THR
1	A	266	ASP
1	A	277	LEU
1	A	292	THR
1	A	302	ASP
1	A	306	GLU

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Mol	Chain	Res	Type
1	A	308	VAL
1	A	321	LEU
1	A	338	ARG
1	A	359	ILE
1	A	368	LYS
1	A	408	VAL
1	A	414	ASP
1	A	416	THR
1	A	430	ARG
1	A	453	VAL
1	B	20	VAL
1	B	49	LYS
1	B	75	ARG
1	B	87	ARG
1	B	117	LEU
1	B	132	ILE
1	B	157	ASN
1	B	161	GLN
1	B	201	VAL
1	B	221	GLN
1	B	292	THR
1	B	306	GLU
1	B	308	VAL
1	B	321	LEU
1	B	344	LYS
1	B	363	GLU
1	B	368	LYS
1	B	382	ARG
1	B	408	VAL
1	B	414	ASP
1	B	416	THR
1	B	429	GLN
1	B	430	ARG
1	B	453	VAL
1	B	467	ARG
1	C	1	MET
1	C	3	THR
1	C	29	GLU
1	C	49	LYS
1	C	75	ARG
1	C	87	ARG
1	C	109	ASP

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Mol	Chain	Res	Type
1	C	116	CYS
1	C	132	ILE
1	C	143	ARG
1	C	157	ASN
1	C	161	GLN
1	C	171	LEU
1	C	201	VAL
1	C	221	GLN
1	C	292	THR
1	C	302	ASP
1	C	306	GLU
1	C	308	VAL
1	C	321	LEU
1	C	344	LYS
1	C	363	GLU
1	C	368	LYS
1	C	408	VAL
1	C	414	ASP
1	C	416	THR
1	C	430	ARG
1	C	453	VAL
1	C	461	LYS
1	C	467	ARG
1	D	29	GLU
1	D	49	LYS
1	D	75	ARG
1	D	87	ARG
1	D	109	ASP
1	D	127	MET
1	D	134	LEU
1	D	157	ASN
1	D	161	GLN
1	D	201	VAL
1	D	221	GLN
1	D	270	ASN
1	D	277	LEU
1	D	292	THR
1	D	306	GLU
1	D	308	VAL
1	D	321	LEU
1	D	338	ARG
1	D	363	GLU

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Mol	Chain	Res	Type
1	D	368	LYS
1	D	408	VAL
1	D	415	THR
1	D	416	THR
1	D	430	ARG
1	D	453	VAL
1	E	1	MET
1	E	29	GLU
1	E	49	LYS
1	E	75	ARG
1	E	87	ARG
1	E	157	ASN
1	E	161	GLN
1	E	164	SER
1	E	201	VAL
1	E	221	GLN
1	E	302	ASP
1	E	306	GLU
1	E	308	VAL
1	E	321	LEU
1	E	363	GLU
1	E	368	LYS
1	E	408	VAL
1	E	414	ASP
1	E	430	ARG
1	E	449	ASN
1	E	453	VAL
1	F	49	LYS
1	F	56	GLN
1	F	75	ARG
1	F	87	ARG
1	F	98	ASN
1	F	99	ASN
1	F	109	ASP
1	F	132	ILE
1	F	157	ASN
1	F	161	GLN
1	F	162	ILE
1	F	180	LYS
1	F	201	VAL
1	F	221	GLN
1	F	261	LEU

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Mol	Chain	Res	Type
1	F	277	LEU
1	F	302	ASP
1	F	306	GLU
1	F	308	VAL
1	F	321	LEU
1	F	344	LYS
1	F	359	ILE
1	F	363	GLU
1	F	367	LEU
1	F	368	LYS
1	F	408	VAL
1	F	416	THR
1	F	430	ARG
1	F	449	ASN
1	F	453	VAL
1	F	462	LYS
1	G	1	MET
1	G	29	GLU
1	G	52	ASN
1	G	56	GLN
1	G	75	ARG
1	G	87	ARG
1	G	102	SER
1	G	109	ASP
1	G	132	ILE
1	G	157	ASN
1	G	161	GLN
1	G	201	VAL
1	G	221	GLN
1	G	270	ASN
1	G	277	LEU
1	G	306	GLU
1	G	308	VAL
1	G	321	LEU
1	G	344	LYS
1	G	359	ILE
1	G	363	GLU
1	G	408	VAL
1	G	414	ASP
1	G	415	THR
1	G	416	THR
1	G	428	ILE

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Mol	Chain	Res	Type
1	G	430	ARG
1	G	449	ASN
1	G	453	VAL
1	G	467	ARG
1	H	49	LYS
1	H	56	GLN
1	H	57	ASN
1	H	75	ARG
1	H	87	ARG
1	H	157	ASN
1	H	161	GLN
1	H	201	VAL
1	H	221	GLN
1	H	277	LEU
1	H	292	THR
1	H	306	GLU
1	H	308	VAL
1	H	321	LEU
1	H	344	LYS
1	H	363	GLU
1	H	368	LYS
1	H	408	VAL
1	H	414	ASP
1	H	416	THR
1	H	428	ILE
1	H	430	ARG
1	H	449	ASN
1	H	453	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	G	270	ASN
1	H	469	ASN

### 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 monosaccharides in this entry.

## 5.6 Ligand geometry [\(i\)](#)

1 ligand is modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	PEG	B	501	-	6,6,6	0.44	0	5,5,5	0.35	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
2	PEG	B	501	-	-	1/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

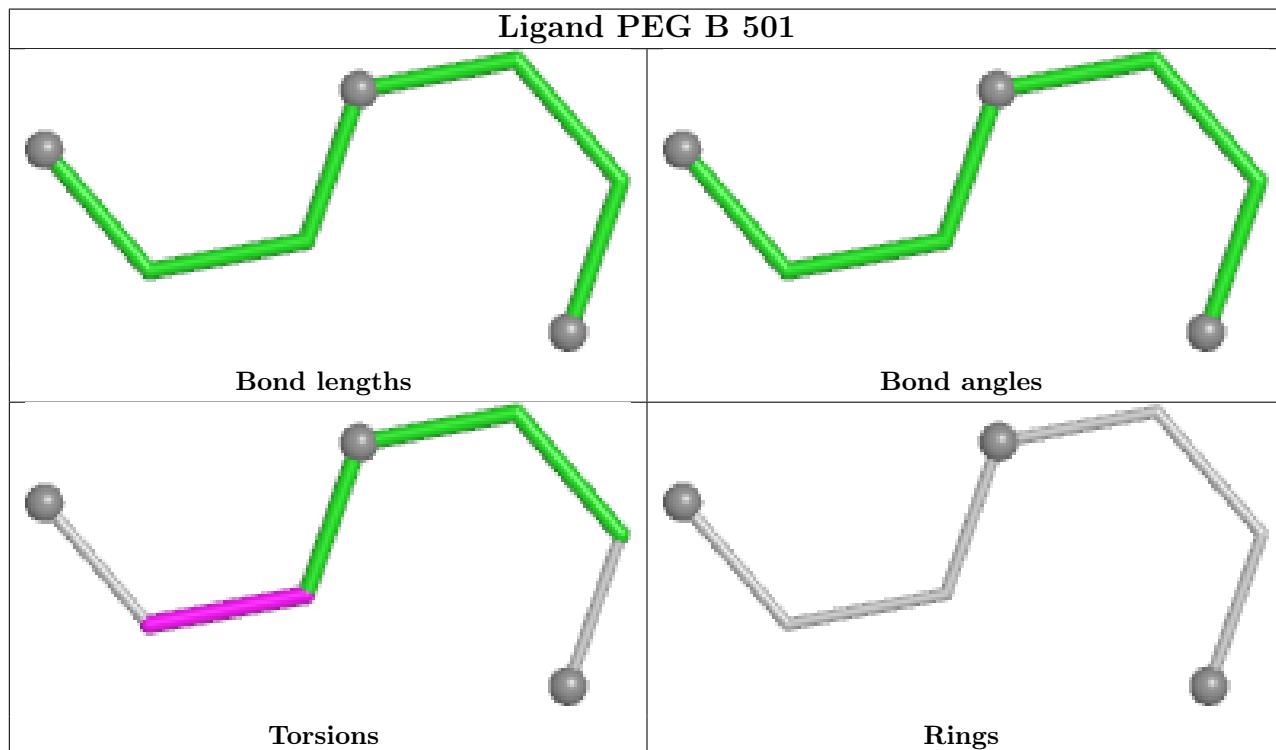
All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	501	PEG	O1-C1-C2-O2

There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



## 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 (i)

### 6.1 Protein, DNA and RNA chains (i)

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	470/508 (92%)	0.30	8 (1%) 70 69	54, 78, 112, 127	0
1	B	469/508 (92%)	0.54	29 (6%) 20 16	53, 87, 116, 132	0
1	C	470/508 (92%)	0.61	44 (9%) 8 6	60, 99, 135, 157	0
1	D	468/508 (92%)	0.24	3 (0%) 89 89	53, 75, 107, 143	0
1	E	465/508 (91%)	0.51	41 (8%) 10 7	54, 86, 133, 167	0
1	F	470/508 (92%)	0.35	17 (3%) 42 37	59, 88, 124, 148	0
1	G	469/508 (92%)	0.52	38 (8%) 12 9	58, 87, 120, 137	0
1	H	468/508 (92%)	0.46	23 (4%) 29 26	61, 90, 123, 141	0
All	All	3749/4064 (92%)	0.44	203 (5%) 25 22	53, 86, 124, 167	0

All (203) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	399	ILE	5.3
1	E	304	PHE	5.3
1	C	304	PHE	5.3
1	C	380	ASN	5.0
1	B	12	LEU	4.5
1	C	400	LEU	4.5
1	H	51	VAL	4.5
1	G	40	ILE	4.5
1	C	262	ILE	4.5
1	C	353	VAL	4.5
1	B	415	THR	4.4
1	H	336	LEU	4.4
1	E	399	ILE	4.3
1	H	12	LEU	4.2
1	C	12	LEU	4.2
1	C	378	LEU	4.1

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Mol	Chain	Res	Type	RSRZ
1	E	378	LEU	4.1
1	D	494	PHE	4.0
1	C	346	ALA	4.0
1	C	403	ASP	3.9
1	B	346	ALA	3.8
1	C	263	ILE	3.8
1	C	379	THR	3.8
1	C	295	PHE	3.7
1	C	398	SER	3.7
1	E	392	ILE	3.7
1	E	400	LEU	3.7
1	C	293	ARG	3.7
1	E	398	SER	3.6
1	C	264	PHE	3.6
1	B	304	PHE	3.6
1	C	352	LYS	3.6
1	G	296	VAL	3.6
1	G	378	LEU	3.6
1	G	398	SER	3.6
1	C	272	ALA	3.5
1	C	387	CYS	3.5
1	C	342	PHE	3.5
1	C	331	ILE	3.4
1	C	423	VAL	3.4
1	E	415	THR	3.4
1	E	387	CYS	3.4
1	G	191	LEU	3.4
1	F	399	ILE	3.4
1	E	393	PHE	3.4
1	B	417	PHE	3.3
1	B	378	LEU	3.3
1	G	342	PHE	3.3
1	G	294	VAL	3.3
1	A	378	LEU	3.3
1	E	300	ILE	3.3
1	G	400	LEU	3.3
1	G	383	ASP	3.3
1	H	378	LEU	3.2
1	E	342	PHE	3.2
1	A	261	LEU	3.2
1	E	281	PHE	3.2
1	C	371	TYR	3.2

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Mol	Chain	Res	Type	RSRZ
1	F	357	GLY	3.1
1	B	6	PHE	3.1
1	E	308	VAL	3.1
1	C	40	ILE	3.1
1	F	304	PHE	3.1
1	F	378	LEU	3.0
1	B	331	ILE	3.0
1	G	264	PHE	3.0
1	B	413	ASN	3.0
1	G	401	SER	3.0
1	C	381	CYS	3.0
1	E	380	ASN	3.0
1	E	389	LYS	3.0
1	E	376	CYS	2.9
1	E	404	THR	2.9
1	E	388	VAL	2.9
1	G	388	VAL	2.9
1	B	371	TYR	2.9
1	C	383	ASP	2.9
1	B	291	GLY	2.8
1	C	275	GLY	2.8
1	E	373	MET	2.8
1	G	460	TYR	2.8
1	C	354	LEU	2.8
1	E	401	SER	2.8
1	B	401	SER	2.8
1	C	32	PHE	2.8
1	E	330	LEU	2.7
1	F	272	ALA	2.7
1	G	389	LYS	2.7
1	C	397	MET	2.7
1	H	304	PHE	2.7
1	B	187	VAL	2.7
1	E	301	LEU	2.7
1	G	295	PHE	2.6
1	E	98	ASN	2.6
1	E	286	GLN	2.6
1	G	382	ARG	2.6
1	E	335	HIS	2.6
1	G	304	PHE	2.6
1	A	306	GLU	2.6
1	C	382	ARG	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	94	MET	2.6
1	C	296	VAL	2.6
1	E	306	GLU	2.6
1	F	327	MET	2.6
1	A	264	PHE	2.6
1	B	32	PHE	2.6
1	C	306	GLU	2.6
1	B	290	ASN	2.6
1	A	296	VAL	2.6
1	E	187	VAL	2.6
1	C	377	VAL	2.5
1	E	296	VAL	2.5
1	G	386	THR	2.5
1	F	338	ARG	2.5
1	B	263	ILE	2.5
1	H	401	SER	2.5
1	A	431	ALA	2.5
1	H	261	LEU	2.5
1	E	1	MET	2.5
1	E	264	PHE	2.5
1	C	290	ASN	2.5
1	G	390	GLU	2.5
1	C	415	THR	2.5
1	C	421	ALA	2.5
1	H	174	GLY	2.5
1	F	330	LEU	2.5
1	G	331	ILE	2.5
1	H	400	LEU	2.4
1	C	298	LYS	2.4
1	H	484	CYS	2.4
1	G	402	PHE	2.4
1	E	346	ALA	2.4
1	E	424	PHE	2.4
1	F	261	LEU	2.4
1	C	273	VAL	2.4
1	H	263	ILE	2.4
1	E	339	VAL	2.4
1	G	376	CYS	2.4
1	E	277	LEU	2.4
1	H	399	ILE	2.4
1	H	342	PHE	2.3
1	G	7	VAL	2.3

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Mol	Chain	Res	Type	RSRZ
1	G	349	GLN	2.3
1	B	99	ASN	2.3
1	G	298	LYS	2.3
1	D	261	LEU	2.3
1	A	434	VAL	2.3
1	G	39	VAL	2.3
1	B	296	VAL	2.3
1	H	262	ILE	2.3
1	B	399	ILE	2.3
1	F	373	MET	2.3
1	G	6	PHE	2.3
1	C	388	VAL	2.2
1	G	399	ILE	2.2
1	B	40	ILE	2.2
1	G	12	LEU	2.2
1	G	346	ALA	2.2
1	A	318	GLY	2.2
1	B	392	ILE	2.2
1	B	308	VAL	2.2
1	B	160	PHE	2.2
1	B	380	ASN	2.2
1	H	300	ILE	2.2
1	H	296	VAL	2.2
1	H	343	VAL	2.2
1	F	306	GLU	2.2
1	B	450	VAL	2.2
1	C	308	VAL	2.2
1	F	302	ASP	2.1
1	E	294	VAL	2.1
1	C	217	GLN	2.1
1	H	298	LYS	2.1
1	E	305	THR	2.1
1	C	297	GLN	2.1
1	E	357	GLY	2.1
1	H	264	PHE	2.1
1	G	461	LYS	2.1
1	F	367	LEU	2.1
1	G	32	PHE	2.1
1	B	191	LEU	2.1
1	H	379	THR	2.1
1	C	269	MET	2.1
1	E	355	CYS	2.1

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Mol	Chain	Res	Type	RSRZ
1	H	224	ASP	2.1
1	G	291	GLY	2.1
1	F	423	VAL	2.1
1	E	434	VAL	2.0
1	F	352	LYS	2.0
1	B	7	VAL	2.0
1	H	294	VAL	2.0
1	F	281	PHE	2.0
1	G	43	PHE	2.0
1	D	300	ILE	2.0
1	G	31	ALA	2.0
1	B	292	THR	2.0
1	E	397	MET	2.0
1	F	230	PHE	2.0
1	E	354	LEU	2.0
1	G	459	GLY	2.0
1	G	1	MET	2.0
1	G	293	ARG	2.0
1	H	338	ARG	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 monosaccharides in this entry.

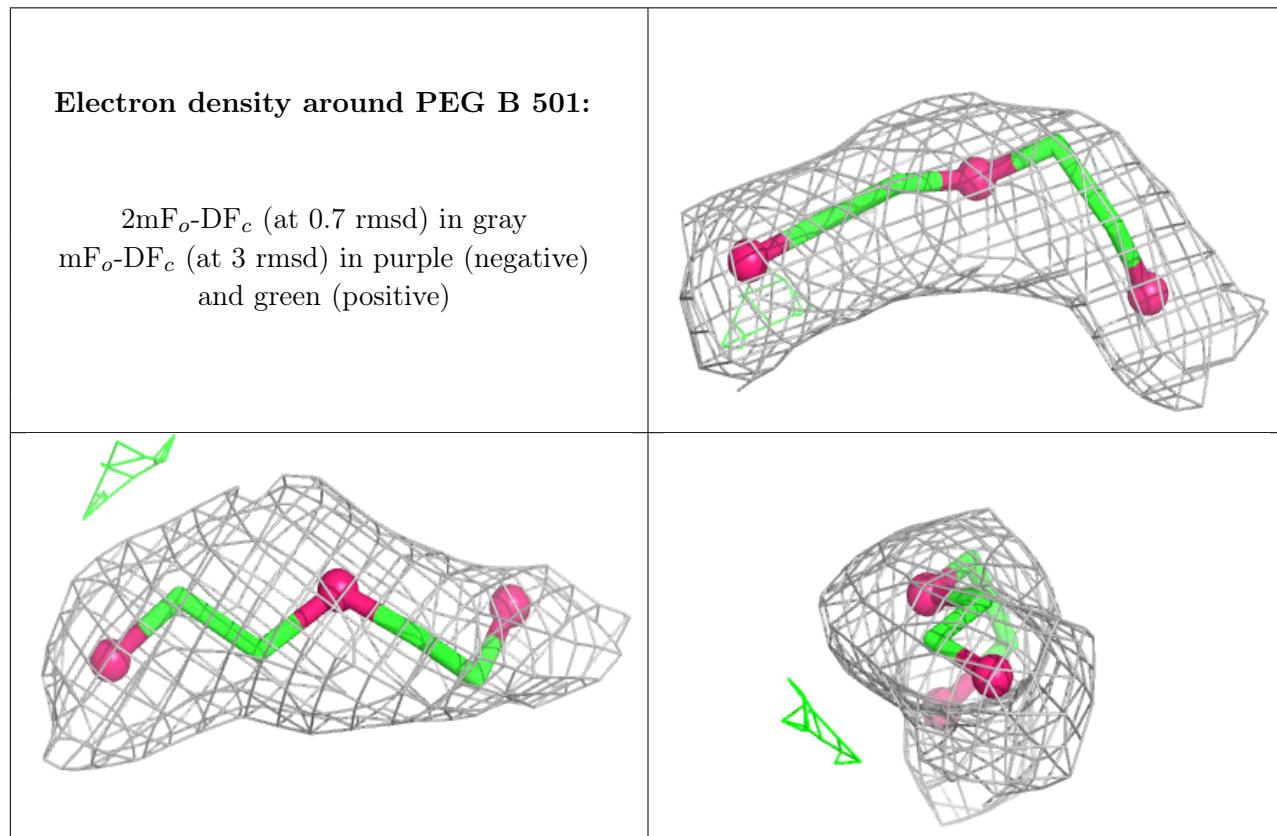
## 6.4 Ligands [\(i\)](#)

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. The B-factors column lists the minimum, median, 95<sup>th</sup> 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	B-factors(Å <sup>2</sup> )	Q<0.9
2	PEG	B	501	7/7	0.72	0.35	92,94,97,97	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers

as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.



## 6.5 Other polymers [\(i\)](#)

There are no such residues in this entry.