



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 02:51 AM UTC

PDB ID : 1M0P / pdb_00001m0p
Title : Structure of Dialkylglycine Decarboxylase Complexed with 1-Amino-1-phenyl ethanephosphonate
Authors : Liu, W.; Rogers, C.J.; Fisher, A.J.; Toney, M.D.
Deposited on : 2002-06-13
Resolution : 2.60 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) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

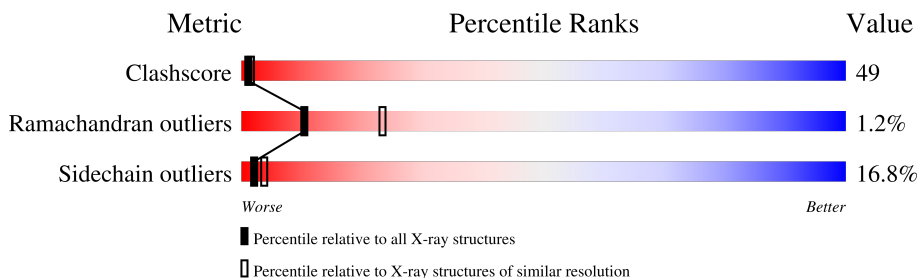
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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))
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)

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 $\leq 5\%$

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	433	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 3420 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 2,2-Dialkylglycine Decarboxylase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	431	Total	C	N	O	S	0	0	0
			3252	2051	576	607	18			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	15	HIS	GLN	SEE REMARK 999	UNP P16932
A	81	GLU	GLY	SEE REMARK 999	UNP P16932

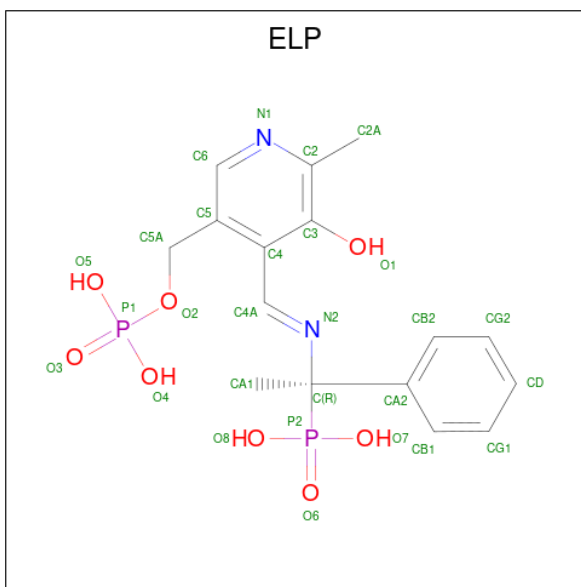
- Molecule 2 is POTASSIUM ION (CCD ID: K) (formula: K).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	K	0	0
			1	1		

- Molecule 3 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Na	0	0
			1	1		

- Molecule 4 is (1R)-1-[[[(1E)-{3-HYDROXY-2-METHYL-5-[(PHOSPHONOOXY)METHYL]PYRIDIN-4-YL}METHYLENE)AMINO]-1-PHENYLETHYLPHOSPHONIC ACID (CCD ID: ELP) (formula: C₁₆H₂₀N₂O₈P₂).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			28	16	2	8	2		

- Molecule 5 is water.

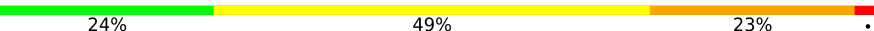
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	138	Total	O	0	0
			138	138		

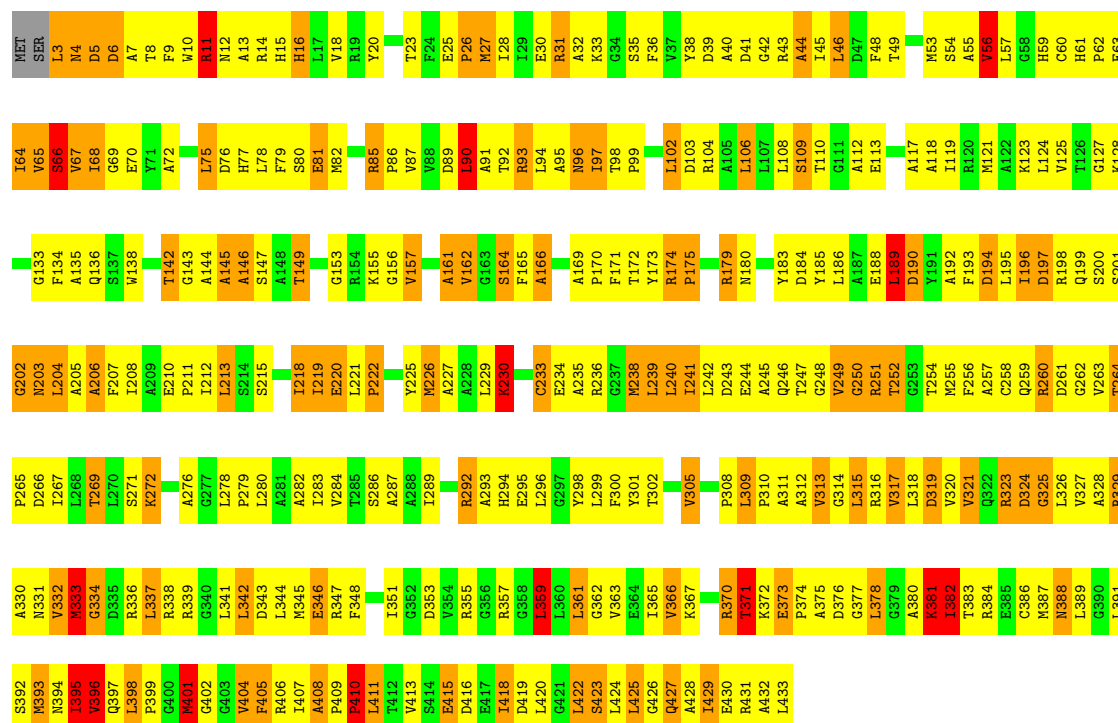
3 Residue-property plots

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. 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.

Note EDS was not executed.

• Molecule 1: 2,2-Dialkylglycine Decarboxylase

Chain A: 



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 64 2 2	Depositor
Cell constants a, b, c, α , β , γ	150.77Å 150.77Å 84.63Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	20.00 – 2.60	Depositor
% Data completeness (in resolution range)	92.1 (20.00-2.60)	Depositor
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	TNT, CNS	Depositor
R, R_{free}	0.173 , 0.230	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	3420	wwPDB-VP
Average B, all atoms (Å ²)	43.0	wwPDB-VP

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: K, NA, ELP

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	2.13	118/3309 (3.6%)	1.61	58/4478 (1.3%)

All (118) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	64	ILE	CA-CB	-11.09	1.40	1.54
1	A	97	ILE	CA-CB	-10.54	1.40	1.54
1	A	103	ASP	CA-C	-9.25	1.43	1.52
1	A	380	ALA	CA-CB	-9.20	1.38	1.53
1	A	299	LEU	C-O	-9.19	1.13	1.23
1	A	118	ALA	C-O	8.89	1.34	1.24
1	A	205	ALA	CA-CB	-8.35	1.40	1.53
1	A	91	ALA	CA-CB	-8.31	1.40	1.53
1	A	149	THR	CA-CB	-8.18	1.42	1.53
1	A	106	LEU	CA-C	8.14	1.62	1.52
1	A	75	LEU	CA-C	-7.92	1.45	1.53
1	A	196	ILE	CA-CB	-7.91	1.45	1.54
1	A	18	VAL	CA-CB	-7.71	1.44	1.54
1	A	241	ILE	CA-CB	7.64	1.63	1.54
1	A	213	LEU	CA-C	-7.53	1.43	1.52
1	A	227	ALA	CA-CB	-7.44	1.41	1.53
1	A	26	PRO	C-O	-7.40	1.14	1.24
1	A	240	LEU	N-CA	-7.39	1.37	1.46
1	A	405	PHE	CA-C	-7.39	1.43	1.52
1	A	324	ASP	CA-C	-7.34	1.41	1.52
1	A	219	ILE	CA-CB	-7.12	1.45	1.54
1	A	284	VAL	C-O	7.07	1.31	1.24
1	A	16	HIS	CA-CB	-6.98	1.43	1.53
1	A	190	ASP	N-CA	-6.96	1.38	1.46
1	A	252	THR	CA-C	6.94	1.62	1.52
1	A	309	LEU	CA-C	6.91	1.61	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	102	LEU	CA-C	-6.87	1.44	1.52
1	A	235	ALA	C-O	-6.85	1.16	1.24
1	A	193	PHE	CA-C	-6.83	1.43	1.52
1	A	382	ILE	CA-CB	-6.83	1.47	1.54
1	A	207	PHE	CA-C	-6.82	1.44	1.52
1	A	20	TYR	CA-C	-6.75	1.44	1.53
1	A	67	VAL	CA-CB	-6.75	1.46	1.54
1	A	169	ALA	CA-CB	6.72	1.62	1.53
1	A	334	GLY	CA-C	-6.70	1.43	1.52
1	A	238	MET	SD-CE	6.68	1.96	1.79
1	A	145	ALA	CA-CB	-6.62	1.43	1.53
1	A	196	ILE	N-CA	-6.61	1.39	1.46
1	A	31	ARG	CA-C	-6.55	1.44	1.52
1	A	260	ARG	C-O	-6.55	1.16	1.24
1	A	423	SER	CA-C	6.47	1.60	1.52
1	A	359	LEU	N-CA	-6.46	1.39	1.46
1	A	13	ALA	CA-CB	-6.46	1.43	1.53
1	A	183	TYR	CA-C	-6.27	1.44	1.52
1	A	112	ALA	CA-C	-6.26	1.44	1.52
1	A	287	ALA	CA-CB	-6.21	1.43	1.53
1	A	165	PHE	CA-CB	-6.18	1.43	1.54
1	A	220	GLU	CA-C	-6.13	1.45	1.52
1	A	230	LYS	CA-C	-6.00	1.45	1.52
1	A	44	ALA	CA-CB	-5.94	1.44	1.53
1	A	416	ASP	CA-C	-5.91	1.45	1.52
1	A	166	ALA	CA-C	-5.87	1.45	1.52
1	A	134	PHE	CA-C	-5.85	1.45	1.52
1	A	415	GLU	CA-C	-5.84	1.45	1.52
1	A	162	VAL	CA-C	5.81	1.60	1.52
1	A	269	THR	CA-C	-5.80	1.45	1.52
1	A	243	ASP	CA-C	5.80	1.60	1.52
1	A	294	HIS	N-CA	-5.76	1.39	1.46
1	A	179	ARG	N-CA	-5.75	1.39	1.46
1	A	321	VAL	CA-CB	-5.74	1.48	1.54
1	A	97	ILE	CA-C	-5.74	1.44	1.52
1	A	180	ASN	CA-C	-5.71	1.46	1.53
1	A	286	SER	N-CA	-5.70	1.38	1.45
1	A	67	VAL	N-CA	-5.68	1.40	1.46
1	A	245	ALA	CA-C	5.66	1.60	1.52
1	A	66	SER	CA-C	5.64	1.59	1.52
1	A	36	PHE	CA-C	-5.61	1.45	1.52
1	A	267	ILE	CA-C	-5.59	1.45	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	4	ASN	N-CA	-5.57	1.38	1.46
1	A	146	ALA	CA-CB	-5.56	1.44	1.53
1	A	90	LEU	C-O	5.54	1.30	1.24
1	A	161	ALA	N-CA	-5.52	1.39	1.46
1	A	230	LYS	N-CA	-5.50	1.39	1.46
1	A	56	VAL	CA-C	5.47	1.60	1.52
1	A	251	ARG	CZ-NH1	5.47	1.40	1.32
1	A	82	MET	SD-CE	-5.45	1.66	1.79
1	A	144	ALA	CA-C	-5.45	1.46	1.52
1	A	56	VAL	CA-CB	-5.40	1.47	1.54
1	A	98	THR	CA-C	-5.39	1.45	1.52
1	A	371	THR	CA-CB	5.39	1.63	1.53
1	A	197	ASP	CA-C	-5.38	1.45	1.52
1	A	218	ILE	CA-CB	-5.38	1.47	1.54
1	A	210	GLU	CA-C	5.37	1.59	1.52
1	A	11	ARG	C-O	5.35	1.30	1.24
1	A	189	LEU	C-N	-5.35	1.27	1.33
1	A	65	VAL	CA-CB	5.34	1.61	1.54
1	A	203	ASN	CA-C	-5.33	1.46	1.53
1	A	410	PRO	CA-C	-5.33	1.46	1.52
1	A	427	GLN	CA-C	-5.33	1.45	1.52
1	A	27	MET	CA-CB	-5.32	1.45	1.53
1	A	247	THR	CA-CB	-5.30	1.44	1.53
1	A	20	TYR	N-CA	-5.30	1.41	1.46
1	A	184	ASP	N-CA	-5.28	1.39	1.46
1	A	144	ALA	N-CA	-5.27	1.40	1.46
1	A	26	PRO	N-CA	-5.26	1.40	1.47
1	A	46	LEU	N-CA	-5.25	1.39	1.46
1	A	95	ALA	CA-CB	-5.25	1.44	1.53
1	A	416	ASP	N-CA	-5.25	1.40	1.46
1	A	397	GLN	CA-C	-5.24	1.46	1.52
1	A	207	PHE	CA-CB	-5.23	1.43	1.53
1	A	162	VAL	CA-CB	5.23	1.61	1.54
1	A	205	ALA	N-CA	-5.17	1.39	1.46
1	A	333	MET	SD-CE	-5.16	1.66	1.79
1	A	408	ALA	C-N	-5.15	1.27	1.33
1	A	87	VAL	CA-C	-5.13	1.46	1.52
1	A	249	VAL	C-O	5.13	1.30	1.24
1	A	395	ILE	C-O	-5.12	1.18	1.24
1	A	317	VAL	N-CA	-5.12	1.40	1.46
1	A	222	PRO	C-O	5.12	1.29	1.23
1	A	226	MET	CA-CB	-5.11	1.45	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	233	CYS	CA-C	-5.11	1.46	1.52
1	A	305	VAL	CA-CB	5.11	1.60	1.54
1	A	396	VAL	CA-CB	5.09	1.60	1.54
1	A	202	GLY	N-CA	-5.08	1.38	1.45
1	A	183	TYR	CA-CB	5.07	1.59	1.52
1	A	384	ARG	N-CA	5.07	1.52	1.46
1	A	44	ALA	N-CA	-5.04	1.39	1.46
1	A	135	ALA	CA-C	-5.02	1.45	1.52

All (58) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	201	SER	N-CA-C	-9.21	101.97	113.02
1	A	64	ILE	CB-CA-C	-8.82	100.23	112.14
1	A	16	HIS	N-CA-C	8.70	123.72	112.41
1	A	5	ASP	N-CA-C	7.93	122.78	113.18
1	A	348	PHE	N-CA-C	7.84	121.30	108.52
1	A	60	CYS	N-CA-C	7.72	122.05	111.54
1	A	112	ALA	N-CA-C	-7.66	102.27	111.69
1	A	96	ASN	N-CA-C	7.38	119.40	111.36
1	A	156	GLY	N-CA-C	7.22	125.70	115.30
1	A	153	GLY	N-CA-C	7.19	125.33	114.61
1	A	429	ILE	N-CA-C	-6.76	104.17	110.53
1	A	250	GLY	N-CA-C	6.75	123.11	115.08
1	A	206	ALA	N-CA-C	6.73	118.42	108.60
1	A	36	PHE	N-CA-C	6.72	120.11	109.50
1	A	127	GLY	N-CA-C	-6.49	105.08	115.08
1	A	401	MET	N-CA-C	6.32	119.81	109.06
1	A	125	VAL	N-CA-C	6.29	119.87	111.44
1	A	388	ASN	N-CA-C	-6.14	103.53	111.02
1	A	293	ALA	N-CA-C	-6.05	104.68	111.28
1	A	4	ASN	N-CA-C	-6.00	105.92	113.18
1	A	179	ARG	CB-CA-C	5.98	119.10	110.79
1	A	404	VAL	N-CA-C	5.93	116.47	108.17
1	A	381	LYS	N-CA-C	-5.87	104.79	111.07
1	A	396	VAL	CA-C-N	-5.83	114.58	122.86
1	A	396	VAL	C-N-CA	-5.83	114.58	122.86
1	A	353	ASP	N-CA-C	5.81	118.69	108.75
1	A	81	GLU	CB-CG-CD	5.80	122.46	112.60
1	A	366	VAL	CB-CA-C	-5.78	101.77	110.55
1	A	75	LEU	CB-CA-C	-5.69	103.96	111.42
1	A	355	ARG	N-CA-C	5.67	117.58	109.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	411	LEU	N-CA-C	-5.66	105.63	112.54
1	A	142	THR	N-CA-C	5.59	118.80	110.52
1	A	103	ASP	N-CA-C	5.57	119.84	112.72
1	A	344	LEU	N-CA-C	-5.54	105.24	111.28
1	A	95	ALA	N-CA-C	-5.51	105.37	111.71
1	A	262	GLY	N-CA-C	-5.46	106.49	114.90
1	A	194	ASP	N-CA-C	-5.40	105.55	111.82
1	A	78	LEU	CA-C-N	5.39	129.00	121.02
1	A	78	LEU	C-N-CA	5.39	129.00	121.02
1	A	10	TRP	N-CA-C	5.38	117.89	111.71
1	A	85	ARG	N-CA-C	5.34	120.02	112.75
1	A	68	ILE	N-CA-C	5.34	115.78	110.23
1	A	109	SER	N-CA-C	5.29	120.09	113.43
1	A	313	VAL	N-CA-C	5.25	115.88	110.36
1	A	365	ILE	N-CA-C	5.25	116.27	108.23
1	A	393	MET	N-CA-C	5.24	117.38	109.41
1	A	251	ARG	N-CA-C	5.23	117.39	111.11
1	A	325	GLY	N-CA-C	-5.17	105.94	113.48
1	A	175	PRO	N-CA-C	5.16	119.19	111.14
1	A	334	GLY	N-CA-C	-5.16	106.48	113.24
1	A	289	ILE	N-CA-C	-5.14	105.38	110.62
1	A	324	ASP	CB-CA-C	5.07	119.12	110.56
1	A	188	GLU	N-CA-C	-5.05	105.67	111.07
1	A	295	GLU	N-CA-C	-5.04	105.92	111.71
1	A	31	ARG	N-CA-C	5.02	115.93	108.60
1	A	174	ARG	CA-C-N	5.02	124.93	119.76
1	A	174	ARG	C-N-CA	5.02	124.93	119.76
1	A	264	THR	N-CA-C	5.01	116.65	109.04

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	3252	0	3279	323	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	1	0	0	0	0
3	A	1	0	0	0	0
4	A	28	0	15	7	0
5	A	138	0	0	13	0
All	All	3420	0	3294	324	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 49.

All (324) 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:3:LEU:HD12	1:A:4:ASN:H	1.05	1.10
1:A:25:GLU:HG3	1:A:27:MET:HE3	1.37	1.07
1:A:328:ALA:HA	1:A:331:ASN:HD22	1.32	0.95
1:A:226:MET:HA	1:A:226:MET:HE3	1.48	0.94
1:A:79:PHE:CE2	1:A:81:GLU:HB2	2.05	0.92
1:A:46:LEU:HD23	1:A:391:LEU:HD13	1.53	0.90
1:A:3:LEU:CD1	1:A:4:ASN:H	1.86	0.89
1:A:11:ARG:HH11	1:A:11:ARG:HB2	1.37	0.89
1:A:174:ARG:CD	1:A:401:MET:HB2	2.05	0.86
1:A:337:LEU:HD13	1:A:361:LEU:HD12	1.55	0.86
1:A:8:THR:HA	1:A:11:ARG:NH1	1.91	0.85
1:A:61:HIS:ND1	1:A:62:PRO:HD2	1.91	0.85
1:A:57:LEU:CD1	1:A:64:ILE:HD11	2.05	0.85
1:A:61:HIS:HE1	1:A:63:GLU:HG2	1.42	0.84
1:A:317:VAL:O	1:A:321:VAL:HG23	1.77	0.84
1:A:246:GLN:HG2	1:A:272:LYS:HD3	1.59	0.84
1:A:3:LEU:HD12	1:A:4:ASN:N	1.90	0.83
1:A:333:MET:HA	1:A:333:MET:HE2	1.61	0.83
1:A:138:TRP:HA	1:A:149:THR:HG23	1.62	0.81
1:A:316:ARG:O	1:A:320:VAL:HG23	1.80	0.81
1:A:3:LEU:HD13	1:A:41:ASP:OD1	1.83	0.79
1:A:61:HIS:CE1	1:A:63:GLU:HG2	2.18	0.78
1:A:85:ARG:HG3	5:A:494:HOH:O	1.82	0.78
1:A:174:ARG:HD2	1:A:401:MET:HB2	1.66	0.77
1:A:61:HIS:O	1:A:65:VAL:HG23	1.85	0.76
1:A:292:ARG:HH11	1:A:292:ARG:HG2	1.51	0.76
1:A:79:PHE:HE2	1:A:81:GLU:HB2	1.49	0.76
1:A:278:LEU:HG	1:A:279:PRO:N	2.01	0.75
1:A:278:LEU:CD1	1:A:279:PRO:HD2	2.18	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:387:MET:HA	1:A:387:MET:HE3	1.69	0.73
1:A:11:ARG:HH11	1:A:11:ARG:CB	2.01	0.72
1:A:11:ARG:HB2	1:A:11:ARG:NH1	2.05	0.71
1:A:80:SER:HB2	1:A:301:TYR:CZ	2.25	0.71
1:A:374:PRO:HB3	1:A:402:GLY:HA2	1.73	0.70
1:A:337:LEU:CD1	1:A:361:LEU:HD12	2.22	0.70
1:A:419:ASP:HA	1:A:422:LEU:HD23	1.72	0.70
1:A:3:LEU:HD13	1:A:41:ASP:CG	2.17	0.69
1:A:367:LYS:HE3	1:A:374:PRO:O	1.92	0.69
1:A:93:ARG:NH1	1:A:93:ARG:HB2	2.08	0.69
1:A:328:ALA:HA	1:A:331:ASN:ND2	2.07	0.69
1:A:420:LEU:HD11	1:A:424:LEU:HD11	1.75	0.68
1:A:321:VAL:HA	1:A:326:LEU:HD12	1.76	0.68
1:A:337:LEU:HD13	1:A:361:LEU:CD1	2.23	0.68
1:A:389:LEU:HD13	1:A:427:GLN:HB2	1.76	0.67
1:A:309:LEU:HB3	1:A:310:PRO:HD3	1.76	0.67
1:A:128:LYS:HD2	1:A:203:ASN:HA	1.76	0.67
1:A:93:ARG:HB2	1:A:93:ARG:HH11	1.58	0.67
1:A:292:ARG:HH11	1:A:292:ARG:CG	2.07	0.67
1:A:325:GLY:HA2	5:A:464:HOH:O	1.94	0.67
1:A:174:ARG:NE	1:A:401:MET:HB2	2.09	0.66
1:A:170:PRO:HB2	1:A:222:PRO:CG	2.25	0.66
1:A:401:MET:HE3	1:A:404:VAL:HG23	1.77	0.66
1:A:121:MET:HB2	1:A:298:TYR:CE1	2.31	0.65
1:A:427:GLN:O	1:A:431:ARG:HG3	1.96	0.65
1:A:90:LEU:CD2	1:A:318:LEU:HD12	2.25	0.64
1:A:246:GLN:HG2	1:A:272:LYS:CD	2.27	0.64
1:A:172:THR:HG23	5:A:548:HOH:O	1.97	0.64
1:A:212:ILE:HD12	1:A:252:THR:HG21	1.79	0.64
1:A:370:ARG:HG3	1:A:370:ARG:HH11	1.61	0.64
1:A:93:ARG:HD2	1:A:97:ILE:HG23	1.77	0.64
1:A:419:ASP:O	1:A:422:LEU:HB2	1.97	0.64
1:A:3:LEU:HA	1:A:41:ASP:OD1	1.97	0.64
1:A:133:GLY:O	1:A:166:ALA:HA	1.98	0.63
1:A:278:LEU:HG	1:A:279:PRO:CD	2.29	0.63
1:A:332:VAL:HG12	1:A:333:MET:N	2.14	0.63
1:A:213:LEU:HD12	1:A:213:LEU:N	2.14	0.63
1:A:278:LEU:HD12	1:A:279:PRO:HD2	1.81	0.63
1:A:332:VAL:HG12	1:A:333:MET:HE3	1.81	0.63
1:A:164:SER:HB3	5:A:465:HOH:O	1.99	0.62
1:A:338:ARG:O	1:A:339:ARG:C	2.40	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:170:PRO:HB2	1:A:222:PRO:HG2	1.81	0.61
1:A:393:MET:HE3	1:A:405:PHE:CD1	2.35	0.61
1:A:57:LEU:HD12	1:A:64:ILE:HD11	1.81	0.61
1:A:26:PRO:HD2	1:A:27:MET:HE3	1.83	0.61
1:A:339:ARG:CA	1:A:342:LEU:HD12	2.30	0.60
4:A:434:ELP:HB1	4:A:434:ELP:O7	2.01	0.60
1:A:66:SER:O	1:A:70:GLU:HB2	2.02	0.60
1:A:8:THR:HA	1:A:11:ARG:HH12	1.66	0.60
1:A:45:ILE:HG21	1:A:387:MET:HE1	1.83	0.60
1:A:68:ILE:HG23	1:A:69:GLY:N	2.16	0.60
1:A:389:LEU:CD1	1:A:427:GLN:HB2	2.32	0.60
1:A:38:TYR:HA	1:A:43:ARG:O	2.02	0.59
1:A:76:ASP:CG	1:A:77:HIS:H	2.10	0.59
1:A:339:ARG:HA	1:A:342:LEU:HD12	1.85	0.59
1:A:194:ASP:O	1:A:198:ARG:HG2	2.02	0.59
1:A:333:MET:HE1	1:A:415:GLU:HG3	1.83	0.59
1:A:220:GLU:HG3	1:A:357:ARG:NH1	2.17	0.59
1:A:410:PRO:O	1:A:413:VAL:HG12	2.01	0.59
1:A:367:LYS:HG3	1:A:373:GLU:HG2	1.84	0.59
1:A:420:LEU:HD12	1:A:420:LEU:O	2.03	0.59
1:A:45:ILE:CG2	1:A:387:MET:HE1	2.33	0.58
1:A:338:ARG:O	1:A:341:LEU:N	2.35	0.58
1:A:256:PHE:HB2	1:A:259:GLN:HG3	1.84	0.58
1:A:420:LEU:HD12	1:A:420:LEU:C	2.28	0.58
1:A:242:LEU:HD12	1:A:265:PRO:HB3	1.84	0.58
1:A:337:LEU:HB2	1:A:418:ILE:HD11	1.85	0.58
1:A:171:PHE:CZ	1:A:173:TYR:HB3	2.39	0.58
1:A:195:LEU:O	1:A:196:ILE:C	2.44	0.58
1:A:211:PRO:HG3	1:A:242:LEU:HD22	1.86	0.58
1:A:242:LEU:HD13	1:A:258:CYS:HB3	1.84	0.58
1:A:124:LEU:HD22	1:A:298:TYR:HA	1.84	0.57
1:A:396:VAL:HG23	1:A:398:LEU:HD23	1.85	0.57
1:A:226:MET:CE	1:A:229:LEU:HD23	2.35	0.57
1:A:206:ALA:HB1	1:A:241:ILE:HD12	1.86	0.57
1:A:239:LEU:HD13	1:A:266:ASP:HB3	1.87	0.57
1:A:278:LEU:HG	1:A:279:PRO:HD2	1.87	0.57
1:A:278:LEU:CG	1:A:279:PRO:HD2	2.35	0.57
1:A:171:PHE:CE1	1:A:173:TYR:HB3	2.39	0.57
1:A:170:PRO:HG2	1:A:222:PRO:HD3	1.86	0.56
1:A:53:MET:HB2	1:A:272:LYS:HE2	1.87	0.56
1:A:204:LEU:HB3	1:A:238:MET:HG2	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:211:PRO:O	1:A:221:LEU:HG	2.06	0.56
1:A:418:ILE:HG23	1:A:422:LEU:CD2	2.35	0.56
1:A:38:TYR:CE1	1:A:44:ALA:HB2	2.41	0.56
1:A:3:LEU:HD13	1:A:41:ASP:OD2	2.05	0.56
1:A:92:THR:O	1:A:93:ARG:C	2.46	0.56
1:A:212:ILE:HA	1:A:219:ILE:O	2.06	0.56
1:A:226:MET:HA	1:A:226:MET:CE	2.30	0.55
1:A:230:LYS:HD2	1:A:240:LEU:CD2	2.36	0.55
1:A:367:LYS:HE2	1:A:376:ASP:H	1.72	0.55
1:A:65:VAL:O	1:A:68:ILE:HG22	2.07	0.55
1:A:81:GLU:HG3	1:A:301:TYR:HE2	1.72	0.55
1:A:408:ALA:N	1:A:409:PRO:HD3	2.22	0.55
1:A:90:LEU:HD21	1:A:318:LEU:HD12	1.88	0.55
1:A:149:THR:HB	5:A:501:HOH:O	2.07	0.55
1:A:61:HIS:CE1	1:A:62:PRO:HD2	2.41	0.55
1:A:39:ASP:OD1	1:A:41:ASP:N	2.39	0.54
1:A:220:GLU:HG3	1:A:357:ARG:HH12	1.73	0.54
1:A:93:ARG:HD2	1:A:97:ILE:CG2	2.38	0.54
1:A:185:TYR:CZ	1:A:222:PRO:HB2	2.42	0.54
1:A:48:PHE:CD2	1:A:407:ILE:HG23	2.42	0.54
1:A:197:ASP:OD2	1:A:236:ARG:NH2	2.36	0.54
1:A:269:THR:HG22	1:A:283:ILE:HG22	1.88	0.54
1:A:93:ARG:O	1:A:96:ASN:HB2	2.08	0.54
1:A:251:ARG:NE	5:A:438:HOH:O	2.26	0.54
1:A:317:VAL:O	1:A:318:LEU:C	2.51	0.54
1:A:215:SER:CB	4:A:434:ELP:HG1	2.38	0.53
1:A:242:LEU:HB2	1:A:265:PRO:HG3	1.90	0.53
1:A:330:ALA:HB2	1:A:411:LEU:HD22	1.90	0.53
1:A:378:LEU:C	1:A:378:LEU:HD12	2.31	0.53
1:A:192:ALA:O	1:A:195:LEU:HB3	2.08	0.53
1:A:323:ARG:HG2	1:A:324:ASP:OD1	2.09	0.53
1:A:418:ILE:O	1:A:422:LEU:HD22	2.08	0.53
1:A:46:LEU:HD23	1:A:391:LEU:CD1	2.32	0.53
1:A:61:HIS:CG	1:A:62:PRO:HD2	2.42	0.53
1:A:69:GLY:O	1:A:72:ALA:HB3	2.09	0.53
1:A:81:GLU:HB3	5:A:519:HOH:O	2.08	0.52
1:A:218:ILE:HG13	1:A:362:GLY:HA3	1.92	0.52
1:A:334:GLY:HA2	1:A:359:LEU:CD1	2.39	0.52
1:A:313:VAL:O	1:A:317:VAL:HG23	2.09	0.52
1:A:67:VAL:O	1:A:70:GLU:HB3	2.09	0.52
1:A:6:ASP:O	1:A:9:PHE:HB3	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:138:TRP:CZ2	4:A:434:ELP:CG2	2.92	0.52
1:A:252:THR:HB	5:A:541:HOH:O	2.08	0.52
1:A:418:ILE:HG22	1:A:419:ASP:N	2.24	0.52
1:A:319:ASP:O	1:A:320:VAL:C	2.51	0.52
1:A:389:LEU:HD12	1:A:428:ALA:HB2	1.90	0.52
1:A:338:ARG:O	1:A:342:LEU:HD12	2.09	0.52
1:A:49:THR:O	1:A:53:MET:HA	2.09	0.52
1:A:119:ILE:CG2	1:A:123:LYS:HE3	2.40	0.52
1:A:28:ILE:O	1:A:40:ALA:N	2.44	0.51
1:A:378:LEU:HD12	1:A:378:LEU:O	2.09	0.51
1:A:161:ALA:O	1:A:164:SER:OG	2.28	0.51
1:A:230:LYS:HD2	1:A:240:LEU:HD22	1.93	0.51
1:A:53:MET:HB2	1:A:272:LYS:CE	2.41	0.51
1:A:61:HIS:CE1	1:A:63:GLU:CG	2.91	0.51
1:A:93:ARG:HG2	1:A:318:LEU:HD13	1.93	0.51
1:A:117:ALA:HA	1:A:300:PHE:CE1	2.46	0.51
1:A:128:LYS:HB3	1:A:203:ASN:O	2.11	0.51
1:A:212:ILE:HD12	1:A:252:THR:CG2	2.41	0.51
1:A:362:GLY:HA2	1:A:405:PHE:O	2.11	0.51
1:A:12:ASN:HA	1:A:15:HIS:HB2	1.93	0.51
1:A:89:ASP:HB3	1:A:315:LEU:HD21	1.93	0.50
1:A:93:ARG:HG3	1:A:94:LEU:N	2.23	0.50
1:A:25:GLU:HG3	1:A:26:PRO:HD2	1.92	0.50
1:A:333:MET:HE2	1:A:333:MET:CA	2.32	0.50
1:A:32:ALA:HB1	1:A:59:HIS:CG	2.46	0.50
1:A:61:HIS:C	1:A:65:VAL:HG23	2.36	0.50
1:A:309:LEU:O	1:A:312:ALA:HB3	2.11	0.50
1:A:76:ASP:OD1	1:A:77:HIS:N	2.41	0.50
1:A:255:MET:HG3	1:A:256:PHE:CE2	2.46	0.50
1:A:260:ARG:NH1	1:A:357:ARG:HG2	2.26	0.50
1:A:338:ARG:C	1:A:342:LEU:HD12	2.37	0.49
1:A:92:THR:HG22	1:A:96:ASN:ND2	2.28	0.49
1:A:124:LEU:HD23	1:A:298:TYR:HB2	1.94	0.49
1:A:250:GLY:HA2	1:A:254:THR:O	2.12	0.49
1:A:318:LEU:O	1:A:319:ASP:C	2.55	0.49
1:A:363:VAL:HG23	1:A:407:ILE:CD1	2.42	0.49
1:A:398:LEU:HD23	1:A:398:LEU:N	2.27	0.49
1:A:246:GLN:NE2	4:A:434:ELP:O1	2.43	0.49
1:A:138:TRP:HD1	4:A:434:ELP:C3	2.25	0.49
1:A:220:GLU:CG	1:A:357:ARG:NH1	2.75	0.49
1:A:258:CYS:HB2	1:A:263:VAL:O	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:337:LEU:O	1:A:341:LEU:HG	2.13	0.49
1:A:419:ASP:O	1:A:420:LEU:C	2.55	0.48
1:A:68:ILE:CG2	1:A:69:GLY:N	2.76	0.48
1:A:9:PHE:CD1	1:A:28:ILE:HD11	2.48	0.48
1:A:398:LEU:N	1:A:398:LEU:CD2	2.77	0.48
1:A:396:VAL:CG1	1:A:406:ARG:HG3	2.44	0.48
1:A:28:ILE:HB	1:A:40:ALA:HB2	1.96	0.48
1:A:93:ARG:O	1:A:96:ASN:N	2.46	0.48
1:A:110:THR:O	1:A:113:GLU:HB3	2.14	0.48
1:A:337:LEU:HB2	1:A:418:ILE:CD1	2.44	0.48
1:A:394:ASN:O	1:A:405:PHE:HA	2.14	0.48
1:A:328:ALA:O	1:A:331:ASN:N	2.39	0.47
1:A:189:LEU:O	1:A:190:ASP:C	2.53	0.47
1:A:64:ILE:HA	1:A:67:VAL:HG12	1.96	0.47
1:A:213:LEU:HB2	1:A:219:ILE:HB	1.96	0.47
1:A:38:TYR:CE1	1:A:44:ALA:CB	2.98	0.47
1:A:155:LYS:O	1:A:157:VAL:HG22	2.15	0.47
1:A:174:ARG:N	1:A:175:PRO:CD	2.78	0.47
1:A:343:ASP:O	1:A:346:GLU:HB2	2.14	0.47
1:A:65:VAL:C	1:A:68:ILE:HG22	2.39	0.47
1:A:93:ARG:HA	1:A:93:ARG:HD3	1.60	0.47
1:A:195:LEU:O	1:A:199:GLN:HG3	2.15	0.46
1:A:8:THR:CA	1:A:11:ARG:HH12	2.29	0.46
1:A:230:LYS:O	1:A:234:GLU:HG3	2.15	0.46
1:A:367:LYS:HG3	1:A:373:GLU:CG	2.45	0.46
1:A:48:PHE:CD2	1:A:407:ILE:CG2	2.98	0.46
1:A:204:LEU:HB3	1:A:238:MET:SD	2.56	0.46
1:A:64:ILE:O	1:A:68:ILE:HG22	2.15	0.46
1:A:196:ILE:O	1:A:199:GLN:N	2.47	0.46
1:A:80:SER:HB3	1:A:305:VAL:CG1	2.46	0.46
1:A:418:ILE:HG23	1:A:422:LEU:HD21	1.98	0.46
1:A:429:ILE:O	1:A:433:LEU:HD12	2.16	0.46
1:A:85:ARG:HB2	1:A:86:PRO:HD3	1.97	0.46
1:A:128:LYS:NZ	5:A:544:HOH:O	2.49	0.46
1:A:292:ARG:HG2	1:A:292:ARG:NH1	2.22	0.46
1:A:200:SER:C	1:A:202:GLY:H	2.24	0.45
1:A:381:LYS:O	1:A:382:ILE:C	2.60	0.45
1:A:326:LEU:HA	1:A:329:ARG:HB3	1.99	0.45
1:A:67:VAL:HG13	1:A:68:ILE:N	2.30	0.45
1:A:170:PRO:CG	1:A:222:PRO:CD	2.95	0.45
1:A:174:ARG:NE	1:A:401:MET:CB	2.78	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:204:LEU:HB3	1:A:238:MET:CG	2.46	0.45
1:A:367:LYS:HG2	1:A:375:ALA:HA	1.99	0.45
1:A:68:ILE:O	1:A:69:GLY:C	2.58	0.45
1:A:99:PRO:HG2	1:A:102:LEU:HD12	1.98	0.45
1:A:72:ALA:HA	1:A:309:LEU:CD1	2.46	0.45
1:A:230:LYS:CD	1:A:240:LEU:HD23	2.46	0.45
1:A:377:GLY:N	5:A:487:HOH:O	2.47	0.45
1:A:61:HIS:HB3	1:A:64:ILE:HG12	1.98	0.45
1:A:195:LEU:HG	1:A:199:GLN:HE21	1.81	0.45
1:A:426:GLY:O	1:A:430:GLU:HG3	2.17	0.45
1:A:276:ALA:HB1	5:A:456:HOH:O	2.15	0.45
1:A:345:MET:HA	1:A:351:ILE:HD12	1.98	0.45
1:A:195:LEU:HG	1:A:199:GLN:NE2	2.31	0.44
1:A:213:LEU:N	1:A:213:LEU:CD1	2.79	0.44
1:A:225:TYR:O	1:A:226:MET:C	2.56	0.44
1:A:394:ASN:O	1:A:406:ARG:N	2.43	0.44
1:A:11:ARG:O	1:A:14:ARG:HB2	2.17	0.44
1:A:401:MET:HG2	1:A:402:GLY:O	2.16	0.44
1:A:310:PRO:O	1:A:311:ALA:C	2.60	0.44
1:A:387:MET:O	1:A:388:ASN:C	2.58	0.44
1:A:398:LEU:HB3	1:A:399:PRO:CD	2.47	0.44
1:A:423:SER:O	1:A:427:GLN:HG3	2.18	0.44
1:A:329:ARG:HD2	1:A:333:MET:CG	2.47	0.44
1:A:383:THR:OG1	1:A:395:ILE:HG21	2.17	0.44
1:A:15:HIS:HB3	1:A:16:HIS:CD2	2.53	0.44
1:A:75:LEU:HD13	1:A:308:PRO:HB3	1.99	0.44
1:A:106:LEU:O	1:A:282:ALA:HA	2.18	0.44
1:A:196:ILE:O	1:A:197:ASP:C	2.59	0.44
1:A:244:GLU:HB3	1:A:248:GLY:N	2.33	0.44
1:A:39:ASP:OD1	1:A:42:GLY:N	2.51	0.44
1:A:374:PRO:CB	1:A:402:GLY:HA2	2.44	0.44
1:A:215:SER:HB2	4:A:434:ELP:HG1	1.99	0.43
1:A:249:VAL:HG12	1:A:249:VAL:O	2.18	0.43
1:A:57:LEU:HD11	1:A:64:ILE:HD11	1.93	0.43
1:A:425:LEU:O	1:A:429:ILE:HD12	2.18	0.43
1:A:76:ASP:CG	1:A:77:HIS:N	2.77	0.43
1:A:347:ARG:HH12	1:A:430:GLU:CD	2.26	0.43
1:A:259:GLN:O	1:A:260:ARG:C	2.59	0.43
1:A:316:ARG:O	1:A:317:VAL:C	2.58	0.43
1:A:339:ARG:HA	1:A:342:LEU:CD1	2.47	0.43
1:A:389:LEU:HA	1:A:389:LEU:HD23	1.74	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:119:ILE:HG22	1:A:123:LYS:HE3	2.01	0.43
1:A:204:LEU:N	1:A:204:LEU:HD13	2.34	0.42
1:A:252:THR:O	1:A:260:ARG:NH1	2.49	0.42
1:A:371:THR:O	1:A:372:LYS:C	2.62	0.42
1:A:170:PRO:CG	1:A:222:PRO:HD3	2.49	0.42
1:A:254:THR:O	1:A:255:MET:C	2.60	0.42
1:A:218:ILE:HG23	1:A:218:ILE:HD12	1.68	0.42
1:A:226:MET:O	1:A:229:LEU:HB3	2.20	0.42
1:A:93:ARG:O	1:A:94:LEU:C	2.61	0.42
1:A:138:TRP:CD2	4:A:434:ELP:CG1	3.03	0.42
1:A:172:THR:O	1:A:175:PRO:HD3	2.20	0.42
1:A:204:LEU:HD22	5:A:471:HOH:O	2.19	0.42
1:A:233:CYS:HB3	1:A:238:MET:O	2.19	0.42
1:A:370:ARG:HG3	1:A:370:ARG:NH1	2.32	0.42
1:A:383:THR:HG21	1:A:395:ILE:HG22	2.02	0.42
1:A:395:ILE:HA	1:A:404:VAL:O	2.20	0.42
1:A:9:PHE:CD1	1:A:28:ILE:CD1	3.03	0.41
1:A:302:THR:O	1:A:305:VAL:HG12	2.20	0.41
1:A:257:ALA:O	1:A:260:ARG:N	2.48	0.41
1:A:5:ASP:O	1:A:7:ALA:N	2.53	0.41
1:A:108:LEU:O	1:A:280:LEU:HD12	2.20	0.41
1:A:213:LEU:N	1:A:219:ILE:O	2.49	0.41
1:A:314:GLY:O	1:A:315:LEU:C	2.61	0.41
1:A:332:VAL:CG1	1:A:333:MET:N	2.80	0.41
1:A:5:ASP:O	1:A:6:ASP:C	2.63	0.41
1:A:8:THR:N	1:A:11:ARG:HH12	2.18	0.41
1:A:142:THR:O	1:A:145:ALA:HB3	2.20	0.41
1:A:170:PRO:HB2	1:A:222:PRO:CD	2.50	0.41
1:A:221:LEU:HA	1:A:222:PRO:HD3	1.83	0.41
1:A:54:SER:O	1:A:56:VAL:N	2.54	0.41
1:A:326:LEU:O	1:A:327:VAL:C	2.64	0.41
1:A:64:ILE:O	1:A:64:ILE:HG22	2.20	0.40
1:A:93:ARG:HH11	1:A:93:ARG:CB	2.29	0.40
1:A:142:THR:O	1:A:146:ALA:N	2.30	0.40
1:A:345:MET:HB2	1:A:351:ILE:HG21	2.02	0.40
1:A:43:ARG:NH1	1:A:388:ASN:O	2.54	0.40
1:A:292:ARG:CG	1:A:292:ARG:NH1	2.72	0.40
1:A:256:PHE:O	1:A:257:ALA:C	2.61	0.40
1:A:337:LEU:CB	1:A:418:ILE:CD1	3.00	0.40
1:A:38:TYR:CD1	1:A:44:ALA:HB2	2.57	0.40
1:A:56:VAL:HG22	1:A:411:LEU:HG	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:334:GLY:CA	1:A:359:LEU:HD13	2.52	0.40
1:A:381:LYS:HD2	1:A:432:ALA:O	2.20	0.40
1:A:392:SER:C	1:A:393:MET:HG2	2.46	0.40
1:A:174:ARG:HH21	1:A:402:GLY:H	1.69	0.40
1:A:200:SER:O	5:A:476:HOH:O	2.22	0.40
1:A:250:GLY:CA	1:A:327:VAL:HG22	2.52	0.40
1:A:386:CYS:SG	1:A:425:LEU:HD23	2.62	0.40
1:A:418:ILE:CG2	1:A:422:LEU:CD2	2.99	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	429/433 (99%)	391 (91%)	33 (8%)	5 (1%)	10	23

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	55	ALA
1	A	6	ASP
1	A	143	GLY
1	A	271	SER
1	A	319	ASP

5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was

analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	334/336 (99%)	278 (83%)	56 (17%)	2 4

All (56) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	LEU
1	A	11	ARG
1	A	23	THR
1	A	30	GLU
1	A	31	ARG
1	A	33	LYS
1	A	35	SER
1	A	56	VAL
1	A	66	SER
1	A	90	LEU
1	A	93	ARG
1	A	104	ARG
1	A	109	SER
1	A	136	GLN
1	A	147	SER
1	A	157	VAL
1	A	162	VAL
1	A	164	SER
1	A	179	ARG
1	A	186	LEU
1	A	189	LEU
1	A	204	LEU
1	A	208	ILE
1	A	230	LYS
1	A	239	LEU
1	A	261	ASP
1	A	264	THR
1	A	272	LYS
1	A	292	ARG
1	A	296	LEU
1	A	315	LEU
1	A	323	ARG
1	A	329	ARG
1	A	332	VAL
1	A	333	MET
1	A	336	ARG

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Mol	Chain	Res	Type
1	A	337	LEU
1	A	342	LEU
1	A	346	GLU
1	A	359	LEU
1	A	361	LEU
1	A	366	VAL
1	A	370	ARG
1	A	371	THR
1	A	373	GLU
1	A	378	LEU
1	A	381	LYS
1	A	382	ILE
1	A	395	ILE
1	A	396	VAL
1	A	398	LEU
1	A	401	MET
1	A	410	PRO
1	A	418	ILE
1	A	422	LEU
1	A	425	LEU

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	136	GLN
1	A	180	ASN
1	A	199	GLN
1	A	331	ASN
1	A	397	GLN

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 [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 3 ligands modelled in this entry, 2 are monoatomic - leaving 1 for Mogul analysis.

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
4	ELP	A	434	-	26,29,29	3.10	17 (65%)	33,44,44	1.55	4 (12%)

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
4	ELP	A	434	-	-	8/21/27/27	0/2/2/2

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	434	ELP	C-CA2	-8.76	1.44	1.53
4	A	434	ELP	CG1-CD	4.37	1.47	1.38
4	A	434	ELP	C6-C5	4.11	1.45	1.37
4	A	434	ELP	C3-C2	3.84	1.45	1.41
4	A	434	ELP	C2-N1	3.72	1.40	1.33
4	A	434	ELP	CD-CG2	3.68	1.46	1.38
4	A	434	ELP	C4-C3	3.59	1.47	1.41
4	A	434	ELP	CB1-CA2	3.37	1.44	1.39
4	A	434	ELP	C4-C4A	3.35	1.53	1.46
4	A	434	ELP	CB2-CA2	2.80	1.44	1.39
4	A	434	ELP	C4-C5	2.78	1.45	1.42
4	A	434	ELP	P1-O4	-2.75	1.44	1.54
4	A	434	ELP	P1-O5	-2.64	1.45	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	434	ELP	P1-O2	-2.42	1.52	1.60
4	A	434	ELP	P2-O8	-2.38	1.48	1.54
4	A	434	ELP	CG2-CB2	2.33	1.42	1.38
4	A	434	ELP	C6-N1	2.23	1.39	1.34

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	434	ELP	C-N2-C4A	4.81	127.95	122.33
4	A	434	ELP	CB1-CA2-CB2	3.19	122.78	118.03
4	A	434	ELP	O4-P1-O2	2.59	113.42	106.67
4	A	434	ELP	O5-P1-O4	2.12	115.76	107.80

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	434	ELP	P2-C-CA2-CB2
4	A	434	ELP	C4-C5-C5A-O2
4	A	434	ELP	C3-C4-C4A-N2
4	A	434	ELP	C5-C4-C4A-N2
4	A	434	ELP	CA1-C-CA2-CB2
4	A	434	ELP	CA1-C-CA2-CB1
4	A	434	ELP	C6-C5-C5A-O2
4	A	434	ELP	N2-C-CA2-CB2

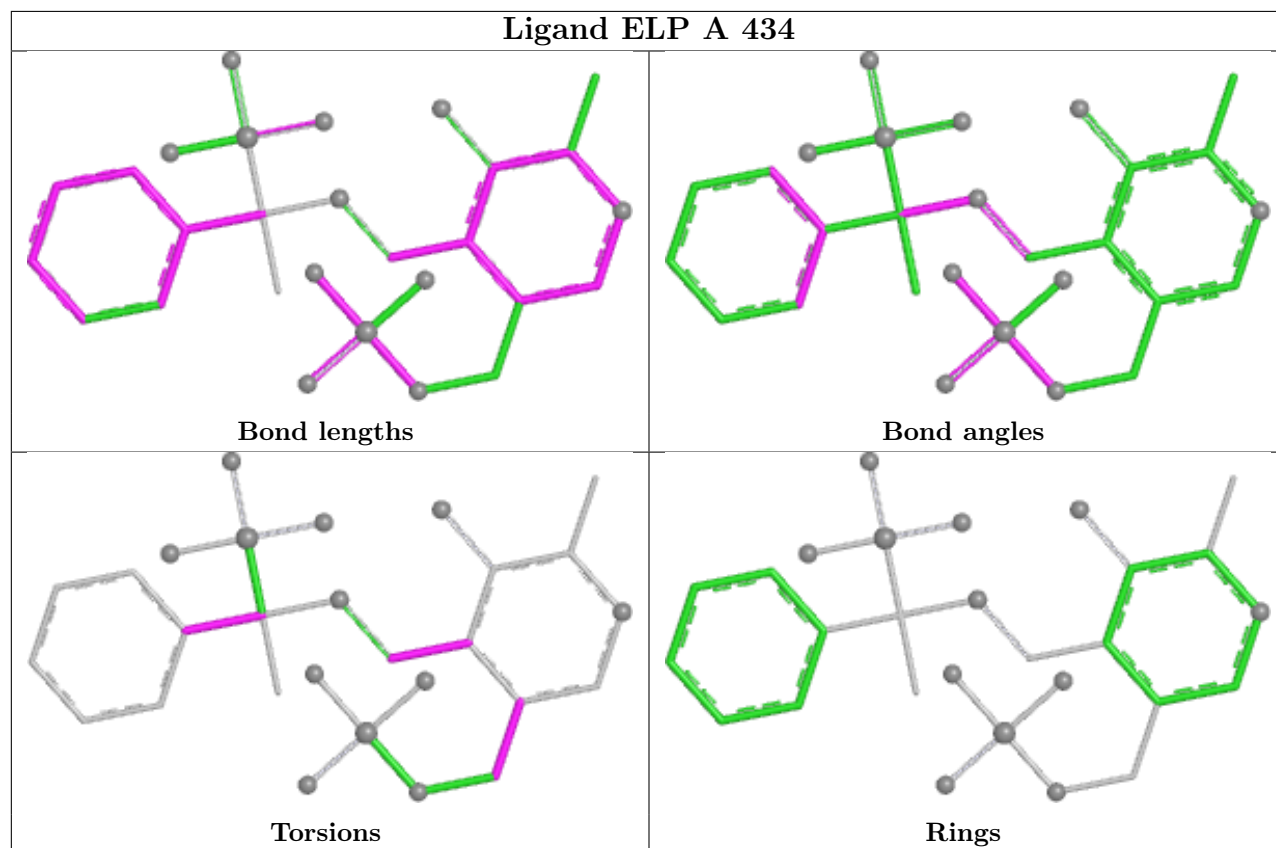
There are no ring outliers.

1 monomer is involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	434	ELP	7	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and

any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.