



# Full wwPDB X-ray Structure Validation Report ⓘ

May 29, 2020 – 10:15 am BST

PDB ID : 1MKD  
Title : crystal structure of PDE4D catalytic domain and zardaverine complex  
Authors : Lee, M.E.; Markowitz, J.; Lee, J.-O.; Lee, H.  
Deposited on : 2002-08-29  
Resolution : 2.90 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.11

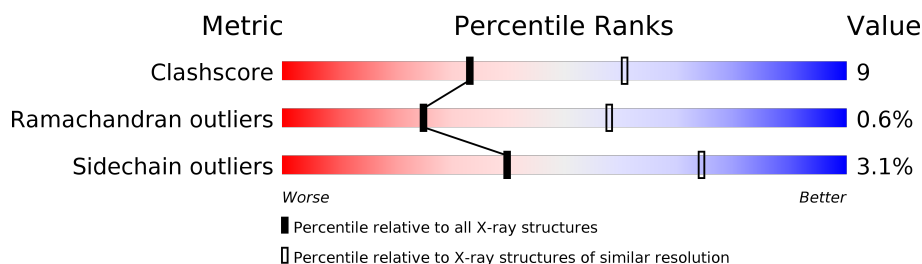
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.90 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ .

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	328	79% 18% .
1	B	328	79% 19% .
1	C	328	78% 20% .
1	D	328	79% 19% .
1	E	328	77% 20% .
1	F	328	77% 21% .
1	G	328	78% 20% .
1	H	328	77% 20% .

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Mol	Chain	Length	Quality of chain
1	I	328	<div><div></div><div>78%</div><div>20%</div><div></div></div>
1	J	328	<div><div></div><div>77%</div><div>19%</div><div></div></div>
1	K	328	<div><div></div><div>77%</div><div>21%</div><div></div></div>
1	L	328	<div><div></div><div>77%</div><div>20%</div><div></div></div>

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 32064 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 Phosphodiesterase 4D.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	328	Total	C	N	O	S	0	0	0
			2650	1675	450	511	14			
1	B	328	Total	C	N	O	S	0	0	0
			2650	1675	450	511	14			
1	C	328	Total	C	N	O	S	0	0	0
			2650	1675	450	511	14			
1	D	328	Total	C	N	O	S	0	0	0
			2650	1675	450	511	14			
1	E	328	Total	C	N	O	S	0	0	0
			2650	1675	450	511	14			
1	F	328	Total	C	N	O	S	0	0	0
			2650	1675	450	511	14			
1	G	328	Total	C	N	O	S	0	0	0
			2650	1675	450	511	14			
1	H	328	Total	C	N	O	S	0	0	0
			2650	1675	450	511	14			
1	I	328	Total	C	N	O	S	0	0	0
			2650	1675	450	511	14			
1	J	328	Total	C	N	O	S	0	0	0
			2650	1675	450	511	14			
1	K	328	Total	C	N	O	S	0	0	0
			2650	1675	450	511	14			
1	L	328	Total	C	N	O	S	0	0	0
			2650	1675	450	511	14			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	439	PRO	ARG	CONFLICT	UNP Q08499
B	439	PRO	ARG	CONFLICT	UNP Q08499
C	439	PRO	ARG	CONFLICT	UNP Q08499
D	439	PRO	ARG	CONFLICT	UNP Q08499
E	439	PRO	ARG	CONFLICT	UNP Q08499

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Chain	Residue	Modelled	Actual	Comment	Reference
F	439	PRO	ARG	CONFLICT	UNP Q08499
G	439	PRO	ARG	CONFLICT	UNP Q08499
H	439	PRO	ARG	CONFLICT	UNP Q08499
I	439	PRO	ARG	CONFLICT	UNP Q08499
J	439	PRO	ARG	CONFLICT	UNP Q08499
K	439	PRO	ARG	CONFLICT	UNP Q08499
L	439	PRO	ARG	CONFLICT	UNP Q08499

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	G	1	Total 1	Zn 1	0	0
2	J	1	Total 1	Zn 1	0	0
2	D	1	Total 1	Zn 1	0	0
2	K	1	Total 1	Zn 1	0	0
2	E	1	Total 1	Zn 1	0	0
2	H	1	Total 1	Zn 1	0	0
2	B	1	Total 1	Zn 1	0	0
2	I	1	Total 1	Zn 1	0	0
2	C	1	Total 1	Zn 1	0	0
2	A	1	Total 1	Zn 1	0	0
2	L	1	Total 1	Zn 1	0	0
2	F	1	Total 1	Zn 1	0	0

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

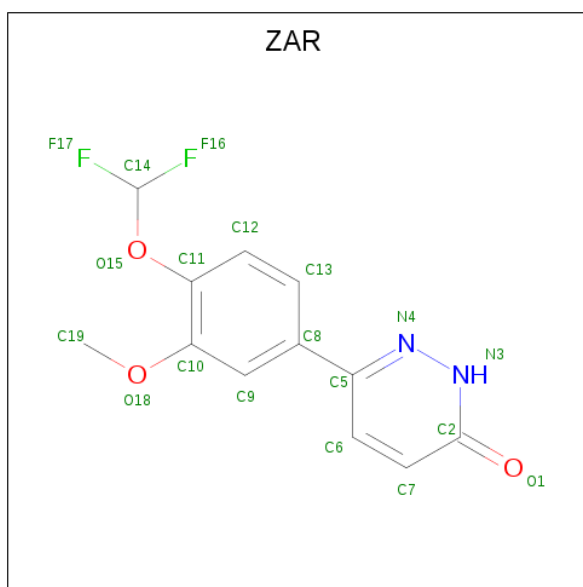
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	G	1	Total 1	Mg 1	0	0
3	J	1	Total 1	Mg 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	D	1	Total	Mg	0	0
			1	1		
3	K	1	Total	Mg	0	0
			1	1		
3	E	1	Total	Mg	0	0
			1	1		
3	H	1	Total	Mg	0	0
			1	1		
3	B	1	Total	Mg	0	0
			1	1		
3	I	1	Total	Mg	0	0
			1	1		
3	C	1	Total	Mg	0	0
			1	1		
3	A	1	Total	Mg	0	0
			1	1		
3	L	1	Total	Mg	0	0
			1	1		
3	F	1	Total	Mg	0	0
			1	1		

- Molecule 4 is 6-(4-DIFLUOROMETHOXY-3-METHOXY-PHENYL)-2H-PYRIDAZIN-3-ONE (three-letter code: ZAR) (formula:  $C_{12}H_{10}F_2N_2O_3$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	F	N	O	0	0
			19	12	2	2	3		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	B	1	Total	C	F	N	O	0	0
			19	12	2	2	3		
4	C	1	Total	C	F	N	O	0	0
			19	12	2	2	3		
4	D	1	Total	C	F	N	O	0	0
			19	12	2	2	3		
4	E	1	Total	C	F	N	O	0	0
			19	12	2	2	3		
4	F	1	Total	C	F	N	O	0	0
			19	12	2	2	3		
4	G	1	Total	C	F	N	O	0	0
			19	12	2	2	3		
4	H	1	Total	C	F	N	O	0	0
			19	12	2	2	3		
4	I	1	Total	C	F	N	O	0	0
			19	12	2	2	3		
4	J	1	Total	C	F	N	O	0	0
			19	12	2	2	3		
4	K	1	Total	C	F	N	O	0	0
			19	12	2	2	3		
4	L	1	Total	C	F	N	O	0	0
			19	12	2	2	3		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	O	0	0
			1	1		
5	B	1	Total	O	0	0
			1	1		
5	C	1	Total	O	0	0
			1	1		
5	D	1	Total	O	0	0
			1	1		
5	E	1	Total	O	0	0
			1	1		
5	F	1	Total	O	0	0
			1	1		
5	G	1	Total	O	0	0
			1	1		
5	H	1	Total	O	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	I	1	Total 1	O 1	0	0
5	J	1	Total 1	O 1	0	0
5	K	1	Total 1	O 1	0	0
5	L	1	Total 1	O 1	0	0

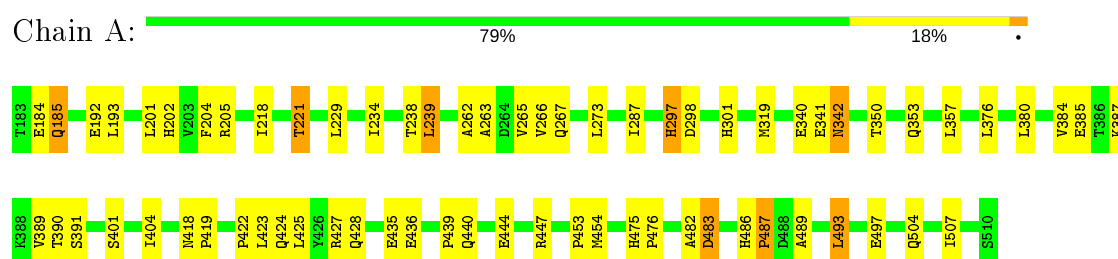


### 3 Residue-property plots [i](#)

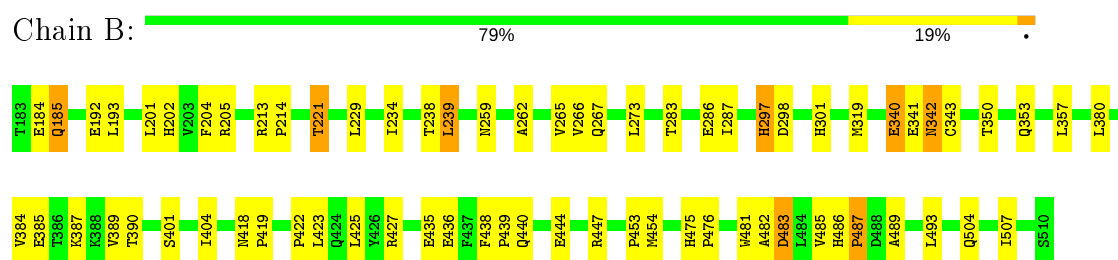
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according 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.

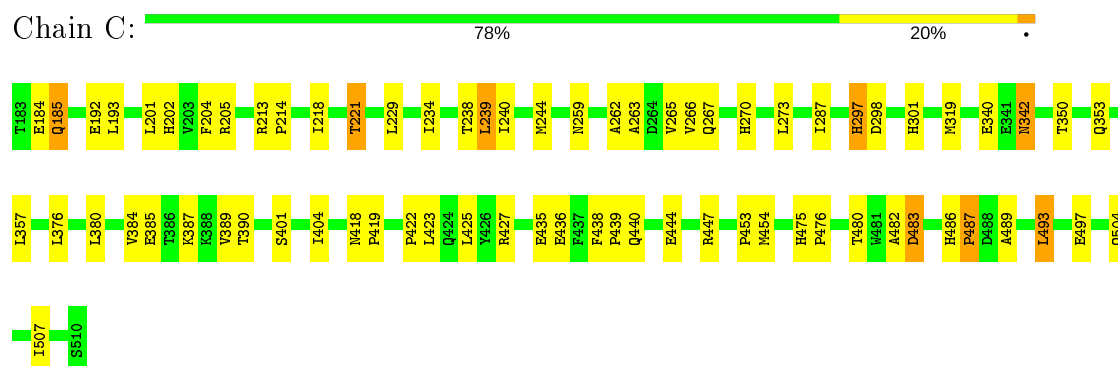
#### • Molecule 1: Phosphodiesterase 4D



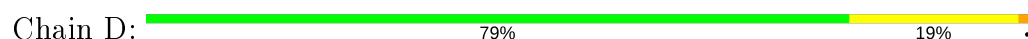
#### • Molecule 1: Phosphodiesterase 4D

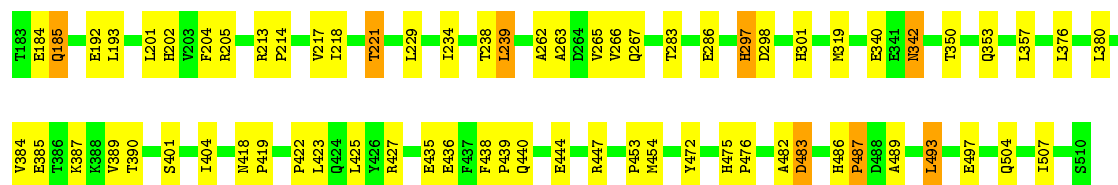


#### • Molecule 1: Phosphodiesterase 4D



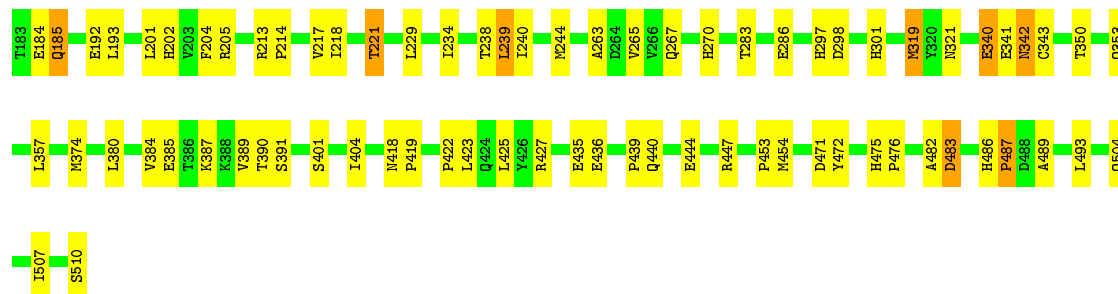
#### • Molecule 1: Phosphodiesterase 4D





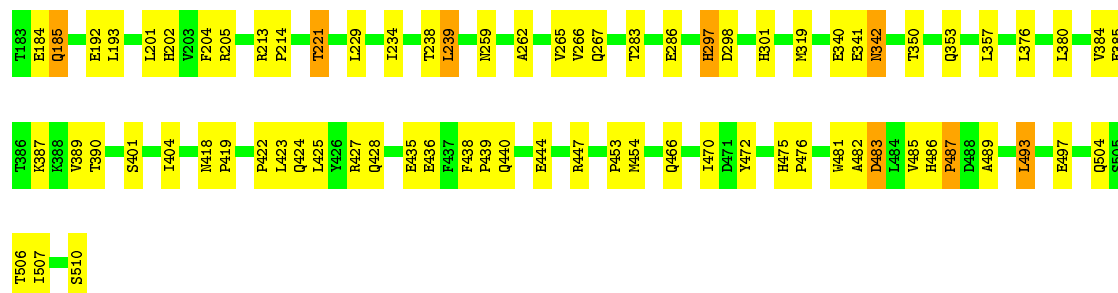
• Molecule 1: Phosphodiesterase 4D

Chain E: 77% 20%



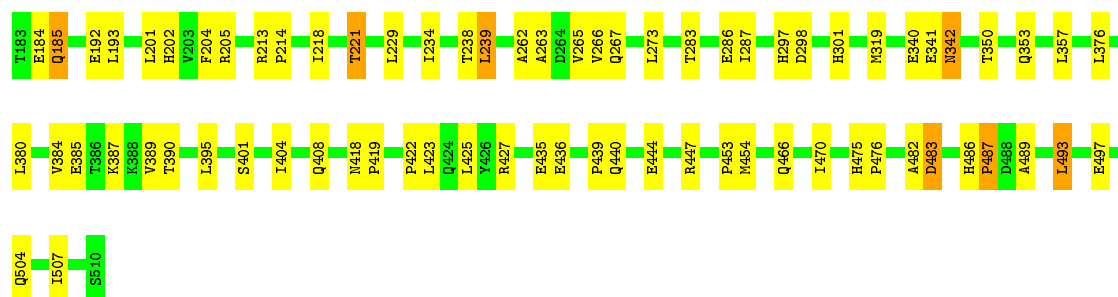
• Molecule 1: Phosphodiesterase 4D

Chain F: 77% 21%



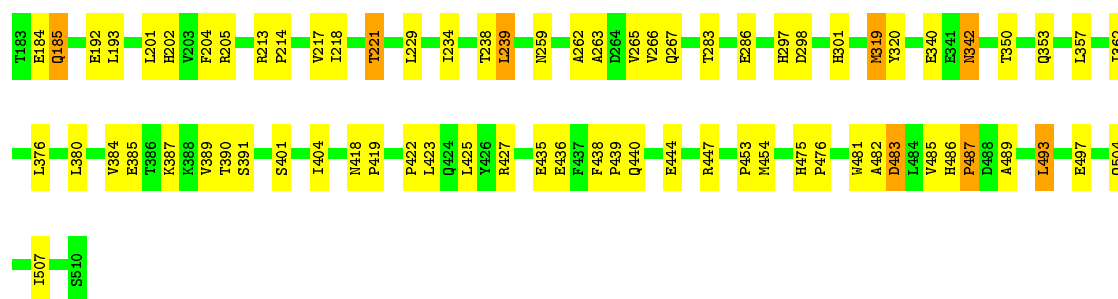
• Molecule 1: Phosphodiesterase 4D

Chain G: 78% 20%



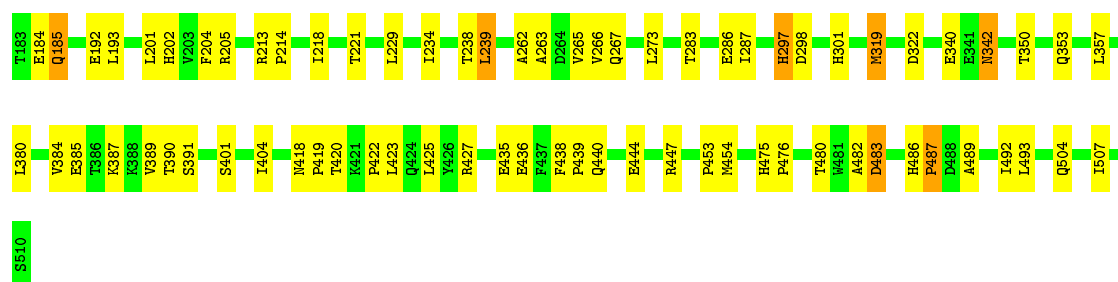
• Molecule 1: Phosphodiesterase 4D

Chain H: 77% 20%



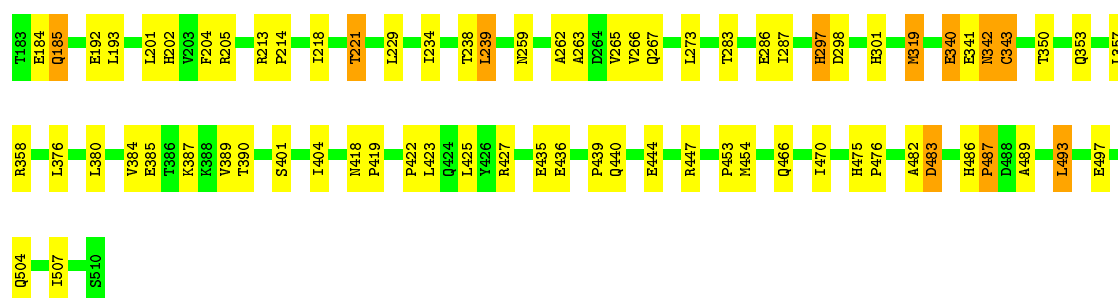
• Molecule 1: Phosphodiesterase 4D

Chain I: 78% 20%



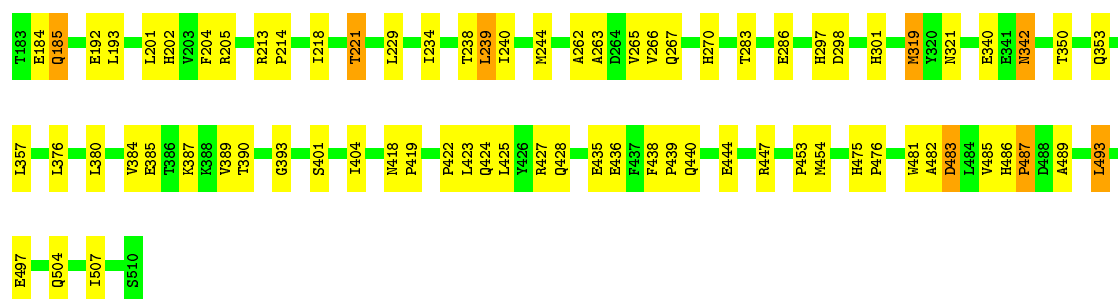
• Molecule 1: Phosphodiesterase 4D

Chain J: 77% 19%



• Molecule 1: Phosphodiesterase 4D

Chain K: 77% 21%

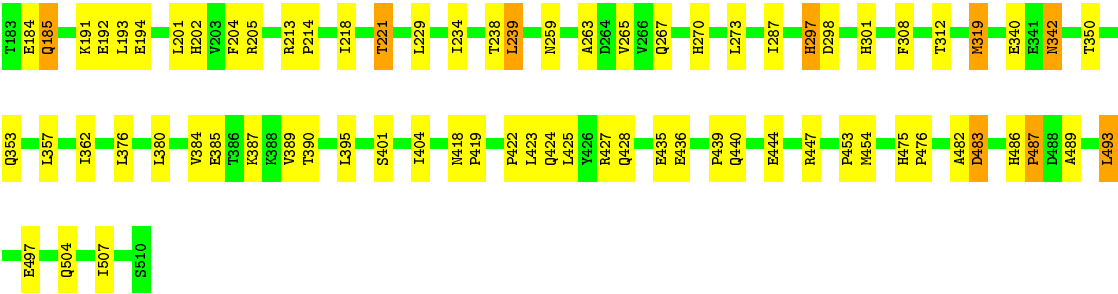


• Molecule 1: Phosphodiesterase 4D

Chain L: 

77%

20%



## 4 Data and refinement statistics

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

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	97.33 Å   164.57 Å   325.54 Å 90.00°   90.00°   90.00°	Depositor
Resolution (Å)	19.98 – 2.90	Depositor
% Data completeness (in resolution range)	94.7 (19.98-2.90)	Depositor
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.07	Depositor
Refinement program	CNS 1.0	Depositor
R, $R_{free}$	0.245 , 0.260	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	32064	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	48.0	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: ZN, ZAR, MG

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	0.40	0/2705	0.59	1/3676 (0.0%)
1	B	0.42	0/2705	0.59	1/3676 (0.0%)
1	C	0.41	0/2705	0.59	1/3676 (0.0%)
1	D	0.42	0/2705	0.59	1/3676 (0.0%)
1	E	0.43	0/2705	0.59	1/3676 (0.0%)
1	F	0.41	0/2705	0.58	1/3676 (0.0%)
1	G	0.42	0/2705	0.59	1/3676 (0.0%)
1	H	0.41	0/2705	0.59	1/3676 (0.0%)
1	I	0.42	0/2705	0.59	1/3676 (0.0%)
1	J	0.42	1/2705 (0.0%)	0.60	1/3676 (0.0%)
1	K	0.43	0/2705	0.58	1/3676 (0.0%)
1	L	0.47	0/2705	0.59	1/3676 (0.0%)
All	All	0.42	1/32460 (0.0%)	0.59	12/44112 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	J	343	CYS	CB-SG	6.94	1.94	1.82

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	K	385	GLU	N-CA-C	-5.27	96.77	111.00
1	F	385	GLU	N-CA-C	-5.24	96.84	111.00
1	J	385	GLU	N-CA-C	-5.11	97.19	111.00
1	E	385	GLU	N-CA-C	-5.11	97.21	111.00
1	D	385	GLU	N-CA-C	-5.10	97.22	111.00
1	C	385	GLU	N-CA-C	-5.10	97.23	111.00
1	G	385	GLU	N-CA-C	-5.08	97.29	111.00
1	B	385	GLU	N-CA-C	-5.07	97.30	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
1	L	385	GLU	N-CA-C	-5.07	97.31	111.00
1	I	385	GLU	N-CA-C	-5.06	97.34	111.00
1	H	385	GLU	N-CA-C	-5.03	97.42	111.00
1	A	385	GLU	N-CA-C	-5.00	97.49	111.00

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	2650	0	2598	42	0
1	B	2650	0	2598	44	0
1	C	2650	0	2598	43	0
1	D	2650	0	2598	43	0
1	E	2650	0	2598	63	0
1	F	2650	0	2598	53	0
1	G	2650	0	2598	42	0
1	H	2650	0	2598	50	0
1	I	2650	0	2598	44	0
1	J	2650	0	2598	62	0
1	K	2650	0	2598	47	0
1	L	2650	0	2598	56	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
2	E	1	0	0	0	0
2	F	1	0	0	0	0
2	G	1	0	0	0	0
2	H	1	0	0	0	0
2	I	1	0	0	0	0
2	J	1	0	0	0	0
2	K	1	0	0	0	0
2	L	1	0	0	0	0
3	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
3	E	1	0	0	0	0
3	F	1	0	0	0	0
3	G	1	0	0	0	0
3	H	1	0	0	0	0
3	I	1	0	0	0	0
3	J	1	0	0	0	0
3	K	1	0	0	0	0
3	L	1	0	0	0	0
4	A	19	0	10	0	0
4	B	19	0	10	0	0
4	C	19	0	10	0	0
4	D	19	0	10	0	0
4	E	19	0	10	0	0
4	F	19	0	10	0	0
4	G	19	0	10	0	0
4	H	19	0	10	0	0
4	I	19	0	10	0	0
4	J	19	0	10	0	0
4	K	19	0	10	0	0
4	L	19	0	10	0	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
5	C	1	0	0	0	0
5	D	1	0	0	0	0
5	E	1	0	0	0	0
5	F	1	0	0	0	0
5	G	1	0	0	0	0
5	H	1	0	0	0	0
5	I	1	0	0	0	0
5	J	1	0	0	0	0
5	K	1	0	0	0	0
5	L	1	0	0	0	0
All	All	32064	0	31296	545	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 9.

All (545) 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:E:472:TYR:CE1	1:J:487:PRO:HD2	1.35	1.58
1:E:472:TYR:CE1	1:J:487:PRO:CD	2.06	1.36
1:F:472:TYR:CE1	1:L:487:PRO:HD3	1.75	1.21
1:F:472:TYR:HE1	1:L:487:PRO:HD3	1.07	1.04
1:E:472:TYR:HE1	1:J:487:PRO:CD	1.55	0.96
1:E:472:TYR:CZ	1:J:487:PRO:HD2	2.01	0.94
1:A:453:PRO:HG3	1:I:391:SER:HB2	1.54	0.90
1:E:472:TYR:CE1	1:J:487:PRO:HD3	2.07	0.89
1:B:202:HIS:HE1	1:B:204:PHE:HB2	1.45	0.81
1:A:202:HIS:HE1	1:A:204:PHE:HB2	1.48	0.79
1:I:202:HIS:HE1	1:I:204:PHE:HB2	1.48	0.79
1:D:202:HIS:HE1	1:D:204:PHE:HB2	1.48	0.78
1:E:202:HIS:HE1	1:E:204:PHE:HB2	1.48	0.78
1:L:202:HIS:HE1	1:L:204:PHE:HB2	1.48	0.78
1:C:202:HIS:HE1	1:C:204:PHE:HB2	1.48	0.78
1:G:202:HIS:HE1	1:G:204:PHE:HB2	1.47	0.77
1:J:229:LEU:HD21	1:J:239:LEU:HD12	1.66	0.77
1:A:229:LEU:HD21	1:A:239:LEU:HD12	1.67	0.77
1:K:202:HIS:HE1	1:K:204:PHE:HB2	1.50	0.77
1:F:472:TYR:OH	1:L:487:PRO:HD2	1.85	0.76
1:B:229:LEU:HD21	1:B:239:LEU:HD12	1.67	0.76
1:F:202:HIS:HE1	1:F:204:PHE:HB2	1.50	0.76
1:H:202:HIS:HE1	1:H:204:PHE:HB2	1.48	0.76
1:G:229:LEU:HD21	1:G:239:LEU:HD12	1.67	0.76
1:J:202:HIS:HE1	1:J:204:PHE:HB2	1.49	0.76
1:B:202:HIS:CE1	1:B:204:PHE:HB2	2.21	0.75
1:F:229:LEU:HD21	1:F:239:LEU:HD12	1.68	0.75
1:I:229:LEU:HD21	1:I:239:LEU:HD12	1.69	0.75
1:L:202:HIS:CE1	1:L:204:PHE:HB2	2.22	0.75
1:C:229:LEU:HD21	1:C:239:LEU:HD12	1.67	0.74
1:L:229:LEU:HD21	1:L:239:LEU:HD12	1.67	0.74
1:G:202:HIS:CE1	1:G:204:PHE:HB2	2.23	0.74
1:K:229:LEU:HD21	1:K:239:LEU:HD12	1.68	0.74
1:D:202:HIS:CE1	1:D:204:PHE:HB2	2.24	0.73
1:J:202:HIS:CE1	1:J:204:PHE:HB2	2.24	0.73
1:A:202:HIS:CE1	1:A:204:PHE:HB2	2.24	0.72
1:I:202:HIS:CE1	1:I:204:PHE:HB2	2.24	0.72
1:C:202:HIS:CE1	1:C:204:PHE:HB2	2.24	0.72
1:E:202:HIS:CE1	1:E:204:PHE:HB2	2.23	0.72
1:F:472:TYR:CE1	1:L:487:PRO:CD	2.66	0.72
1:H:202:HIS:CE1	1:H:204:PHE:HB2	2.24	0.72
1:D:229:LEU:HD21	1:D:239:LEU:HD12	1.70	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:202:HIS:CE1	1:F:204:PHE:HB2	2.25	0.71
1:H:229:LEU:HD21	1:H:239:LEU:HD12	1.71	0.71
1:E:472:TYR:CD1	1:J:487:PRO:HD3	2.25	0.70
1:K:202:HIS:CE1	1:K:204:PHE:HB2	2.25	0.70
1:E:229:LEU:HD21	1:E:239:LEU:HD12	1.73	0.70
1:I:319:MET:SD	1:J:319:MET:SD	2.91	0.69
1:E:472:TYR:HE1	1:J:487:PRO:HD2	0.93	0.68
1:E:472:TYR:CD1	1:J:487:PRO:CD	2.76	0.67
1:F:472:TYR:CZ	1:L:487:PRO:HD3	2.27	0.67
1:F:472:TYR:OH	1:L:487:PRO:CD	2.42	0.67
1:B:238:THR:HG23	1:B:342:ASN:O	1.95	0.66
1:F:472:TYR:HE1	1:L:487:PRO:CD	1.97	0.66
1:H:238:THR:HG23	1:H:342:ASN:O	1.94	0.65
1:A:391:SER:OG	1:H:453:PRO:HG3	1.96	0.65
1:K:238:THR:HG23	1:K:342:ASN:O	1.95	0.65
1:A:238:THR:HG23	1:A:342:ASN:O	1.96	0.65
1:J:238:THR:HG23	1:J:342:ASN:O	1.96	0.65
1:L:238:THR:HG23	1:L:342:ASN:O	1.97	0.64
1:E:238:THR:HG23	1:E:342:ASN:O	1.97	0.63
1:C:238:THR:HG23	1:C:342:ASN:O	1.99	0.62
1:C:447:ARG:HH11	1:C:447:ARG:HG2	1.64	0.62
1:I:447:ARG:HG2	1:I:447:ARG:HH11	1.65	0.62
1:D:238:THR:HG23	1:D:342:ASN:O	2.00	0.61
1:E:447:ARG:HH11	1:E:447:ARG:HG2	1.64	0.61
1:I:238:THR:HG23	1:I:342:ASN:O	2.00	0.61
1:D:447:ARG:HG2	1:D:447:ARG:HH11	1.64	0.61
1:K:447:ARG:HH11	1:K:447:ARG:HG2	1.66	0.61
1:F:238:THR:HG23	1:F:342:ASN:O	2.02	0.60
1:H:447:ARG:HH11	1:H:447:ARG:HG2	1.66	0.60
1:B:447:ARG:HG2	1:B:447:ARG:HH11	1.67	0.60
1:C:418:ASN:HB2	1:C:419:PRO:HD3	1.83	0.60
1:L:447:ARG:HG2	1:L:447:ARG:HH11	1.66	0.59
1:F:447:ARG:HH11	1:F:447:ARG:HG2	1.67	0.59
1:G:238:THR:HG23	1:G:342:ASN:O	2.02	0.59
1:L:440:GLN:O	1:L:444:GLU:HG3	2.03	0.58
1:K:440:GLN:O	1:K:444:GLU:HG3	2.04	0.58
1:G:447:ARG:HH11	1:G:447:ARG:HG2	1.68	0.58
1:H:418:ASN:HB2	1:H:419:PRO:HD3	1.85	0.58
1:A:435:GLU:O	1:A:439:PRO:CD	2.52	0.58
1:J:418:ASN:HB2	1:J:419:PRO:HD3	1.85	0.58
1:D:418:ASN:HB2	1:D:419:PRO:HD3	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:418:ASN:HB2	1:F:419:PRO:HD3	1.85	0.57
1:G:440:GLN:O	1:G:444:GLU:HG3	2.05	0.57
1:H:440:GLN:O	1:H:444:GLU:HG3	2.05	0.57
1:A:440:GLN:O	1:A:444:GLU:HG3	2.05	0.56
1:L:201:LEU:HD22	1:L:267:GLN:HG3	1.87	0.56
1:J:447:ARG:HG2	1:J:447:ARG:HH11	1.68	0.56
1:I:453:PRO:O	1:I:454:MET:HB2	2.05	0.56
1:K:350:THR:OG1	1:K:353:GLN:HG3	2.05	0.56
1:I:418:ASN:HB2	1:I:419:PRO:HD3	1.87	0.56
1:K:229:LEU:HD23	1:K:234:ILE:HB	1.88	0.56
1:G:435:GLU:O	1:G:439:PRO:CD	2.54	0.56
1:G:453:PRO:O	1:G:454:MET:HB2	2.06	0.56
1:A:350:THR:OG1	1:A:353:GLN:HG3	2.06	0.56
1:D:201:LEU:HD22	1:D:267:GLN:HG3	1.88	0.56
1:B:350:THR:OG1	1:B:353:GLN:HG3	2.06	0.55
1:L:418:ASN:HB2	1:L:419:PRO:HD3	1.88	0.55
1:F:435:GLU:O	1:F:439:PRO:CD	2.54	0.55
1:J:440:GLN:O	1:J:444:GLU:HG3	2.05	0.55
1:L:192:GLU:OE2	1:L:205:ARG:HD2	2.06	0.55
1:C:435:GLU:O	1:C:439:PRO:CD	2.53	0.55
1:E:435:GLU:O	1:E:439:PRO:CD	2.54	0.55
1:G:201:LEU:HD22	1:G:267:GLN:HG3	1.89	0.55
1:A:391:SER:OG	1:H:453:PRO:CG	2.55	0.55
1:B:435:GLU:O	1:B:439:PRO:CD	2.55	0.55
1:H:229:LEU:HD23	1:H:234:ILE:HB	1.88	0.55
1:H:391:SER:OG	1:I:453:PRO:HG3	2.07	0.55
1:D:435:GLU:O	1:D:439:PRO:CD	2.55	0.55
1:E:510:SER:HB2	1:L:205:ARG:HH22	1.72	0.55
1:G:350:THR:OG1	1:G:353:GLN:HG3	2.07	0.55
1:L:350:THR:OG1	1:L:353:GLN:HG3	2.07	0.55
1:B:418:ASN:HB2	1:B:419:PRO:HD3	1.88	0.54
1:C:440:GLN:O	1:C:444:GLU:HG3	2.07	0.54
1:L:229:LEU:HD23	1:L:234:ILE:HB	1.89	0.54
1:C:192:GLU:OE2	1:C:205:ARG:HD2	2.08	0.54
1:D:453:PRO:O	1:D:454:MET:HB2	2.07	0.54
1:J:435:GLU:O	1:J:439:PRO:CD	2.55	0.54
1:B:453:PRO:O	1:B:454:MET:HB2	2.07	0.54
1:E:453:PRO:O	1:E:454:MET:HB2	2.08	0.54
1:F:453:PRO:O	1:F:454:MET:HB2	2.06	0.54
1:I:229:LEU:HD23	1:I:234:ILE:HB	1.89	0.54
1:J:453:PRO:O	1:J:454:MET:HB2	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:435:GLU:O	1:L:439:PRO:CD	2.56	0.54
1:G:192:GLU:OE2	1:G:205:ARG:HD2	2.07	0.54
1:A:418:ASN:HB2	1:A:419:PRO:HD3	1.90	0.54
1:G:504:GLN:OE1	1:G:507:ILE:HD12	2.08	0.54
1:E:440:GLN:O	1:E:444:GLU:HG3	2.08	0.54
1:A:447:ARG:HH11	1:A:447:ARG:HG2	1.72	0.53
1:C:453:PRO:O	1:C:454:MET:HB2	2.07	0.53
1:E:418:ASN:HB2	1:E:419:PRO:HD3	1.89	0.53
1:K:192:GLU:OE2	1:K:205:ARG:HD2	2.08	0.53
1:L:453:PRO:O	1:L:454:MET:HB2	2.08	0.53
1:H:350:THR:OG1	1:H:353:GLN:HG3	2.08	0.53
1:G:418:ASN:HB2	1:G:419:PRO:HD3	1.89	0.53
1:D:440:GLN:O	1:D:444:GLU:HG3	2.08	0.53
1:I:440:GLN:O	1:I:444:GLU:HG3	2.09	0.53
1:J:229:LEU:HD23	1:J:234:ILE:HB	1.90	0.53
1:K:435:GLU:O	1:K:439:PRO:CD	2.55	0.53
1:K:504:GLN:OE1	1:K:507:ILE:HD12	2.09	0.53
1:A:453:PRO:O	1:A:454:MET:HB2	2.09	0.53
1:C:504:GLN:OE1	1:C:507:ILE:HD12	2.09	0.53
1:K:201:LEU:HD22	1:K:267:GLN:HG3	1.89	0.53
1:L:384:VAL:HG11	1:L:483:ASP:HB3	1.91	0.53
1:F:192:GLU:OE2	1:F:205:ARG:HD2	2.08	0.53
1:F:229:LEU:HD23	1:F:234:ILE:HB	1.91	0.53
1:C:422:PRO:HD2	1:C:425:LEU:HD12	1.91	0.53
1:D:229:LEU:HD23	1:D:234:ILE:HB	1.90	0.53
1:E:229:LEU:HD23	1:E:234:ILE:HB	1.91	0.53
1:G:229:LEU:HD23	1:G:234:ILE:HB	1.91	0.53
1:J:350:THR:OG1	1:J:353:GLN:HG3	2.09	0.53
1:J:504:GLN:OE1	1:J:507:ILE:HD12	2.09	0.53
1:H:435:GLU:O	1:H:439:PRO:CD	2.56	0.52
1:J:192:GLU:OE2	1:J:205:ARG:HD2	2.09	0.52
1:D:192:GLU:OE2	1:D:205:ARG:HD2	2.09	0.52
1:F:440:GLN:O	1:F:444:GLU:HG3	2.09	0.52
1:H:201:LEU:HD22	1:H:267:GLN:HG3	1.92	0.52
1:H:192:GLU:OE2	1:H:205:ARG:HD2	2.10	0.52
1:I:350:THR:OG1	1:I:353:GLN:HG3	2.09	0.52
1:I:435:GLU:O	1:I:439:PRO:CD	2.57	0.52
1:L:504:GLN:OE1	1:L:507:ILE:HD12	2.09	0.52
1:B:229:LEU:HD23	1:B:234:ILE:HB	1.92	0.52
1:H:504:GLN:OE1	1:H:507:ILE:HD12	2.09	0.52
1:K:418:ASN:HB2	1:K:419:PRO:HD3	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:453:PRO:O	1:K:454:MET:HB2	2.09	0.52
1:F:201:LEU:HD22	1:F:267:GLN:HG3	1.91	0.52
1:I:201:LEU:HD22	1:I:267:GLN:HG3	1.90	0.52
1:I:423:LEU:O	1:I:427:ARG:HG3	2.10	0.52
1:F:504:GLN:OE1	1:F:507:ILE:HD12	2.10	0.52
1:A:504:GLN:OE1	1:A:507:ILE:HD12	2.09	0.51
1:H:422:PRO:HD2	1:H:425:LEU:HD12	1.92	0.51
1:K:298:ASP:O	1:K:301:HIS:HB2	2.10	0.51
1:C:350:THR:OG1	1:C:353:GLN:HG3	2.10	0.51
1:A:201:LEU:HD22	1:A:267:GLN:HG3	1.92	0.51
1:D:422:PRO:HD2	1:D:425:LEU:HD12	1.91	0.51
1:L:486:HIS:CE1	1:L:487:PRO:HB3	2.45	0.51
1:F:350:THR:OG1	1:F:353:GLN:HG3	2.10	0.51
1:I:504:GLN:OE1	1:I:507:ILE:HD12	2.09	0.51
1:E:504:GLN:OE1	1:E:507:ILE:HD12	2.11	0.51
1:F:422:PRO:HD2	1:F:425:LEU:HD12	1.93	0.51
1:I:192:GLU:OE2	1:I:205:ARG:HD2	2.11	0.51
1:A:229:LEU:HD23	1:A:234:ILE:HB	1.92	0.51
1:C:229:LEU:HD23	1:C:234:ILE:HB	1.92	0.51
1:G:389:VAL:HG12	1:G:390:THR:O	2.11	0.51
1:A:435:GLU:O	1:A:439:PRO:HD3	2.11	0.51
1:E:471:ASP:O	1:J:486:HIS:HE1	1.94	0.51
1:F:510:SER:HB3	1:J:205:ARG:HH22	1.75	0.51
1:K:422:PRO:HD2	1:K:425:LEU:HD12	1.93	0.51
1:C:298:ASP:O	1:C:301:HIS:HB2	2.11	0.51
1:E:298:ASP:O	1:E:301:HIS:HB2	2.11	0.51
1:F:423:LEU:O	1:F:427:ARG:HG3	2.11	0.51
1:H:453:PRO:O	1:H:454:MET:HB2	2.11	0.51
1:B:389:VAL:HG12	1:B:390:THR:O	2.11	0.51
1:F:298:ASP:O	1:F:301:HIS:HB2	2.11	0.50
1:J:422:PRO:HD2	1:J:425:LEU:HD12	1.93	0.50
1:K:423:LEU:O	1:K:427:ARG:HG3	2.11	0.50
1:B:201:LEU:HD22	1:B:267:GLN:HG3	1.93	0.50
1:B:504:GLN:OE1	1:B:507:ILE:HD12	2.11	0.50
1:C:384:VAL:HG11	1:C:483:ASP:HB3	1.92	0.50
1:D:384:VAL:HG11	1:D:483:ASP:HB3	1.92	0.50
1:L:422:PRO:HD2	1:L:425:LEU:HD12	1.92	0.50
1:E:422:PRO:HD2	1:E:425:LEU:HD12	1.93	0.50
1:G:435:GLU:O	1:G:439:PRO:HD3	2.11	0.50
1:J:423:LEU:O	1:J:427:ARG:HG3	2.12	0.50
1:D:350:THR:OG1	1:D:353:GLN:HG3	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:384:VAL:HG11	1:I:483:ASP:HB3	1.93	0.50
1:D:298:ASP:O	1:D:301:HIS:HB2	2.11	0.50
1:G:423:LEU:O	1:G:427:ARG:HG3	2.12	0.50
1:B:482:ALA:HA	1:B:489:ALA:HB3	1.93	0.50
1:L:436:GLU:O	1:L:439:PRO:HD2	2.12	0.50
1:B:440:GLN:O	1:B:444:GLU:HG3	2.11	0.50
1:L:482:ALA:HA	1:L:489:ALA:HB3	1.94	0.50
1:I:389:VAL:HG12	1:I:390:THR:O	2.12	0.49
1:I:422:PRO:HD2	1:I:425:LEU:HD12	1.93	0.49
1:D:262:ALA:O	1:D:266:VAL:HG23	2.12	0.49
1:L:380:LEU:O	1:L:384:VAL:HG23	2.12	0.49
1:G:384:VAL:HG11	1:G:483:ASP:HB3	1.93	0.49
1:G:486:HIS:CE1	1:G:487:PRO:HB3	2.47	0.49
1:B:298:ASP:O	1:B:301:HIS:HB2	2.11	0.49
1:F:472:TYR:CZ	1:L:487:PRO:CD	2.92	0.49
1:E:350:THR:OG1	1:E:353:GLN:HG3	2.12	0.49
1:I:436:GLU:O	1:I:439:PRO:HD2	2.13	0.49
1:J:201:LEU:HD22	1:J:267:GLN:HG3	1.94	0.49
1:A:192:GLU:OE2	1:A:205:ARG:HD2	2.12	0.49
1:A:384:VAL:HG11	1:A:483:ASP:HB3	1.95	0.49
1:F:193:LEU:HD13	1:F:221:THR:HG21	1.94	0.49
1:G:298:ASP:O	1:G:301:HIS:HB2	2.11	0.49
1:J:482:ALA:HA	1:J:489:ALA:HB3	1.94	0.49
1:D:504:GLN:OE1	1:D:507:ILE:HD12	2.12	0.49
1:E:192:GLU:OE2	1:E:205:ARG:HD2	2.12	0.49
1:G:422:PRO:HD2	1:G:425:LEU:HD12	1.95	0.49
1:K:384:VAL:HG11	1:K:483:ASP:HB3	1.94	0.49
1:B:475:HIS:HB3	1:B:476:PRO:HD3	1.95	0.49
1:C:201:LEU:HD22	1:C:267:GLN:HG3	1.95	0.49
1:D:193:LEU:HD13	1:D:221:THR:HG21	1.94	0.49
1:L:298:ASP:O	1:L:301:HIS:HB2	2.13	0.49
1:B:192:GLU:OE2	1:B:205:ARG:HD2	2.13	0.48
1:B:486:HIS:CE1	1:B:487:PRO:HB3	2.48	0.48
1:J:193:LEU:HD13	1:J:221:THR:HG21	1.94	0.48
1:K:265:VAL:HG21	1:K:297:HIS:CE1	2.48	0.48
1:A:422:PRO:HD2	1:A:425:LEU:HD12	1.95	0.48
1:H:298:ASP:O	1:H:301:HIS:HB2	2.13	0.48
1:L:193:LEU:HD13	1:L:221:THR:HG21	1.95	0.48
1:H:436:GLU:O	1:H:439:PRO:HD2	2.14	0.48
1:I:482:ALA:HA	1:I:489:ALA:HB3	1.95	0.48
1:C:193:LEU:HD13	1:C:221:THR:HG21	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:201:LEU:HD22	1:E:267:GLN:HG3	1.94	0.48
1:E:472:TYR:HE1	1:J:487:PRO:N	2.08	0.48
1:I:380:LEU:O	1:I:384:VAL:HG23	2.14	0.48
1:I:486:HIS:CE1	1:I:487:PRO:HB3	2.49	0.48
1:K:482:ALA:HA	1:K:489:ALA:HB3	1.96	0.48
1:I:298:ASP:O	1:I:301:HIS:HB2	2.14	0.48
1:H:380:LEU:O	1:H:384:VAL:HG23	2.12	0.48
1:F:380:LEU:O	1:F:384:VAL:HG23	2.14	0.48
1:K:262:ALA:O	1:K:266:VAL:HG23	2.14	0.48
1:B:423:LEU:O	1:B:427:ARG:HG3	2.14	0.48
1:E:482:ALA:HA	1:E:489:ALA:HB3	1.96	0.48
1:G:436:GLU:O	1:G:439:PRO:HD2	2.13	0.48
1:E:265:VAL:HG21	1:E:297:HIS:CE1	2.49	0.48
1:A:391:SER:HG	1:H:453:PRO:HG3	1.79	0.48
1:H:384:VAL:HG11	1:H:483:ASP:HB3	1.96	0.48
1:J:384:VAL:HG11	1:J:483:ASP:HB3	1.95	0.48
1:D:380:LEU:O	1:D:384:VAL:HG23	2.14	0.47
1:K:475:HIS:HB3	1:K:476:PRO:HD3	1.95	0.47
1:A:389:VAL:HG12	1:A:390:THR:O	2.14	0.47
1:A:436:GLU:O	1:A:439:PRO:HD2	2.14	0.47
1:C:482:ALA:HA	1:C:489:ALA:HB3	1.96	0.47
1:H:401:SER:HA	1:H:404:ILE:HG22	1.96	0.47
1:I:193:LEU:HD13	1:I:221:THR:HG21	1.96	0.47
1:D:486:HIS:CE1	1:D:487:PRO:HB3	2.48	0.47
1:E:319:MET:SD	1:H:319:MET:SD	3.12	0.47
1:J:298:ASP:O	1:J:301:HIS:HB2	2.14	0.47
1:L:265:VAL:HG21	1:L:297:HIS:CE1	2.49	0.47
1:A:423:LEU:O	1:A:427:ARG:HG3	2.13	0.47
1:A:475:HIS:HB3	1:A:476:PRO:HD3	1.96	0.47
1:G:482:ALA:HA	1:G:489:ALA:HB3	1.95	0.47
1:A:384:VAL:O	1:A:387:LYS:HB2	2.15	0.47
1:F:262:ALA:O	1:F:266:VAL:HG23	2.15	0.47
1:F:475:HIS:HB3	1:F:476:PRO:HD3	1.96	0.47
1:J:475:HIS:HB3	1:J:476:PRO:HD3	1.96	0.47
1:A:298:ASP:O	1:A:301:HIS:HB2	2.14	0.47
1:D:482:ALA:HA	1:D:489:ALA:HB3	1.96	0.47
1:E:389:VAL:HG12	1:E:390:THR:O	2.14	0.47
1:H:384:VAL:O	1:H:387:LYS:HB2	2.14	0.47
1:H:423:LEU:O	1:H:427:ARG:HG3	2.14	0.47
1:B:193:LEU:HD13	1:B:221:THR:HG21	1.96	0.47
1:J:380:LEU:O	1:J:384:VAL:HG23	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:486:HIS:CE1	1:H:487:PRO:HB3	2.50	0.47
1:I:218:ILE:HD12	1:I:263:ALA:HB1	1.97	0.47
1:I:265:VAL:HG21	1:I:297:HIS:CE1	2.49	0.47
1:J:436:GLU:O	1:J:439:PRO:HD2	2.15	0.47
1:F:384:VAL:HG11	1:F:483:ASP:HB3	1.96	0.47
1:J:262:ALA:O	1:J:266:VAL:HG23	2.15	0.47
1:E:510:SER:CB	1:L:205:ARG:HH22	2.27	0.47
1:A:380:LEU:O	1:A:384:VAL:HG23	2.14	0.47
1:B:422:PRO:HD2	1:B:425:LEU:HD12	1.97	0.47
1:D:389:VAL:HG12	1:D:390:THR:O	2.15	0.46
1:G:193:LEU:HD13	1:G:221:THR:HG21	1.97	0.46
1:C:265:VAL:HG21	1:C:297:HIS:CE1	2.51	0.46
1:C:389:VAL:HG12	1:C:390:THR:O	2.14	0.46
1:D:401:SER:HA	1:D:404:ILE:HG22	1.96	0.46
1:E:374:MET:CE	1:J:389:VAL:HB	2.46	0.46
1:J:384:VAL:O	1:J:387:LYS:HB2	2.14	0.46
1:K:389:VAL:HG12	1:K:390:THR:O	2.14	0.46
1:A:218:ILE:HD12	1:A:263:ALA:HB1	1.97	0.46
1:C:380:LEU:O	1:C:384:VAL:HG23	2.15	0.46
1:D:423:LEU:O	1:D:427:ARG:HG3	2.14	0.46
1:E:435:GLU:O	1:E:439:PRO:HD3	2.13	0.46
1:E:384:VAL:HG11	1:E:483:ASP:HB3	1.97	0.46
1:H:193:LEU:HD13	1:H:221:THR:HG21	1.97	0.46
1:L:435:GLU:O	1:L:439:PRO:HD3	2.15	0.46
1:E:486:HIS:CE1	1:E:487:PRO:HB3	2.50	0.46
1:F:384:VAL:O	1:F:387:LYS:HB2	2.15	0.46
1:A:436:GLU:C	1:A:439:PRO:HD2	2.36	0.46
1:C:435:GLU:O	1:C:439:PRO:HD3	2.14	0.46
1:E:193:LEU:HD13	1:E:221:THR:HG21	1.96	0.46
1:E:475:HIS:HB3	1:E:476:PRO:HD3	1.97	0.46
1:J:389:VAL:HG12	1:J:390:THR:O	2.16	0.46
1:B:436:GLU:O	1:B:439:PRO:HD2	2.16	0.46
1:D:218:ILE:HD12	1:D:263:ALA:HB1	1.97	0.46
1:D:384:VAL:O	1:D:387:LYS:HB2	2.15	0.46
1:F:435:GLU:O	1:F:439:PRO:HD3	2.16	0.46
1:K:384:VAL:O	1:K:387:LYS:HB2	2.15	0.46
1:D:472:TYR:CZ	1:K:393:GLY:HA2	2.50	0.46
1:E:321:ASN:HB3	1:H:362:ILE:HD13	1.97	0.46
1:K:193:LEU:HD13	1:K:221:THR:HG21	1.97	0.46
1:A:486:HIS:CE1	1:A:487:PRO:HB3	2.51	0.46
1:E:340:GLU:HB2	1:E:343:CYS:SG	2.56	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:401:SER:HA	1:E:404:ILE:HG22	1.98	0.46
1:L:401:SER:HA	1:L:404:ILE:HG22	1.98	0.46
1:E:471:ASP:O	1:J:486:HIS:CE1	2.69	0.46
1:F:486:HIS:HA	1:F:487:PRO:HA	1.75	0.46
1:G:218:ILE:HD12	1:G:263:ALA:HB1	1.98	0.46
1:G:380:LEU:O	1:G:384:VAL:HG23	2.16	0.46
1:G:401:SER:HA	1:G:404:ILE:HG22	1.99	0.46
1:K:486:HIS:CE1	1:K:487:PRO:HB3	2.51	0.46
1:H:283:THR:OG1	1:H:286:GLU:HG3	2.16	0.45
1:H:436:GLU:C	1:H:439:PRO:HD2	2.37	0.45
1:J:265:VAL:HG21	1:J:297:HIS:CE1	2.50	0.45
1:L:436:GLU:C	1:L:439:PRO:HD2	2.36	0.45
1:A:262:ALA:O	1:A:266:VAL:HG23	2.17	0.45
1:E:423:LEU:O	1:E:427:ARG:HG3	2.15	0.45
1:J:283:THR:OG1	1:J:286:GLU:HG3	2.17	0.45
1:B:265:VAL:HG21	1:B:297:HIS:CE1	2.51	0.45
1:E:380:LEU:O	1:E:384:VAL:HG23	2.16	0.45
1:F:401:SER:HA	1:F:404:ILE:HG22	1.98	0.45
1:G:384:VAL:O	1:G:387:LYS:HB2	2.16	0.45
1:H:435:GLU:O	1:H:439:PRO:HD3	2.15	0.45
1:J:435:GLU:O	1:J:439:PRO:HD3	2.17	0.45
1:K:401:SER:HA	1:K:404:ILE:HG22	1.98	0.45
1:G:213:ARG:N	1:G:214:PRO:CD	2.79	0.45
1:G:436:GLU:C	1:G:439:PRO:HD2	2.37	0.45
1:H:482:ALA:HA	1:H:489:ALA:HB3	1.98	0.45
1:B:340:GLU:HB2	1:B:343:CYS:SG	2.56	0.45
1:B:384:VAL:HG11	1:B:483:ASP:HB3	1.97	0.45
1:C:384:VAL:O	1:C:387:LYS:HB2	2.16	0.45
1:F:389:VAL:HG12	1:F:390:THR:O	2.17	0.45
1:G:262:ALA:O	1:G:266:VAL:HG23	2.16	0.45
1:G:265:VAL:HG21	1:G:297:HIS:CE1	2.51	0.45
1:I:401:SER:HA	1:I:404:ILE:HG22	1.98	0.45
1:I:436:GLU:C	1:I:439:PRO:HD2	2.36	0.45
1:E:374:MET:HE2	1:J:389:VAL:HB	1.98	0.45
1:L:423:LEU:O	1:L:427:ARG:HG3	2.15	0.45
1:B:435:GLU:O	1:B:439:PRO:HD3	2.16	0.45
1:F:482:ALA:HA	1:F:489:ALA:HB3	1.97	0.45
1:L:218:ILE:HD12	1:L:263:ALA:HB1	1.98	0.45
1:D:475:HIS:HB3	1:D:476:PRO:HD3	1.99	0.45
1:H:214:PRO:HD2	1:H:259:ASN:ND2	2.31	0.45
1:J:401:SER:HA	1:J:404:ILE:HG22	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:218:ILE:HD12	1:K:263:ALA:HB1	1.98	0.45
1:A:482:ALA:HA	1:A:489:ALA:HB3	1.99	0.45
1:B:384:VAL:O	1:B:387:LYS:HB2	2.17	0.45
1:C:213:ARG:N	1:C:214:PRO:CD	2.79	0.45
1:L:389:VAL:HG12	1:L:390:THR:O	2.17	0.45
1:A:193:LEU:HD13	1:A:221:THR:HG21	1.98	0.45
1:J:486:HIS:HA	1:J:487:PRO:HA	1.74	0.45
1:A:486:HIS:HA	1:A:487:PRO:HA	1.75	0.44
1:F:213:ARG:N	1:F:214:PRO:CD	2.80	0.44
1:I:435:GLU:O	1:I:439:PRO:HD3	2.17	0.44
1:K:213:ARG:N	1:K:214:PRO:CD	2.80	0.44
1:K:436:GLU:C	1:K:439:PRO:HD2	2.37	0.44
1:K:436:GLU:O	1:K:439:PRO:HD2	2.16	0.44
1:F:486:HIS:CE1	1:F:487:PRO:HB3	2.52	0.44
1:K:283:THR:OG1	1:K:286:GLU:HG3	2.17	0.44
1:K:435:GLU:O	1:K:439:PRO:HD3	2.17	0.44
1:L:384:VAL:O	1:L:387:LYS:HB2	2.17	0.44
1:H:389:VAL:HG12	1:H:390:THR:O	2.16	0.44
1:I:384:VAL:O	1:I:387:LYS:HB2	2.17	0.44
1:K:321:ASN:O	1:L:362:ILE:HD13	2.18	0.44
1:B:380:LEU:O	1:B:384:VAL:HG23	2.17	0.44
1:D:493:LEU:O	1:D:497:GLU:HG3	2.17	0.44
1:I:213:ARG:N	1:I:214:PRO:CD	2.81	0.44
1:K:240:ILE:O	1:K:244:MET:HG2	2.18	0.44
1:L:267:GLN:O	1:L:270:HIS:HB3	2.17	0.44
1:B:262:ALA:O	1:B:266:VAL:HG23	2.17	0.44
1:B:401:SER:HA	1:B:404:ILE:HG22	2.00	0.44
1:C:401:SER:HA	1:C:404:ILE:HG22	1.99	0.44
1:D:435:GLU:O	1:D:439:PRO:HD3	2.17	0.44
1:E:341:GLU:O	1:E:342:ASN:C	2.56	0.44
1:I:322:ASP:OD2	1:J:358:ARG:NE	2.46	0.44
1:I:475:HIS:HB3	1:I:476:PRO:HD3	1.99	0.44
1:L:475:HIS:HB3	1:L:476:PRO:HD3	1.99	0.44
1:B:486:HIS:HA	1:B:487:PRO:HA	1.76	0.44
1:C:486:HIS:CE1	1:C:487:PRO:HB3	2.52	0.44
1:D:486:HIS:HA	1:D:487:PRO:HA	1.74	0.44
1:E:184:GLU:HG3	1:E:185:GLN:N	2.33	0.44
1:H:265:VAL:HG21	1:H:297:HIS:CE1	2.53	0.44
1:D:265:VAL:HG21	1:D:297:HIS:CE1	2.53	0.44
1:I:184:GLU:HG3	1:I:185:GLN:N	2.33	0.44
1:J:493:LEU:O	1:J:497:GLU:HG3	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:424:GLN:O	1:L:428:GLN:HG3	2.17	0.44
1:E:436:GLU:O	1:E:439:PRO:HD2	2.17	0.44
1:F:265:VAL:HG21	1:F:297:HIS:CE1	2.53	0.44
1:H:475:HIS:HB3	1:H:476:PRO:HD3	2.00	0.44
1:J:436:GLU:C	1:J:439:PRO:HD2	2.38	0.44
1:E:436:GLU:C	1:E:439:PRO:HD2	2.38	0.43
1:F:436:GLU:O	1:F:439:PRO:HD2	2.18	0.43
1:F:466:GLN:O	1:F:470:ILE:HG13	2.18	0.43
1:L:213:ARG:N	1:L:214:PRO:CD	2.80	0.43
1:K:481:TRP:O	1:K:485:VAL:HG22	2.18	0.43
1:A:401:SER:HA	1:A:404:ILE:HG22	1.99	0.43
1:B:213:ARG:N	1:B:214:PRO:CD	2.81	0.43
1:C:262:ALA:O	1:C:266:VAL:HG23	2.18	0.43
1:C:436:GLU:C	1:C:439:PRO:HD2	2.39	0.43
1:G:475:HIS:HB3	1:G:476:PRO:HD3	2.00	0.43
1:L:184:GLU:HG3	1:L:185:GLN:N	2.34	0.43
1:B:436:GLU:C	1:B:439:PRO:HD2	2.38	0.43
1:C:447:ARG:NH1	1:C:447:ARG:HG2	2.32	0.43
1:E:472:TYR:CD1	1:J:486:HIS:O	2.71	0.43
1:L:486:HIS:HA	1:L:487:PRO:HA	1.77	0.43
1:L:493:LEU:O	1:L:497:GLU:HG3	2.19	0.43
1:D:213:ARG:N	1:D:214:PRO:CD	2.82	0.43
1:D:472:TYR:CE2	1:K:393:GLY:HA2	2.54	0.43
1:E:267:GLN:O	1:E:270:HIS:HB3	2.18	0.43
1:J:214:PRO:HD2	1:J:259:ASN:ND2	2.34	0.43
1:J:486:HIS:CE1	1:J:487:PRO:HB3	2.53	0.43
1:B:453:PRO:CG	1:E:391:SER:OG	2.67	0.43
1:F:436:GLU:C	1:F:439:PRO:HD2	2.38	0.43
1:F:481:TRP:O	1:F:485:VAL:HG22	2.18	0.43
1:A:184:GLU:HG3	1:A:185:GLN:N	2.33	0.43
1:C:423:LEU:O	1:C:427:ARG:HG3	2.18	0.43
1:G:273:LEU:HD13	1:G:287:ILE:HG23	2.01	0.43
1:K:267:GLN:O	1:K:270:HIS:HB3	2.19	0.43
1:L:191:LYS:HA	1:L:194:GLU:OE2	2.19	0.43
1:K:438:PHE:HB2	1:K:439:PRO:HD3	2.01	0.42
1:E:447:ARG:HG2	1:E:447:ARG:NH1	2.32	0.42
1:H:218:ILE:HD12	1:H:263:ALA:HB1	2.00	0.42
1:J:218:ILE:HD12	1:J:263:ALA:HB1	2.01	0.42
1:J:273:LEU:HD13	1:J:287:ILE:HG23	2.01	0.42
1:L:214:PRO:HD2	1:L:259:ASN:HD22	1.85	0.42
1:A:493:LEU:O	1:A:497:GLU:HG3	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:184:GLU:HG3	1:B:185:GLN:N	2.34	0.42
1:B:453:PRO:HG3	1:E:391:SER:OG	2.19	0.42
1:E:213:ARG:N	1:E:214:PRO:CD	2.82	0.42
1:L:273:LEU:HD13	1:L:287:ILE:HG23	2.02	0.42
1:H:214:PRO:HD2	1:H:259:ASN:HD22	1.84	0.42
1:I:283:THR:OG1	1:I:286:GLU:HG3	2.20	0.42
1:L:308:PHE:CZ	1:L:312:THR:HG21	2.55	0.42
1:A:265:VAL:HG21	1:A:297:HIS:CE1	2.54	0.42
1:E:384:VAL:O	1:E:387:LYS:HB2	2.19	0.42
1:F:447:ARG:HG2	1:F:447:ARG:NH1	2.33	0.42
1:J:341:GLU:O	1:J:342:ASN:C	2.57	0.42
1:L:214:PRO:HD2	1:L:259:ASN:ND2	2.35	0.42
1:G:486:HIS:HA	1:G:487:PRO:HA	1.75	0.42
1:H:184:GLU:HG3	1:H:185:GLN:N	2.34	0.42
1:H:493:LEU:O	1:H:497:GLU:HG3	2.20	0.42
1:I:420:THR:HB	1:I:492:ILE:HG23	2.02	0.42
1:C:218:ILE:HD12	1:C:263:ALA:HB1	2.01	0.42
1:D:184:GLU:HG3	1:D:185:GLN:N	2.34	0.42
1:D:213:ARG:O	1:D:217:VAL:HG23	2.19	0.42
1:D:283:THR:OG1	1:D:286:GLU:HG3	2.19	0.42
1:E:218:ILE:HD12	1:E:263:ALA:HB1	2.01	0.42
1:F:493:LEU:O	1:F:497:GLU:HG3	2.19	0.42
1:E:240:ILE:O	1:E:244:MET:HG2	2.20	0.42
1:I:262:ALA:O	1:I:266:VAL:HG23	2.20	0.42
1:A:273:LEU:HD13	1:A:287:ILE:HG23	2.02	0.42
1:C:475:HIS:HB3	1:C:476:PRO:HD3	2.01	0.42
1:H:213:ARG:N	1:H:214:PRO:CD	2.82	0.42
1:K:424:GLN:O	1:K:428:GLN:HG3	2.20	0.42
1:E:283:THR:OG1	1:E:286:GLU:HG3	2.20	0.41
1:G:493:LEU:O	1:G:497:GLU:HG3	2.19	0.41
1:H:262:ALA:O	1:H:266:VAL:HG23	2.20	0.41
1:K:297:HIS:NE2	1:K:298:ASP:OD2	2.53	0.41
1:D:447:ARG:HG2	1:D:447:ARG:NH1	2.31	0.41
1:H:447:ARG:NH1	1:H:447:ARG:HG2	2.34	0.41
1:J:213:ARG:N	1:J:214:PRO:CD	2.83	0.41
1:K:447:ARG:NH1	1:K:447:ARG:HG2	2.33	0.41
1:B:341:GLU:O	1:B:342:ASN:C	2.58	0.41
1:E:319:MET:CE	1:H:320:TYR:OH	2.68	0.41
1:F:184:GLU:HG3	1:F:185:GLN:N	2.34	0.41
1:H:438:PHE:HB2	1:H:439:PRO:HD3	2.02	0.41
1:I:273:LEU:HD13	1:I:287:ILE:HG23	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:493:LEU:O	1:K:497:GLU:HG3	2.21	0.41
1:A:424:GLN:O	1:A:428:GLN:HG3	2.21	0.41
1:B:273:LEU:HD13	1:B:287:ILE:HG23	2.02	0.41
1:C:267:GLN:O	1:C:270:HIS:HB3	2.21	0.41
1:C:273:LEU:HD13	1:C:287:ILE:HG23	2.01	0.41
1:C:493:LEU:O	1:C:497:GLU:HG3	2.20	0.41
1:H:391:SER:OG	1:I:453:PRO:CG	2.67	0.41
1:D:438:PHE:HB2	1:D:439:PRO:HD3	2.02	0.41
1:D:436:GLU:O	1:D:439:PRO:HD2	2.21	0.41
1:F:424:GLN:O	1:F:428:GLN:HG3	2.21	0.41
1:G:184:GLU:HG3	1:G:185:GLN:N	2.35	0.41
1:J:340:GLU:HB2	1:J:343:CYS:SG	2.60	0.41
1:F:214:PRO:HD2	1:F:259:ASN:ND2	2.36	0.41
1:F:341:GLU:O	1:F:342:ASN:C	2.59	0.41
1:F:438:PHE:HB2	1:F:439:PRO:HD3	2.03	0.41
1:G:341:GLU:O	1:G:342:ASN:C	2.59	0.41
1:J:447:ARG:NH1	1:J:447:ARG:HG2	2.35	0.41
1:B:214:PRO:HD2	1:B:259:ASN:ND2	2.36	0.41
1:B:481:TRP:O	1:B:485:VAL:HG22	2.20	0.41
1:C:436:GLU:O	1:C:439:PRO:HD2	2.21	0.41
1:D:436:GLU:C	1:D:439:PRO:HD2	2.40	0.41
1:F:283:THR:OG1	1:F:286:GLU:HG3	2.21	0.41
1:H:213:ARG:O	1:H:217:VAL:HG23	2.21	0.41
1:K:184:GLU:HG3	1:K:185:GLN:N	2.36	0.41
1:K:380:LEU:O	1:K:384:VAL:HG23	2.21	0.41
1:L:389:VAL:HG22	1:L:395:LEU:HD23	2.02	0.41
1:C:480:THR:O	1:C:483:ASP:HB2	2.20	0.41
1:C:486:HIS:HA	1:C:487:PRO:HA	1.75	0.41
1:G:283:THR:OG1	1:G:286:GLU:HG3	2.21	0.41
1:J:184:GLU:HG3	1:J:185:GLN:N	2.35	0.41
1:B:438:PHE:HB2	1:B:439:PRO:HD3	2.03	0.41
1:C:214:PRO:HD2	1:C:259:ASN:ND2	2.36	0.41
1:G:466:GLN:O	1:G:470:ILE:HG13	2.21	0.41
1:I:480:THR:O	1:I:483:ASP:HB2	2.21	0.41
1:E:213:ARG:O	1:E:217:VAL:HG23	2.20	0.41
1:F:506:THR:HG23	1:J:427:ARG:HH12	1.86	0.41
1:B:283:THR:OG1	1:B:286:GLU:HG3	2.21	0.40
1:J:466:GLN:O	1:J:470:ILE:HG13	2.21	0.40
1:L:447:ARG:HG2	1:L:447:ARG:NH1	2.34	0.40
1:D:193:LEU:HD11	1:D:217:VAL:CG1	2.52	0.40
1:G:408:GLN:HB2	1:G:408:GLN:HE21	1.71	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:471:ASP:HB3	1:J:487:PRO:HG3	2.03	0.40
1:B:447:ARG:NH1	1:B:447:ARG:HG2	2.34	0.40
1:C:438:PHE:HB2	1:C:439:PRO:HD3	2.03	0.40
1:G:389:VAL:HG22	1:G:395:LEU:HD23	2.04	0.40
1:H:481:TRP:O	1:H:485:VAL:HG22	2.21	0.40
1:C:184:GLU:HG3	1:C:185:GLN:N	2.37	0.40
1:E:341:GLU:O	1:E:343:CYS:N	2.55	0.40
1:K:319:MET:SD	1:L:319:MET:SD	3.19	0.40
1:A:341:GLU:O	1:A:342:ASN:C	2.60	0.40
1:C:240:ILE:O	1:C:244:MET:HG2	2.21	0.40
1:I:438:PHE:HB2	1:I:439:PRO:HD3	2.03	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	326/328 (99%)	302 (93%)	22 (7%)	2 (1%)	25	58
1	B	326/328 (99%)	302 (93%)	22 (7%)	2 (1%)	25	58
1	C	326/328 (99%)	305 (94%)	19 (6%)	2 (1%)	25	58
1	D	326/328 (99%)	305 (94%)	19 (6%)	2 (1%)	25	58
1	E	326/328 (99%)	305 (94%)	19 (6%)	2 (1%)	25	58
1	F	326/328 (99%)	305 (94%)	19 (6%)	2 (1%)	25	58
1	G	326/328 (99%)	305 (94%)	19 (6%)	2 (1%)	25	58
1	H	326/328 (99%)	304 (93%)	20 (6%)	2 (1%)	25	58
1	I	326/328 (99%)	305 (94%)	19 (6%)	2 (1%)	25	58
1	J	326/328 (99%)	305 (94%)	19 (6%)	2 (1%)	25	58
1	K	326/328 (99%)	303 (93%)	21 (6%)	2 (1%)	25	58

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	L	326/328 (99%)	305 (94%)	19 (6%)	2 (1%)	25	58
All	All	3912/3936 (99%)	3651 (93%)	237 (6%)	24 (1%)	25	58

All (24) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	342	ASN
1	B	340	GLU
1	B	342	ASN
1	C	342	ASN
1	D	342	ASN
1	E	340	GLU
1	E	342	ASN
1	F	342	ASN
1	G	342	ASN
1	H	342	ASN
1	I	342	ASN
1	J	340	GLU
1	J	342	ASN
1	K	342	ASN
1	L	342	ASN
1	A	340	GLU
1	H	340	GLU
1	I	340	GLU
1	K	340	GLU
1	L	340	GLU
1	C	340	GLU
1	D	340	GLU
1	F	340	GLU
1	G	340	GLU

### 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	300/300 (100%)	290 (97%)	10 (3%)	38	72
1	B	300/300 (100%)	291 (97%)	9 (3%)	41	75
1	C	300/300 (100%)	290 (97%)	10 (3%)	38	72
1	D	300/300 (100%)	290 (97%)	10 (3%)	38	72
1	E	300/300 (100%)	292 (97%)	8 (3%)	44	77
1	F	300/300 (100%)	290 (97%)	10 (3%)	38	72
1	G	300/300 (100%)	291 (97%)	9 (3%)	41	75
1	H	300/300 (100%)	291 (97%)	9 (3%)	41	75
1	I	300/300 (100%)	292 (97%)	8 (3%)	44	77
1	J	300/300 (100%)	290 (97%)	10 (3%)	38	72
1	K	300/300 (100%)	291 (97%)	9 (3%)	41	75
1	L	300/300 (100%)	290 (97%)	10 (3%)	38	72
All	All	3600/3600 (100%)	3488 (97%)	112 (3%)	40	74

All (112) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	185	GLN
1	A	221	THR
1	A	239	LEU
1	A	297	HIS
1	A	319	MET
1	A	357	LEU
1	A	376	LEU
1	A	483	ASP
1	A	487	PRO
1	A	493	LEU
1	B	185	GLN
1	B	221	THR
1	B	239	LEU
1	B	297	HIS
1	B	319	MET
1	B	357	LEU
1	B	483	ASP
1	B	487	PRO
1	B	493	LEU
1	C	185	GLN
1	C	221	THR
1	C	239	LEU

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Mol	Chain	Res	Type
1	C	297	HIS
1	C	319	MET
1	C	357	LEU
1	C	376	LEU
1	C	483	ASP
1	C	487	PRO
1	C	493	LEU
1	D	185	GLN
1	D	221	THR
1	D	239	LEU
1	D	297	HIS
1	D	319	MET
1	D	357	LEU
1	D	376	LEU
1	D	483	ASP
1	D	487	PRO
1	D	493	LEU
1	E	185	GLN
1	E	221	THR
1	E	239	LEU
1	E	319	MET
1	E	357	LEU
1	E	483	ASP
1	E	487	PRO
1	E	493	LEU
1	F	185	GLN
1	F	221	THR
1	F	239	LEU
1	F	297	HIS
1	F	319	MET
1	F	357	LEU
1	F	376	LEU
1	F	483	ASP
1	F	487	PRO
1	F	493	LEU
1	G	185	GLN
1	G	221	THR
1	G	239	LEU
1	G	319	MET
1	G	357	LEU
1	G	376	LEU
1	G	483	ASP

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Mol	Chain	Res	Type
1	G	487	PRO
1	G	493	LEU
1	H	185	GLN
1	H	221	THR
1	H	239	LEU
1	H	319	MET
1	H	357	LEU
1	H	376	LEU
1	H	483	ASP
1	H	487	PRO
1	H	493	LEU
1	I	185	GLN
1	I	239	LEU
1	I	297	HIS
1	I	319	MET
1	I	357	LEU
1	I	483	ASP
1	I	487	PRO
1	I	493	LEU
1	J	185	GLN
1	J	221	THR
1	J	239	LEU
1	J	297	HIS
1	J	319	MET
1	J	357	LEU
1	J	376	LEU
1	J	483	ASP
1	J	487	PRO
1	J	493	LEU
1	K	185	GLN
1	K	221	THR
1	K	239	LEU
1	K	319	MET
1	K	357	LEU
1	K	376	LEU
1	K	483	ASP
1	K	487	PRO
1	K	493	LEU
1	L	185	GLN
1	L	221	THR
1	L	239	LEU
1	L	297	HIS

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Mol	Chain	Res	Type
1	L	319	MET
1	L	357	LEU
1	L	376	LEU
1	L	483	ASP
1	L	487	PRO
1	L	493	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (88) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	185	GLN
1	A	307	GLN
1	A	311	ASN
1	A	321	ASN
1	A	339	GLN
1	A	355	GLN
1	A	399	ASN
1	A	408	GLN
1	A	424	GLN
1	A	466	GLN
1	B	185	GLN
1	B	328	ASN
1	B	339	GLN
1	B	355	GLN
1	B	399	ASN
1	B	408	GLN
1	B	424	GLN
1	C	185	GLN
1	C	339	GLN
1	C	355	GLN
1	C	399	ASN
1	C	408	GLN
1	C	424	GLN
1	D	185	GLN
1	D	339	GLN
1	D	355	GLN
1	D	399	ASN
1	D	408	GLN
1	D	424	GLN
1	E	185	GLN
1	E	321	ASN
1	E	339	GLN

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Mol	Chain	Res	Type
1	E	355	GLN
1	E	399	ASN
1	E	408	GLN
1	E	424	GLN
1	F	185	GLN
1	F	339	GLN
1	F	355	GLN
1	F	399	ASN
1	F	408	GLN
1	F	424	GLN
1	G	185	GLN
1	G	307	GLN
1	G	311	ASN
1	G	339	GLN
1	G	355	GLN
1	G	399	ASN
1	G	408	GLN
1	G	424	GLN
1	H	185	GLN
1	H	328	ASN
1	H	339	GLN
1	H	355	GLN
1	H	399	ASN
1	H	408	GLN
1	H	424	GLN
1	I	185	GLN
1	I	307	GLN
1	I	311	ASN
1	I	339	GLN
1	I	355	GLN
1	I	399	ASN
1	I	408	GLN
1	I	424	GLN
1	J	185	GLN
1	J	307	GLN
1	J	311	ASN
1	J	339	GLN
1	J	355	GLN
1	J	399	ASN
1	J	408	GLN
1	J	424	GLN
1	J	486	HIS

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Mol	Chain	Res	Type
1	K	185	GLN
1	K	307	GLN
1	K	311	ASN
1	K	339	GLN
1	K	355	GLN
1	K	399	ASN
1	K	408	GLN
1	K	424	GLN
1	L	185	GLN
1	L	339	GLN
1	L	355	GLN
1	L	399	ASN
1	L	408	GLN
1	L	424	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 carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 36 ligands modelled in this entry, 24 are monoatomic - leaving 12 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	ZAR	J	3010	-	19,20,20	2.68	8 (42%)	25,27,27	2.09	5 (20%)
4	ZAR	G	3007	-	19,20,20	2.72	8 (42%)	25,27,27	2.14	6 (24%)
4	ZAR	F	3006	-	19,20,20	2.63	8 (42%)	25,27,27	2.11	5 (20%)
4	ZAR	K	3011	-	19,20,20	2.73	9 (47%)	25,27,27	2.09	5 (20%)
4	ZAR	E	3005	-	19,20,20	2.68	9 (47%)	25,27,27	2.09	5 (20%)
4	ZAR	A	3001	-	19,20,20	2.74	8 (42%)	25,27,27	2.08	5 (20%)
4	ZAR	D	3004	-	19,20,20	2.62	8 (42%)	25,27,27	2.15	6 (24%)
4	ZAR	L	3012	-	19,20,20	2.70	9 (47%)	25,27,27	2.13	6 (24%)
4	ZAR	I	3009	-	19,20,20	2.67	9 (47%)	25,27,27	2.08	5 (20%)
4	ZAR	B	3002	-	19,20,20	2.66	7 (36%)	25,27,27	2.12	6 (24%)
4	ZAR	C	3003	-	19,20,20	2.70	7 (36%)	25,27,27	2.09	5 (20%)
4	ZAR	H	3008	-	19,20,20	2.69	8 (42%)	25,27,27	2.12	5 (20%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	ZAR	J	3010	-	-	0/10/10/10	0/2/2/2
4	ZAR	G	3007	-	-	0/10/10/10	0/2/2/2
4	ZAR	F	3006	-	-	0/10/10/10	0/2/2/2
4	ZAR	K	3011	-	-	0/10/10/10	0/2/2/2
4	ZAR	E	3005	-	-	0/10/10/10	0/2/2/2
4	ZAR	A	3001	-	-	0/10/10/10	0/2/2/2
4	ZAR	D	3004	-	-	0/10/10/10	0/2/2/2
4	ZAR	L	3012	-	-	0/10/10/10	0/2/2/2
4	ZAR	I	3009	-	-	0/10/10/10	0/2/2/2
4	ZAR	B	3002	-	-	0/10/10/10	0/2/2/2
4	ZAR	C	3003	-	-	0/10/10/10	0/2/2/2
4	ZAR	H	3008	-	-	0/10/10/10	0/2/2/2

All (98) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	3001	ZAR	C8-C5	-7.48	1.37	1.48
4	B	3002	ZAR	C8-C5	-7.34	1.37	1.48
4	C	3003	ZAR	C8-C5	-7.31	1.37	1.48
4	G	3007	ZAR	C8-C5	-7.23	1.37	1.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	J	3010	ZAR	C8-C5	-7.21	1.37	1.48
4	L	3012	ZAR	C8-C5	-7.13	1.37	1.48
4	K	3011	ZAR	C8-C5	-7.11	1.37	1.48
4	H	3008	ZAR	C8-C5	-6.89	1.38	1.48
4	E	3005	ZAR	C8-C5	-6.86	1.38	1.48
4	F	3006	ZAR	C8-C5	-6.77	1.38	1.48
4	I	3009	ZAR	C8-C5	-6.72	1.38	1.48
4	D	3004	ZAR	C8-C5	-6.71	1.38	1.48
4	H	3008	ZAR	C6-C5	6.08	1.52	1.38
4	L	3012	ZAR	C6-C5	6.02	1.52	1.38
4	E	3005	ZAR	C6-C5	6.01	1.52	1.38
4	D	3004	ZAR	C6-C5	6.00	1.52	1.38
4	J	3010	ZAR	C6-C5	5.95	1.52	1.38
4	G	3007	ZAR	C6-C5	5.95	1.52	1.38
4	F	3006	ZAR	C6-C5	5.94	1.52	1.38
4	A	3001	ZAR	C6-C5	5.89	1.52	1.38
4	C	3003	ZAR	C6-C5	5.85	1.52	1.38
4	K	3011	ZAR	C6-C5	5.85	1.52	1.38
4	I	3009	ZAR	C6-C5	5.84	1.52	1.38
4	B	3002	ZAR	C6-C5	5.82	1.52	1.38
4	I	3009	ZAR	C9-C8	3.22	1.45	1.39
4	H	3008	ZAR	C9-C8	3.05	1.45	1.39
4	K	3011	ZAR	C9-C8	2.93	1.44	1.39
4	D	3004	ZAR	C9-C8	2.88	1.44	1.39
4	F	3006	ZAR	C9-C8	2.82	1.44	1.39
4	E	3005	ZAR	C9-C8	2.81	1.44	1.39
4	H	3008	ZAR	N3-N4	2.79	1.41	1.34
4	G	3007	ZAR	C9-C8	2.79	1.44	1.39
4	K	3011	ZAR	C5-N4	-2.77	1.29	1.34
4	C	3003	ZAR	C9-C8	2.76	1.44	1.39
4	A	3001	ZAR	C9-C8	2.75	1.44	1.39
4	L	3012	ZAR	N3-N4	2.73	1.41	1.34
4	B	3002	ZAR	C9-C8	2.72	1.44	1.39
4	C	3003	ZAR	C9-C10	2.72	1.43	1.38
4	J	3010	ZAR	C9-C8	2.68	1.44	1.39
4	E	3005	ZAR	C9-C10	2.68	1.43	1.38
4	E	3005	ZAR	N3-N4	2.67	1.41	1.34
4	A	3001	ZAR	C9-C10	2.66	1.43	1.38
4	K	3011	ZAR	C9-C10	2.66	1.43	1.38
4	G	3007	ZAR	C9-C10	2.65	1.43	1.38
4	D	3004	ZAR	N3-N4	2.64	1.41	1.34
4	A	3001	ZAR	N3-N4	2.64	1.41	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	3003	ZAR	N3-N4	2.62	1.41	1.34
4	I	3009	ZAR	C9-C10	2.61	1.43	1.38
4	J	3010	ZAR	C9-C10	2.61	1.43	1.38
4	G	3007	ZAR	C5-N4	-2.60	1.29	1.34
4	C	3003	ZAR	C5-N4	-2.59	1.29	1.34
4	L	3012	ZAR	C9-C10	2.57	1.43	1.38
4	J	3010	ZAR	N3-N4	2.56	1.40	1.34
4	L	3012	ZAR	C9-C8	2.55	1.44	1.39
4	G	3007	ZAR	N3-N4	2.55	1.40	1.34
4	E	3005	ZAR	C5-N4	-2.53	1.29	1.34
4	B	3002	ZAR	N3-N4	2.52	1.40	1.34
4	F	3006	ZAR	C9-C10	2.48	1.43	1.38
4	H	3008	ZAR	C9-C10	2.46	1.43	1.38
4	B	3002	ZAR	C5-N4	-2.45	1.29	1.34
4	I	3009	ZAR	N3-N4	2.44	1.40	1.34
4	F	3006	ZAR	N3-N4	2.38	1.40	1.34
4	K	3011	ZAR	N3-N4	2.37	1.40	1.34
4	D	3004	ZAR	C9-C10	2.32	1.43	1.38
4	I	3009	ZAR	C5-N4	-2.31	1.29	1.34
4	B	3002	ZAR	C9-C10	2.27	1.42	1.38
4	K	3011	ZAR	C13-C8	2.27	1.44	1.39
4	F	3006	ZAR	C12-C11	2.26	1.44	1.39
4	I	3009	ZAR	C2-N3	2.26	1.40	1.31
4	L	3012	ZAR	C5-N4	-2.25	1.30	1.34
4	A	3001	ZAR	C5-N4	-2.24	1.30	1.34
4	E	3005	ZAR	C13-C8	2.22	1.44	1.39
4	G	3007	ZAR	C12-C11	2.22	1.44	1.39
4	D	3004	ZAR	C13-C8	2.22	1.44	1.39
4	F	3006	ZAR	C5-N4	-2.21	1.30	1.34
4	H	3008	ZAR	C5-N4	-2.21	1.30	1.34
4	D	3004	ZAR	C5-N4	-2.21	1.30	1.34
4	B	3002	ZAR	C2-N3	2.20	1.40	1.31
4	J	3010	ZAR	C5-N4	-2.19	1.30	1.34
4	I	3009	ZAR	C12-C11	2.19	1.44	1.39
4	H	3008	ZAR	C2-N3	2.19	1.40	1.31
4	K	3011	ZAR	C2-N3	2.18	1.40	1.31
4	I	3009	ZAR	C13-C8	2.18	1.44	1.39
4	L	3012	ZAR	C2-N3	2.17	1.40	1.31
4	E	3005	ZAR	C12-C11	2.17	1.44	1.39
4	F	3006	ZAR	C2-N3	2.16	1.40	1.31
4	G	3007	ZAR	C2-N3	2.15	1.40	1.31
4	A	3001	ZAR	C2-N3	2.13	1.39	1.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	E	3005	ZAR	C2-N3	2.12	1.39	1.31
4	K	3011	ZAR	C12-C11	2.09	1.44	1.39
4	C	3003	ZAR	C2-N3	2.09	1.39	1.31
4	L	3012	ZAR	C13-C8	2.08	1.43	1.39
4	A	3001	ZAR	C12-C11	2.07	1.43	1.39
4	L	3012	ZAR	C12-C11	2.05	1.43	1.39
4	D	3004	ZAR	C2-N3	2.03	1.39	1.31
4	J	3010	ZAR	C12-C11	2.02	1.43	1.39
4	H	3008	ZAR	C12-C11	2.02	1.43	1.39
4	J	3010	ZAR	C2-N3	2.00	1.39	1.31

All (64) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	3004	ZAR	C19-O18-C10	7.04	128.16	117.53
4	L	3012	ZAR	C19-O18-C10	6.99	128.09	117.53
4	J	3010	ZAR	C19-O18-C10	6.94	128.00	117.53
4	G	3007	ZAR	C19-O18-C10	6.93	127.99	117.53
4	H	3008	ZAR	C19-O18-C10	6.92	127.97	117.53
4	B	3002	ZAR	C19-O18-C10	6.91	127.96	117.53
4	A	3001	ZAR	C19-O18-C10	6.89	127.93	117.53
4	K	3011	ZAR	C19-O18-C10	6.88	127.91	117.53
4	F	3006	ZAR	C19-O18-C10	6.78	127.76	117.53
4	E	3005	ZAR	C19-O18-C10	6.76	127.74	117.53
4	I	3009	ZAR	C19-O18-C10	6.76	127.73	117.53
4	C	3003	ZAR	C19-O18-C10	6.53	127.38	117.53
4	F	3006	ZAR	C5-N4-N3	4.29	123.99	119.93
4	C	3003	ZAR	C5-N4-N3	4.26	123.97	119.93
4	I	3009	ZAR	C5-N4-N3	4.25	123.96	119.93
4	K	3011	ZAR	C5-N4-N3	4.24	123.95	119.93
4	H	3008	ZAR	C5-N4-N3	4.22	123.93	119.93
4	G	3007	ZAR	C5-N4-N3	4.21	123.92	119.93
4	E	3005	ZAR	C5-N4-N3	4.19	123.90	119.93
4	D	3004	ZAR	C5-N4-N3	4.11	123.82	119.93
4	B	3002	ZAR	C5-N4-N3	4.10	123.82	119.93
4	J	3010	ZAR	C5-N4-N3	4.10	123.81	119.93
4	L	3012	ZAR	C5-N4-N3	4.08	123.80	119.93
4	A	3001	ZAR	C5-N4-N3	4.06	123.78	119.93
4	B	3002	ZAR	C11-O15-C14	3.57	131.36	118.77
4	E	3005	ZAR	C11-O15-C14	3.49	131.08	118.77
4	H	3008	ZAR	C11-O15-C14	3.48	131.06	118.77
4	L	3012	ZAR	C11-O15-C14	3.47	131.03	118.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	3004	ZAR	C11-O15-C14	3.46	130.99	118.77
4	J	3010	ZAR	C11-O15-C14	3.42	130.83	118.77
4	C	3003	ZAR	C11-O15-C14	3.40	130.78	118.77
4	A	3001	ZAR	C11-O15-C14	3.39	130.72	118.77
4	G	3007	ZAR	C11-O15-C14	3.30	130.43	118.77
4	F	3006	ZAR	C11-O15-C14	3.29	130.38	118.77
4	K	3011	ZAR	C11-O15-C14	3.24	130.22	118.77
4	I	3009	ZAR	C11-O15-C14	3.19	130.04	118.77
4	C	3003	ZAR	C6-C5-N4	-2.91	117.35	121.54
4	H	3008	ZAR	C6-C5-N4	-2.89	117.38	121.54
4	D	3004	ZAR	C6-C5-N4	-2.89	117.39	121.54
4	F	3006	ZAR	C6-C5-N4	-2.81	117.50	121.54
4	L	3012	ZAR	C6-C5-N4	-2.79	117.53	121.54
4	G	3007	ZAR	C6-C5-N4	-2.76	117.56	121.54
4	J	3010	ZAR	C6-C5-N4	-2.76	117.57	121.54
4	E	3005	ZAR	C6-C5-N4	-2.76	117.57	121.54
4	A	3001	ZAR	C6-C5-N4	-2.65	117.73	121.54
4	I	3009	ZAR	C6-C5-N4	-2.65	117.73	121.54
4	B	3002	ZAR	C6-C5-N4	-2.61	117.79	121.54
4	K	3011	ZAR	C6-C5-N4	-2.60	117.80	121.54
4	C	3003	ZAR	C7-C6-C5	2.59	122.64	118.88
4	L	3012	ZAR	C7-C6-C5	2.55	122.58	118.88
4	G	3007	ZAR	C7-C6-C5	2.53	122.56	118.88
4	H	3008	ZAR	C7-C6-C5	2.52	122.55	118.88
4	D	3004	ZAR	C7-C6-C5	2.51	122.53	118.88
4	B	3002	ZAR	C7-C6-C5	2.48	122.49	118.88
4	K	3011	ZAR	C7-C6-C5	2.48	122.48	118.88
4	F	3006	ZAR	C7-C6-C5	2.46	122.45	118.88
4	I	3009	ZAR	C7-C6-C5	2.45	122.44	118.88
4	E	3005	ZAR	C7-C6-C5	2.41	122.38	118.88
4	A	3001	ZAR	C7-C6-C5	2.41	122.38	118.88
4	J	3010	ZAR	C7-C6-C5	2.36	122.31	118.88
4	B	3002	ZAR	O18-C10-C11	2.11	118.35	115.41
4	L	3012	ZAR	O18-C10-C11	2.09	118.32	115.41
4	G	3007	ZAR	O18-C10-C11	2.07	118.30	115.41
4	D	3004	ZAR	O18-C10-C11	2.04	118.25	115.41

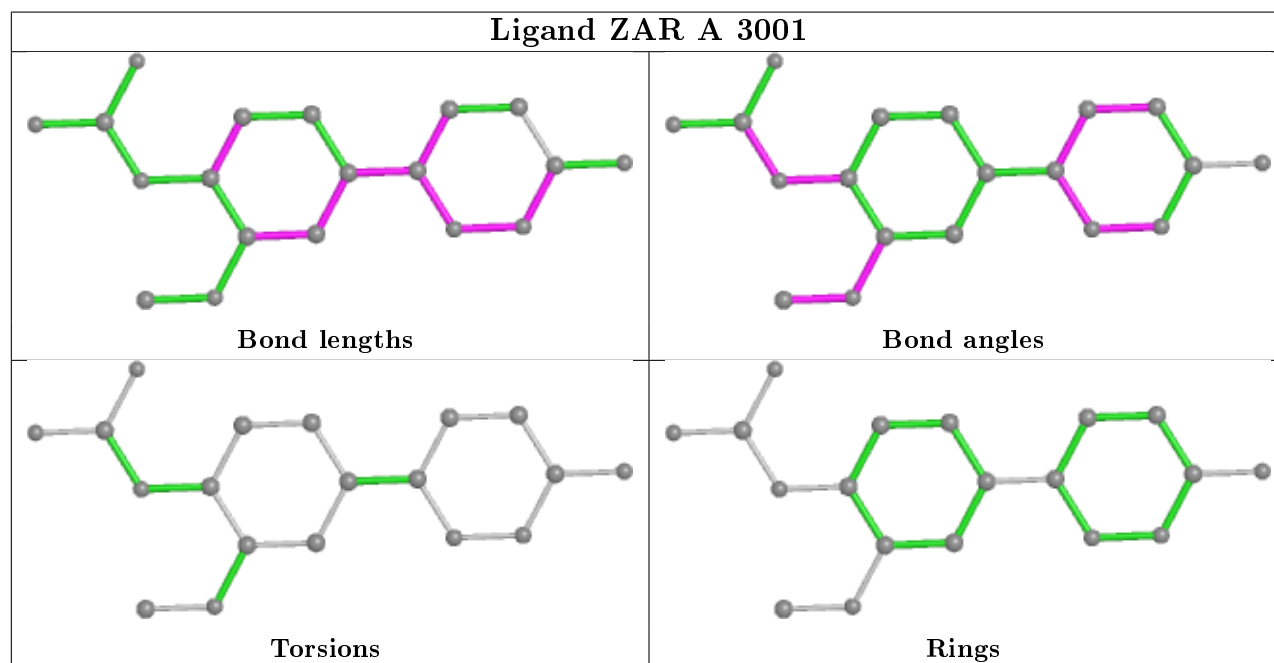
There are no chirality outliers.

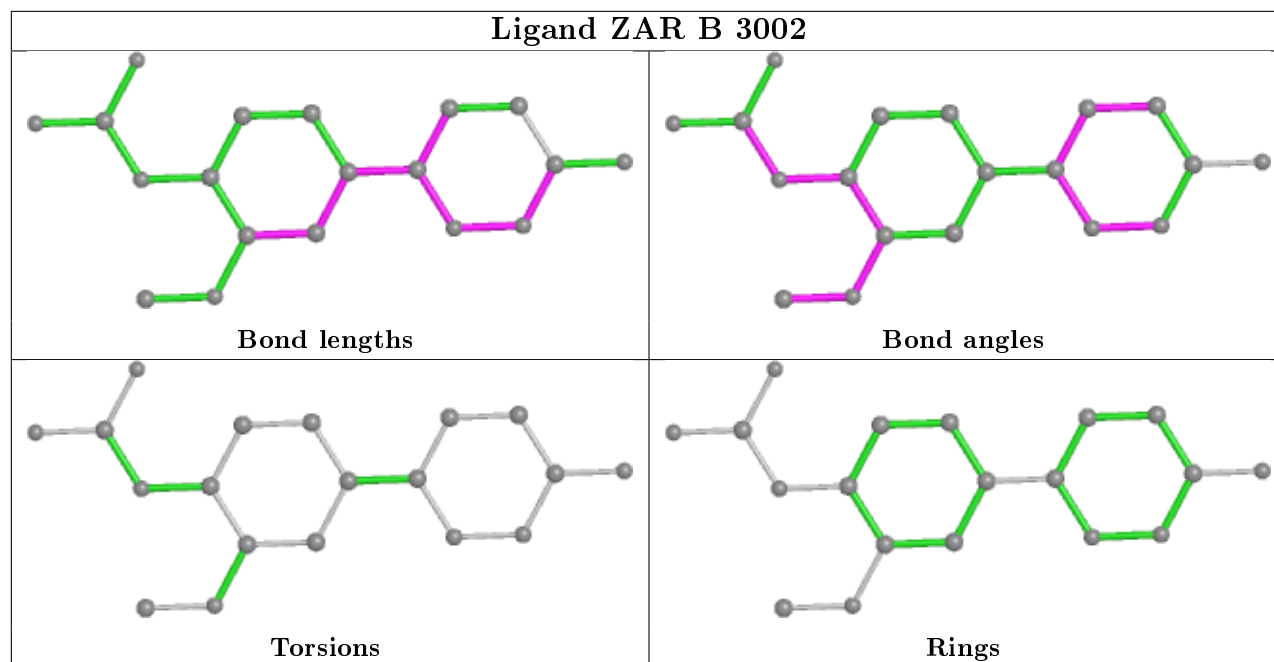
There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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.