



# Full wwPDB X-ray Structure Validation Report ⓘ

Nov 16, 2023 – 10:12 AM JST

PDB ID : 6LL9  
Title : Crystal structure of D-alanine-D-alanine ligase from *Aeromonas hydrophila*  
Authors : Zhang, H.  
Deposited on : 2019-12-22  
Resolution : 2.70 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)  
Xtrriage (Phenix) : 1.13  
EDS : 2.36  
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) : 2.36

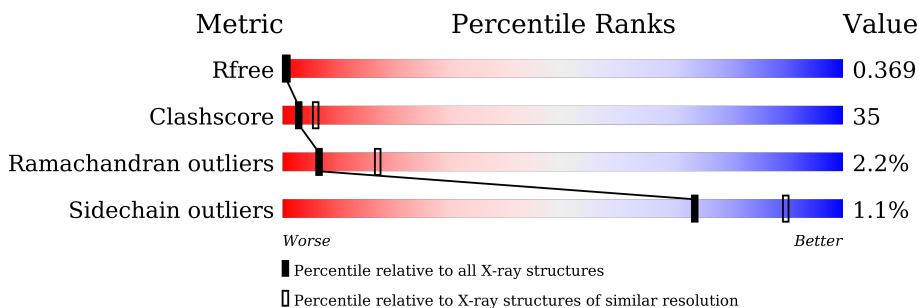
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.70 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	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)

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  $\leq 5\%$ .

Mol	Chain	Length	Quality of chain
1	A	374	 45% 32% 21%
1	B	374	 45% 26% 29%

## 2 Entry composition i

There are 3 unique types of molecules in this entry. The entry contains 4279 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 D-alanine–D-alanine ligase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	297	2236	1425	375	426	10	0	0	0
1	B	266	2026	1300	340	377	9	0	0	0

There are 90 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-44	MET	-	initiating methionine	UNP A0A3S8RJF8
A	-43	GLY	-	expression tag	UNP A0A3S8RJF8
A	-42	SER	-	expression tag	UNP A0A3S8RJF8
A	-41	SER	-	expression tag	UNP A0A3S8RJF8
A	-40	HIS	-	expression tag	UNP A0A3S8RJF8
A	-39	HIS	-	expression tag	UNP A0A3S8RJF8
A	-38	HIS	-	expression tag	UNP A0A3S8RJF8
A	-37	HIS	-	expression tag	UNP A0A3S8RJF8
A	-36	HIS	-	expression tag	UNP A0A3S8RJF8
A	-35	HIS	-	expression tag	UNP A0A3S8RJF8
A	-34	SER	-	expression tag	UNP A0A3S8RJF8
A	-33	SER	-	expression tag	UNP A0A3S8RJF8
A	-32	GLY	-	expression tag	UNP A0A3S8RJF8
A	-31	LEU	-	expression tag	UNP A0A3S8RJF8
A	-30	VAL	-	expression tag	UNP A0A3S8RJF8
A	-29	PRO	-	expression tag	UNP A0A3S8RJF8
A	-28	ARG	-	expression tag	UNP A0A3S8RJF8
A	-27	GLY	-	expression tag	UNP A0A3S8RJF8
A	-26	SER	-	expression tag	UNP A0A3S8RJF8
A	-25	HIS	-	expression tag	UNP A0A3S8RJF8
A	-24	MET	-	expression tag	UNP A0A3S8RJF8
A	-23	ALA	-	expression tag	UNP A0A3S8RJF8
A	-22	SER	-	expression tag	UNP A0A3S8RJF8
A	-21	MET	-	expression tag	UNP A0A3S8RJF8
A	-20	THR	-	expression tag	UNP A0A3S8RJF8

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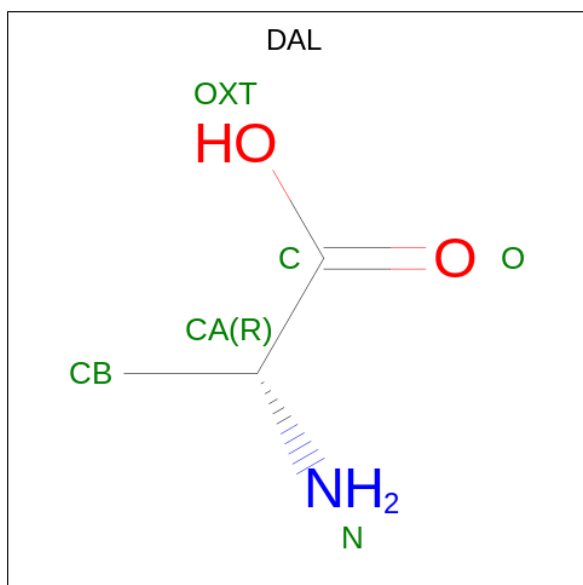
Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	GLY	-	expression tag	UNP A0A3S8RJF8
A	-18	GLY	-	expression tag	UNP A0A3S8RJF8
A	-17	GLN	-	expression tag	UNP A0A3S8RJF8
A	-16	GLN	-	expression tag	UNP A0A3S8RJF8
A	-15	MET	-	expression tag	UNP A0A3S8RJF8
A	-14	GLY	-	expression tag	UNP A0A3S8RJF8
A	-13	ARG	-	expression tag	UNP A0A3S8RJF8
A	-12	GLY	-	expression tag	UNP A0A3S8RJF8
A	-11	SER	-	expression tag	UNP A0A3S8RJF8
A	-10	GLU	-	expression tag	UNP A0A3S8RJF8
A	-9	PHE	-	expression tag	UNP A0A3S8RJF8
A	-8	GLU	-	expression tag	UNP A0A3S8RJF8
A	-7	LEU	-	expression tag	UNP A0A3S8RJF8
A	-6	ARG	-	expression tag	UNP A0A3S8RJF8
A	-5	ARG	-	expression tag	UNP A0A3S8RJF8
A	-4	GLN	-	expression tag	UNP A0A3S8RJF8
A	-3	ALA	-	expression tag	UNP A0A3S8RJF8
A	-2	CYS	-	expression tag	UNP A0A3S8RJF8
A	-1	GLY	-	expression tag	UNP A0A3S8RJF8
A	0	ARG	-	expression tag	UNP A0A3S8RJF8
B	-44	MET	-	initiating methionine	UNP A0A3S8RJF8
B	-43	GLY	-	expression tag	UNP A0A3S8RJF8
B	-42	SER	-	expression tag	UNP A0A3S8RJF8
B	-41	SER	-	expression tag	UNP A0A3S8RJF8
B	-40	HIS	-	expression tag	UNP A0A3S8RJF8
B	-39	HIS	-	expression tag	UNP A0A3S8RJF8
B	-38	HIS	-	expression tag	UNP A0A3S8RJF8
B	-37	HIS	-	expression tag	UNP A0A3S8RJF8
B	-36	HIS	-	expression tag	UNP A0A3S8RJF8
B	-35	HIS	-	expression tag	UNP A0A3S8RJF8
B	-34	SER	-	expression tag	UNP A0A3S8RJF8
B	-33	SER	-	expression tag	UNP A0A3S8RJF8
B	-32	GLY	-	expression tag	UNP A0A3S8RJF8
B	-31	LEU	-	expression tag	UNP A0A3S8RJF8
B	-30	VAL	-	expression tag	UNP A0A3S8RJF8
B	-29	PRO	-	expression tag	UNP A0A3S8RJF8
B	-28	ARG	-	expression tag	UNP A0A3S8RJF8
B	-27	GLY	-	expression tag	UNP A0A3S8RJF8
B	-26	SER	-	expression tag	UNP A0A3S8RJF8
B	-25	HIS	-	expression tag	UNP A0A3S8RJF8
B	-24	MET	-	expression tag	UNP A0A3S8RJF8
B	-23	ALA	-	expression tag	UNP A0A3S8RJF8

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-22	SER	-	expression tag	UNP A0A3S8RJF8
B	-21	MET	-	expression tag	UNP A0A3S8RJF8
B	-20	THR	-	expression tag	UNP A0A3S8RJF8
B	-19	GLY	-	expression tag	UNP A0A3S8RJF8
B	-18	GLY	-	expression tag	UNP A0A3S8RJF8
B	-17	GLN	-	expression tag	UNP A0A3S8RJF8
B	-16	GLN	-	expression tag	UNP A0A3S8RJF8
B	-15	MET	-	expression tag	UNP A0A3S8RJF8
B	-14	GLY	-	expression tag	UNP A0A3S8RJF8
B	-13	ARG	-	expression tag	UNP A0A3S8RJF8
B	-12	GLY	-	expression tag	UNP A0A3S8RJF8
B	-11	SER	-	expression tag	UNP A0A3S8RJF8
B	-10	GLU	-	expression tag	UNP A0A3S8RJF8
B	-9	PHE	-	expression tag	UNP A0A3S8RJF8
B	-8	GLU	-	expression tag	UNP A0A3S8RJF8
B	-7	LEU	-	expression tag	UNP A0A3S8RJF8
B	-6	ARG	-	expression tag	UNP A0A3S8RJF8
B	-5	ARG	-	expression tag	UNP A0A3S8RJF8
B	-4	GLN	-	expression tag	UNP A0A3S8RJF8
B	-3	ALA	-	expression tag	UNP A0A3S8RJF8
B	-2	CYS	-	expression tag	UNP A0A3S8RJF8
B	-1	GLY	-	expression tag	UNP A0A3S8RJF8
B	0	ARG	-	expression tag	UNP A0A3S8RJF8

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



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

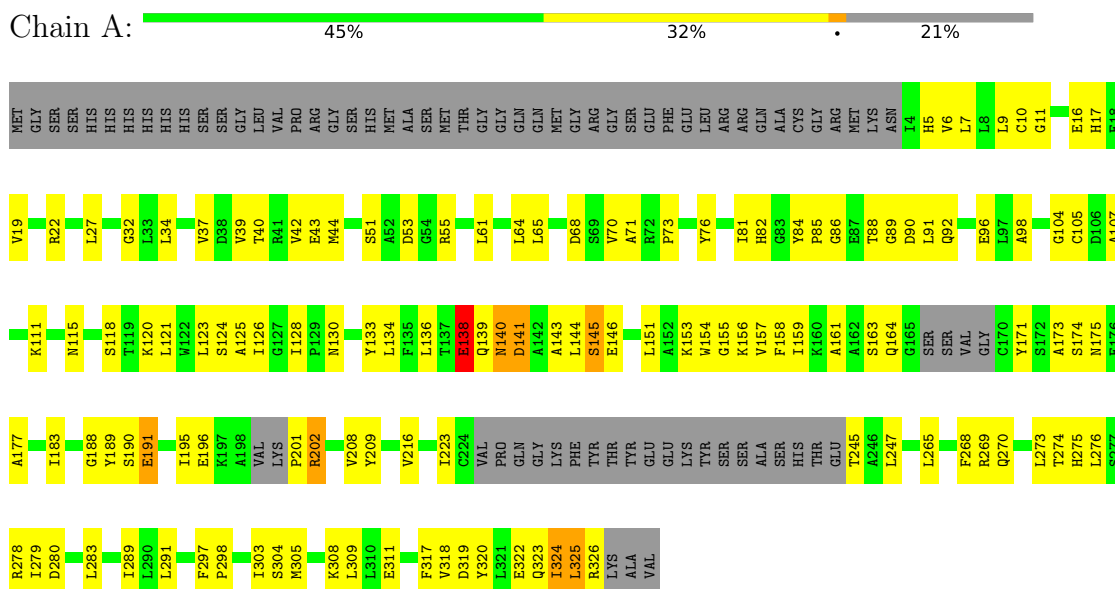
- Molecule 3 is water.

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

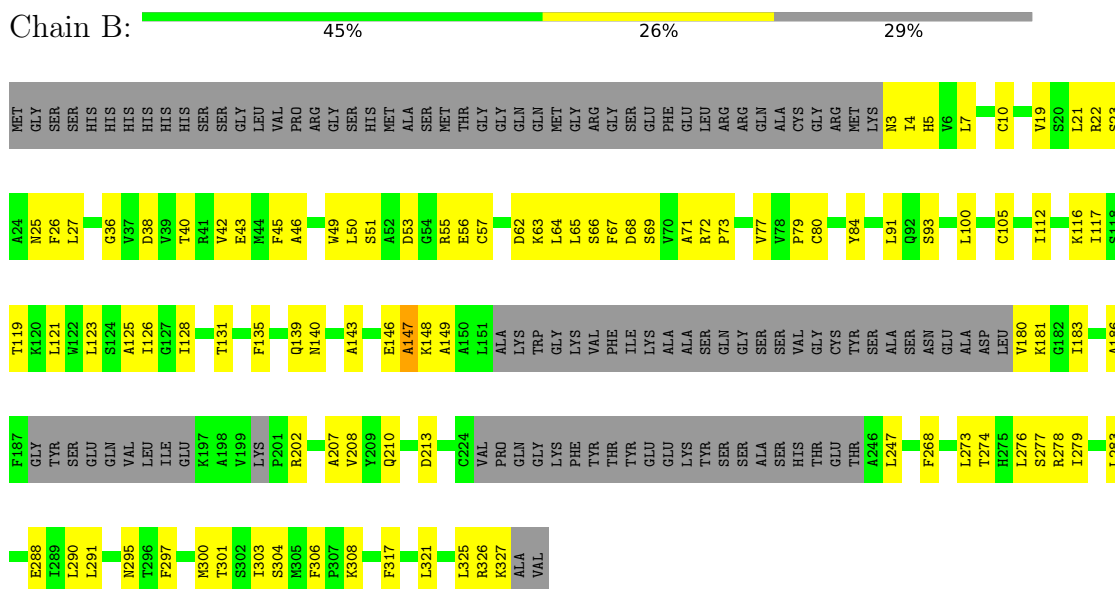
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: D-alanine–D-alanine ligase



- Molecule 1: D-alanine–D-alanine ligase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	62.00Å 93.59Å 110.81Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	55.41 – 2.70 71.50 – 2.53	Depositor EDS
% Data completeness (in resolution range)	99.5 (55.41-2.70) 98.0 (71.50-2.53)	Depositor EDS
$R_{merge}$	0.14	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.55 (at 2.51Å)	Xtrriage
Refinement program	PHENIX 1.14_3260	Depositor
R, $R_{free}$	0.295 , 0.350 0.322 , 0.369	Depositor DCC
$R_{free}$ test set	1113 reflections (5.10%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	55.5	Xtrriage
Anisotropy	1.067	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 49.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.34$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.89	EDS
Total number of atoms	4279	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	85.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.84% 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: DAL

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	0.43	0/2278	0.79	2/3090 (0.1%)
1	B	0.42	0/2064	0.69	0/2796
All	All	0.42	0/4342	0.75	2/5886 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	138	GLU	N-CA-C	-5.49	96.18	111.00
1	A	140	ASN	C-N-CA	5.27	134.88	121.70

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	2236	0	2162	186	0
1	B	2026	0	1995	121	0
2	A	6	0	6	1	0
2	B	6	0	6	0	0
3	A	5	0	0	2	0
All	All	4279	0	4169	297	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 35.

All (297) 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:125:ALA:HB1	1:B:135:PHE:CE2	1.41	1.52
1:A:157:VAL:HG11	1:A:195:ILE:CG2	1.55	1.34
1:A:19:VAL:HG12	1:A:22:ARG:NH2	1.56	1.21
1:B:57:CYS:HB3	1:B:67:PHE:CE2	1.79	1.18
1:A:157:VAL:CG1	1:A:195:ILE:CG2	2.24	1.15
1:A:151:LEU:HD11	1:A:154:TRP:CZ3	1.84	1.11
1:B:140:ASN:HB3	1:B:183:ILE:CG2	1.82	1.09
1:A:125:ALA:HB1	1:B:135:PHE:CZ	1.86	1.09
1:A:157:VAL:HG13	1:A:196:GLU:O	1.49	1.09
1:A:125:ALA:CB	1:B:135:PHE:HE2	1.67	1.07
1:A:157:VAL:HG11	1:A:195:ILE:HG22	1.38	1.06
1:A:126:ILE:HD11	1:A:128:ILE:HD12	1.38	1.05
1:A:125:ALA:CB	1:B:135:PHE:CE2	2.37	1.05
1:B:143:ALA:HB3	1:B:146:GLU:HA	1.36	1.04
1:A:279:ILE:HG23	1:A:291:LEU:HD11	1.36	1.02
1:A:157:VAL:H	1:A:173:ALA:CB	1.71	1.02
1:A:126:ILE:CD1	1:A:128:ILE:HD12	1.92	1.00
1:B:66:SER:HA	1:B:71:ALA:CB	1.92	0.99
1:B:279:ILE:HG23	1:B:291:LEU:HD11	1.45	0.98
1:B:268:PHE:HA	1:B:273:LEU:HD12	1.44	0.98
1:A:105:CYS:HA	1:A:274:THR:OG1	1.63	0.96
1:A:157:VAL:CG1	1:A:195:ILE:HG23	1.96	0.96
1:A:157:VAL:CG1	1:A:195:ILE:HG22	1.89	0.95
1:A:141:ASP:OD1	1:A:183:ILE:HG22	1.67	0.94
1:B:300:MET:HE3	1:B:317:PHE:HZ	1.30	0.94
1:A:42:VAL:HG22	1:A:51:SER:OG	1.68	0.93
1:A:157:VAL:H	1:A:173:ALA:HB3	1.30	0.93
1:B:19:VAL:HG13	1:B:301:THR:HG21	1.49	0.93
1:A:164:GLN:HE22	1:A:189:TYR:HB3	1.33	0.92
1:B:140:ASN:HB3	1:B:183:ILE:HG21	1.52	0.92
1:A:19:VAL:HG12	1:A:22:ARG:HH22	1.31	0.90
1:A:320:TYR:O	1:A:324:ILE:HG13	1.70	0.90
1:A:88:THR:O	1:A:111:LYS:CE	2.21	0.89
1:A:305:MET:O	1:A:309:LEU:HG	1.72	0.88
1:B:208:VAL:HG21	1:B:279:ILE:HD12	1.53	0.88
1:B:57:CYS:HB3	1:B:67:PHE:CD2	2.09	0.87
1:B:300:MET:CE	1:B:317:PHE:HZ	1.85	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:7:LEU:HB3	1:B:77:VAL:HG22	1.54	0.87
1:B:140:ASN:OD1	1:B:183:ILE:HD13	1.74	0.87
1:B:300:MET:HE3	1:B:317:PHE:CZ	2.11	0.86
1:B:66:SER:HA	1:B:71:ALA:HB2	1.54	0.86
1:B:27:LEU:HD11	1:B:300:MET:HE2	1.56	0.86
1:A:279:ILE:HG23	1:A:291:LEU:CD1	2.06	0.86
1:A:268:PHE:HA	1:A:273:LEU:HD12	1.57	0.85
1:B:140:ASN:CB	1:B:183:ILE:HG21	2.06	0.85
1:A:318:VAL:HG23	3:A:501:HOH:O	1.77	0.85
1:B:27:LEU:HD11	1:B:300:MET:CE	2.06	0.84
1:A:64:LEU:HD23	1:A:73:PRO:HA	1.60	0.84
1:A:157:VAL:HG11	1:A:195:ILE:HG23	1.56	0.84
1:A:275:HIS:CE1	1:A:324:ILE:CG2	2.60	0.83
1:A:134:LEU:HD12	1:A:134:LEU:O	1.78	0.83
1:B:121:LEU:HD21	1:B:135:PHE:HZ	1.42	0.83
1:A:11:GLY:HA3	1:A:17:HIS:CE1	2.14	0.82
1:A:121:LEU:HD21	1:B:125:ALA:HB2	1.62	0.82
1:A:279:ILE:CG2	1:A:291:LEU:CD1	2.57	0.82
1:B:247:LEU:HD21	1:B:308:LYS:HB3	1.61	0.82
1:A:123:LEU:CD1	1:A:291:LEU:HD23	2.08	0.82
1:B:57:CYS:CB	1:B:67:PHE:CE2	2.61	0.82
1:B:140:ASN:CB	1:B:183:ILE:CG2	2.57	0.82
1:A:320:TYR:O	1:A:324:ILE:CG1	2.27	0.81
1:B:121:LEU:HD21	1:B:135:PHE:CZ	2.16	0.81
1:A:88:THR:O	1:A:111:LYS:HD3	1.81	0.80
1:B:126:ILE:HD11	1:B:128:ILE:HD12	1.64	0.80
1:B:300:MET:CE	1:B:317:PHE:CZ	2.64	0.80
1:B:45:PHE:CE2	1:B:50:LEU:HD12	2.17	0.79
1:A:5:HIS:NE2	1:A:40:THR:HG21	1.98	0.79
1:B:40:THR:O	1:B:40:THR:HG22	1.81	0.79
1:A:151:LEU:HD23	1:A:195:ILE:HG21	1.65	0.78
1:B:140:ASN:OD1	1:B:183:ILE:HG21	1.83	0.78
1:B:66:SER:HA	1:B:71:ALA:HB1	1.66	0.78
1:A:157:VAL:N	1:A:173:ALA:HB3	1.99	0.77
1:B:279:ILE:HG23	1:B:291:LEU:CD1	2.14	0.77
1:A:157:VAL:HG12	1:A:195:ILE:HG23	1.67	0.77
1:A:279:ILE:CG2	1:A:291:LEU:HD11	2.15	0.76
1:A:151:LEU:HD11	1:A:154:TRP:HZ3	1.49	0.75
1:A:164:GLN:HE22	1:A:189:TYR:CB	1.99	0.74
1:A:141:ASP:OD1	1:A:183:ILE:CG2	2.35	0.74
1:A:123:LEU:HD11	1:A:291:LEU:HD23	1.69	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:19:VAL:HG13	1:B:301:THR:CG2	2.17	0.74
1:A:89:GLY:HA2	1:A:92:GLN:OE1	1.86	0.73
1:A:88:THR:O	1:A:111:LYS:CD	2.36	0.73
1:A:125:ALA:CB	1:B:135:PHE:CZ	2.69	0.73
1:A:156:LYS:HA	1:A:173:ALA:HB3	1.71	0.73
1:B:21:LEU:O	1:B:25:ASN:ND2	2.22	0.73
1:A:151:LEU:HD11	1:A:154:TRP:CH2	2.24	0.72
1:A:317:PHE:O	1:A:320:TYR:HB3	1.89	0.72
1:A:151:LEU:CD1	1:A:154:TRP:CZ3	2.68	0.72
1:A:157:VAL:HG11	1:A:195:ILE:HG21	1.64	0.72
1:B:62:ASP:OD2	1:B:64:LEU:HD12	1.89	0.71
1:B:279:ILE:CG2	1:B:291:LEU:CD1	2.69	0.71
1:A:322:GLU:O	1:A:326:ARG:HG3	1.90	0.70
1:A:141:ASP:CG	1:A:183:ILE:HG22	2.12	0.69
1:B:10:CYS:SG	1:B:43:GLU:HG2	2.32	0.69
1:B:57:CYS:HB3	1:B:67:PHE:CZ	2.28	0.69
1:A:44:MET:SD	1:A:81:ILE:HD11	2.32	0.69
1:A:247:LEU:HD12	1:A:247:LEU:N	2.08	0.69
1:B:183:ILE:O	1:B:186:ALA:HB3	1.93	0.68
1:A:84:TYR:HB2	1:A:88:THR:HG21	1.74	0.67
1:B:56:GLU:O	1:B:67:PHE:CD2	2.46	0.67
1:A:70:VAL:HG12	1:A:71:ALA:N	2.10	0.67
1:A:11:GLY:CA	1:A:17:HIS:CE1	2.78	0.67
1:B:67:PHE:O	1:B:69:SER:N	2.26	0.67
1:A:123:LEU:HD13	1:A:291:LEU:HD23	1.76	0.67
1:A:139:GLN:CB	1:A:191:GLU:OE2	2.43	0.67
1:B:38:ASP:OD2	1:B:72:ARG:NH2	2.23	0.67
1:A:247:LEU:HD12	1:A:247:LEU:H	1.61	0.66
1:A:61:LEU:HA	1:A:98:ALA:HB2	1.78	0.66
1:B:143:ALA:CB	1:B:146:GLU:HA	2.18	0.66
1:B:45:PHE:HE2	1:B:50:LEU:HD12	1.61	0.66
1:A:32:GLY:HA2	1:A:37:VAL:HG21	1.78	0.66
1:A:275:HIS:CE1	1:A:324:ILE:HG22	2.30	0.65
1:A:107:ALA:O	1:A:111:LYS:HG2	1.96	0.65
1:A:64:LEU:HD23	1:A:73:PRO:CA	2.27	0.65
1:B:140:ASN:HB3	1:B:183:ILE:HG22	1.76	0.65
1:A:157:VAL:HG12	1:A:158:PHE:N	2.12	0.64
1:B:117:ILE:O	1:B:121:LEU:HG	1.97	0.64
1:B:140:ASN:CG	1:B:183:ILE:HG21	2.18	0.64
1:A:317:PHE:HB3	3:A:501:HOH:O	1.96	0.64
1:B:56:GLU:O	1:B:67:PHE:HD2	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:125:ALA:HB1	1:B:135:PHE:HE2	0.86	0.64
1:A:305:MET:O	1:A:309:LEU:CG	2.46	0.64
1:A:88:THR:O	1:A:111:LYS:HE2	1.98	0.63
1:B:22:ARG:HA	1:B:25:ASN:HD22	1.63	0.63
1:A:278:ARG:NH2	1:A:280:ASP:OD2	2.32	0.63
1:A:81:ILE:HG21	1:A:85:PRO:O	1.98	0.62
1:A:134:LEU:HD12	1:A:134:LEU:C	2.20	0.62
1:A:88:THR:O	1:A:111:LYS:NZ	2.32	0.62
1:A:158:PHE:O	1:A:195:ILE:HA	2.00	0.61
1:A:317:PHE:O	1:A:320:TYR:N	2.33	0.61
1:A:247:LEU:H	1:A:247:LEU:CD1	2.13	0.61
1:A:279:ILE:CG2	1:A:291:LEU:HD13	2.31	0.60
1:A:265:LEU:O	1:A:269:ARG:HG3	2.01	0.60
1:A:151:LEU:CD2	1:A:195:ILE:HG21	2.30	0.60
1:A:275:HIS:ND1	1:A:324:ILE:HG21	2.17	0.60
1:A:19:VAL:CG1	1:A:22:ARG:NH2	2.49	0.60
1:B:27:LEU:HD11	1:B:300:MET:SD	2.43	0.59
1:A:126:ILE:CD1	1:A:128:ILE:CD1	2.76	0.59
1:A:164:GLN:NE2	1:A:189:TYR:HB3	2.13	0.59
1:A:154:TRP:HE3	1:A:157:VAL:HG22	1.67	0.58
1:A:144:LEU:C	1:A:146:GLU:H	2.04	0.58
1:A:223:ILE:CD1	1:A:245:THR:HG21	2.33	0.58
1:B:57:CYS:SG	1:B:67:PHE:CE2	2.97	0.57
1:B:5:HIS:ND1	1:B:73:PRO:O	2.31	0.57
1:B:143:ALA:HB3	1:B:146:GLU:CA	2.23	0.57
1:A:151:LEU:CD2	1:A:195:ILE:CG2	2.82	0.57
1:A:159:ILE:HG12	1:A:195:ILE:CD1	2.34	0.57
1:B:27:LEU:CD1	1:B:300:MET:HE2	2.33	0.57
1:B:57:CYS:CB	1:B:67:PHE:CZ	2.87	0.57
1:A:70:VAL:HG12	1:A:71:ALA:H	1.70	0.56
1:A:208:VAL:HA	1:A:216:VAL:O	2.05	0.56
1:A:209:TYR:CZ	1:A:216:VAL:HG11	2.40	0.56
1:B:64:LEU:CD2	1:B:73:PRO:HG3	2.36	0.56
1:B:65:LEU:O	1:B:71:ALA:HB1	2.05	0.56
1:A:275:HIS:ND1	1:A:324:ILE:CG2	2.69	0.55
1:A:126:ILE:HG22	1:A:270:GLN:NE2	2.21	0.55
1:B:56:GLU:OE1	1:B:56:GLU:N	2.35	0.55
1:B:202:ARG:HB3	1:B:283:LEU:HB3	1.89	0.55
1:A:5:HIS:NE2	1:A:40:THR:CG2	2.68	0.55
1:B:123:LEU:CD1	1:B:291:LEU:HD23	2.36	0.55
1:A:44:MET:SD	1:A:81:ILE:CD1	2.95	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:164:GLN:NE2	1:A:189:TYR:C	2.60	0.55
1:A:157:VAL:CG1	1:A:196:GLU:O	2.40	0.54
1:A:6:VAL:HG22	1:A:76:TYR:HB3	1.90	0.54
1:A:151:LEU:O	1:A:151:LEU:HG	2.07	0.54
1:A:70:VAL:CG1	1:A:71:ALA:N	2.71	0.54
1:A:86:GLY:O	1:A:89:GLY:N	2.39	0.54
1:B:57:CYS:SG	1:B:67:PHE:CZ	3.01	0.53
1:A:81:ILE:CG2	1:A:85:PRO:O	2.56	0.53
1:A:151:LEU:HD23	1:A:195:ILE:CG2	2.35	0.53
1:A:161:ALA:HB2	1:A:190:SER:O	2.08	0.53
1:A:320:TYR:O	1:A:324:ILE:HG12	2.09	0.53
1:A:61:LEU:HD12	1:A:61:LEU:H	1.73	0.53
1:A:223:ILE:HD11	1:A:305:MET:HG3	1.90	0.53
1:A:70:VAL:CG1	1:A:71:ALA:H	2.21	0.52
1:A:175:ASN:ND2	1:A:177:ALA:HB3	2.23	0.52
1:A:157:VAL:CG1	1:A:158:PHE:N	2.73	0.52
1:B:247:LEU:CD2	1:B:308:LYS:HB3	2.36	0.52
1:A:276:LEU:CD2	1:A:297:PHE:CD2	2.93	0.51
1:B:19:VAL:HG12	1:B:19:VAL:O	2.09	0.51
1:A:201:PRO:O	1:A:283:LEU:O	2.28	0.51
1:A:138:GLU:HA	1:A:138:GLU:OE2	2.10	0.51
1:B:126:ILE:CD1	1:B:128:ILE:HD12	2.39	0.51
1:A:278:ARG:HB2	1:A:298:PRO:HG3	1.93	0.51
1:A:151:LEU:C	1:A:153:LYS:H	2.14	0.51
1:B:55:ARG:HH12	1:B:69:SER:HB2	1.75	0.51
1:B:208:VAL:CG2	1:B:279:ILE:HD12	2.34	0.51
1:A:164:GLN:NE2	1:A:189:TYR:CB	2.73	0.51
1:A:9:LEU:HD12	1:A:91:LEU:HD21	1.93	0.51
1:B:131:THR:O	1:B:131:THR:OG1	2.22	0.51
1:A:105:CYS:CA	1:A:274:THR:OG1	2.48	0.50
1:A:275:HIS:HE1	1:A:324:ILE:HG22	1.73	0.50
1:B:288:GLU:OE2	1:B:290:LEU:HD21	2.12	0.50
1:A:157:VAL:N	1:A:173:ALA:CB	2.56	0.50
1:B:36:GLY:HA3	1:B:326:ARG:NH2	2.26	0.50
1:A:39:VAL:HG13	1:A:39:VAL:O	2.12	0.50
1:A:120:LYS:HD3	1:A:133:TYR:CD1	2.47	0.50
1:B:66:SER:CA	1:B:71:ALA:HB2	2.35	0.50
1:A:151:LEU:CD2	1:A:195:ILE:HB	2.42	0.50
1:A:96:GLU:OE1	1:B:84:TYR:OH	2.21	0.49
1:A:123:LEU:HD11	1:A:291:LEU:CD2	2.41	0.49
1:B:23:SER:O	1:B:27:LEU:HD13	2.11	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:161:ALA:CB	1:A:190:SER:O	2.61	0.49
1:A:304:SER:HA	2:A:400:DAL:HB3	1.95	0.49
1:A:322:GLU:HG2	1:A:326:ARG:NH1	2.27	0.49
1:B:147:ALA:C	1:B:149:ALA:H	2.16	0.49
1:A:247:LEU:N	1:A:247:LEU:CD1	2.73	0.48
1:A:324:ILE:C	1:A:326:ARG:H	2.16	0.48
1:A:303:ILE:O	1:A:303:ILE:HG22	2.13	0.48
1:B:140:ASN:HD21	1:B:143:ALA:HB2	1.77	0.48
1:B:63:LYS:HB3	1:B:100:LEU:HD21	1.95	0.48
1:B:148:LYS:CB	1:B:180:VAL:HG13	2.43	0.48
1:B:140:ASN:OD1	1:B:183:ILE:CD1	2.53	0.48
1:B:140:ASN:ND2	1:B:143:ALA:HB2	2.29	0.48
1:A:209:TYR:HB2	1:A:320:TYR:CE1	2.49	0.48
1:B:57:CYS:HA	1:B:66:SER:O	2.13	0.48
1:B:123:LEU:HD13	1:B:291:LEU:HD23	1.95	0.48
1:B:288:GLU:HG2	1:B:290:LEU:HG	1.96	0.47
1:A:42:VAL:HG22	1:A:51:SER:HG	1.73	0.47
1:A:51:SER:H	1:A:55:ARG:HA	1.80	0.47
1:B:303:ILE:HG22	1:B:303:ILE:O	2.14	0.47
1:A:157:VAL:HG12	1:A:158:PHE:H	1.79	0.47
1:B:207:ALA:HB1	1:B:306:PHE:CE1	2.50	0.47
1:A:10:CYS:SG	1:A:43:GLU:HG2	2.54	0.47
1:A:124:SER:OG	1:A:130:ASN:ND2	2.43	0.47
1:A:283:LEU:HD13	1:A:289:ILE:HD11	1.95	0.47
1:B:278:ARG:NH2	1:B:295:ASN:OD1	2.47	0.47
1:B:210:GLN:NE2	1:B:213:ASP:HA	2.29	0.47
1:B:19:VAL:CG1	1:B:301:THR:HG21	2.34	0.46
1:A:16:GLU:OE1	1:A:82:HIS:HB2	2.16	0.46
1:A:19:VAL:CG1	1:A:22:ARG:HH22	2.16	0.46
1:B:49:TRP:O	1:B:56:GLU:HA	2.16	0.46
1:B:105:CYS:HA	1:B:274:THR:HB	1.97	0.46
1:B:112:ILE:O	1:B:119:THR:OG1	2.25	0.46
1:A:157:VAL:CG1	1:A:158:PHE:H	2.28	0.46
1:A:7:LEU:HD13	1:A:65:LEU:HD22	1.97	0.46
1:A:223:ILE:HD12	1:A:245:THR:HG21	1.98	0.46
1:A:90:ASP:OD1	1:B:93:SER:OG	2.25	0.46
1:A:157:VAL:HG13	1:A:195:ILE:HG22	1.88	0.46
1:B:279:ILE:CG2	1:B:291:LEU:HD13	2.44	0.46
1:A:86:GLY:HA2	1:A:92:GLN:HE22	1.79	0.46
1:A:136:LEU:CD1	1:A:183:ILE:HD12	2.45	0.46
1:A:161:ALA:HB1	1:A:191:GLU:O	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:146:GLU:OE1	1:A:146:GLU:HA	2.16	0.46
1:A:145:SER:O	1:A:145:SER:OG	2.24	0.45
1:A:151:LEU:HD21	1:A:195:ILE:CG2	2.47	0.45
1:B:51:SER:OG	1:B:67:PHE:CE2	2.69	0.45
1:A:10:CYS:SG	1:A:43:GLU:CG	3.05	0.45
1:A:6:VAL:HA	1:A:76:TYR:O	2.17	0.45
1:A:308:LYS:O	1:A:311:GLU:HG3	2.17	0.45
1:B:51:SER:HB2	1:B:53:ASP:OD2	2.17	0.45
1:B:116:LYS:HA	1:B:119:THR:HB	1.99	0.45
1:A:104:GLY:O	1:A:274:THR:OG1	2.32	0.45
1:A:115:ASN:HB3	1:A:118:SER:HB2	1.98	0.45
1:A:275:HIS:CE1	1:A:324:ILE:HG23	2.51	0.45
1:B:276:LEU:O	1:B:277:SER:OG	2.30	0.45
1:A:115:ASN:O	1:A:118:SER:HB2	2.17	0.44
1:A:151:LEU:HD21	1:A:195:ILE:HB	1.99	0.44
1:B:49:TRP:HB2	1:B:57:CYS:O	2.18	0.44
1:A:126:ILE:CG1	1:A:128:ILE:HD12	2.46	0.44
1:B:3:ASN:OD1	1:B:4:ILE:N	2.48	0.44
1:A:158:PHE:CE1	1:A:171:TYR:HA	2.52	0.44
1:B:79:PRO:HB3	1:B:91:LEU:CD2	2.48	0.44
1:B:326:ARG:HA	1:B:327:LYS:HA	1.65	0.44
1:A:84:TYR:HA	1:A:85:PRO:HA	1.71	0.43
1:B:42:VAL:HG13	1:B:50:LEU:O	2.17	0.43
1:B:40:THR:O	1:B:40:THR:CG2	2.52	0.43
1:B:321:LEU:O	1:B:325:LEU:HD23	2.18	0.43
1:B:7:LEU:HD22	1:B:65:LEU:HD22	1.99	0.43
1:B:19:VAL:O	1:B:19:VAL:CG1	2.67	0.43
1:B:45:PHE:O	1:B:46:ALA:HB3	2.19	0.42
1:A:53:ASP:O	1:A:55:ARG:HG3	2.19	0.42
1:A:303:ILE:O	1:A:303:ILE:CG2	2.68	0.42
1:A:319:ASP:O	1:A:323:GLN:HG3	2.19	0.42
1:A:208:VAL:CG1	1:A:268:PHE:CD2	3.02	0.42
1:A:223:ILE:HD13	1:A:245:THR:HG21	2.01	0.42
1:A:269:ARG:O	1:B:139:GLN:NE2	2.53	0.42
1:B:80:CYS:HA	1:B:297:PHE:CZ	2.54	0.42
1:A:64:LEU:HD21	1:A:73:PRO:HG3	2.02	0.42
1:B:180:VAL:HG23	1:B:181:LYS:N	2.34	0.42
1:A:164:GLN:HE21	1:A:189:TYR:C	2.23	0.41
1:A:208:VAL:HG12	1:A:268:PHE:CD2	2.55	0.41
1:B:274:THR:O	1:B:276:LEU:N	2.47	0.41
1:B:19:VAL:CG1	1:B:301:THR:CG2	2.93	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:26:PHE:HB3	1:B:300:MET:O	2.20	0.41
1:A:64:LEU:HD23	1:A:64:LEU:HA	1.81	0.41
1:A:188:GLY:C	1:A:190:SER:H	2.24	0.41
1:A:320:TYR:CE1	1:A:324:ILE:HD11	2.56	0.41
1:B:301:THR:H	1:B:304:SER:HB2	1.85	0.41
1:A:34:LEU:O	1:A:37:VAL:HG12	2.21	0.41
1:A:151:LEU:O	1:A:157:VAL:HG21	2.22	0.40
1:A:202:ARG:HD2	1:A:283:LEU:HD23	2.03	0.40
1:A:27:LEU:HD23	1:A:27:LEU:HA	1.84	0.40
1:A:89:GLY:CA	1:A:92:GLN:OE1	2.65	0.40
1:B:27:LEU:HD11	1:B:300:MET:HB3	2.03	0.40
1:A:308:LYS:HA	1:A:311:GLU:HG3	2.04	0.40
1:B:45:PHE:CE2	1:B:50:LEU:CD1	2.98	0.40
1:B:27:LEU:CD1	1:B:300:MET:CE	2.90	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	289/374 (77%)	255 (88%)	24 (8%)	10 (4%)	<b>3</b> <b>8</b>
1	B	256/374 (68%)	240 (94%)	14 (6%)	2 (1%)	<b>19</b> <b>43</b>
All	All	545/748 (73%)	495 (91%)	38 (7%)	12 (2%)	<b>6</b> <b>17</b>

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	141	ASP
1	A	163	SER
1	B	68	ASP
1	A	138	GLU

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Mol	Chain	Res	Type
1	A	140	ASN
1	A	325	LEU
1	A	143	ALA
1	A	155	GLY
1	B	147	ALA
1	A	68	ASP
1	A	174	SER
1	A	202	ARG

### 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	227/306 (74%)	222 (98%)	5 (2%)	52	79
1	B	210/306 (69%)	210 (100%)	0	100	100
All	All	437/612 (71%)	432 (99%)	5 (1%)	73	90

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	138	GLU
1	A	145	SER
1	A	191	GLU
1	A	324	ILE
1	A	325	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	164	GLN
1	B	25	ASN
1	B	139	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

## 5.5 Carbohydrates [i](#)

There are no 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	DAL	B	400	-	5,5,5	1.14	1 (20%)	6,6,6	1.42	1 (16%)
2	DAL	A	400	-	5,5,5	1.18	1 (20%)	6,6,6	1.36	1 (16%)

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	DAL	B	400	-	-	0/4/4/4	-
2	DAL	A	400	-	-	3/4/4/4	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	400	DAL	OXT-C	-2.17	1.23	1.30

*Continued on next page...*

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	400	DAL	OXT-C	-2.12	1.23	1.30

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	400	DAL	OXT-C-O	-2.70	117.96	124.09
2	A	400	DAL	OXT-C-O	-2.63	118.12	124.09

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	400	DAL	O-C-CA-CB
2	A	400	DAL	OXT-C-CA-CB
2	A	400	DAL	OXT-C-CA-N

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	400	DAL	1	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

Unable to reproduce the depositors R factor - this section is therefore empty.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

### 6.3 Carbohydrates

Unable to reproduce the depositors R factor - this section is therefore empty.

### 6.4 Ligands

Unable to reproduce the depositors R factor - this section is therefore empty.

### 6.5 Other polymers

Unable to reproduce the depositors R factor - this section is therefore empty.