



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 20, 2023 – 11:41 AM EDT

PDB ID : 2HUU  
Title : Crystal structure of Aedes aegypti alanine glyoxylate aminotransferase in complex with alanine  
Authors : Han, Q.; Robinson, H.; Gao, Y.G.; Vogelaar, N.; Wilson, S.R.; Rizzi, M.; Li, J.  
Deposited on : 2006-07-27  
Resolution : 2.10 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.

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 ⓘ](#)) 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 : 2.35  
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) : 2.35

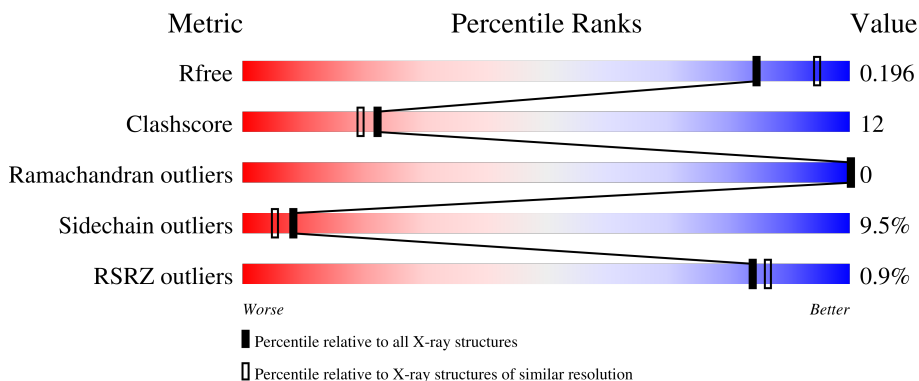
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*


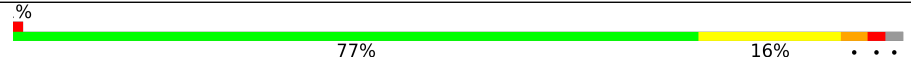
The reported resolution of this entry is 2.10 Å.

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	5197 (2.10-2.10)
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (2.10-2.10)

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.

Mol	Chain	Length	Quality of chain
1	A	393	 77% 16% . . .
1	B	393	 77% 16% . . .

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
3	1BO	B	801	-	-	X	-

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 6604 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.

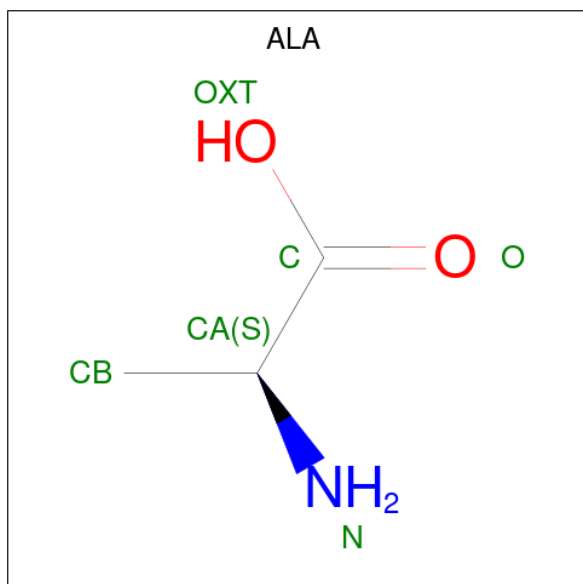
- Molecule 1 is a protein called Alanine glyoxylate aminotransferase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	P	S			
1	A	385	2978	1885	523	549	1	20	0	0	0
1	B	385	2978	1885	523	549	1	20	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

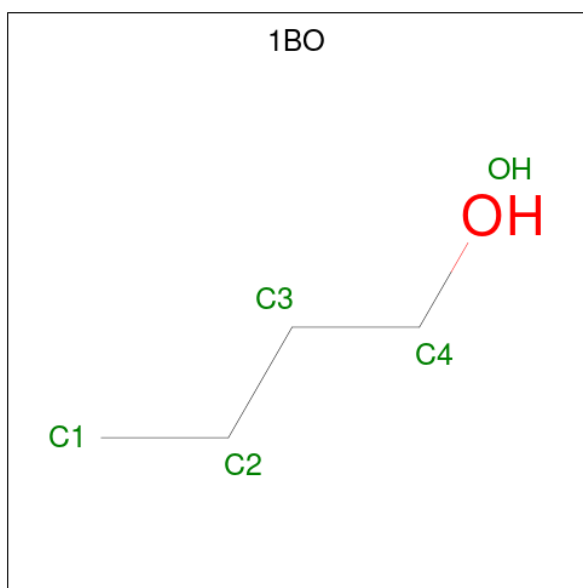
Chain	Residue	Modelled	Actual	Comment	Reference
A	206	LLP	LYS	modified residue	UNP Q3LSM4
B	206	LLP	LYS	modified residue	UNP Q3LSM4

- Molecule 2 is ALANINE (three-letter code: ALA) (formula: C<sub>3</sub>H<sub>7</sub>NO<sub>2</sub>).



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

- Molecule 3 is 1-BUTANOL (three-letter code: 1BO) (formula: C<sub>4</sub>H<sub>10</sub>O).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	B	1	Total	C	O	0	0
			5	4	1		

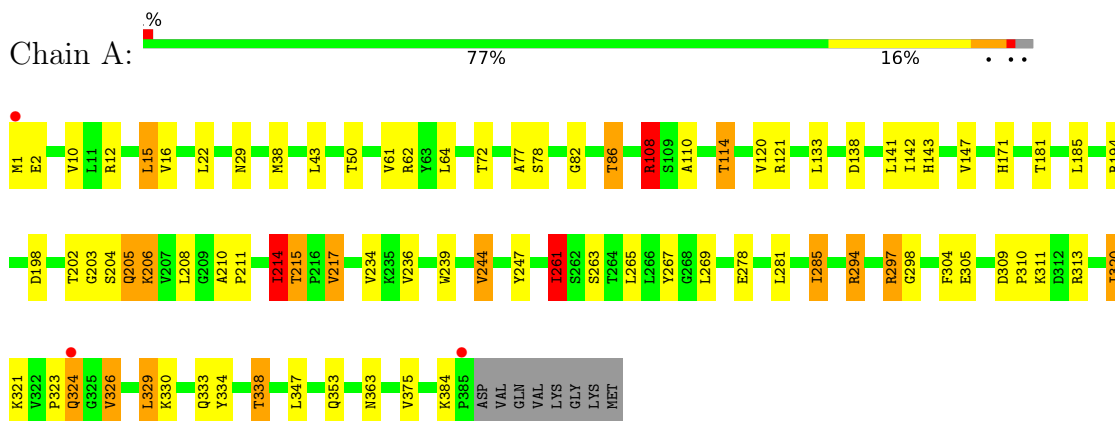
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	323	Total	O	0	0
			323	323		
4	B	314	Total	O	0	0
			314	314		

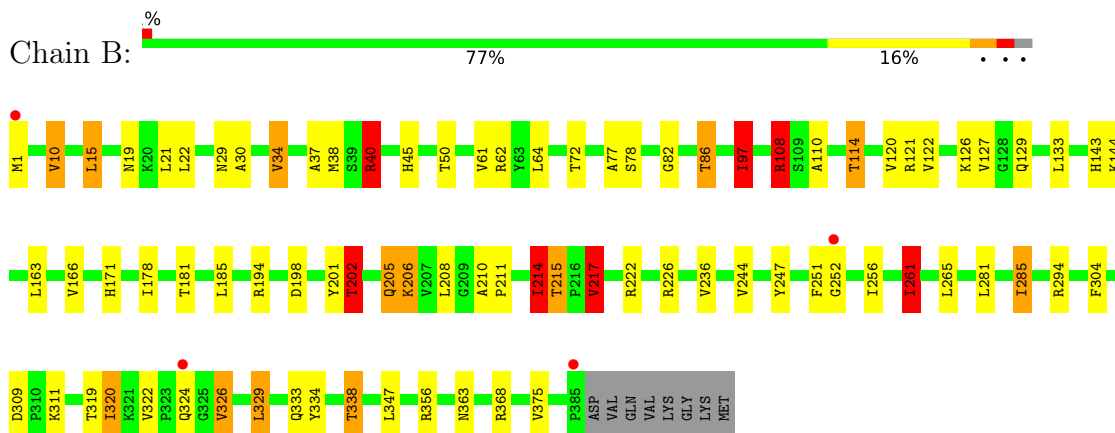
### 3 Residue-property plots [i](#)

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: Alanine glyoxylate aminotransferase



- Molecule 1: Alanine glyoxylate aminotransferase



## 4 Data and refinement statistics

Property	Value	Source
Space group	H 3	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	137.12Å 137.12Å 120.30Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	29.16 – 2.10 29.15 – 2.10	Depositor EDS
% Data completeness (in resolution range)	100.0 (29.16-2.10) 100.0 (29.15-2.10)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.91 (at 2.10Å)	Xtrriage
Refinement program	REFMAC 5.2.0005	Depositor
R, $R_{free}$	0.150 , 0.195 0.152 , 0.196	Depositor DCC
$R_{free}$ test set	2493 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	24.5	Xtrriage
Anisotropy	0.045	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 50.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	0.021 for h,-h-k,-l	Xtrriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	6604	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	25.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.02% 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: 1BO, LLP

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	0.81	1/3017 (0.0%)	0.94	9/4092 (0.2%)
1	B	0.84	0/3017	0.99	14/4092 (0.3%)
All	All	0.83	1/6034 (0.0%)	0.96	23/8184 (0.3%)

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

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	244	VAL	CB-CG1	-5.50	1.41	1.52

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	108	ARG	NE-CZ-NH1	12.67	126.64	120.30
1	B	108	ARG	NE-CZ-NH2	-12.09	114.26	120.30
1	A	108	ARG	NE-CZ-NH1	10.15	125.38	120.30
1	B	40	ARG	NE-CZ-NH2	-8.44	116.08	120.30
1	A	294	ARG	NE-CZ-NH2	-8.14	116.23	120.30
1	A	108	ARG	NE-CZ-NH2	-8.12	116.24	120.30
1	B	294	ARG	NE-CZ-NH2	-7.85	116.37	120.30
1	A	217	VAL	CB-CA-C	-7.66	96.84	111.40
1	B	62	ARG	NE-CZ-NH2	-7.56	116.52	120.30
1	B	217	VAL	CB-CA-C	-7.37	97.39	111.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	214	ILE	CB-CA-C	-6.66	98.28	111.60
1	A	62	ARG	NE-CZ-NH2	-6.39	117.11	120.30
1	B	97	ILE	CB-CA-C	-6.27	99.06	111.60
1	A	214	ILE	CB-CA-C	-6.08	99.43	111.60
1	B	40	ARG	NE-CZ-NH1	6.01	123.30	120.30
1	B	202	THR	CB-CA-C	-5.95	95.54	111.60
1	B	10	VAL	CG1-CB-CG2	5.75	120.09	110.90
1	B	251	PHE	C-N-CA	-5.54	110.67	122.30
1	A	239	TRP	CA-CB-CG	5.46	124.07	113.70
1	A	294	ARG	NE-CZ-NH1	5.41	123.01	120.30
1	B	15	LEU	CB-CG-CD2	5.25	119.93	111.00
1	A	261	ILE	CB-CA-C	-5.12	101.36	111.60
1	B	261	ILE	CB-CA-C	-5.08	101.44	111.60

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	252	GLY	Peptide

## 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	2978	0	2985	69	0
1	B	2978	0	2985	71	0
2	A	6	0	4	3	0
3	B	5	0	10	4	0
4	A	323	0	0	10	0
4	B	314	0	0	10	0
All	All	6604	0	5984	140	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 12.

All (140) 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:B:22:LEU:H	1:B:29:ASN:HD21	1.14	0.96
1:B:334:TYR:O	1:B:338:THR:HG23	1.68	0.93
1:B:37:ALA:O	1:B:40:ARG:HG2	1.69	0.92
1:A:110:ALA:O	1:A:114:THR:HG23	1.73	0.87
1:A:304:PHE:HB3	1:A:320:ILE:CD1	2.04	0.87
1:A:22:LEU:H	1:A:29:ASN:HD21	1.21	0.86
1:A:334:TYR:O	1:A:338:THR:HG23	1.77	0.84
1:A:205:GLN:HE21	1:A:205:GLN:H	1.28	0.81
1:A:384:LYS:HE2	4:A:968:HOH:O	1.80	0.79
1:A:294:ARG:O	1:A:297:ARG:HD3	1.85	0.77
1:B:97:ILE:HD12	1:B:120:VAL:HA	1.66	0.77
1:B:50:THR:HG21	1:B:261:ILE:HD11	1.66	0.77
1:A:114:THR:HG22	1:A:120:VAL:HG21	1.65	0.77
1:A:202:THR:HG22	1:A:203:GLY:H	1.47	0.76
1:A:171:HIS:HE1	1:A:198:ASP:OD2	1.70	0.75
1:A:121:ARG:HH11	1:A:143:HIS:HD2	1.35	0.74
1:B:97:ILE:HD11	1:B:120:VAL:HG22	1.68	0.74
1:A:304:PHE:HB3	1:A:320:ILE:HD11	1.69	0.73
1:B:97:ILE:CD1	1:B:120:VAL:HG22	2.19	0.73
1:B:356:ARG:HH22	3:B:801:1BO:H31	1.54	0.73
1:A:194:ARG:HH11	1:A:194:ARG:HG3	1.53	0.73
1:B:356:ARG:HH22	3:B:801:1BO:C3	2.03	0.72
1:B:205:GLN:HE21	1:B:205:GLN:H	1.39	0.71
1:A:181:THR:O	1:A:202:THR:HG23	1.90	0.71
1:B:77:ALA:O	1:B:215:THR:HG23	1.90	0.71
1:B:114:THR:HG22	1:B:120:VAL:HG21	1.72	0.71
1:A:29:ASN:HD22	1:A:363:ASN:HD21	1.36	0.70
1:B:37:ALA:O	1:B:40:ARG:CG	2.40	0.70
1:B:171:HIS:HE1	1:B:198:ASP:OD2	1.75	0.70
1:B:194:ARG:NH2	4:B:1112:HOH:O	2.25	0.69
1:A:77:ALA:O	1:A:215:THR:HG23	1.92	0.69
1:A:205:GLN:HE21	1:A:205:GLN:N	1.90	0.68
1:B:19:ASN:HB2	4:B:1085:HOH:O	1.94	0.67
1:B:108:ARG:HD2	4:B:808:HOH:O	1.94	0.67
1:A:330:LYS:HD2	4:A:994:HOH:O	1.95	0.66
1:A:247:TYR:OH	1:A:261:ILE:HG13	1.95	0.66
1:B:29:ASN:HD22	1:B:363:ASN:HD21	1.43	0.66
1:B:77:ALA:O	1:B:215:THR:CG2	2.44	0.66
1:A:77:ALA:O	1:A:215:THR:CG2	2.44	0.65
1:A:206:LLP:NZ	1:A:206:LLP:O3	2.30	0.65
1:A:82:GLY:O	1:A:86:THR:HB	1.98	0.64
1:A:210:ALA:HB1	1:A:211:PRO:HD2	1.79	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:801:1BO:H13	4:B:1082:HOH:O	1.99	0.63
1:A:304:PHE:HB3	1:A:320:ILE:HD13	1.81	0.62
1:A:214:ILE:HG12	1:A:265:LEU:HB3	1.82	0.62
1:A:205:GLN:H	1:A:205:GLN:NE2	1.98	0.61
1:B:194:ARG:NE	4:B:1112:HOH:O	2.33	0.61
1:A:108:ARG:HD2	4:A:721:HOH:O	2.01	0.60
1:B:82:GLY:O	1:B:86:THR:HB	2.01	0.60
1:A:121:ARG:HH11	1:A:143:HIS:CD2	2.19	0.60
1:B:121:ARG:HH11	1:B:143:HIS:HD2	1.50	0.60
1:B:206:LLP:O3	1:B:206:LLP:NZ	2.34	0.59
1:A:194:ARG:NE	4:A:1018:HOH:O	2.30	0.59
1:B:247:TYR:OH	1:B:261:ILE:HG13	2.03	0.59
1:A:309:ASP:OD1	1:A:311:LYS:HG2	2.03	0.58
1:B:329:LEU:O	1:B:333:GLN:HG3	2.03	0.58
1:B:205:GLN:HE21	1:B:205:GLN:N	2.01	0.58
1:A:281:LEU:O	1:A:285:ILE:HG23	2.04	0.58
1:A:294:ARG:O	1:A:297:ARG:CD	2.52	0.58
1:A:324:GLN:H	1:A:324:GLN:CD	2.07	0.58
1:A:29:ASN:ND2	1:A:363:ASN:HD21	2.03	0.56
1:A:78:SER:O	1:A:215:THR:HG21	2.05	0.56
1:A:202:THR:HG22	1:A:203:GLY:N	2.19	0.55
1:A:110:ALA:O	1:A:114:THR:CG2	2.50	0.55
4:A:1018:HOH:O	1:B:1:MET:HE1	2.07	0.55
1:B:304:PHE:HB3	1:B:320:ILE:HD13	1.89	0.55
1:A:61:VAL:HG22	1:A:72:THR:CG2	2.37	0.55
1:A:247:TYR:OH	1:A:261:ILE:CG1	2.54	0.55
1:B:194:ARG:CZ	4:B:1112:HOH:O	2.55	0.54
1:B:205:GLN:H	1:B:205:GLN:NE2	2.05	0.54
1:B:181:THR:O	1:B:202:THR:HG23	2.08	0.54
1:A:353:GLN:HG2	4:A:1014:HOH:O	2.07	0.54
1:B:110:ALA:O	1:B:114:THR:HG23	2.08	0.54
1:B:29:ASN:ND2	1:B:363:ASN:HD21	2.05	0.53
1:A:50:THR:HG21	1:A:261:ILE:HD11	1.89	0.53
1:B:222:ARG:NE	4:B:1108:HOH:O	2.26	0.53
1:B:86:THR:HG23	1:B:178:ILE:HD13	1.91	0.53
1:B:110:ALA:O	1:B:114:THR:CG2	2.57	0.53
1:B:247:TYR:OH	1:B:261:ILE:CG1	2.57	0.53
1:B:38:MET:SD	1:B:211:PRO:HG3	2.49	0.53
1:B:185:LEU:HB3	1:B:202:THR:HG21	1.91	0.52
1:A:278:GLU:HG3	4:A:1019:HOH:O	2.11	0.51
1:A:12:ARG:HD2	4:A:851:HOH:O	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:701:ALA:HB2	1:B:45:HIS:NE2	2.26	0.50
1:B:356:ARG:HH22	3:B:801:1BO:H32	1.76	0.50
1:B:181:THR:O	1:B:202:THR:CG2	2.59	0.50
1:B:61:VAL:HG22	1:B:72:THR:CG2	2.41	0.50
1:B:129:GLN:HE21	1:B:311:LYS:NZ	2.10	0.50
1:B:126:LYS:HZ2	1:B:127:VAL:H	1.60	0.50
1:B:319:THR:HG22	1:B:356:ARG:HG2	1.94	0.49
1:B:144:LYS:HD2	4:B:930:HOH:O	2.11	0.49
1:B:210:ALA:HB1	1:B:211:PRO:HD2	1.93	0.49
1:A:214:ILE:HD13	1:A:269:LEU:HB2	1.94	0.49
1:B:78:SER:C	1:B:215:THR:HG21	2.33	0.49
1:B:21:LEU:HD11	1:B:368:ARG:HD3	1.94	0.49
1:A:38:MET:SD	1:A:211:PRO:HG3	2.53	0.49
2:A:701:ALA:HB2	1:B:45:HIS:HE2	1.78	0.49
1:A:78:SER:C	1:A:215:THR:HG21	2.33	0.48
1:A:138:ASP:O	1:A:142:ILE:HG12	2.12	0.48
1:A:324:GLN:CD	1:A:324:GLN:N	2.67	0.48
1:B:78:SER:O	1:B:215:THR:HG21	2.13	0.48
1:A:310:PRO:HG3	1:A:313:ARG:NH2	2.29	0.47
1:B:50:THR:CG2	1:B:261:ILE:HD11	2.42	0.47
1:B:309:ASP:OD1	1:B:311:LYS:HG2	2.14	0.47
1:A:297:ARG:HD3	1:A:298:GLY:N	2.31	0.46
1:B:163:LEU:O	1:B:166:VAL:HG13	2.16	0.46
1:A:15:LEU:O	1:B:40:ARG:NH2	2.48	0.46
1:B:201:TYR:HB3	1:B:217:VAL:HG13	1.97	0.46
1:A:261:ILE:HD12	1:A:261:ILE:O	2.16	0.45
1:A:261:ILE:HG13	1:A:261:ILE:H	1.64	0.45
1:A:329:LEU:O	1:A:333:GLN:HG3	2.16	0.45
1:B:143:HIS:HE1	4:B:937:HOH:O	1.98	0.45
1:B:86:THR:CG2	1:B:178:ILE:HG21	2.47	0.45
1:A:305:GLU:HG2	1:A:321:LYS:HD2	1.98	0.44
1:B:256:ILE:HG13	4:B:831:HOH:O	2.17	0.44
1:B:30:ALA:HB1	1:B:34:VAL:HG22	1.99	0.44
1:A:22:LEU:H	1:A:29:ASN:ND2	2.03	0.44
1:B:281:LEU:O	1:B:285:ILE:HG23	2.18	0.44
1:B:304:PHE:CD2	1:B:320:ILE:HD11	2.53	0.44
1:A:204:SER:HB3	1:A:214:ILE:HD12	1.98	0.44
1:A:384:LYS:CE	4:A:968:HOH:O	2.55	0.43
1:A:297:ARG:HD3	1:A:298:GLY:H	1.82	0.43
1:A:171:HIS:CE1	1:A:198:ASP:OD2	2.61	0.43
1:B:126:LYS:HZ2	1:B:127:VAL:HG12	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:86:THR:HG23	1:B:178:ILE:HG21	2.00	0.43
1:A:61:VAL:HG22	1:A:72:THR:HG21	2.01	0.43
1:B:261:ILE:HG13	1:B:261:ILE:H	1.71	0.43
1:A:304:PHE:CD2	1:A:320:ILE:HD11	2.54	0.42
1:A:353:GLN:CG	4:A:1014:HOH:O	2.65	0.42
1:A:194:ARG:HH11	1:A:194:ARG:CG	2.28	0.42
1:A:263:SER:HB3	1:A:267:TYR:CZ	2.55	0.42
1:B:171:HIS:CE1	1:B:198:ASP:OD2	2.65	0.42
1:A:214:ILE:HD13	1:A:269:LEU:HD22	2.02	0.42
1:A:214:ILE:CG1	1:A:265:LEU:HB3	2.50	0.42
1:A:323:PRO:O	1:A:326:VAL:HG13	2.20	0.41
1:B:322:VAL:CG1	1:B:326:VAL:HG22	2.51	0.41
1:B:214:ILE:HG12	1:B:265:LEU:HB3	2.03	0.41
1:A:185:LEU:HB3	1:A:202:THR:HG21	2.01	0.41
2:A:701:ALA:HB2	1:B:45:HIS:CE1	2.56	0.41
1:B:126:LYS:NZ	1:B:127:VAL:H	2.18	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	382/393 (97%)	378 (99%)	4 (1%)	0	100	100
1	B	382/393 (97%)	379 (99%)	3 (1%)	0	100	100
All	All	764/786 (97%)	757 (99%)	7 (1%)	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	315/322 (98%)	284 (90%)	31 (10%)	8 5
1	B	315/322 (98%)	286 (91%)	29 (9%)	9 6
All	All	630/644 (98%)	570 (90%)	60 (10%)	8 5

All (60) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	2	GLU
1	A	10	VAL
1	A	15	LEU
1	A	16	VAL
1	A	43	LEU
1	A	64	LEU
1	A	86	THR
1	A	108	ARG
1	A	114	THR
1	A	133	LEU
1	A	141	LEU
1	A	147	VAL
1	A	205	GLN
1	A	208	LEU
1	A	214	ILE
1	A	215	THR
1	A	217	VAL
1	A	234	VAL
1	A	236	VAL
1	A	244	VAL
1	A	261	ILE
1	A	285	ILE
1	A	297	ARG
1	A	320	ILE
1	A	324	GLN
1	A	326	VAL

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Mol	Chain	Res	Type
1	A	329	LEU
1	A	338	THR
1	A	347	LEU
1	A	375	VAL
1	B	10	VAL
1	B	15	LEU
1	B	34	VAL
1	B	40	ARG
1	B	64	LEU
1	B	86	THR
1	B	97	ILE
1	B	108	ARG
1	B	114	THR
1	B	122	VAL
1	B	133	LEU
1	B	202	THR
1	B	205	GLN
1	B	208	LEU
1	B	214	ILE
1	B	215	THR
1	B	217	VAL
1	B	226	ARG
1	B	236	VAL
1	B	244	VAL
1	B	261	ILE
1	B	285	ILE
1	B	320	ILE
1	B	324	GLN
1	B	326	VAL
1	B	329	LEU
1	B	338	THR
1	B	347	LEU
1	B	375	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	29	ASN
1	A	69	ASN
1	A	101	HIS
1	A	129	GLN
1	A	143	HIS

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Mol	Chain	Res	Type
1	A	171	HIS
1	A	205	GLN
1	A	333	GLN
1	B	29	ASN
1	B	69	ASN
1	B	101	HIS
1	B	129	GLN
1	B	143	HIS
1	B	152	GLN
1	B	171	HIS
1	B	172	GLN
1	B	205	GLN
1	B	333	GLN
1	B	362	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](#)

2 non-standard protein/DNA/RNA residues 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
1	LLP	A	206	1	23,24,25	1.83	4 (17%)	25,32,34	2.06	6 (24%)
1	LLP	B	206	1	23,24,25	1.91	8 (34%)	25,32,34	1.98	5 (20%)

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
1	LLP	A	206	1	-	3/16/17/19	0/1/1/1
1	LLP	B	206	1	-	4/16/17/19	0/1/1/1

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	206	LLP	O3-C3	-5.31	1.24	1.37
1	A	206	LLP	O3-C3	-4.78	1.25	1.37
1	A	206	LLP	C4-C4'	4.04	1.54	1.46
1	B	206	LLP	C4-C4'	3.14	1.52	1.46
1	A	206	LLP	C4'-NZ	3.03	1.37	1.27
1	B	206	LLP	C4'-NZ	2.97	1.37	1.27
1	B	206	LLP	C2-N1	2.93	1.39	1.33
1	B	206	LLP	CD-CE	2.42	1.59	1.51
1	A	206	LLP	CD-CE	2.41	1.59	1.51
1	B	206	LLP	C6-N1	2.25	1.39	1.34
1	B	206	LLP	CE-NZ	2.23	1.51	1.46
1	B	206	LLP	P-OP3	-2.08	1.46	1.54

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	206	LLP	OP4-C5'-C5	6.46	121.66	109.35
1	A	206	LLP	OP4-C5'-C5	5.94	120.67	109.35
1	A	206	LLP	OP2-P-OP4	-3.70	96.89	106.73
1	A	206	LLP	C4-C4'-NZ	-3.69	107.39	124.31
1	B	206	LLP	OP2-P-OP4	-3.39	97.70	106.73
1	B	206	LLP	C4-C4'-NZ	-3.30	109.18	124.31
1	A	206	LLP	C5-C6-N1	-3.10	118.66	123.82
1	B	206	LLP	C5-C6-N1	-2.18	120.19	123.82
1	A	206	LLP	CD-CG-CB	2.17	121.29	113.62
1	B	206	LLP	C5'-C5-C6	-2.14	115.85	119.37
1	A	206	LLP	OP3-P-OP2	2.02	115.35	107.64

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	206	LLP	O-C-CA-CB
1	B	206	LLP	O-C-CA-CB
1	A	206	LLP	C4-C4'-NZ-CE
1	B	206	LLP	C4-C4'-NZ-CE

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Mol	Chain	Res	Type	Atoms
1	B	206	LLP	C6-C5-C5'-OP4
1	B	206	LLP	CG-CD-CE-NZ
1	A	206	LLP	CG-CD-CE-NZ

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	206	LLP	1	0
1	B	206	LLP	1	0

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

2 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
2	ALA	A	701	-	5,5,5	1.58	2 (40%)	6,6,6	1.10	1 (16%)
3	1BO	B	801	-	4,4,4	0.38	0	3,3,3	0.31	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	ALA	A	701	-	-	2/4/4/4	-
3	1BO	B	801	-	-	2/2/2/2	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	701	ALA	OXT-C	-2.45	1.22	1.30
2	A	701	ALA	CA-C	-2.23	1.51	1.54

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	701	ALA	OXT-C-O	-2.02	119.49	124.09

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	701	ALA	O-C-CA-CB
2	A	701	ALA	OXT-C-CA-CB
3	B	801	1BO	C1-C2-C3-C4
3	B	801	1BO	C2-C3-C4-OH

There are no ring outliers.

2 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	701	ALA	3	0
3	B	801	1BO	4	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	384/393 (97%)	-0.39	3 (0%) 86 88	17, 23, 35, 61	0
1	B	384/393 (97%)	-0.39	4 (1%) 82 85	17, 22, 34, 62	0
All	All	768/786 (97%)	-0.39	7 (0%) 84 86	17, 23, 35, 62	0

All (7) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1	MET	5.2
1	B	1	MET	5.2
1	B	385	PRO	2.5
1	A	385	PRO	2.3
1	B	324	GLN	2.3
1	B	252	GLY	2.3
1	A	324	GLN	2.2

### 6.2 Non-standard residues in protein, DNA, RNA chains [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
1	LLP	A	206	24/25	0.98	0.15	18,20,22,28	0
1	LLP	B	206	24/25	0.98	0.17	20,21,24,25	0

### 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	ALA	A	701	6/6	0.81	0.31	55,56,56,57	0
3	1BO	B	801	5/5	0.93	0.19	29,30,32,34	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.