



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 1, 2026 – 12:00 PM UTC

PDB ID : 4D2V / pdb_00004d2v
Title : Structure of MELK in complex with inhibitors
Authors : Johnson, C.N.; Berdini, V.; Beke, L.; Bonnet, P.; Brehmer, D.; Coyle, J.E.;
Day, P.J.; Frederickson, M.; Freyne, E.J.E.; Gilissen, R.A.H.J.; Hamlett,
C.C.F.; Howard, S.; Meerpoel, L.; McMenemy, R.; Patel, S.; Rees, D.C.;
Sharff, A.; Sommen, F.; Wu, T.; Linders, J.T.M.
Deposited on : 2014-05-13
Resolution : 2.45 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](#) ①) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

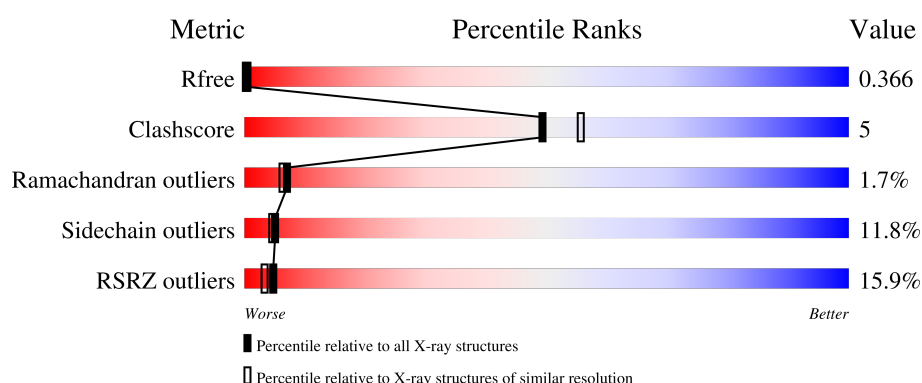
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.45 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1190 (2.46-2.46)
Clashscore	190562	1229 (2.46-2.46)
Ramachandran outliers	187476	1218 (2.46-2.46)
Sidechain outliers	187428	1218 (2.46-2.46)
RSRZ outliers	180081	1190 (2.46-2.46)

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

Mol	Chain	Length	Quality of chain
1	A	356	13% 68% 16% • 12%
1	B	356	16% 71% 16% • • 10%
1	C	356	13% 70% 17% • 11%
1	D	356	15% 67% 18% • • 11%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 11042 atoms, of which 92 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 MATERNAL EMBRYONIC LEUCINE ZIPPER KINASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	313	Total	C	N	O	S	0	1	0
			2550	1645	429	459	17			
1	B	322	Total	C	N	O	S	0	1	0
			2609	1679	442	471	17			
1	C	316	Total	C	N	O	S	0	0	0
			2564	1655	431	461	17			
1	D	318	Total	C	N	O	S	0	0	0
			2575	1662	436	461	16			

There are 108 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	expression tag	UNP Q14680
A	-18	GLY	-	expression tag	UNP Q14680
A	-17	SER	-	expression tag	UNP Q14680
A	-16	SER	-	expression tag	UNP Q14680
A	-15	HIS	-	expression tag	UNP Q14680
A	-14	HIS	-	expression tag	UNP Q14680
A	-13	HIS	-	expression tag	UNP Q14680
A	-12	HIS	-	expression tag	UNP Q14680
A	-11	HIS	-	expression tag	UNP Q14680
A	-10	HIS	-	expression tag	UNP Q14680
A	-9	SER	-	expression tag	UNP Q14680
A	-8	SER	-	expression tag	UNP Q14680
A	-7	GLY	-	expression tag	UNP Q14680
A	-6	LEU	-	expression tag	UNP Q14680
A	-5	VAL	-	expression tag	UNP Q14680
A	-4	PRO	-	expression tag	UNP Q14680
A	-3	ARG	-	expression tag	UNP Q14680
A	-2	GLY	-	expression tag	UNP Q14680
A	-1	SER	-	expression tag	UNP Q14680
A	0	HIS	-	expression tag	UNP Q14680
A	167	ALA	THR	engineered mutation	UNP Q14680

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Chain	Residue	Modelled	Actual	Comment	Reference
A	171	ALA	SER	engineered mutation	UNP Q14680
A	213	THR	ASN	engineered mutation	UNP Q14680
A	214	ALA	VAL	engineered mutation	UNP Q14680
A	215	ALA	MET	engineered mutation	UNP Q14680
A	218	VAL	TYR	engineered mutation	UNP Q14680
A	219	ALA	LYS	engineered mutation	UNP Q14680
B	-19	MET	-	expression tag	UNP Q14680
B	-18	GLY	-	expression tag	UNP Q14680
B	-17	SER	-	expression tag	UNP Q14680
B	-16	SER	-	expression tag	UNP Q14680
B	-15	HIS	-	expression tag	UNP Q14680
B	-14	HIS	-	expression tag	UNP Q14680
B	-13	HIS	-	expression tag	UNP Q14680
B	-12	HIS	-	expression tag	UNP Q14680
B	-11	HIS	-	expression tag	UNP Q14680
B	-10	HIS	-	expression tag	UNP Q14680
B	-9	SER	-	expression tag	UNP Q14680
B	-8	SER	-	expression tag	UNP Q14680
B	-7	GLY	-	expression tag	UNP Q14680
B	-6	LEU	-	expression tag	UNP Q14680
B	-5	VAL	-	expression tag	UNP Q14680
B	-4	PRO	-	expression tag	UNP Q14680
B	-3	ARG	-	expression tag	UNP Q14680
B	-2	GLY	-	expression tag	UNP Q14680
B	-1	SER	-	expression tag	UNP Q14680
B	0	HIS	-	expression tag	UNP Q14680
B	167	ALA	THR	engineered mutation	UNP Q14680
B	171	ALA	SER	engineered mutation	UNP Q14680
B	213	THR	ASN	engineered mutation	UNP Q14680
B	214	ALA	VAL	engineered mutation	UNP Q14680
B	215	ALA	MET	engineered mutation	UNP Q14680
B	218	VAL	TYR	engineered mutation	UNP Q14680
B	219	ALA	LYS	engineered mutation	UNP Q14680
C	-19	MET	-	expression tag	UNP Q14680
C	-18	GLY	-	expression tag	UNP Q14680
C	-17	SER	-	expression tag	UNP Q14680
C	-16	SER	-	expression tag	UNP Q14680
C	-15	HIS	-	expression tag	UNP Q14680
C	-14	HIS	-	expression tag	UNP Q14680
C	-13	HIS	-	expression tag	UNP Q14680
C	-12	HIS	-	expression tag	UNP Q14680
C	-11	HIS	-	expression tag	UNP Q14680

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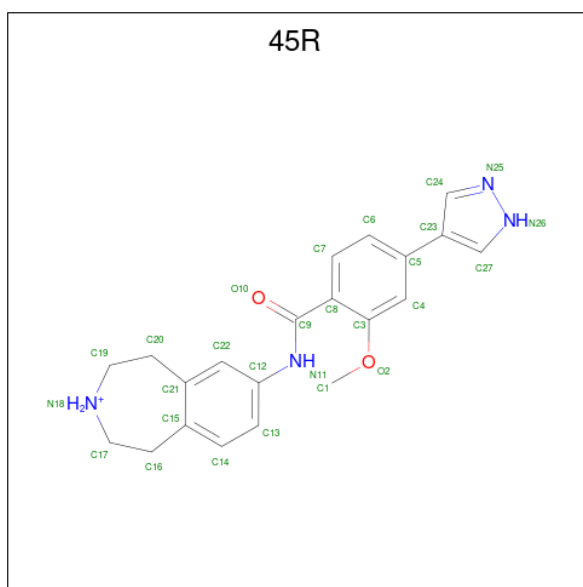
Chain	Residue	Modelled	Actual	Comment	Reference
C	-10	HIS	-	expression tag	UNP Q14680
C	-9	SER	-	expression tag	UNP Q14680
C	-8	SER	-	expression tag	UNP Q14680
C	-7	GLY	-	expression tag	UNP Q14680
C	-6	LEU	-	expression tag	UNP Q14680
C	-5	VAL	-	expression tag	UNP Q14680
C	-4	PRO	-	expression tag	UNP Q14680
C	-3	ARG	-	expression tag	UNP Q14680
C	-2	GLY	-	expression tag	UNP Q14680
C	-1	SER	-	expression tag	UNP Q14680
C	0	HIS	-	expression tag	UNP Q14680
C	167	ALA	THR	engineered mutation	UNP Q14680
C	171	ALA	SER	engineered mutation	UNP Q14680
C	213	THR	ASN	engineered mutation	UNP Q14680
C	214	ALA	VAL	engineered mutation	UNP Q14680
C	215	ALA	MET	engineered mutation	UNP Q14680
C	218	VAL	TYR	engineered mutation	UNP Q14680
C	219	ALA	LYS	engineered mutation	UNP Q14680
D	-19	MET	-	expression tag	UNP Q14680
D	-18	GLY	-	expression tag	UNP Q14680
D	-17	SER	-	expression tag	UNP Q14680
D	-16	SER	-	expression tag	UNP Q14680
D	-15	HIS	-	expression tag	UNP Q14680
D	-14	HIS	-	expression tag	UNP Q14680
D	-13	HIS	-	expression tag	UNP Q14680
D	-12	HIS	-	expression tag	UNP Q14680
D	-11	HIS	-	expression tag	UNP Q14680
D	-10	HIS	-	expression tag	UNP Q14680
D	-9	SER	-	expression tag	UNP Q14680
D	-8	SER	-	expression tag	UNP Q14680
D	-7	GLY	-	expression tag	UNP Q14680
D	-6	LEU	-	expression tag	UNP Q14680
D	-5	VAL	-	expression tag	UNP Q14680
D	-4	PRO	-	expression tag	UNP Q14680
D	-3	ARG	-	expression tag	UNP Q14680
D	-2	GLY	-	expression tag	UNP Q14680
D	-1	SER	-	expression tag	UNP Q14680
D	0	HIS	-	expression tag	UNP Q14680
D	167	ALA	THR	engineered mutation	UNP Q14680
D	171	ALA	SER	engineered mutation	UNP Q14680
D	213	THR	ASN	engineered mutation	UNP Q14680
D	214	ALA	VAL	engineered mutation	UNP Q14680

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Chain	Residue	Modelled	Actual	Comment	Reference
D	215	ALA	MET	engineered mutation	UNP Q14680
D	218	VAL	TYR	engineered mutation	UNP Q14680
D	219	ALA	LYS	engineered mutation	UNP Q14680

- Molecule 2 is 7-{{2-methoxy-4-(1H-pyrazol-4-yl)benzoyl}amino}-2,3,4,5-tetrahydro-1H-3-benzazepinium (CCD ID: 45R) (formula: C₂₁H₂₃N₄O₂).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	H	N	O	0	0
			50	21	23	4	2		
2	B	1	Total	C	H	N	O	0	0
			50	21	23	4	2		
2	C	1	Total	C	H	N	O	0	0
			50	21	23	4	2		
2	D	1	Total	C	H	N	O	0	0
			50	21	23	4	2		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	136	Total	O	0	0
			136	136		
3	B	147	Total	O	0	0
			147	147		
3	C	123	Total	O	0	0
			123	123		

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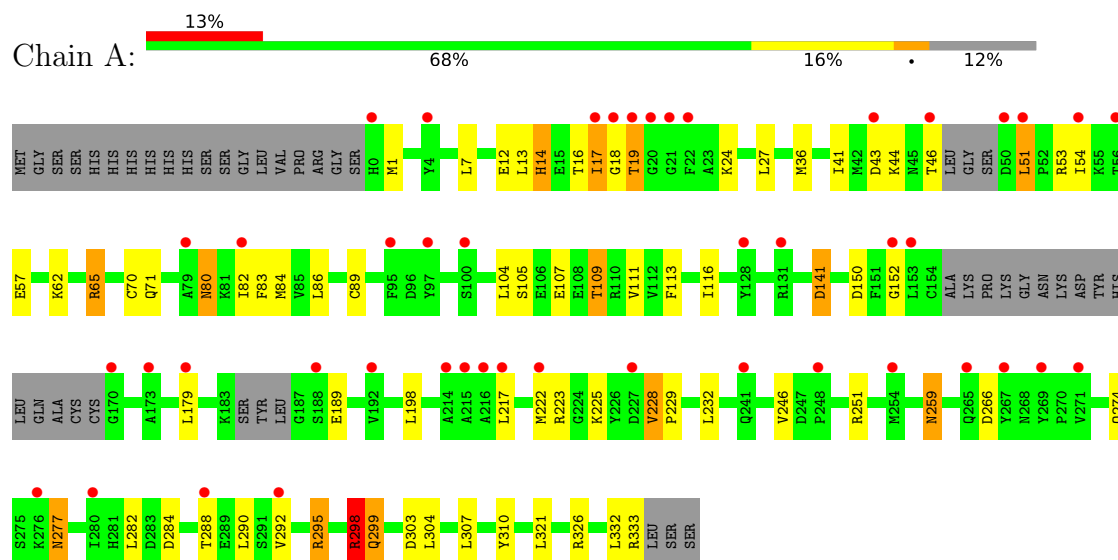
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	D	138	Total 138	O 138	0	0

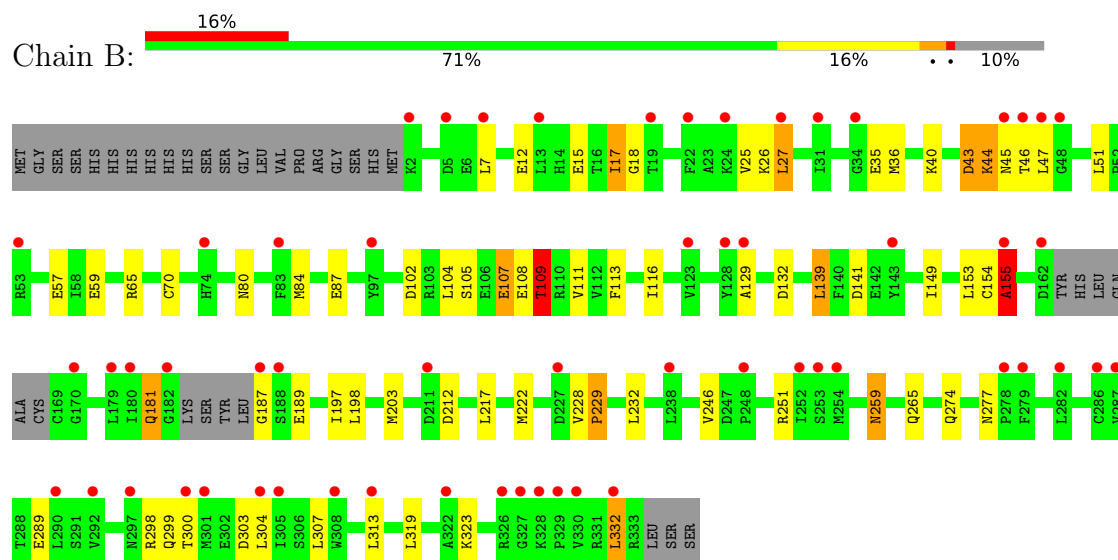
3 Residue-property plots

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

• Molecule 1: MATERNAL EMBRYONIC LEUCINE ZIPPER KINASE

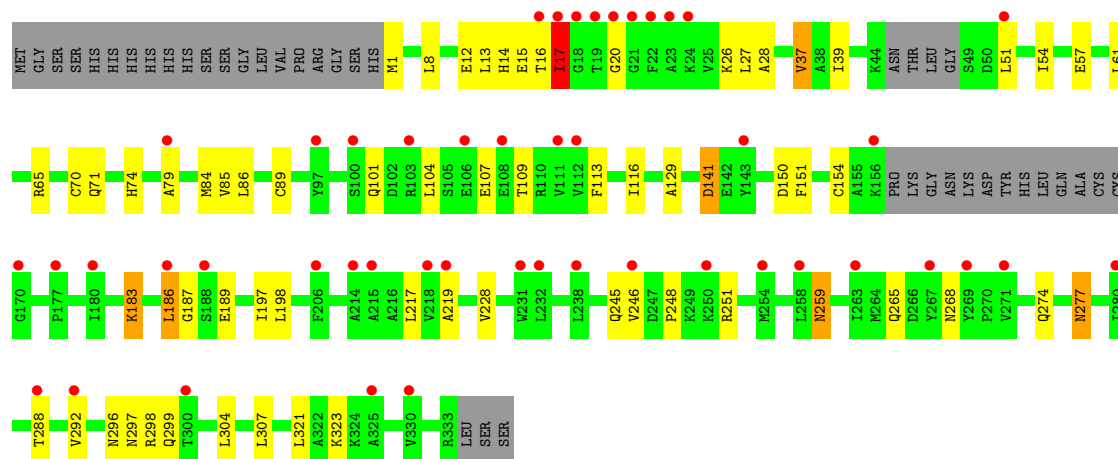


• Molecule 1: MATERNAL EMBRYONIC LEUCINE ZIPPER KINASE

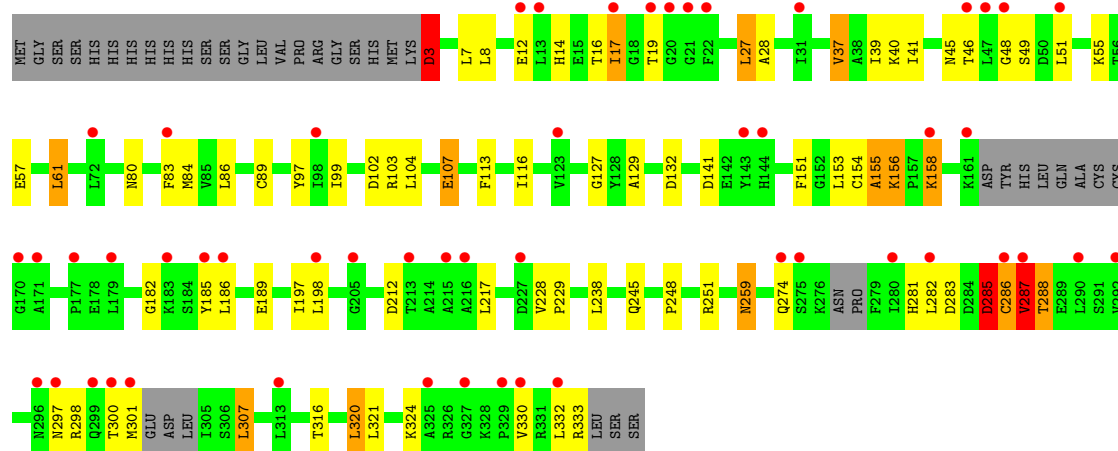


• Molecule 1: MATERNAL EMBRYONIC LEUCINE ZIPPER KINASE





• Molecule 1: MATERNAL EMBRYONIC LEUCINE ZIPPER KINASE



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	66.65Å 75.86Å 79.07Å 86.08° 69.45° 89.87°	Depositor
Resolution (Å)	48.69 – 2.45 48.69 – 2.45	Depositor EDS
% Data completeness (in resolution range)	94.6 (48.69-2.45) 94.6 (48.69-2.45)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.67 (at 2.45Å)	Xtriage
Refinement program	BUSTER 2.11.5	Depositor
R, R_{free}	0.291 , 0.357 0.286 , 0.366	Depositor DCC
R_{free} test set	2512 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	55.0	Xtriage
Anisotropy	0.368	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 117.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.54$, $\langle L^2 \rangle = 0.38$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	11042	wwPDB-VP
Average B, all atoms (Å ²)	69.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.73% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 45R

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	0.95	0/2607	1.38	11/3525 (0.3%)
1	B	0.98	0/2670	1.41	17/3609 (0.5%)
1	C	0.96	0/2622	1.38	14/3545 (0.4%)
1	D	0.98	1/2632 (0.0%)	1.44	22/3555 (0.6%)
All	All	0.97	1/10531 (0.0%)	1.40	64/14234 (0.4%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1
1	D	0	1
All	All	0	2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	155	ALA	CA-C	-5.06	1.50	1.52

All (64) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	14	HIS	CA-C-N	7.48	131.75	121.05
1	C	14	HIS	C-N-CA	7.48	131.75	121.05
1	A	18	GLY	CA-C-N	7.38	135.65	121.54
1	A	18	GLY	C-N-CA	7.38	135.65	121.54
1	B	141	ASP	CA-CB-CG	7.31	119.91	112.60
1	A	141	ASP	CA-CB-CG	7.05	119.65	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	277	ASN	CA-CB-CG	6.97	119.57	112.60
1	B	70	CYS	CA-C-N	6.79	130.34	120.71
1	B	70	CYS	C-N-CA	6.79	130.34	120.71
1	B	187	GLY	CA-C-N	6.27	130.63	120.60
1	B	187	GLY	C-N-CA	6.27	130.63	120.60
1	C	323	LYS	CA-C-N	6.26	128.96	120.38
1	C	323	LYS	C-N-CA	6.26	128.96	120.38
1	A	277	ASN	CA-CB-CG	6.23	118.83	112.60
1	B	87	GLU	CA-C-N	6.20	130.16	121.24
1	B	87	GLU	C-N-CA	6.20	130.16	121.24
1	A	222	MET	CA-C-N	6.20	128.58	120.28
1	A	222	MET	C-N-CA	6.20	128.58	120.28
1	D	155	ALA	N-CA-C	6.12	117.85	108.30
1	D	55	LYS	CA-C-N	5.97	128.77	120.29
1	D	55	LYS	C-N-CA	5.97	128.77	120.29
1	D	287	VAL	N-CA-CB	5.87	120.91	111.23
1	C	277	ASN	CA-CB-CG	5.82	118.42	112.60
1	C	141	ASP	CA-CB-CG	5.80	118.40	112.60
1	D	286	CYS	CA-C-N	5.79	132.39	121.97
1	D	286	CYS	C-N-CA	5.79	132.39	121.97
1	D	3	ASP	CA-C-N	5.76	131.27	122.23
1	D	3	ASP	C-N-CA	5.76	131.27	122.23
1	B	303	ASP	CA-CB-CG	5.68	118.28	112.60
1	D	229	PRO	CA-C-N	5.66	128.64	120.38
1	D	229	PRO	C-N-CA	5.66	128.64	120.38
1	D	283	ASP	CA-C-N	5.65	129.73	121.31
1	D	283	ASP	C-N-CA	5.65	129.73	121.31
1	D	151	PHE	CA-C-N	5.63	126.23	119.98
1	D	151	PHE	C-N-CA	5.63	126.23	119.98
1	B	155	ALA	N-CA-C	5.61	117.06	108.30
1	B	197	ILE	CA-C-N	5.60	127.72	120.44
1	B	197	ILE	C-N-CA	5.60	127.72	120.44
1	B	109	THR	N-CA-CB	5.53	118.25	110.12
1	D	155	ALA	O-C-N	5.45	124.86	120.83
1	C	16	THR	CA-C-N	5.41	131.71	121.97
1	C	16	THR	C-N-CA	5.41	131.71	121.97
1	C	197	ILE	CA-C-N	5.39	127.45	120.44
1	C	197	ILE	C-N-CA	5.39	127.45	120.44
1	D	197	ILE	CA-C-N	5.33	127.37	120.44
1	D	197	ILE	C-N-CA	5.33	127.37	120.44
1	D	297	ASN	CA-CB-CG	5.26	117.86	112.60
1	D	46	THR	CA-C-N	5.24	127.73	120.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	46	THR	C-N-CA	5.24	127.73	120.29
1	A	111	VAL	CA-C-N	5.22	127.25	120.56
1	A	111	VAL	C-N-CA	5.22	127.25	120.56
1	A	303	ASP	CA-CB-CG	5.17	117.78	112.60
1	A	70	CYS	CA-C-N	5.15	128.19	120.87
1	A	70	CYS	C-N-CA	5.15	128.19	120.87
1	B	229	PRO	CA-C-N	5.12	127.86	120.38
1	B	229	PRO	C-N-CA	5.12	127.86	120.38
1	D	19	THR	N-CA-C	-5.10	102.77	110.06
1	C	70	CYS	CA-C-N	5.09	128.10	120.87
1	C	70	CYS	C-N-CA	5.09	128.10	120.87
1	D	102	ASP	CA-CB-CG	5.09	117.69	112.60
1	B	303	ASP	CA-C-N	5.02	127.27	120.44
1	B	303	ASP	C-N-CA	5.02	127.27	120.44
1	C	129	ALA	CA-C-N	5.02	126.97	120.44
1	C	129	ALA	C-N-CA	5.02	126.97	120.44

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	155	ALA	Peptide
1	D	285	ASP	Peptide

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	2550	0	2556	25	0
1	B	2609	0	2629	32	0
1	C	2564	0	2582	25	0
1	D	2575	0	2602	32	0
2	A	27	23	23	2	0
2	B	27	23	23	3	0
2	C	27	23	23	2	0
2	D	27	23	23	4	0
3	A	136	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	147	0	0	3	0
3	C	123	0	0	0	0
3	D	138	0	0	3	0
All	All	10950	92	10461	112	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 5.

All (112) 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:C:248:PRO:HA	1:C:251:ARG:HG3	1.64	0.78
1:D:248:PRO:HA	1:D:251:ARG:HG3	1.67	0.77
1:B:43:ASP:HB3	1:B:46:THR:HB	1.70	0.73
1:D:129:ALA:H	1:D:155:ALA:CB	2.03	0.72
1:A:105:SER:O	1:A:109:THR:HG23	1.90	0.70
1:C:186:LEU:CB	1:C:187:GLY:HA2	2.23	0.68
1:D:129:ALA:H	1:D:155:ALA:HB3	1.59	0.68
1:D:3:ASP:HA	3:D:2003:HOH:O	1.94	0.68
1:B:17:ILE:CD1	1:B:27:LEU:HD13	2.26	0.66
1:A:17:ILE:HA	1:D:17:ILE:HD12	1.80	0.64
1:C:245:GLN:HB2	1:C:251:ARG:HG2	1.79	0.63
1:D:245:GLN:HB2	1:D:251:ARG:HG2	1.79	0.63
1:B:129:ALA:H	1:B:155:ALA:CB	2.11	0.62
1:B:139:LEU:CD2	1:B:149:ILE:HG12	2.29	0.62
1:C:186:LEU:HB3	1:C:187:GLY:HA2	1.80	0.62
1:A:288:THR:HG22	1:A:298:ARG:HG3	1.81	0.62
2:B:1334:45R:H16	3:B:2034:HOH:O	2.00	0.61
1:B:129:ALA:H	1:B:155:ALA:HB3	1.65	0.61
1:D:17:ILE:HD11	2:D:1334:45R:H1A	1.83	0.60
1:D:17:ILE:O	1:D:17:ILE:HG13	2.02	0.59
1:C:183:LYS:HG2	1:C:186:LEU:HD13	1.85	0.59
1:B:108:GLU:HG2	3:B:2062:HOH:O	2.03	0.58
1:C:259:ASN:HD22	1:C:259:ASN:H	1.50	0.58
1:D:158:LYS:HE2	1:D:186:LEU:HD22	1.86	0.58
1:A:86:LEU:HD13	2:A:1334:45R:C27	2.33	0.58
1:B:18:GLY:HA3	1:B:25:VAL:H	1.69	0.58
1:B:104:LEU:HB2	1:B:109:THR:HG22	1.86	0.57
1:A:19:THR:HB	3:A:2012:HOH:O	2.03	0.57
1:A:44:LYS:HB3	1:A:82:ILE:HD11	1.87	0.56
1:D:57:GLU:HG3	1:D:61:LEU:HD23	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:259:ASN:HD22	1:D:259:ASN:H	1.53	0.56
1:B:212:ASP:O	1:C:79:ALA:HB2	2.06	0.55
1:B:17:ILE:HD11	1:B:27:LEU:HD13	1.89	0.55
1:C:186:LEU:CG	1:C:187:GLY:HA2	2.37	0.54
1:B:35:GLU:HB2	1:B:319:LEU:HD22	1.89	0.54
1:A:27:LEU:HD11	2:A:1334:45R:C13	2.38	0.53
1:A:65:ARG:HD2	1:A:71:GLN:HE22	1.73	0.53
1:B:105:SER:O	1:B:109:THR:HG23	2.08	0.53
1:D:288:THR:HG23	1:D:298:ARG:HE	1.75	0.52
1:B:181:GLN:HG2	1:B:222:MET:HE1	1.92	0.52
1:B:139:LEU:HD21	1:B:149:ILE:CD1	2.40	0.52
1:A:259:ASN:HD22	1:A:259:ASN:H	1.57	0.52
1:C:104:LEU:HB2	1:C:109:THR:CG2	2.40	0.52
1:D:89:CYS:HA	1:D:141:ASP:HA	1.92	0.52
1:B:259:ASN:H	1:B:259:ASN:HD22	1.56	0.51
1:D:113:PHE:HA	1:D:116:ILE:HD12	1.92	0.51
1:C:113:PHE:HA	1:C:116:ILE:HD12	1.92	0.51
1:B:139:LEU:HD21	1:B:149:ILE:HG12	1.93	0.51
1:D:212:ASP:HB2	3:D:2097:HOH:O	2.10	0.51
1:C:51:LEU:HA	1:C:54:ILE:HG12	1.93	0.50
1:A:62:LYS:HG2	1:A:310:TYR:CD2	2.47	0.50
1:B:289:GLU:HG3	1:B:332:LEU:HD22	1.94	0.50
1:A:113:PHE:HA	1:A:116:ILE:HD12	1.93	0.49
1:D:132:ASP:HB2	1:D:153:LEU:HD12	1.94	0.49
1:A:228:VAL:HG21	3:A:2040:HOH:O	2.13	0.48
1:A:89:CYS:HA	1:A:141:ASP:HA	1.95	0.48
1:C:65:ARG:HG2	1:C:277:ASN:HB3	1.94	0.48
1:B:107:GLU:O	1:B:111:VAL:HG23	2.14	0.48
1:D:86:LEU:HD13	2:D:1334:45R:C14	2.45	0.47
1:B:17:ILE:HG21	2:B:1334:45R:H24	1.96	0.47
1:A:19:THR:HA	1:A:24:LYS:HB3	1.96	0.47
1:C:288:THR:O	1:C:292:VAL:HG13	2.14	0.47
1:B:109:THR:HG21	1:B:203:MET:CG	2.44	0.47
1:B:132:ASP:HB2	1:B:153:LEU:HD12	1.96	0.47
1:B:17:ILE:HG23	1:C:17:ILE:HG22	1.95	0.47
1:B:57:GLU:HG2	1:B:84:MET:HE1	1.97	0.47
1:C:89:CYS:HA	1:C:141:ASP:HA	1.97	0.46
1:B:17:ILE:HD13	1:B:27:LEU:HD13	1.98	0.46
1:C:28:ALA:HB3	1:C:37:VAL:HG12	1.97	0.46
1:A:43:ASP:HA	1:A:80:ASN:O	2.15	0.46
1:D:14:HIS:HB2	1:D:27:LEU:HB3	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:229:PRO:HD2	1:B:232:LEU:HD22	1.98	0.45
1:B:139:LEU:HD22	1:B:139:LEU:N	2.30	0.45
1:C:186:LEU:HG	1:C:187:GLY:HA2	1.97	0.45
1:D:127:GLY:O	1:D:156:LYS:HA	2.17	0.45
1:D:286:CYS:O	1:D:287:VAL:HG23	2.16	0.45
2:D:1334:45R:H13	2:D:1334:45R:O10	2.15	0.45
1:A:57:GLU:HG2	1:A:84:MET:HE1	2.00	0.44
1:A:14:HIS:CD2	1:A:36:MET:HE1	2.51	0.44
1:C:57:GLU:HG2	1:C:84:MET:HE1	1.99	0.44
1:B:36:MET:HB2	3:B:2016:HOH:O	2.16	0.44
1:C:186:LEU:HB3	1:C:187:GLY:CA	2.47	0.44
1:C:65:ARG:HG3	1:C:71:GLN:HE22	1.82	0.44
1:D:129:ALA:HB3	1:D:155:ALA:HB2	2.00	0.44
1:D:28:ALA:HB3	1:D:37:VAL:HG12	2.00	0.43
1:B:113:PHE:HA	1:B:116:ILE:HD12	2.00	0.43
1:D:97:TYR:CE2	1:D:104:LEU:HD11	2.53	0.43
1:D:57:GLU:HG2	1:D:84:MET:HE1	2.01	0.43
1:A:284:ASP:O	1:A:288:THR:HG23	2.19	0.43
1:C:219:ALA:HB1	1:D:107:GLU:HB2	2.00	0.43
1:A:41:ILE:HG12	1:A:83:PHE:CD1	2.54	0.43
1:A:53:ARG:HD3	1:A:152:GLY:O	2.18	0.43
1:D:129:ALA:H	1:D:155:ALA:HB2	1.78	0.43
1:C:17:ILE:HD13	2:C:1334:45R:C22	2.49	0.43
1:C:86:LEU:HD13	2:C:1334:45R:C24	2.49	0.43
1:A:51:LEU:HA	1:A:54:ILE:HG12	2.00	0.42
1:A:223:ARG:HE	1:A:225:LYS:HB2	1.83	0.42
1:B:40:LYS:HE3	2:B:1334:45R:H19	2.00	0.42
1:D:285:ASP:HB3	1:D:330:VAL:HG11	2.02	0.42
1:B:129:ALA:HB3	1:B:155:ALA:HB2	2.02	0.42
1:D:316:THR:O	1:D:320:LEU:HB2	2.20	0.41
1:B:109:THR:HG21	1:B:203:MET:HG2	2.03	0.41
1:A:229:PRO:HD2	1:A:232:LEU:HD22	2.02	0.41
1:A:288:THR:O	1:A:292:VAL:HG13	2.19	0.41
1:D:7:LEU:HD11	1:D:39:ILE:HD13	2.02	0.41
1:C:61:LEU:HD11	1:C:151:PHE:CD1	2.55	0.41
1:C:74:HIS:HB3	1:C:85:VAL:CG2	2.50	0.41
1:B:109:THR:HG21	1:B:203:MET:HG3	2.03	0.41
1:D:40:LYS:HD2	2:D:1334:45R:H17	2.02	0.41
1:D:307:LEU:HB2	3:D:2132:HOH:O	2.19	0.41
1:D:41:ILE:HG12	1:D:83:PHE:CD1	2.56	0.40
1:A:65:ARG:HG2	1:A:277:ASN:O	2.21	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	306/356 (86%)	289 (94%)	12 (4%)	5 (2%)	7	7
1	B	317/356 (89%)	288 (91%)	26 (8%)	3 (1%)	14	17
1	C	310/356 (87%)	287 (93%)	17 (6%)	6 (2%)	6	5
1	D	310/356 (87%)	280 (90%)	23 (7%)	7 (2%)	5	3
All	All	1243/1424 (87%)	1144 (92%)	78 (6%)	21 (2%)	7	6

All (21) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	19	THR
1	A	298	ARG
1	C	17	ILE
1	D	287	VAL
1	B	15	GLU
1	D	48	GLY
1	D	103	ARG
1	A	299	GLN
1	B	44	LYS
1	B	102	ASP
1	C	297	ASN
1	C	298	ARG
1	D	285	ASP
1	A	295	ARG
1	C	183	LYS
1	D	281	HIS
1	A	150	ASP
1	C	150	ASP
1	D	49	SER
1	C	20	GLY

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Mol	Chain	Res	Type
1	D	182	GLY

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	277/314 (88%)	242 (87%)	35 (13%)	4	4
1	B	285/314 (91%)	250 (88%)	35 (12%)	4	4
1	C	279/314 (89%)	251 (90%)	28 (10%)	7	7
1	D	280/314 (89%)	246 (88%)	34 (12%)	5	4
All	All	1121/1256 (89%)	989 (88%)	132 (12%)	5	4

All (132) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	7	LEU
1	A	12	GLU
1	A	13	LEU
1	A	14	HIS
1	A	16	THR
1	A	17	ILE
1	A	46	THR
1	A	51	LEU
1	A	65	ARG
1	A	80	ASN
1	A	104	LEU
1	A	107	GLU
1	A	109	THR
1	A	179	LEU
1	A	189	GLU
1	A	198	LEU
1	A	217	LEU
1	A	228	VAL
1	A	246	VAL

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Mol	Chain	Res	Type
1	A	251	ARG
1	A	259	ASN
1	A	266	ASP
1	A	274	GLN
1	A	282	LEU
1	A	290	LEU
1	A	295	ARG
1	A	298	ARG
1	A	299	GLN
1	A	304	LEU
1	A	307	LEU
1	A	321	LEU
1	A	326	ARG
1	A	332	LEU
1	A	333	ARG
1	B	7	LEU
1	B	12	GLU
1	B	17	ILE
1	B	26	LYS
1	B	27	LEU
1	B	43	ASP
1	B	44	LYS
1	B	45	ASN
1	B	47	LEU
1	B	51	LEU
1	B	59	GLU
1	B	65	ARG
1	B	80	ASN
1	B	107	GLU
1	B	109	THR
1	B	139	LEU
1	B	154	CYS
1	B	181	GLN
1	B	189	GLU
1	B	198	LEU
1	B	217	LEU
1	B	228	VAL
1	B	246	VAL
1	B	251	ARG
1	B	259	ASN
1	B	265	GLN
1	B	274	GLN

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Mol	Chain	Res	Type
1	B	298	ARG
1	B	299	GLN
1	B	300	THR
1	B	304	LEU
1	B	307	LEU
1	B	313	LEU
1	B	323	LYS
1	B	332	LEU
1	C	1	MET
1	C	8	LEU
1	C	12	GLU
1	C	13	LEU
1	C	15	GLU
1	C	17	ILE
1	C	26	LYS
1	C	27	LEU
1	C	37	VAL
1	C	39	ILE
1	C	101	GLN
1	C	107	GLU
1	C	154	CYS
1	C	186	LEU
1	C	189	GLU
1	C	198	LEU
1	C	217	LEU
1	C	228	VAL
1	C	246	VAL
1	C	259	ASN
1	C	265	GLN
1	C	268	ASN
1	C	274	GLN
1	C	296	ASN
1	C	299	GLN
1	C	304	LEU
1	C	307	LEU
1	C	321	LEU
1	D	3	ASP
1	D	8	LEU
1	D	12	GLU
1	D	16	THR
1	D	17	ILE
1	D	27	LEU

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Mol	Chain	Res	Type
1	D	37	VAL
1	D	45	ASN
1	D	51	LEU
1	D	61	LEU
1	D	80	ASN
1	D	99	ILE
1	D	107	GLU
1	D	154	CYS
1	D	156	LYS
1	D	158	LYS
1	D	185	TYR
1	D	189	GLU
1	D	198	LEU
1	D	217	LEU
1	D	228	VAL
1	D	238	LEU
1	D	259	ASN
1	D	274	GLN
1	D	282	LEU
1	D	288	THR
1	D	300	THR
1	D	301	MET
1	D	307	LEU
1	D	320	LEU
1	D	321	LEU
1	D	324	LYS
1	D	332	LEU
1	D	333	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (37) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	71	GLN
1	A	137	ASN
1	A	181	GLN
1	A	242	GLN
1	A	245	GLN
1	A	259	ASN
1	A	265	GLN
1	A	294	HIS
1	A	312	HIS
1	B	45	ASN

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Mol	Chain	Res	Type
1	B	71	GLN
1	B	137	ASN
1	B	242	GLN
1	B	256	ASN
1	B	259	ASN
1	B	293	HIS
1	B	299	GLN
1	B	312	HIS
1	C	68	HIS
1	C	71	GLN
1	C	80	ASN
1	C	101	GLN
1	C	137	ASN
1	C	245	GLN
1	C	256	ASN
1	C	259	ASN
1	C	265	GLN
1	C	281	HIS
1	C	293	HIS
1	C	312	HIS
1	D	45	ASN
1	D	137	ASN
1	D	245	GLN
1	D	256	ASN
1	D	259	ASN
1	D	293	HIS
1	D	312	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

4 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	45R	B	1334	-	30,30,30	0.43	0	40,41,41	0.71	0
2	45R	C	1334	-	30,30,30	0.51	0	40,41,41	0.62	0
2	45R	A	1334	-	30,30,30	0.43	0	40,41,41	0.69	0
2	45R	D	1334	-	30,30,30	0.59	0	40,41,41	0.92	2 (5%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	45R	B	1334	-	-	0/14/22/22	0/4/4/4
2	45R	C	1334	-	-	0/14/22/22	0/4/4/4
2	45R	A	1334	-	-	0/14/22/22	0/4/4/4
2	45R	D	1334	-	-	1/14/22/22	0/4/4/4

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	1334	45R	O2-C3-C8	2.16	119.70	116.55
2	D	1334	45R	O2-C3-C4	-2.09	120.47	124.08

There are no chirality outliers.

All (1) torsion outliers are listed below:

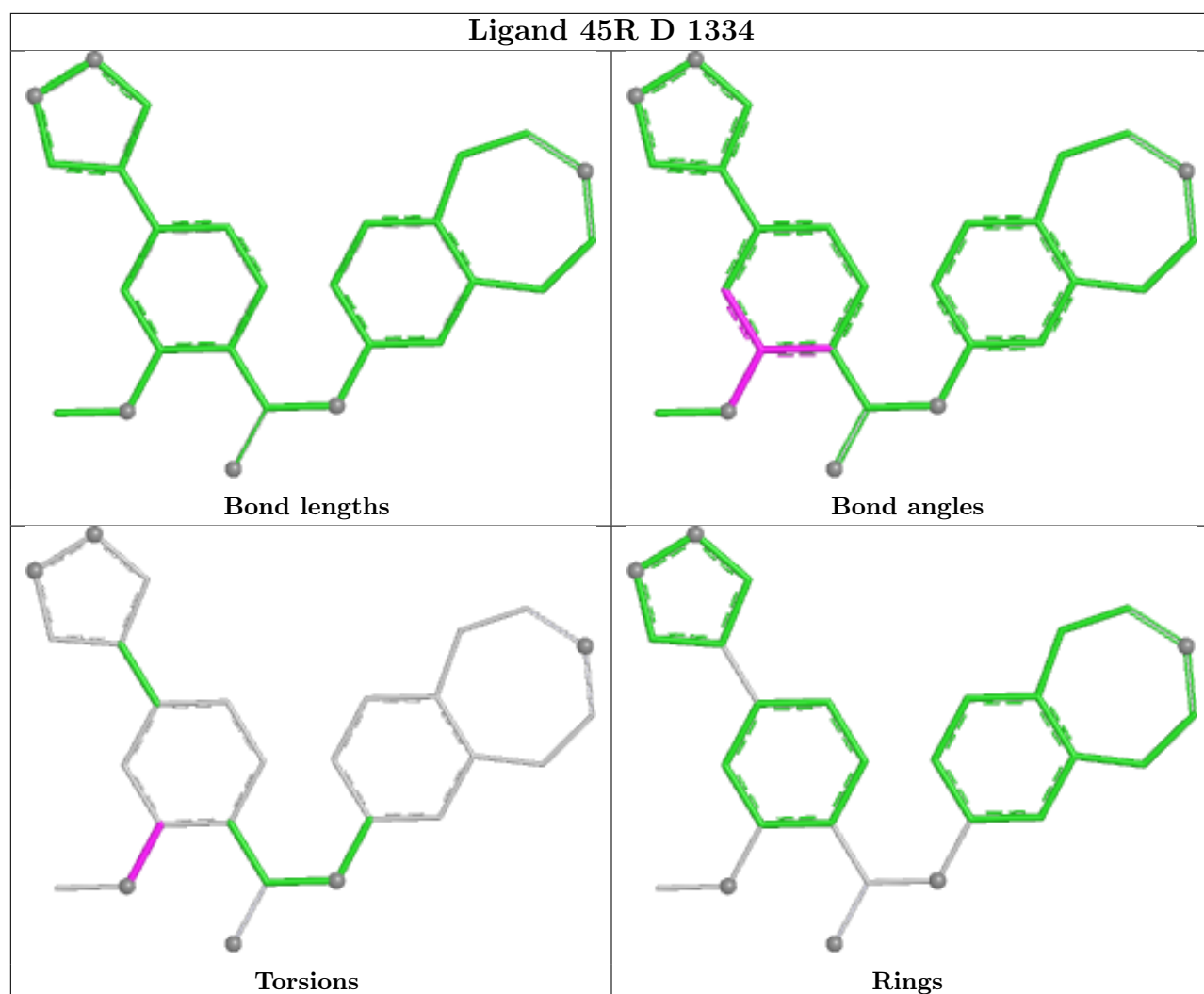
Mol	Chain	Res	Type	Atoms
2	D	1334	45R	C4-C3-O2-C1

There are no ring outliers.

4 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	1334	45R	3	0
2	C	1334	45R	2	0
2	A	1334	45R	2	0
2	D	1334	45R	4	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

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	313/356 (87%)	1.23	45 (14%) 6 4	31, 68, 101, 127	1 (0%)
1	B	322/356 (90%)	1.27	58 (18%) 3 3	34, 67, 102, 123	1 (0%)
1	C	316/356 (88%)	1.31	47 (14%) 5 4	42, 72, 105, 128	0
1	D	318/356 (89%)	1.27	52 (16%) 4 3	36, 65, 106, 131	0
All	All	1269/1424 (89%)	1.27	202 (15%) 5 3	31, 68, 105, 131	2 (0%)

All (202) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	292	VAL	6.4
1	D	186	LEU	5.6
1	D	185	TYR	4.6
1	B	180	ILE	4.3
1	B	179	LEU	4.2
1	C	19	THR	4.2
1	B	19	THR	4.2
1	D	19	THR	4.1
1	D	21	GLY	4.1
1	D	300	THR	4.0
1	D	144	HIS	4.0
1	A	97[A]	TYR	3.9
1	C	143	TYR	3.9
1	D	297	ASN	3.9
1	C	263	ILE	3.8
1	A	215	ALA	3.8
1	C	111	VAL	3.7
1	B	286	CYS	3.6
1	A	179	LEU	3.6
1	C	180	ILE	3.6
1	D	205	GLY	3.5

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Mol	Chain	Res	Type	RSRZ
1	A	22	PHE	3.5
1	C	16	THR	3.5
1	C	170	GLY	3.5
1	D	292	VAL	3.4
1	B	290	LEU	3.4
1	D	179	LEU	3.4
1	C	22	PHE	3.4
1	B	300	THR	3.3
1	A	54	ILE	3.3
1	A	18	GLY	3.2
1	A	288	THR	3.2
1	B	305	ILE	3.2
1	D	332	LEU	3.2
1	A	19	THR	3.2
1	D	330	VAL	3.1
1	A	20	GLY	3.1
1	A	292	VAL	3.1
1	A	248	PRO	3.1
1	B	330	VAL	3.1
1	A	0	HIS	3.1
1	B	297	ASN	3.1
1	D	161	LYS	3.0
1	C	215	ALA	3.0
1	A	269	TYR	3.0
1	A	51	LEU	3.0
1	A	100	SER	3.0
1	B	278	PRO	3.0
1	D	22	PHE	3.0
1	C	156	LYS	3.0
1	A	280	ILE	2.9
1	A	214	ALA	2.9
1	C	17	ILE	2.9
1	D	280	ILE	2.9
1	C	288	THR	2.8
1	C	97	TYR	2.8
1	D	17	ILE	2.8
1	D	296	ASN	2.8
1	A	153	LEU	2.8
1	B	282	LEU	2.8
1	B	279	PHE	2.8
1	A	267	TYR	2.7
1	C	51	LEU	2.7

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Mol	Chain	Res	Type	RSRZ
1	C	186	LEU	2.7
1	D	301	MET	2.7
1	B	74	HIS	2.7
1	B	48	GLY	2.7
1	C	219	ALA	2.7
1	D	46	THR	2.7
1	C	330	VAL	2.6
1	B	129	ALA	2.6
1	A	43	ASP	2.6
1	D	48	GLY	2.6
1	A	222	MET	2.6
1	D	286	CYS	2.6
1	B	13	LEU	2.6
1	D	143	TYR	2.6
1	B	162	ASP	2.6
1	B	22	PHE	2.6
1	D	51	LEU	2.6
1	D	275	SER	2.6
1	B	182	GLY	2.6
1	C	280	ILE	2.6
1	C	206	PHE	2.6
1	A	217	LEU	2.6
1	B	328	LYS	2.6
1	A	21	GLY	2.5
1	B	170	GLY	2.5
1	D	290	LEU	2.5
1	D	325	ALA	2.5
1	B	27	LEU	2.5
1	C	246	VAL	2.5
1	A	56	THR	2.5
1	B	252	ILE	2.5
1	A	46	THR	2.5
1	B	31	ILE	2.4
1	A	241	GLN	2.4
1	B	308	TRP	2.4
1	C	188	SER	2.4
1	C	106	GLU	2.4
1	A	188	SER	2.4
1	C	269	TYR	2.4
1	B	287	VAL	2.4
1	B	24	LYS	2.4
1	C	24	LYS	2.4

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Mol	Chain	Res	Type	RSRZ
1	C	18	GLY	2.4
1	B	47	LEU	2.4
1	A	128	TYR	2.4
1	B	332	LEU	2.3
1	D	282	LEU	2.3
1	B	123	VAL	2.3
1	B	292	VAL	2.3
1	C	214	ALA	2.3
1	D	171	ALA	2.3
1	A	152	GLY	2.3
1	B	34	GLY	2.3
1	A	276	LYS	2.3
1	C	108	GLU	2.3
1	B	248	PRO	2.3
1	B	304	LEU	2.3
1	A	95	PHE	2.3
1	A	4	TYR	2.3
1	D	177	PRO	2.3
1	A	265	GLN	2.3
1	B	187	GLY	2.3
1	D	170	GLY	2.3
1	D	274	GLN	2.3
1	B	253	SER	2.3
1	C	231	TRP	2.3
1	A	227	ASP	2.3
1	C	112	VAL	2.3
1	C	218	VAL	2.3
1	A	131	ARG	2.3
1	B	329	PRO	2.3
1	C	267	TYR	2.3
1	A	271	VAL	2.2
1	A	79	ALA	2.2
1	C	79	ALA	2.2
1	B	2	LYS	2.2
1	D	183	LYS	2.2
1	B	128	TYR	2.2
1	B	7	LEU	2.2
1	B	327	GLY	2.2
1	B	326	ARG	2.2
1	D	299	GLN	2.2
1	A	170	GLY	2.2
1	C	20	GLY	2.2

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Mol	Chain	Res	Type	RSRZ
1	D	198	LEU	2.2
1	D	227	ASP	2.2
1	C	250	LYS	2.2
1	D	83	PHE	2.2
1	A	216	ALA	2.1
1	B	45	ASN	2.1
1	B	143	TYR	2.1
1	D	31	ILE	2.1
1	B	188	SER	2.1
1	C	100	SER	2.1
1	D	287	VAL	2.1
1	B	254	MET	2.1
1	A	173	ALA	2.1
1	C	23	ALA	2.1
1	B	46	THR	2.1
1	C	232	LEU	2.1
1	C	258	LEU	2.1
1	C	300	THR	2.1
1	D	13	LEU	2.1
1	D	47	LEU	2.1
1	B	97	TYR	2.1
1	C	177	PRO	2.1
1	D	329	PRO	2.1
1	D	123	VAL	2.1
1	B	155	ALA	2.1
1	B	322	ALA	2.1
1	D	216	ALA	2.1
1	D	213	THR	2.1
1	B	5	ASP	2.1
1	B	211	ASP	2.1
1	D	158	LYS	2.1
1	A	192	VAL	2.1
1	B	53	ARG	2.1
1	C	103	ARG	2.1
1	D	327	GLY	2.1
1	D	98	ILE	2.1
1	C	325	ALA	2.0
1	B	238	LEU	2.0
1	B	313	LEU	2.0
1	C	238	LEU	2.0
1	D	72	LEU	2.0
1	D	12	GLU	2.0

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Mol	Chain	Res	Type	RSRZ
1	D	20	GLY	2.0
1	B	227	ASP	2.0
1	A	254	MET	2.0
1	B	301	MET	2.0
1	B	83	PHE	2.0
1	C	271	VAL	2.0
1	D	215	ALA	2.0
1	D	313	LEU	2.0
1	C	21	GLY	2.0
1	A	17	ILE	2.0
1	A	82	ILE	2.0
1	A	50	ASP	2.0
1	C	254	MET	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

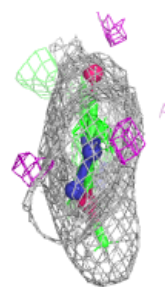
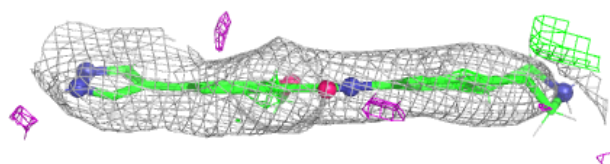
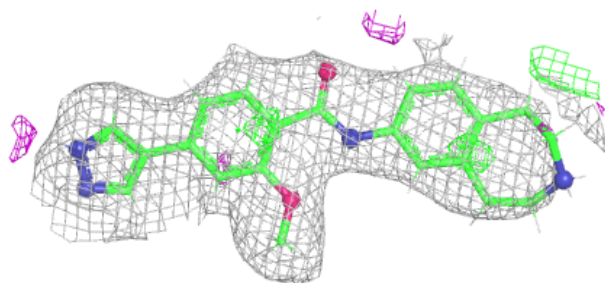
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	45R	B	1334	27/27	0.83	0.16	48,56,72,76	50
2	45R	D	1334	27/27	0.83	0.17	39,58,72,74	0
2	45R	C	1334	27/27	0.89	0.15	27,48,59,62	50
2	45R	A	1334	27/27	0.89	0.15	36,48,60,61	50

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around 45R D 1334:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers [i](#)

There are no such residues in this entry.