



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 20, 2020 – 12:46 PM BST

PDB ID : 4GBG  
Title : Crystal structure of Ethyl acetoacetate treated lipase from *Thermomyces lanuginosa* at 2.9 Å resolution  
Authors : Yamini, S.; Mukherjee, J.; Gupta, M.N.; Sinha, M.; Kaur, P.; Sharma, S.; Singh, T.P.  
Deposited on : 2012-07-27  
Resolution : 2.90 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 ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.13.1  
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) : 2.13.1

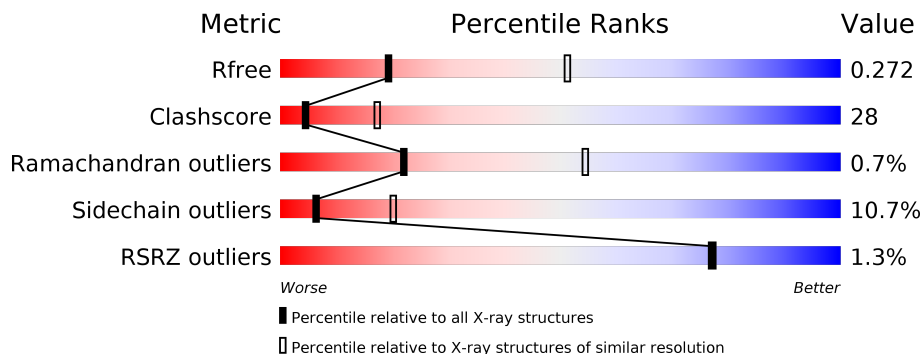
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.90 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 on 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.

Mol	Chain	Length	Quality of chain
1	A	269	
1	B	269	

## 2 Entry composition [i](#)

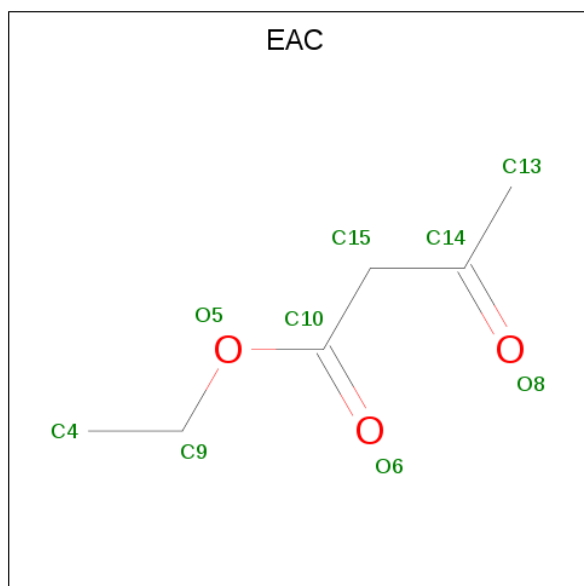
There are 4 unique types of molecules in this entry. The entry contains 4527 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Lipase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	269	Total 2070	C 1303	N 359	O 402	S 6	0	0	0
1	B	269	Total 2070	C 1303	N 359	O 402	S 6	0	0	0

- Molecule 2 is ethyl 3-oxobutanoate (three-letter code: EAC) (formula:  $C_6H_{10}O_3$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
2	A	1	Total 9	C 6	O 3	0	0

- Molecule 3 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula:  $C_8H_{15}NO_6$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
3	A	1	14	8	1	5	0	0
3	B	1	14	8	1	5	0	0

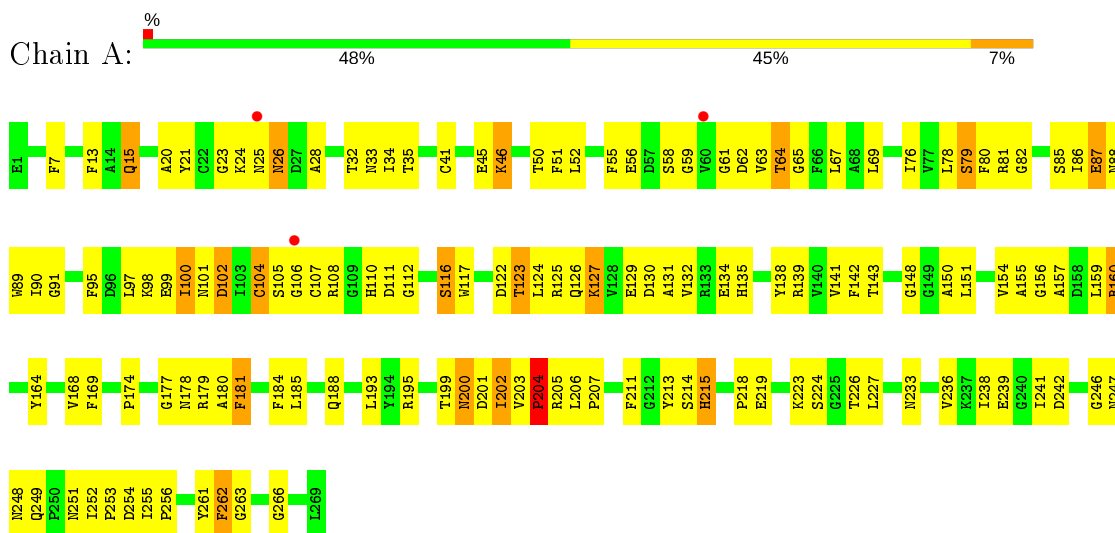
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
4	A	175	175	175	0	0
4	B	175	175	175	0	0

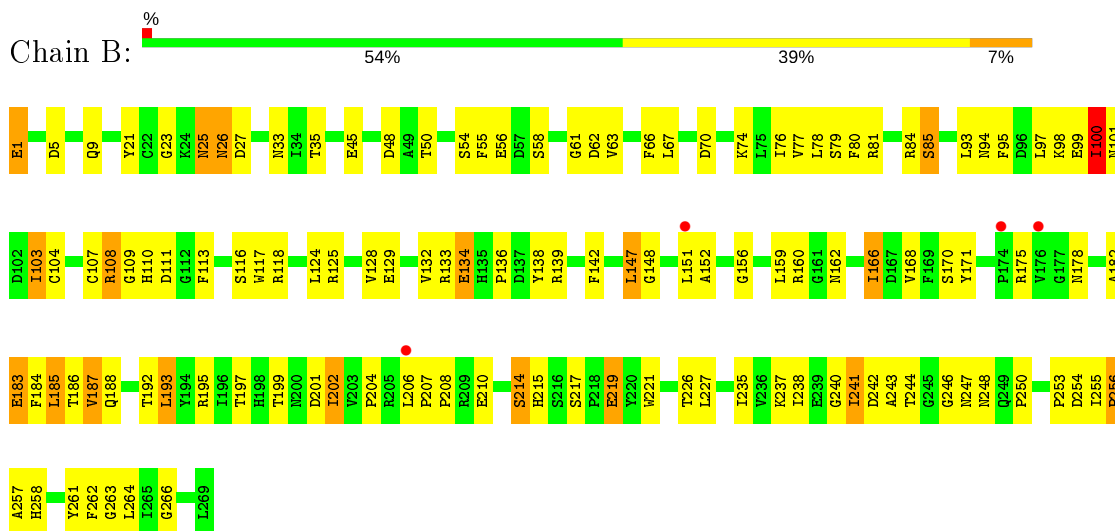
### 3 Residue-property plots [i](#)

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 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: Lipase



- Molecule 1: Lipase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 61	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	140.49 Å 140.49 Å 80.69 Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	40.56 – 2.90 40.56 – 2.90	Depositor EDS
% Data completeness (in resolution range)	99.9 (40.56-2.90) 100.0 (40.56-2.90)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.83 (at 2.90 Å)	Xtrriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.226 , 0.247 0.235 , 0.272	Depositor DCC
$R_{free}$ test set	1036 reflections (5.11%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	53.5	Xtrriage
Anisotropy	0.063	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 39.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtrriage
Estimated twinning fraction	0.084 for h,-h-k,-l	Xtrriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	4527	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	50.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.04% 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  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  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: EAC, NAG

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	0/2120	0.78	3/2887 (0.1%)
1	B	0.54	0/2120	0.83	3/2887 (0.1%)
All	All	0.54	0/4240	0.80	6/5774 (0.1%)

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
1	B	0	1

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
1	B	187	VAL	CB-CA-C	-11.20	90.12	111.40
1	A	262	PHE	CB-CA-C	-6.84	96.71	110.40
1	A	76	ILE	N-CA-C	-6.02	94.75	111.00
1	B	76	ILE	N-CA-C	-5.57	95.97	111.00
1	A	104	CYS	CA-CB-SG	5.23	123.41	114.00
1	B	85	SER	N-CA-C	-5.01	97.48	111.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	171	TYR	Sidechain

## 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	2070	0	1963	125	0
1	B	2070	0	1964	107	0
2	A	9	0	10	1	0
3	A	14	0	13	0	0
3	B	14	0	13	0	0
4	A	175	0	0	7	0
4	B	175	0	0	4	0
All	All	4527	0	3963	232	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 28.

All (232) 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:101:ASN:OD1	1:A:104:CYS:O	1.80	0.99
1:B:195:ARG:NH2	1:B:219:GLU:HG3	1.78	0.97
1:A:202:ILE:HG13	1:A:253:PRO:HB2	1.48	0.91
1:A:252:ILE:HD12	1:A:253:PRO:HD2	1.53	0.90
1:A:201:ASP:OD1	1:A:202:ILE:N	2.05	0.89
1:A:61:GLY:HA3	1:A:116:SER:HB3	1.54	0.88
1:B:254:ASP:OD1	1:B:256:PRO:HD2	1.75	0.86
1:A:56:GLU:HA	1:A:64:THR:HG23	1.57	0.86
1:B:182:ALA:HB2	1:B:214:SER:HB3	1.58	0.85
1:A:101:ASN:OD1	1:A:106:GLY:N	2.09	0.85
1:A:131:ALA:HA	1:A:134:GLU:HG3	1.58	0.84
1:B:23:GLY:HA3	1:B:25:ASN:HD21	1.46	0.81
1:B:195:ARG:HH22	1:B:219:GLU:HG3	1.44	0.79
1:B:26:ASN:N	1:B:26:ASN:HD22	1.81	0.79
1:B:117:TRP:HZ3	1:B:124:LEU:HD12	1.48	0.77
1:B:101:ASN:HA	1:B:104:CYS:O	1.85	0.77
1:A:261:TYR:O	1:A:262:PHE:HB2	1.85	0.76
1:A:248:ASN:HB2	4:A:515:HOH:O	1.86	0.74
1:A:32:THR:HG22	1:A:33:ASN:H	1.54	0.73
1:B:156:GLY:O	1:B:160:ARG:HG3	1.89	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:195:ARG:NH2	1:A:219:GLU:HB2	2.04	0.72
1:A:254:ASP:OD2	1:A:256:PRO:HD2	1.89	0.72
1:A:223:LYS:HD2	1:A:236:VAL:CG2	2.21	0.70
1:B:175:ARG:HG3	1:B:215:HIS:CD2	2.26	0.70
1:B:254:ASP:CG	1:B:256:PRO:HD2	2.11	0.70
1:A:15:GLN:HG2	1:A:41:CYS:HA	1.74	0.69
1:B:226:THR:O	1:B:227:LEU:HB2	1.91	0.68
1:A:81:ARG:HG2	1:A:82:GLY:N	2.09	0.68
1:B:128:VAL:O	1:B:132:VAL:HG23	1.94	0.68
1:A:20:ALA:HB1	1:A:81:ARG:HB2	1.74	0.68
1:A:32:THR:HG22	1:A:33:ASN:N	2.09	0.68
1:B:133:ARG:O	1:B:136:PRO:HD3	1.94	0.68
1:B:95:PHE:HE2	1:B:208:PRO:HD3	1.59	0.67
1:B:1:GLU:HG2	1:B:1:GLU:O	1.93	0.67
1:B:81:ARG:NH2	1:B:84:ARG:HG2	2.10	0.67
1:A:87:GLU:HB2	2:A:301:EAC:O6	1.94	0.66
1:A:101:ASN:HA	1:A:104:CYS:O	1.94	0.66
1:A:201:ASP:OD1	1:A:201:ASP:C	2.30	0.65
1:A:254:ASP:CG	1:A:256:PRO:HD2	2.17	0.65
1:B:67:LEU:HD12	1:B:77:VAL:O	1.97	0.64
1:B:219:GLU:HB3	1:B:238:ILE:HB	1.80	0.64
1:A:168:VAL:HG12	1:A:193:LEU:HD12	1.80	0.64
1:A:202:ILE:CG1	1:A:253:PRO:HB2	2.23	0.64
1:A:104:CYS:SG	1:A:184:PHE:CD2	2.91	0.64
1:A:226:THR:O	1:A:227:LEU:HB2	1.96	0.63
1:B:61:GLY:HA3	1:B:116:SER:OG	1.99	0.63
1:A:200:ASN:O	1:A:201:ASP:O	2.16	0.62
1:A:205:ARG:NH2	1:A:251:ASN:OD1	2.20	0.62
1:A:135:HIS:ND1	4:A:517:HOH:O	2.31	0.62
1:A:202:ILE:HG13	1:A:253:PRO:CB	2.26	0.62
1:A:117:TRP:CD1	1:A:154:VAL:HG12	2.36	0.61
1:A:200:ASN:O	1:A:201:ASP:C	2.39	0.61
1:A:101:ASN:CG	1:A:106:GLY:H	2.03	0.61
1:A:21:TYR:CZ	1:A:266:GLY:HA2	2.35	0.61
1:B:110:HIS:HB3	1:B:113:PHE:CD2	2.35	0.61
1:B:80:PHE:HD2	1:B:152:ALA:HB2	1.66	0.60
1:B:85:SER:HB3	4:B:434:HOH:O	2.01	0.60
1:B:175:ARG:HD2	1:B:207:PRO:O	2.02	0.59
1:B:100:ILE:HG13	1:B:107:CYS:O	2.03	0.59
1:B:183:GLU:HA	1:B:241:ILE:HD11	1.83	0.59
1:B:206:LEU:HA	1:B:207:PRO:C	2.21	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:182:ALA:CB	1:B:214:SER:HB3	2.31	0.59
1:A:95:PHE:HD2	1:A:211:PHE:CE1	2.20	0.58
1:A:107:CYS:SG	1:A:181:PHE:HA	2.45	0.57
1:A:168:VAL:CG1	1:A:193:LEU:HD12	2.34	0.57
1:B:103:ILE:HG22	1:B:104:CYS:SG	2.45	0.56
1:B:109:GLY:O	1:B:110:HIS:C	2.39	0.56
1:B:195:ARG:CZ	1:B:219:GLU:HG3	2.35	0.56
1:B:98:LYS:HB2	1:B:111:ASP:OD1	2.05	0.56
1:B:237:LYS:O	1:B:238:ILE:HD13	2.06	0.56
1:A:59:GLY:HA2	4:A:411:HOH:O	2.06	0.56
1:B:254:ASP:OD2	1:B:256:PRO:HB2	2.06	0.56
1:B:125:ARG:HD3	1:B:159:LEU:HD22	1.88	0.55
1:A:203:VAL:C	1:A:205:ARG:H	2.08	0.55
1:A:100:ILE:HD12	1:A:107:CYS:O	2.06	0.55
1:B:95:PHE:CE2	1:B:208:PRO:HD3	2.40	0.55
1:B:93:LEU:HB3	4:B:512:HOH:O	2.07	0.55
1:A:88:ASN:O	1:A:91:GLY:N	2.40	0.54
1:A:80:PHE:O	1:A:148:GLY:HA3	2.07	0.54
1:B:261:TYR:O	1:B:262:PHE:HB2	2.08	0.54
1:B:26:ASN:ND2	1:B:26:ASN:N	2.52	0.54
1:A:203:VAL:HB	1:A:204:PRO:HD3	1.90	0.54
1:B:117:TRP:CZ3	1:B:124:LEU:HD12	2.37	0.54
1:B:80:PHE:O	1:B:148:GLY:HA3	2.07	0.54
1:A:179:ARG:O	1:A:179:ARG:HG3	2.08	0.54
1:A:107:CYS:HA	1:A:180:ALA:HB3	1.90	0.54
1:A:157:ALA:HB2	1:A:185:LEU:CD2	2.38	0.54
1:A:101:ASN:OD1	1:A:105:SER:CA	2.56	0.53
1:A:130:ASP:O	1:A:134:GLU:HG3	2.08	0.53
1:A:223:LYS:HD2	1:A:236:VAL:HG23	1.89	0.53
1:A:34:ILE:HG12	1:A:51:PHE:CZ	2.43	0.53
1:B:23:GLY:HA3	1:B:25:ASN:ND2	2.21	0.53
1:A:102:ASP:OD2	1:A:102:ASP:N	2.30	0.53
1:A:58:SER:HA	4:A:497:HOH:O	2.09	0.53
1:B:201:ASP:CG	1:B:258:HIS:HD1	2.12	0.52
1:B:204:PRO:HB2	1:B:247:ASN:OD1	2.08	0.52
1:A:34:ILE:HG12	1:A:51:PHE:CE2	2.45	0.52
1:A:101:ASN:OD1	1:A:105:SER:HA	2.09	0.52
1:A:88:ASN:O	1:A:89:TRP:C	2.47	0.52
1:A:238:ILE:HD12	1:A:246:GLY:HA3	1.92	0.52
1:A:204:PRO:HB2	1:A:247:ASN:OD1	2.09	0.52
1:A:238:ILE:HD12	1:A:246:GLY:CA	2.40	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:156:GLY:O	1:A:160:ARG:HG3	2.10	0.52
1:B:80:PHE:HB2	1:B:148:GLY:O	2.10	0.51
1:A:178:ASN:OD1	1:A:180:ALA:HB3	2.10	0.51
1:A:223:LYS:HD2	1:A:236:VAL:HG21	1.91	0.51
1:A:25:ASN:HA	1:A:28:ALA:HB2	1.93	0.51
1:A:206:LEU:HA	1:A:207:PRO:C	2.31	0.51
1:A:101:ASN:ND2	1:A:106:GLY:H	2.09	0.51
1:B:108:ARG:CG	1:B:108:ARG:HH11	2.22	0.51
1:A:215:HIS:HB2	4:A:522:HOH:O	2.11	0.51
1:A:78:LEU:HB3	1:A:142:PHE:CD2	2.46	0.50
1:A:98:LYS:HB2	1:A:111:ASP:OD1	2.12	0.50
1:A:242:ASP:HA	4:A:416:HOH:O	2.10	0.50
1:B:26:ASN:HA	1:B:56:GLU:OE2	2.12	0.50
1:B:78:LEU:HB3	1:B:142:PHE:CD1	2.47	0.49
1:B:125:ARG:O	1:B:129:GLU:HG3	2.13	0.49
1:A:150:ALA:HB2	1:A:174:PRO:HD2	1.95	0.49
1:A:143:THR:HA	1:A:169:PHE:O	2.12	0.49
1:A:52:LEU:HB2	1:A:67:LEU:O	2.12	0.49
1:A:81:ARG:HG2	1:A:82:GLY:O	2.12	0.49
1:B:26:ASN:O	1:B:27:ASP:OD2	2.30	0.49
1:B:99:GLU:HB2	1:B:108:ARG:NH1	2.27	0.49
1:A:130:ASP:O	1:A:134:GLU:CG	2.60	0.49
1:B:104:CYS:O	1:B:107:CYS:HB2	2.12	0.49
1:A:32:THR:O	1:A:50:THR:HB	2.13	0.48
1:B:25:ASN:O	1:B:26:ASN:C	2.49	0.48
1:B:254:ASP:OD2	1:B:257:ALA:N	2.43	0.48
1:A:255:ILE:N	1:A:256:PRO:CD	2.76	0.48
1:B:61:GLY:O	1:B:62:ASP:C	2.52	0.48
1:B:100:ILE:HD12	1:B:107:CYS:HB3	1.95	0.48
1:B:244:THR:HG22	1:B:248:ASN:O	2.13	0.48
1:B:201:ASP:OD2	1:B:258:HIS:HB2	2.14	0.47
1:A:7:PHE:CE1	1:A:262:PHE:HE1	2.32	0.47
1:B:175:ARG:NH1	4:B:404:HOH:O	2.36	0.47
1:B:186:THR:HG23	1:B:217:SER:HB3	1.96	0.47
1:B:97:LEU:N	1:B:97:LEU:HD12	2.30	0.47
1:A:203:VAL:C	1:A:205:ARG:N	2.68	0.47
1:A:85:SER:O	1:A:88:ASN:HB2	2.15	0.47
1:B:184:PHE:CE1	1:B:188:GLN:HG3	2.50	0.47
1:A:81:ARG:CG	1:A:82:GLY:N	2.77	0.47
1:B:208:PRO:HB2	1:B:210:GLU:OE2	2.14	0.47
1:B:94:ASN:O	1:B:110:HIS:NE2	2.42	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:124:LEU:O	1:A:127:LYS:N	2.49	0.46
1:B:184:PHE:O	1:B:185:LEU:C	2.51	0.46
1:B:197:THR:HB	1:B:247:ASN:HB2	1.98	0.46
1:B:26:ASN:H	1:B:26:ASN:HD22	1.60	0.46
1:A:122:ASP:O	1:A:123:THR:C	2.53	0.46
1:A:88:ASN:O	1:A:90:ILE:N	2.48	0.46
1:A:252:ILE:CD1	1:A:253:PRO:HD2	2.37	0.46
1:A:25:ASN:HB3	1:A:51:PHE:CZ	2.51	0.46
1:A:184:PHE:O	1:A:188:GLN:HB2	2.16	0.46
1:A:203:VAL:O	1:A:205:ARG:N	2.49	0.46
1:B:100:ILE:CD1	1:B:107:CYS:HB3	2.46	0.46
1:B:175:ARG:HG3	1:B:215:HIS:NE2	2.31	0.46
1:A:127:LYS:HA	1:A:130:ASP:OD1	2.17	0.45
1:B:21:TYR:CZ	1:B:266:GLY:HA2	2.50	0.45
1:B:183:GLU:O	1:B:187:VAL:HG22	2.17	0.45
1:B:160:ARG:HG2	1:B:166:ILE:HG13	1.99	0.45
1:A:69:LEU:HD11	1:A:138:TYR:CE2	2.51	0.45
1:A:174:PRO:HB3	1:A:203:VAL:HG12	1.99	0.45
1:A:45:GLU:O	1:A:46:LYS:C	2.54	0.45
1:A:117:TRP:NE1	1:A:155:ALA:HA	2.32	0.45
1:B:48:ASP:CG	1:B:48:ASP:O	2.53	0.45
1:B:97:LEU:H	1:B:97:LEU:HD12	1.82	0.45
1:B:33:ASN:HA	1:B:50:THR:HG22	1.99	0.44
1:B:84:ARG:HB2	4:B:503:HOH:O	2.16	0.44
1:A:101:ASN:OD1	1:A:105:SER:C	2.56	0.44
1:B:255:ILE:N	1:B:256:PRO:CD	2.80	0.44
1:B:134:GLU:HG2	1:B:134:GLU:H	1.42	0.44
1:A:110:HIS:CE1	1:A:112:GLY:HA3	2.52	0.44
1:A:261:TYR:C	1:A:263:GLY:H	2.20	0.44
1:B:110:HIS:CB	1:B:113:PHE:CD2	3.00	0.44
1:B:99:GLU:HG2	1:B:100:ILE:N	2.33	0.44
1:A:56:GLU:HG2	1:A:64:THR:CG2	2.48	0.44
1:A:110:HIS:HE1	1:A:112:GLY:HA3	1.83	0.44
1:A:125:ARG:O	1:A:129:GLU:HG3	2.17	0.44
1:A:131:ALA:CA	1:A:134:GLU:HG3	2.39	0.44
1:A:23:GLY:HA2	1:A:35:THR:O	2.18	0.43
1:B:118:ARG:HD3	1:B:118:ARG:HA	1.57	0.43
1:B:192:THR:HG22	1:B:193:LEU:N	2.33	0.43
1:B:35:THR:HA	1:B:45:GLU:HG2	2.01	0.43
1:A:25:ASN:ND2	1:A:51:PHE:CZ	2.87	0.43
1:B:104:CYS:SG	1:B:184:PHE:CD2	3.11	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:241:ILE:HG22	1:A:242:ASP:OD1	2.19	0.43
1:B:255:ILE:O	1:B:258:HIS:HB3	2.19	0.43
1:B:240:GLY:O	1:B:243:ALA:HB2	2.19	0.43
1:A:155:ALA:O	1:A:159:LEU:HG	2.19	0.42
1:B:108:ARG:NH1	1:B:108:ARG:CG	2.80	0.42
1:B:55:PHE:HE1	1:B:63:VAL:HG12	1.85	0.42
1:A:199:THR:HB	1:A:200:ASN:H	1.62	0.42
1:A:56:GLU:HG2	1:A:64:THR:HG23	2.01	0.42
1:A:21:TYR:CE1	1:A:266:GLY:HA2	2.55	0.42
1:A:86:ILE:O	1:A:90:ILE:HG13	2.18	0.42
1:B:74:LYS:HD2	1:B:138:TYR:CE1	2.54	0.42
1:B:9:GLN:OE1	1:B:139:ARG:NH2	2.45	0.42
1:A:151:LEU:O	1:A:154:VAL:N	2.53	0.42
1:B:185:LEU:H	1:B:185:LEU:HG	1.66	0.42
1:B:221:TRP:CD2	1:B:246:GLY:HA2	2.55	0.42
1:B:21:TYR:CE2	1:B:266:GLY:HA2	2.54	0.42
1:A:132:VAL:HG11	1:A:164:TYR:CD2	2.55	0.42
1:A:126:GLN:O	1:A:130:ASP:OD1	2.37	0.42
1:B:5:ASP:O	1:B:9:GLN:HG3	2.19	0.42
1:A:246:GLY:O	1:A:249:GLN:NE2	2.49	0.42
1:B:186:THR:HG22	1:B:186:THR:O	2.19	0.42
1:B:263:GLY:O	1:B:264:LEU:C	2.58	0.42
1:A:61:GLY:O	1:A:62:ASP:C	2.58	0.42
1:A:65:GLY:HA3	1:A:79:SER:O	2.20	0.42
1:B:142:PHE:O	1:B:168:VAL:HA	2.19	0.41
1:A:52:LEU:HA	1:A:52:LEU:HD23	1.74	0.41
1:A:26:ASN:N	1:A:26:ASN:OD1	2.52	0.41
1:B:201:ASP:OD2	1:B:258:HIS:ND1	2.54	0.41
1:B:214:SER:OG	1:B:242:ASP:OD1	2.23	0.41
1:A:55:PHE:HE1	1:A:63:VAL:HG12	1.86	0.41
1:A:101:ASN:HD21	1:A:106:GLY:H	1.69	0.41
1:B:66:PHE:CE2	1:B:79:SER:HB3	2.56	0.41
1:B:95:PHE:CD1	1:B:95:PHE:N	2.88	0.41
1:B:182:ALA:HB1	1:B:241:ILE:HD13	2.03	0.41
1:B:70:ASP:OD1	1:B:70:ASP:C	2.59	0.41
1:A:124:LEU:O	1:A:125:ARG:C	2.58	0.41
1:A:95:PHE:HD2	1:A:211:PHE:CD1	2.39	0.41
1:A:108:ARG:O	1:A:178:ASN:N	2.51	0.41
1:A:218:PRO:HA	4:A:412:HOH:O	2.20	0.41
1:B:170:SER:OG	1:B:195:ARG:HA	2.21	0.41
1:A:52:LEU:HB2	1:A:67:LEU:HD23	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:13:PHE:CE1	1:A:141:VAL:HG11	2.56	0.40
1:A:177:GLY:O	1:A:213:TYR:HA	2.22	0.40
1:A:88:ASN:C	1:A:90:ILE:N	2.72	0.40
1:B:147:LEU:HG	1:B:147:LEU:O	2.20	0.40
1:B:125:ARG:CD	1:B:159:LEU:HD22	2.52	0.40
1:B:202:ILE:HA	1:B:253:PRO:HB2	2.04	0.40
1:A:98:LYS:HG2	1:A:99:GLU:N	2.37	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	267/269 (99%)	239 (90%)	27 (10%)	1 (0%)	34	66
1	B	267/269 (99%)	245 (92%)	19 (7%)	3 (1%)	14	42
All	All	534/538 (99%)	484 (91%)	46 (9%)	4 (1%)	22	54

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	199	THR
1	B	100	ILE
1	A	204	PRO
1	B	250	PRO

### 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	220/220 (100%)	196 (89%)	24 (11%)	6	19
1	B	220/220 (100%)	197 (90%)	23 (10%)	7	21
All	All	440/440 (100%)	393 (89%)	47 (11%)	6	20

All (47) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	15	GLN
1	A	24	LYS
1	A	26	ASN
1	A	46	LYS
1	A	64	THR
1	A	79	SER
1	A	87	GLU
1	A	97	LEU
1	A	100	ILE
1	A	102	ASP
1	A	116	SER
1	A	123	THR
1	A	127	LYS
1	A	139	ARG
1	A	160	ARG
1	A	181	PHE
1	A	200	ASN
1	A	202	ILE
1	A	204	PRO
1	A	214	SER
1	A	215	HIS
1	A	224	SER
1	A	233	ASN
1	A	239	GLU
1	B	1	GLU
1	B	25	ASN
1	B	26	ASN
1	B	54	SER
1	B	58	SER
1	B	100	ILE
1	B	103	ILE
1	B	108	ARG
1	B	134	GLU

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Mol	Chain	Res	Type
1	B	147	LEU
1	B	151	LEU
1	B	162	ASN
1	B	166	ILE
1	B	178	ASN
1	B	183	GLU
1	B	185	LEU
1	B	193	LEU
1	B	202	ILE
1	B	214	SER
1	B	219	GLU
1	B	235	ILE
1	B	241	ILE
1	B	256	PRO

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	25	ASN
1	A	88	ASN
1	A	248	ASN
1	B	25	ASN
1	B	26	ASN
1	B	88	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](#)

3 ligands are 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
3	NAG	A	302	1	14,14,15	0.41	0	17,19,21	1.16	1 (5%)
3	NAG	B	301	1	14,14,15	0.42	0	17,19,21	1.17	2 (11%)
2	EAC	A	301	-	8,8,8	3.06	2 (25%)	9,9,9	2.10	3 (33%)

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
3	NAG	A	302	1	-	0/6/23/26	0/1/1/1
3	NAG	B	301	1	-	2/6/23/26	0/1/1/1
2	EAC	A	301	-	-	4/7/7/7	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	301	EAC	O5-C10	7.04	1.53	1.33
2	A	301	EAC	C15-C10	4.27	1.58	1.51

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	301	EAC	C9-O5-C10	3.83	127.85	116.73
2	A	301	EAC	C14-C15-C10	3.11	118.51	112.55
2	A	301	EAC	O5-C10-C15	2.79	118.90	111.39
3	A	302	NAG	C8-C7-N2	2.33	120.05	116.10
3	B	301	NAG	C8-C7-N2	2.32	120.03	116.10
3	B	301	NAG	C2-N2-C7	-2.01	120.04	122.90

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	301	EAC	C13-C14-C15-C10
2	A	301	EAC	O8-C14-C15-C10
3	B	301	NAG	O5-C5-C6-O6
3	B	301	NAG	C4-C5-C6-O6
2	A	301	EAC	C15-C10-O5-C9
2	A	301	EAC	O6-C10-O5-C9

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	301	EAC	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 [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	269/269 (100%)	0.20	3 (1%) 80 80	22, 48, 74, 88	1 (0%)
1	B	269/269 (100%)	0.19	4 (1%) 73 73	22, 52, 72, 92	1 (0%)
All	All	538/538 (100%)	0.19	7 (1%) 77 77	22, 50, 74, 92	2 (0%)

All (7) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	176	VAL	3.6
1	B	206	LEU	3.4
1	A	25	ASN	3.0
1	A	106	GLY	2.8
1	B	151	LEU	2.4
1	A	60	VAL	2.3
1	B	174	PRO	2.1

### 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( $\text{\AA}^2$ )	Q<0.9
3	NAG	A	302	14/15	0.80	0.28	41,43,46,47	0
2	EAC	A	301	9/9	0.82	0.38	50,51,54,58	0
3	NAG	B	301	14/15	0.84	0.24	40,42,43,43	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.