



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 11:07 AM UTC

PDB ID : 6LL9 / pdb_00006ll9
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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

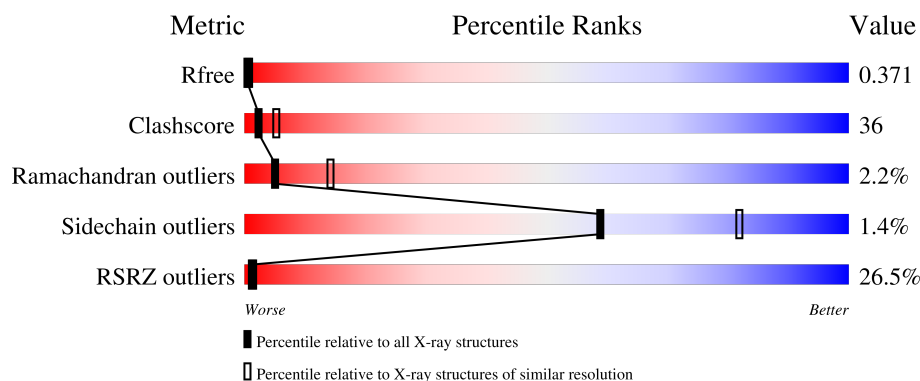
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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}	180053	3538 (2.70-2.70)
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (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 ≥ 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	374	
1	B	374	

2 Entry composition

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
1	A	297	Total	C	N	O	S	0	0	0
			2236	1425	375	426	10			
1	B	266	Total	C	N	O	S	0	0	0
			2026	1300	340	377	9			

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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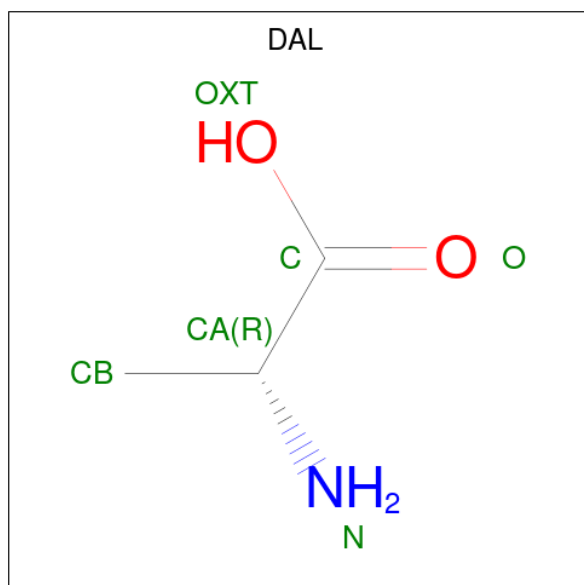
Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	GLY	-	expression tag	UNP A0A3S8RJF8
A	-18	GLY	-	expression tag	UNP A0A3S8RJF8
A	-17	GLN	-	expression tag	UNP A0A3S8RJF8
A	-16	GLN	-	expression tag	UNP A0A3S8RJF8
A	-15	MET	-	expression tag	UNP A0A3S8RJF8
A	-14	GLY	-	expression tag	UNP A0A3S8RJF8
A	-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 (CCD ID: DAL) (formula: $C_3H_7NO_2$).



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		

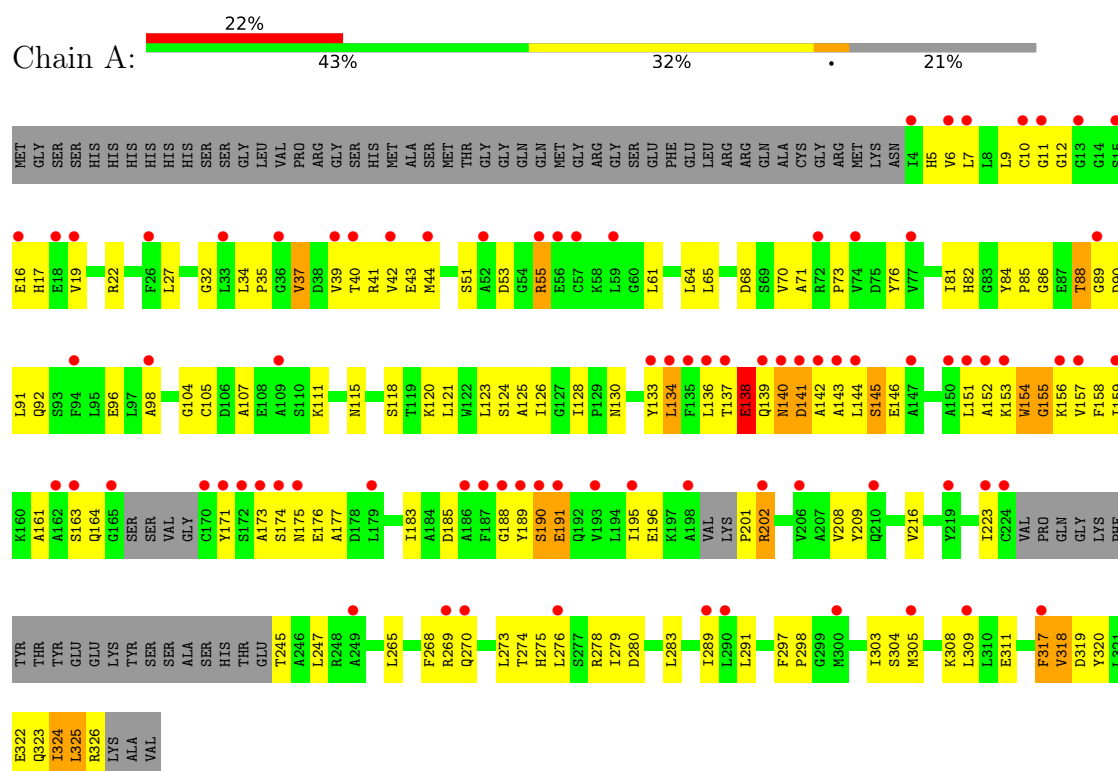
- Molecule 3 is water.

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

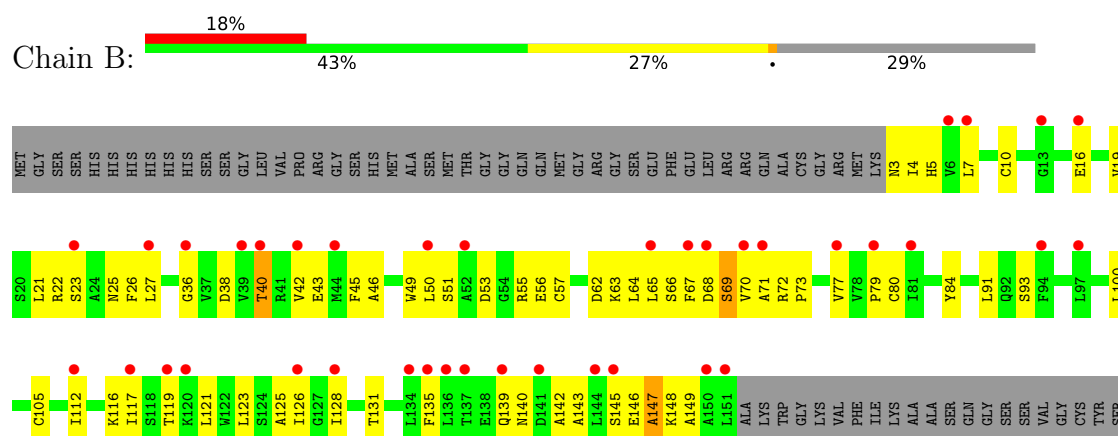
3 Residue-property plots

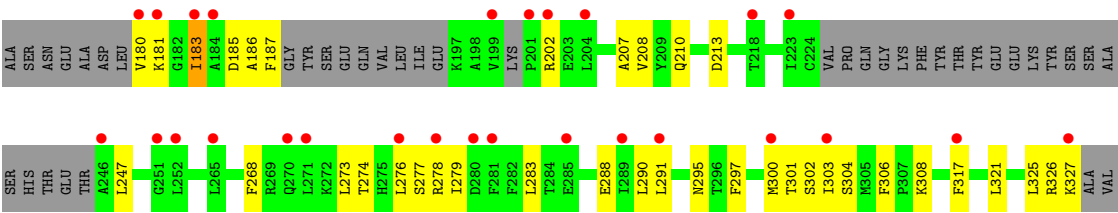
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: 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, α , β , γ	62.00Å 93.59Å 110.81Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	55.41 – 2.70 55.41 – 2.70	Depositor EDS
% Data completeness (in resolution range)	99.5 (55.41-2.70) 99.9 (55.41-2.70)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.55 (at 2.51Å)	Xtriage
Refinement program	PHENIX 1.14_3260	Depositor
R, R_{free}	0.295 , 0.350 0.322 , 0.371	Depositor DCC
R_{free} test set	1113 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	55.5	Xtriage
Anisotropy	1.067	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 52.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	4279	wwPDB-VP
Average B, all atoms (Å ²)	85.0	wwPDB-VP

Xtriage'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.*

¹Intensities estimated from amplitudes.

²Theoretical 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 ⓘ

5.1 Standard geometry ⓘ

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	0.53	0/2278	1.10	27/3090 (0.9%)
1	B	0.50	0/2064	0.92	9/2796 (0.3%)
All	All	0.52	0/4342	1.02	36/5886 (0.6%)

There are no bond length outliers.

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	318	VAL	N-CA-C	-13.06	97.88	110.42
1	B	145	SER	N-CA-C	-12.35	97.73	112.92
1	B	69	SER	N-CA-C	-9.91	99.31	111.40
1	A	176	GLU	N-CA-C	-9.61	101.56	113.38
1	A	12	GLY	N-CA-C	-7.67	103.90	114.64
1	A	185	ASP	N-CA-C	-7.46	104.14	112.57
1	B	142	ALA	N-CA-C	-7.39	102.01	113.02
1	A	155	GLY	CA-C-N	7.39	133.60	123.11
1	A	155	GLY	C-N-CA	7.39	133.60	123.11
1	B	185	ASP	N-CA-C	-7.19	103.60	112.88
1	A	140	ASN	CA-C-N	6.99	134.88	121.54
1	A	140	ASN	C-N-CA	6.99	134.88	121.54
1	A	138	GLU	N-CA-C	-6.87	96.18	110.80
1	B	183	ILE	N-CA-C	-6.56	103.10	112.35
1	A	190	SER	CA-C-N	6.32	133.15	122.15
1	A	190	SER	C-N-CA	6.32	133.15	122.15
1	B	40	THR	N-CA-C	6.17	119.87	111.17
1	A	317	PHE	CA-C-N	6.05	128.18	120.56
1	A	317	PHE	C-N-CA	6.05	128.18	120.56
1	A	137	THR	CA-C-N	6.02	133.03	121.54
1	A	137	THR	C-N-CA	6.02	133.03	121.54
1	A	154	TRP	N-CA-C	-5.80	101.06	109.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	145	SER	N-CA-C	-5.71	106.64	113.21
1	A	152	ALA	N-CA-C	-5.61	106.52	113.19
1	A	154	TRP	CA-C-O	-5.53	114.17	120.58
1	B	185	ASP	O-C-N	5.50	128.79	122.25
1	A	142	ALA	O-C-N	5.47	125.57	121.47
1	A	137	THR	O-C-N	5.28	130.03	123.01
1	B	302	SER	N-CA-C	5.19	118.39	111.75
1	A	55	ARG	CB-CA-C	-5.17	110.60	116.54
1	A	37	VAL	CA-C-N	5.13	130.24	123.00
1	A	37	VAL	C-N-CA	5.13	130.24	123.00
1	A	88	THR	CA-CB-OG1	-5.10	101.95	109.60
1	A	35	PRO	CB-CA-C	-5.09	104.22	112.62
1	A	55	ARG	N-CA-C	5.04	115.97	108.31
1	B	16	GLU	CB-CA-C	-5.02	102.88	111.02

There are no chirality outliers.

There are no planarity outliers.

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	2236	0	2162	188	0
1	B	2026	0	1995	124	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	302	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 36.

All (302) 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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:27:LEU:HD11	1:B:300:MET:HE2	1.43	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: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
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:66:SER:HA	1:B:71:ALA:HB2	1.54	0.86
1:B:300:MET:HE3	1:B:317:PHE:HZ	1.40	0.86
1:A:279:ILE:HG23	1:A:291:LEU:CD1	2.06	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:HE3	1:B:317:PHE:CZ	2.15	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
1:A:141:ASP:CG	1:A:183:ILE:HG22	2.12	0.74
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:27:LEU:CD1	1:B:300:MET:HE2	2.18	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:B:10:CYS:SG	1:B:43:GLU:HG2	2.32	0.69
1:B:140:ASN:CG	1:B:183:ILE:HG21	2.18	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:134:LEU:HD12	1:A:134:LEU:C	2.20	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:A:144:LEU:C	1:A:146:GLU:H	2.04	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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:A:164:GLN:NE2	1:A:189:TYR:C	2.60	0.59
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: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: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:151:LEU:C	1:A:153:LYS:H	2.14	0.56
1:A:275:HIS:ND1	1:A:324:ILE:CG2	2.69	0.55
1:A:145:SER:O	1:A:145:SER:OG	2.24	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:151:LEU:O	1:A:151:LEU:HG	2.07	0.54
1:B:300:MET:HE1	1:B:317:PHE:HZ	1.70	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:147:ALA:C	1:B:149:ALA:H	2.16	0.53
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:324:ILE:C	1:A:326:ARG:H	2.16	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: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:B:112:ILE:O	1:B:119:THR:OG1	2.25	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:A:247:LEU:N	1:A:247:LEU:CD1	2.73	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:A:303:ILE:O	1:A:303:ILE:HG22	2.13	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:A:164:GLN:HE21	1:A:189:TYR:C	2.23	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
1:A:146:GLU:OE1	1:A:146:GLU:HA	2.16	0.46
1:A:188:GLY:C	1:A:190:SER:H	2.24	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:41:ARG:C	1:A:42:VAL:HG23	2.42	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:56:GLU:N	1:B:56:GLU:CD	2.76	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:B:186:ALA:O	1:B:187:PHE:C	2.62	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: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:A:188:GLY:C	1:A:190:SER:N	2.78	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:300:MET:HE1	1:B:317:PHE:CZ	2.50	0.41
1:B:19:VAL:CG1	1:B:301:THR:CG2	2.93	0.41
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: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

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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%)	3	6
1	B	256/374 (68%)	240 (94%)	14 (6%)	2 (1%)	16	37
All	All	545/748 (73%)	495 (91%)	38 (7%)	12 (2%)	5	14

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 ⓘ

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%)	45	74
1	B	210/306 (69%)	209 (100%)	1 (0%)	81	92
All	All	437/612 (71%)	431 (99%)	6 (1%)	59	82

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	134	LEU
1	A	138	GLU
1	A	191	GLU
1	A	324	ILE
1	A	325	LEU
1	B	70	VAL

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

Mol	Chain	Res	Type
1	A	30	GLN
1	A	164	GLN
1	A	313	HIS
1	B	139	GLN

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Mol	Chain	Res	Type
1	B	261	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

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	1.17	1 (20%)	6,6,6	1.46	2 (33%)
2	DAL	A	400	-	5,5,5	1.21	1 (20%)	6,6,6	1.39	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	-2.26	1.23	1.30
2	B	400	DAL	OXT-C	-2.21	1.23	1.30

All (3) 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	124.08
2	A	400	DAL	OXT-C-O	-2.63	118.12	124.08
2	B	400	DAL	OXT-C-CA	2.13	121.13	113.79

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

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, 95th 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 ²)	Q<0.9
1	A	297/374 (79%)	1.57	83 (27%)  	30, 85, 119, 140	0
1	B	266/374 (71%)	1.44	66 (24%)  	30, 80, 120, 137	0
All	All	563/748 (75%)	1.51	149 (26%)  	30, 83, 120, 140	0

All (149) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	137	THR	7.9
1	B	135	PHE	7.7
1	A	170	CYS	5.2
1	A	136	LEU	4.9
1	A	141	ASP	4.8
1	A	171	TYR	4.5
1	A	305	MET	4.4
1	A	300	MET	4.3
1	B	136	LEU	4.3
1	A	270	GLN	4.2
1	A	147	ALA	4.2
1	B	300	MET	4.2
1	A	11	GLY	4.1
1	B	39	VAL	4.1
1	A	172	SER	4.0
1	B	68	ASP	4.0
1	A	140	ASN	4.0
1	B	94	PHE	3.9
1	B	126	ILE	3.9
1	A	26	PHE	3.9
1	B	289	ILE	3.8
1	A	109	ALA	3.8
1	A	206	VAL	3.8
1	B	67	PHE	3.8

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Mol	Chain	Res	Type	RSRZ
1	A	16	GLU	3.8
1	B	137	THR	3.8
1	A	139	GLN	3.7
1	A	151	LEU	3.7
1	A	52	ALA	3.7
1	A	42	VAL	3.6
1	B	71	ALA	3.5
1	A	174	SER	3.5
1	A	156	LYS	3.5
1	A	195	ILE	3.4
1	B	181	LYS	3.4
1	B	16	GLU	3.4
1	B	65	LEU	3.4
1	B	144	LEU	3.4
1	A	269	ARG	3.4
1	A	289	ILE	3.4
1	A	59	LEU	3.3
1	A	152	ALA	3.3
1	A	36	GLY	3.3
1	A	10	CYS	3.2
1	A	13	GLY	3.2
1	A	249	ALA	3.1
1	A	190	SER	3.1
1	A	163	SER	3.1
1	B	77	VAL	3.1
1	A	202	ARG	3.1
1	A	186	ALA	3.0
1	A	6	VAL	3.0
1	A	159	ILE	3.0
1	B	40	THR	3.0
1	A	19	VAL	3.0
1	B	42	VAL	3.0
1	A	188	GLY	2.9
1	A	74	VAL	2.9
1	B	6	VAL	2.9
1	A	223	ILE	2.9
1	B	251	GLY	2.9
1	A	317	PHE	2.9
1	A	98	ALA	2.8
1	B	52	ALA	2.8
1	A	77	VAL	2.8
1	A	40	THR	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	193	VAL	2.8
1	A	134	LEU	2.8
1	B	13	GLY	2.8
1	B	281	PHE	2.7
1	B	204	LEU	2.7
1	B	271	LEU	2.7
1	A	135	PHE	2.7
1	B	81	ILE	2.7
1	A	144	LEU	2.7
1	A	179	LEU	2.7
1	A	55	ARG	2.7
1	A	162	ALA	2.7
1	A	173	ALA	2.7
1	B	291	LEU	2.7
1	A	150	ALA	2.7
1	B	303	ILE	2.6
1	A	142	ALA	2.6
1	A	198	ALA	2.6
1	B	150	ALA	2.6
1	B	145	SER	2.5
1	B	117	ILE	2.5
1	B	285	GLU	2.5
1	A	94	PHE	2.5
1	B	252	LEU	2.5
1	B	44	MET	2.5
1	A	15	SER	2.5
1	A	157	VAL	2.5
1	B	278	ARG	2.4
1	A	189	TYR	2.4
1	B	199	VAL	2.4
1	B	128	ILE	2.4
1	B	23	SER	2.4
1	B	270	GLN	2.4
1	A	33	LEU	2.4
1	A	18	GLU	2.4
1	A	56	GLU	2.4
1	B	139	GLN	2.4
1	B	317	PHE	2.4
1	B	7	LEU	2.3
1	A	4	ILE	2.3
1	A	191	GLU	2.3
1	B	201	PRO	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	180	VAL	2.3
1	B	27	LEU	2.3
1	B	223	ILE	2.3
1	B	119	THR	2.3
1	A	175	ASN	2.3
1	B	97	LEU	2.3
1	B	134	LEU	2.3
1	B	202	ARG	2.3
1	B	141	ASP	2.2
1	A	89	GLY	2.2
1	A	219	TYR	2.2
1	B	79	PRO	2.2
1	A	276	LEU	2.2
1	B	151	LEU	2.2
1	A	39	VAL	2.2
1	A	143	ALA	2.2
1	A	133	TYR	2.2
1	A	165	GLY	2.2
1	B	112	ILE	2.2
1	A	290	LEU	2.2
1	A	44	MET	2.2
1	B	184	ALA	2.1
1	A	153	LYS	2.1
1	B	50	LEU	2.1
1	B	327	LYS	2.1
1	A	210	GLN	2.1
1	B	218	THR	2.1
1	A	57	CYS	2.1
1	A	224	CYS	2.1
1	B	70	VAL	2.1
1	B	280	ASP	2.1
1	B	246	ALA	2.1
1	B	120	LYS	2.1
1	A	187	PHE	2.1
1	A	7	LEU	2.0
1	A	309	LEU	2.0
1	B	265	LEU	2.0
1	B	276	LEU	2.0
1	B	36	GLY	2.0
1	B	183	ILE	2.0
1	A	72	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 oligosaccharides 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, 95th 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
2	DAL	B	400	6/6	0.27	0.28	66,67,67,68	0
2	DAL	A	400	6/6	0.79	0.12	68,69,69,69	0

6.5 Other polymers [i](#)

There are no such residues in this entry.