



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 7, 2026 – 04:16 AM UTC

PDB ID : 1BHQ / pdb_00001bhq
Title : MAC-1 I DOMAIN CADMIUM COMPLEX
Authors : Baldwin, E.T.
Deposited on : 1998-06-10
Resolution : 2.70 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

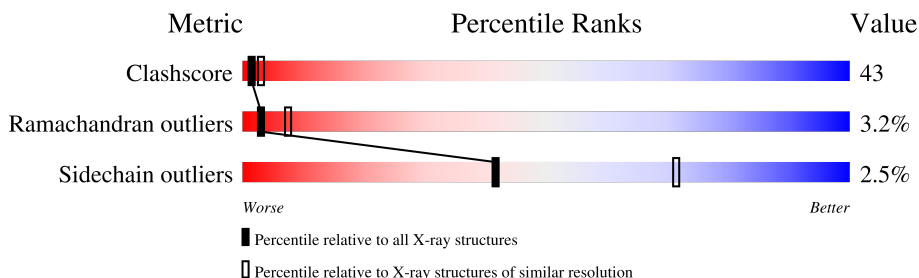
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)

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

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	1	189	30% 46% 23% .
1	2	189	22% 49% 28% .

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 3200 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.

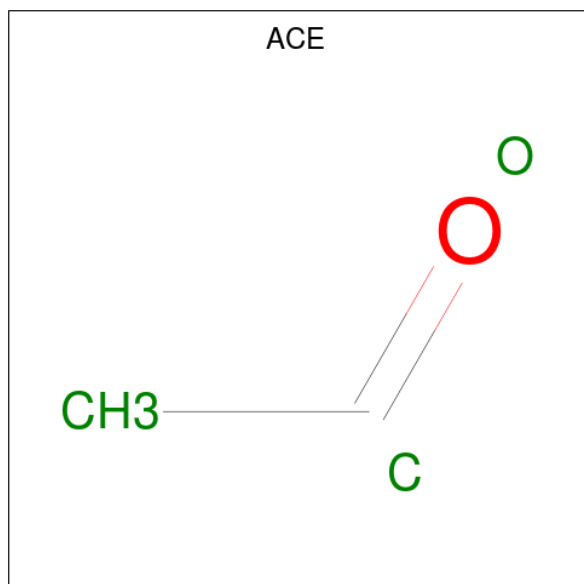
- Molecule 1 is a protein called CD11B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	1	189	Total	C	N	O	S	0	0	0
			1527	973	271	280	3			
1	2	189	Total	C	N	O	S	0	0	0
			1527	973	271	280	3			

- Molecule 2 is CADMIUM ION (CCD ID: CD) (formula: Cd).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	1	1	Total	Cd	0	0
			1	1		
2	2	2	Total	Cd	0	0
			2	2		

- Molecule 3 is ACETYL GROUP (CCD ID: ACE) (formula: C₂H₄O).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	1	1	Total	C	O	0	0
			3	2	1		
3	2	1	Total	C	O	0	0
			3	2	1		

- Molecule 4 is water.

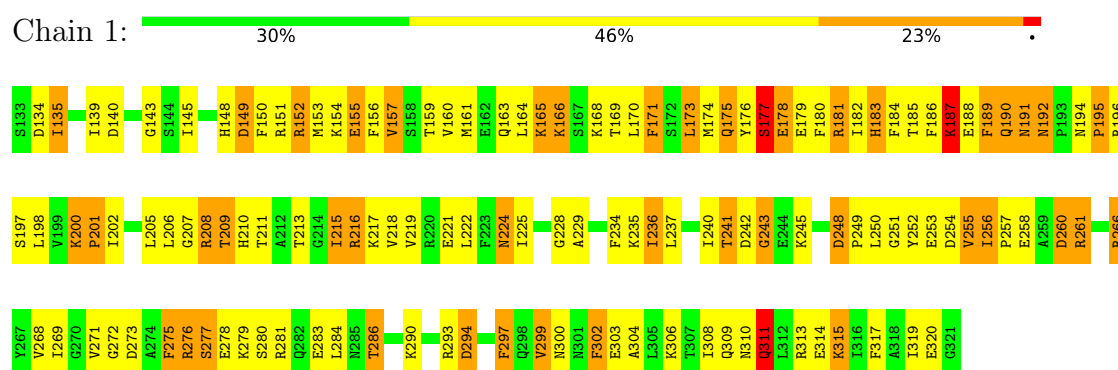
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	1	97	Total	O	0	0
			97	97		
4	2	40	Total	O	0	0
			40	40		

3 Residue-property plots

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

Note EDS was not executed.

• Molecule 1: CD11B



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 2	Depositor
Cell constants a, b, c, α , β , γ	48.42Å 122.39Å 75.36Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	10.00 – 2.70	Depositor
% Data completeness (in resolution range)	43.9 (10.00-2.70)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.10	Depositor
Refinement program	PROLSQ	Depositor
R, R_{free}	0.175 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	3200	wwPDB-VP
Average B, all atoms (Å ²)	10.0	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: CD, ACE

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	1	1.35	3/1556 (0.2%)	2.48	96/2093 (4.6%)
1	2	1.32	3/1556 (0.2%)	2.43	107/2093 (5.1%)
All	All	1.33	6/3112 (0.2%)	2.45	203/4186 (4.8%)

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	2	0	1

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1	208	ARG	CA-CB	-6.24	1.43	1.53
1	2	478	GLU	CA-CB	-5.58	1.45	1.54
1	1	299	VAL	N-CA	5.34	1.52	1.46
1	2	445	ILE	CA-CB	5.19	1.59	1.53
1	2	509	THR	CA-CB	5.15	1.60	1.53
1	1	179	GLU	CA-CB	-5.07	1.45	1.53

All (203) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2	593	ARG	CD-NE-CZ	24.92	159.28	124.40
1	2	521	GLU	CA-CB-CG	14.50	143.10	114.10
1	1	317	PHE	CA-CB-CG	13.30	127.10	113.80
1	1	276	ARG	CD-NE-CZ	12.93	142.50	124.40
1	1	208	ARG	CA-CB-CG	12.24	138.59	114.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	191	ASN	CA-CB-CG	11.72	124.33	112.60
1	1	315	LYS	CB-CG-CD	11.25	137.18	111.30
1	2	478	GLU	N-CA-C	-10.77	100.89	114.56
1	2	585	ASN	CA-CB-CG	10.68	123.28	112.60
1	1	184	PHE	CA-CB-CG	10.57	124.38	113.80
1	1	260	ASP	CA-CB-CG	10.47	123.07	112.60
1	2	480	PHE	CA-C-N	10.33	137.21	122.85
1	2	480	PHE	C-N-CA	10.33	137.21	122.85
1	1	293	ARG	CD-NE-CZ	10.31	138.83	124.40
1	1	216	ARG	CD-NE-CZ	10.10	138.53	124.40
1	2	562	GLU	CA-CB-CG	9.92	133.94	114.10
1	1	253	GLU	CA-CB-CG	9.67	133.44	114.10
1	2	548	ASP	CA-CB-CG	9.59	122.19	112.60
1	2	617	PHE	CA-CB-CG	9.59	123.39	113.80
1	2	494	ASN	CA-CB-CG	9.47	122.08	112.60
1	1	315	LYS	CA-CB-CG	9.34	132.78	114.10
1	1	175	GLN	N-CA-CB	9.31	125.75	110.85
1	1	248	ASP	CA-CB-CG	9.29	121.89	112.60
1	2	515	ILE	N-CA-CB	9.01	121.09	110.55
1	1	179	GLU	CA-CB-CG	8.94	131.98	114.10
1	2	590	LYS	CA-CB-CG	8.93	131.95	114.10
1	2	449	ASP	CA-CB-CG	8.83	121.43	112.60
1	1	299	VAL	CB-CA-C	8.76	126.38	110.71
1	2	571	VAL	N-CA-C	8.66	121.04	107.28
1	1	235	LYS	CA-CB-CG	8.59	131.27	114.10
1	2	521	GLU	CB-CG-CD	8.55	127.13	112.60
1	2	590	LYS	CB-CG-CD	8.54	130.95	111.30
1	1	179	GLU	N-CA-CB	8.38	123.33	110.60
1	1	276	ARG	NE-CZ-NH1	8.32	129.82	121.50
1	2	571	VAL	N-CA-CB	-8.15	101.63	111.90
1	2	491	ASN	CA-CB-CG	8.02	120.62	112.60
1	1	235	LYS	CB-CG-CD	7.90	129.47	111.30
1	1	182	ILE	N-CA-CB	7.88	121.25	111.41
1	1	266	ARG	N-CA-C	7.81	121.46	108.73
1	1	243	GLY	N-CA-C	7.81	124.16	110.80
1	2	478	GLU	CA-CB-CG	7.80	129.69	114.10
1	2	553	GLU	CA-CB-CG	7.68	129.45	114.10
1	1	317	PHE	N-CA-CB	7.65	121.64	110.47
1	1	178	GLU	N-CA-C	-7.65	104.44	114.31
1	1	143	GLY	N-CA-C	7.55	122.97	114.67
1	2	465	LYS	CB-CG-CD	7.47	128.48	111.30
1	1	216	ARG	NE-CZ-NH1	7.46	128.96	121.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2	593	ARG	NE-CZ-NH2	7.42	125.88	119.20
1	1	200	LYS	CA-CB-CG	7.38	128.86	114.10
1	1	209	THR	N-CA-C	7.37	122.30	107.41
1	1	297	PHE	CA-CB-CG	7.34	121.14	113.80
1	1	261	ARG	N-CA-CB	7.29	122.81	110.49
1	1	293	ARG	CA-CB-CG	7.19	128.48	114.10
1	2	602	PHE	CA-CB-CG	-7.18	106.62	113.80
1	2	531	LYS	N-CA-C	7.17	119.09	111.28
1	2	444	SER	CA-C-N	7.16	131.83	122.95
1	2	444	SER	C-N-CA	7.16	131.83	122.95
1	2	446	ILE	CA-C-N	7.13	128.75	119.84
1	2	446	ILE	C-N-CA	7.13	128.75	119.84
1	2	541	THR	CA-C-N	7.07	133.51	122.26
1	2	541	THR	C-N-CA	7.07	133.51	122.26
1	2	474	MET	N-CA-CB	7.02	124.57	111.52
1	2	554	ASP	CA-CB-CG	7.00	119.60	112.60
1	1	290	LYS	CB-CA-C	6.94	118.65	108.87
1	2	593	ARG	NH1-CZ-NH2	-6.92	110.31	119.30
1	2	451	ARG	O-C-N	6.90	129.54	122.09
1	2	558	GLU	CA-CB-CG	6.86	127.82	114.10
1	2	591	PRO	CA-C-N	6.82	126.42	119.19
1	2	591	PRO	C-N-CA	6.82	126.42	119.19
1	1	200	LYS	CA-C-N	6.79	126.41	119.56
1	1	200	LYS	C-N-CA	6.79	126.41	119.56
1	2	546	PHE	CA-CB-CG	6.75	120.55	113.80
1	1	191	ASN	N-CA-C	-6.72	105.70	114.04
1	1	165	LYS	N-CA-CB	6.72	121.24	110.16
1	1	171	PHE	CA-CB-CG	6.67	120.47	113.80
1	1	134	ASP	CA-CB-CG	6.66	119.26	112.60
1	2	478	GLU	CB-CA-C	6.66	119.52	109.13
1	1	253	GLU	CB-CG-CD	6.58	123.78	112.60
1	1	256	ILE	CB-CA-C	6.55	119.92	113.70
1	2	530	ARG	CD-NE-CZ	-6.53	115.26	124.40
1	2	524	ASN	CB-CA-C	6.52	120.55	109.80
1	1	224	ASN	CA-CB-CG	6.52	119.12	112.60
1	2	514	GLY	N-CA-C	-6.51	104.44	112.77
1	2	523	PHE	CA-CB-CG	6.49	120.29	113.80
1	2	446	ILE	CB-CA-C	6.49	118.14	110.68
1	1	175	GLN	N-CA-C	-6.47	99.67	109.95
1	1	276	ARG	NE-CZ-NH2	-6.46	113.39	119.20
1	2	451	ARG	N-CA-C	-6.45	104.17	111.14
1	1	300	ASN	N-CA-C	6.45	117.97	111.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	149	ASP	CA-CB-CG	6.44	119.04	112.60
1	1	317	PHE	N-CA-C	-6.40	105.60	113.41
1	1	135	ILE	N-CA-C	6.40	117.07	107.80
1	1	293	ARG	CG-CD-NE	6.40	126.07	112.00
1	1	258	GLU	N-CA-CB	6.37	119.30	110.07
1	1	134	ASP	CA-C-O	-6.36	114.11	120.98
1	2	444	SER	CA-C-O	6.35	126.04	119.05
1	1	192	ASN	CB-CA-C	6.33	122.65	110.17
1	1	155	GLU	CA-C-O	6.31	127.25	120.24
1	2	613	ARG	CD-NE-CZ	6.30	133.23	124.40
1	2	520	ARG	CD-NE-CZ	6.19	133.06	124.40
1	2	481	ARG	N-CA-C	6.18	119.25	107.75
1	1	236	ILE	CA-C-O	-6.17	113.64	121.48
1	1	215	ILE	CA-C-N	6.13	128.41	120.44
1	1	215	ILE	C-N-CA	6.13	128.41	120.44
1	1	294	ASP	N-CA-C	6.12	118.75	111.71
1	1	206	LEU	CA-C-O	-6.10	113.25	120.81
1	2	562	GLU	CB-CG-CD	6.08	122.94	112.60
1	2	598	GLN	CB-CG-CD	6.06	122.90	112.60
1	2	566	ARG	CA-C-N	6.01	131.96	122.94
1	2	566	ARG	C-N-CA	6.01	131.96	122.94
1	2	525	ILE	N-CA-C	6.00	116.18	110.42
1	1	254	ASP	CA-CB-CG	-5.99	106.61	112.60
1	2	521	GLU	N-CA-CB	5.99	122.34	110.48
1	2	597	PHE	CA-C-O	-5.96	113.89	120.33
1	2	593	ARG	CA-CB-CG	5.96	126.02	114.10
1	2	509	THR	N-CA-C	5.95	118.51	107.99
1	2	560	ASP	CA-CB-CG	5.94	118.54	112.60
1	2	617	PHE	N-CA-CB	5.93	119.50	110.42
1	2	579	LYS	N-CA-CB	5.92	120.50	110.49
1	1	157	VAL	CB-CA-C	5.89	119.42	111.88
1	1	241	THR	CA-CB-OG1	-5.83	100.85	109.60
1	2	614	GLU	CB-CG-CD	5.81	122.48	112.60
1	2	599	VAL	CB-CA-C	5.78	119.47	111.38
1	2	518	VAL	N-CA-C	-5.73	105.03	110.42
1	2	589	SER	N-CA-C	-5.71	101.57	110.42
1	1	216	ARG	NE-CZ-NH2	-5.69	114.08	119.20
1	2	444	SER	N-CA-C	-5.69	106.32	113.72
1	2	500	LYS	O-C-N	5.68	125.53	120.48
1	2	609	GLN	O-C-N	5.62	128.08	122.12
1	2	452	ARG	CD-NE-CZ	-5.62	116.53	124.40
1	2	602	PHE	CB-CA-C	5.61	120.21	110.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2	589	SER	CB-CA-C	5.59	119.03	109.80
1	1	256	ILE	O-C-N	5.57	123.98	120.42
1	2	515	ILE	O-C-N	5.57	127.36	121.91
1	1	255	VAL	CA-C-O	-5.57	115.85	120.80
1	2	593	ARG	CG-CD-NE	5.56	124.24	112.00
1	1	187	LYS	CB-CA-C	5.56	120.39	109.72
1	1	248	ASP	O-C-N	5.55	128.18	121.29
1	1	181	ARG	CB-CA-C	-5.54	100.13	109.72
1	2	542	ASP	N-CA-CB	-5.53	102.52	110.65
1	1	286	THR	CA-CB-OG1	-5.52	101.33	109.60
1	2	586	THR	N-CA-C	5.51	120.11	112.45
1	2	455	GLU	CB-CG-CD	5.50	121.95	112.60
1	1	183	HIS	CA-CB-CG	-5.47	108.33	113.80
1	2	537	LEU	CA-C-N	5.47	130.38	123.10
1	2	537	LEU	C-N-CA	5.47	130.38	123.10
1	2	555	VAL	N-CA-C	5.45	116.32	111.90
1	1	211	THR	N-CA-C	5.45	117.30	111.36
1	2	457	VAL	N-CA-C	5.43	115.63	110.42
1	2	550	LEU	CA-C-N	5.41	126.99	122.17
1	2	550	LEU	C-N-CA	5.41	126.99	122.17
1	2	460	VAL	CB-CA-C	5.39	119.42	112.14
1	1	208	ARG	CD-NE-CZ	-5.38	116.86	124.40
1	2	605	LEU	N-CA-C	-5.38	106.56	113.23
1	2	603	GLU	CA-CB-CG	5.38	124.86	114.10
1	2	544	GLU	CB-CG-CD	5.38	121.74	112.60
1	1	201	PRO	N-CA-C	5.38	120.58	113.86
1	2	608	ILE	N-CA-C	5.38	118.31	113.10
1	2	569	ILE	N-CA-C	-5.36	100.66	108.17
1	1	155	GLU	CA-C-N	5.36	127.40	120.44
1	1	155	GLU	C-N-CA	5.36	127.40	120.44
1	1	229	ALA	CA-C-N	5.34	129.14	121.50
1	1	229	ALA	C-N-CA	5.34	129.14	121.50
1	2	478	GLU	CA-C-O	5.33	124.63	118.55
1	2	479	GLU	CG-CD-OE1	5.33	130.65	118.40
1	2	551	GLY	N-CA-C	-5.32	103.87	111.42
1	2	562	GLU	N-CA-CB	5.31	119.69	110.39
1	1	190	GLN	CA-CB-CG	5.30	124.69	114.10
1	1	151	ARG	NH1-CZ-NH2	5.26	126.14	119.30
1	1	310	ASN	OD1-CG-ND2	5.26	127.86	122.60
1	1	177	SER	N-CA-CB	5.25	119.37	110.49
1	1	178	GLU	CA-CB-CG	5.23	124.56	114.10
1	2	501	PRO	N-CA-C	5.23	120.12	114.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2	553	GLU	CB-CA-C	-5.22	100.97	110.63
1	1	234	PHE	CA-C-O	-5.21	115.88	121.56
1	1	225	ILE	CB-CA-C	5.20	119.81	111.29
1	1	302	PHE	CA-C-O	5.19	125.75	119.11
1	1	311	GLN	N-CA-CB	5.19	118.21	110.22
1	1	152	ARG	N-CA-CB	5.17	117.82	110.16
1	2	460	VAL	CA-C-O	-5.17	115.57	120.95
1	2	572	GLY	CA-C-N	5.17	127.92	120.38
1	2	572	GLY	C-N-CA	5.17	127.92	120.38
1	1	179	GLU	N-CA-C	-5.17	102.51	109.95
1	1	184	PHE	CB-CA-C	5.16	119.14	109.86
1	2	613	ARG	O-C-N	5.16	127.66	122.09
1	1	275	PHE	CA-CB-CG	-5.15	108.65	113.80
1	2	437	PHE	CA-CB-CG	5.15	118.95	113.80
1	2	597	PHE	CA-CB-CG	5.13	118.93	113.80
1	2	550	LEU	CA-C-O	5.12	127.81	121.87
1	2	548	ASP	O-C-N	5.11	125.94	121.39
1	1	189	PHE	CA-CB-CG	5.11	118.91	113.80
1	2	614	GLU	CG-CD-OE2	-5.09	106.70	118.40
1	1	277	SER	N-CA-C	5.08	117.53	109.50
1	2	555	VAL	CA-C-O	-5.07	115.53	120.30
1	1	272	GLY	N-CA-C	5.06	119.26	112.17
1	2	594	ASP	CA-CB-CG	5.06	117.66	112.60
1	2	614	GLU	CG-CD-OE1	5.06	130.04	118.40
1	1	186	PHE	O-C-N	5.01	127.44	122.12
1	1	299	VAL	CA-C-O	-5.01	115.97	121.28
1	1	175	GLN	O-C-N	5.01	129.47	123.16
1	1	225	ILE	CA-C-N	5.01	127.49	120.28
1	1	225	ILE	C-N-CA	5.01	127.49	120.28
1	2	581	ARG	O-C-N	5.00	127.42	122.12

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	2	593	ARG	Sidechain

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	1	1527	0	1545	123	0
1	2	1527	0	1544	146	0
2	1	1	0	0	0	0
2	2	2	0	0	0	0
3	1	3	0	3	0	0
3	2	3	0	3	0	0
4	1	97	0	0	16	1
4	2	40	0	0	16	0
All	All	3200	0	3095	267	1

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 43.

All (267) 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)
1:2:510:HIS:HD2	4:2:26:HOH:O	1.34	1.09
1:1:196:ARG:NH1	4:1:57:HOH:O	1.86	1.07
1:2:510:HIS:CD2	4:2:26:HOH:O	2.09	1.03
1:1:320:GLU:OE2	4:1:1:HOH:O	1.81	0.98
1:1:306:LYS:H	1:1:306:LYS:HD2	1.27	0.96
1:2:467:SER:O	4:2:29:HOH:O	1.86	0.93
1:2:556:ILE:HB	1:2:557:PRO:HD3	1.51	0.91
1:2:569:ILE:HD11	1:2:612:LEU:HD22	1.53	0.90
1:1:187:LYS:HB3	1:1:228:GLY:HA3	1.54	0.88
1:1:277:SER:C	1:1:279:LYS:H	1.81	0.87
1:2:439:ILE:HD11	1:2:473:LEU:HD21	1.56	0.87
1:1:181:ARG:HG2	1:1:205:LEU:HD11	1.57	0.87
1:2:459:THR:HG22	1:2:463:GLN:HE21	1.37	0.86
1:1:299:VAL:HG22	1:1:304:ALA:HB3	1.57	0.86
1:1:178:GLU:HG3	1:1:208:ARG:H	1.42	0.84
1:2:459:THR:CG2	1:2:463:GLN:HE21	1.93	0.80
1:2:518:VAL:HG11	1:2:537:LEU:HD13	1.62	0.80
1:2:497:SER:HA	1:2:500:LYS:NZ	1.97	0.79
1:1:294:ASP:HB3	4:1:15:HOH:O	1.83	0.79
1:1:153:MET:HE3	1:1:302:PHE:HE2	1.47	0.78
1:1:306:LYS:HD2	1:1:306:LYS:N	1.98	0.78
1:1:145:ILE:HA	4:1:950:HOH:O	1.83	0.77
1:1:294:ASP:O	1:1:315:LYS:NZ	2.15	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:545:LYS:NZ	1:2:551:GLY:HA2	2.00	0.76
1:1:208:ARG:HA	4:1:801:HOH:O	1.85	0.76
1:2:454:LYS:HD2	1:2:499:VAL:O	1.84	0.76
1:1:260:ASP:HB2	4:1:848:HOH:O	1.86	0.75
1:2:610:ASN:OD1	4:2:42:HOH:O	2.04	0.75
1:1:153:MET:HE3	1:1:302:PHE:CE2	2.22	0.73
1:1:266:ARG:NH2	4:1:858:HOH:O	2.21	0.73
1:1:135:ILE:O	1:1:171:PHE:HA	1.88	0.72
1:1:218:VAL:HG11	1:1:237:LEU:HD13	1.72	0.72
1:1:173:LEU:HD23	1:1:174:MET:N	2.04	0.72
1:1:168:LYS:HE2	1:1:168:LYS:HA	1.72	0.71
1:1:273:ASP:O	1:1:276:ARG:HD2	1.90	0.71
1:1:320:GLU:CD	4:1:1:HOH:O	2.26	0.71
1:2:445:ILE:HG22	1:2:450:PHE:HB2	1.71	0.71
1:1:276:ARG:H	1:1:276:ARG:CD	2.05	0.70
1:1:276:ARG:H	1:1:276:ARG:HD3	1.57	0.70
1:2:591:PRO:O	1:2:595:HIS:ND1	2.23	0.69
1:1:161:MET:HE3	1:1:171:PHE:CB	2.22	0.69
1:1:161:MET:O	1:1:165:LYS:HG3	1.92	0.69
1:1:277:SER:O	1:1:279:LYS:N	2.25	0.69
1:2:439:ILE:CD1	1:2:473:LEU:HD21	2.23	0.69
1:2:449:ASP:HB3	1:2:602:PHE:CD2	2.28	0.68
1:2:483:HIS:HA	4:2:37:HOH:O	1.94	0.68
1:2:459:THR:HG22	1:2:463:GLN:NE2	2.09	0.68
1:2:516:ARG:HB2	1:2:555:VAL:CG1	2.25	0.67
1:1:200:LYS:N	1:1:201:PRO:HD2	2.10	0.66
1:2:620:GLU:HB2	4:2:17:HOH:O	1.93	0.66
1:1:218:VAL:HG11	1:1:237:LEU:CD1	2.26	0.66
1:1:181:ARG:HE	1:1:205:LEU:HD21	1.60	0.66
1:1:178:GLU:HG3	1:1:208:ARG:N	2.12	0.65
1:2:474:MET:HE2	1:2:482:ILE:HG12	1.79	0.65
1:1:303:GLU:HB2	4:1:53:HOH:O	1.97	0.64
1:2:610:ASN:HA	1:2:613:ARG:HH21	1.62	0.64
1:1:163:GLN:NE2	1:1:309:GLN:HE21	1.94	0.64
1:2:610:ASN:CG	4:2:42:HOH:O	2.40	0.64
1:2:453:MET:HE2	1:2:540:ILE:HG21	1.79	0.64
1:2:516:ARG:HB2	1:2:555:VAL:HG12	1.79	0.64
1:1:299:VAL:HG22	1:1:304:ALA:CB	2.28	0.64
1:2:497:SER:HA	1:2:500:LYS:HZ3	1.60	0.64
1:2:439:ILE:HG22	1:2:540:ILE:HD12	1.79	0.63
1:2:609:GLN:HB2	4:2:42:HOH:O	1.98	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:539:VAL:HB	1:2:568:VAL:HG22	1.81	0.62
1:2:492:ASN:N	1:2:493:PRO:HD3	2.15	0.61
1:1:320:GLU:HG3	4:1:1:HOH:O	2.00	0.61
1:1:194:ASN:HD22	1:1:197:SER:CB	2.13	0.61
1:1:163:GLN:HE22	1:1:309:GLN:HE21	1.47	0.61
1:2:506:LEU:O	1:2:507:GLY:O	2.19	0.61
1:2:588:ALA:HB1	1:2:595:HIS:HB2	1.82	0.60
1:2:515:ILE:HD11	1:2:587:ILE:HG23	1.83	0.60
1:2:466:LYS:HG3	4:2:16:HOH:O	2.01	0.60
1:1:213:THR:HG22	1:1:217:LYS:HE2	1.83	0.60
1:2:545:LYS:HZ2	1:2:551:GLY:HA2	1.66	0.59
1:2:439:ILE:HG12	1:2:473:LEU:HD11	1.83	0.59
1:1:245:LYS:HD2	1:1:248:ASP:OD2	2.01	0.59
1:2:487:LYS:HB2	1:2:527:ASN:C	2.28	0.59
1:1:299:VAL:CG2	1:1:304:ALA:HB3	2.32	0.59
1:1:175:GLN:HG3	1:1:205:LEU:HD12	1.84	0.58
1:1:163:GLN:OE1	1:1:313:ARG:HD3	2.03	0.58
1:2:472:SER:OG	1:2:522:LEU:HD22	2.04	0.58
1:2:478:GLU:HG2	1:2:507:GLY:HA3	1.86	0.58
1:2:500:LYS:HG3	1:2:501:PRO:HD3	1.86	0.58
1:1:161:MET:HE3	1:1:171:PHE:CG	2.39	0.58
1:1:252:TYR:HA	1:1:255:VAL:HG22	1.85	0.58
1:1:308:ILE:HA	1:1:311:GLN:NE2	2.19	0.58
1:1:166:LYS:HB2	1:1:166:LYS:NZ	2.19	0.57
1:2:453:MET:HE2	1:2:540:ILE:CG2	2.34	0.57
1:2:545:LYS:HZ1	1:2:551:GLY:HA2	1.67	0.57
1:1:275:PHE:HA	1:1:280:SER:OG	2.03	0.57
1:1:306:LYS:H	1:1:306:LYS:CD	2.07	0.57
1:1:153:MET:CE	1:1:302:PHE:HE2	2.17	0.57
1:1:215:ILE:O	1:1:219:VAL:HG23	2.05	0.57
1:1:140:ASP:HB2	1:1:241:THR:HB	1.87	0.56
1:1:299:VAL:CG2	1:1:304:ALA:CB	2.84	0.56
1:2:571:VAL:HG11	1:2:602:PHE:CE1	2.40	0.56
1:2:518:VAL:HG11	1:2:537:LEU:CD1	2.32	0.56
1:2:492:ASN:H	1:2:493:PRO:HD3	1.69	0.55
1:2:500:LYS:CG	1:2:501:PRO:HD3	2.35	0.55
1:1:252:TYR:OH	1:1:283:GLU:OE2	2.18	0.55
1:1:189:PHE:C	1:1:191:ASN:H	2.13	0.55
1:1:148:HIS:CD2	1:1:152:ARG:HH21	2.24	0.55
1:2:452:ARG:O	1:2:453:MET:C	2.49	0.55
1:2:436:ALA:O	1:2:537:LEU:HA	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:153:MET:HE2	1:1:240:ILE:HG22	1.89	0.55
1:2:481:ARG:HG3	1:2:505:LEU:HD21	1.90	0.54
1:2:446:ILE:HD12	1:2:448:HIS:HE1	1.71	0.54
1:2:442:SER:O	1:2:504:GLN:NE2	2.41	0.54
1:1:286:THR:HG21	4:1:845:HOH:O	2.07	0.54
1:2:453:MET:O	1:2:456:PHE:HB3	2.08	0.54
1:2:475:GLN:OE1	1:2:504:GLN:HA	2.07	0.54
1:2:513:THR:O	1:2:517:LYS:HG3	2.08	0.53
1:1:308:ILE:HA	1:1:311:GLN:CD	2.33	0.53
1:2:524:ASN:OD1	1:2:525:ILE:N	2.41	0.53
1:2:461:MET:HE3	1:2:471:PHE:HB3	1.90	0.53
1:1:303:GLU:O	1:1:306:LYS:HD3	2.09	0.53
1:2:478:GLU:OE1	1:2:508:ARG:N	2.41	0.53
1:1:163:GLN:HE22	1:1:309:GLN:NE2	2.07	0.53
1:2:556:ILE:CB	1:2:557:PRO:HD3	2.29	0.53
1:2:606:LYS:HA	1:2:609:GLN:NE2	2.24	0.53
1:1:157:VAL:O	1:1:161:MET:HG3	2.09	0.53
1:2:599:VAL:HG11	1:2:605:LEU:HD23	1.91	0.52
1:2:446:ILE:HD12	1:2:448:HIS:CE1	2.44	0.52
1:2:560:ASP:O	1:2:563:GLY:N	2.42	0.52
1:1:148:HIS:HD2	1:1:152:ARG:HE	1.57	0.52
1:2:464:LEU:HA	1:2:617:PHE:CZ	2.45	0.52
1:2:439:ILE:CG2	1:2:540:ILE:HD12	2.40	0.52
1:1:185:THR:HG23	1:1:188:GLU:OE1	2.10	0.52
1:1:277:SER:O	1:1:281:ARG:HG2	2.10	0.52
1:1:313:ARG:NH2	1:1:314:GLU:OE2	2.41	0.52
1:1:149:ASP:HA	1:1:152:ARG:HG3	1.92	0.52
1:2:438:LEU:HD13	1:2:518:VAL:CG2	2.39	0.52
1:1:308:ILE:C	1:1:308:ILE:HD12	2.35	0.51
1:1:269:ILE:HA	1:1:297:PHE:O	2.09	0.51
1:1:192:ASN:O	1:1:198:LEU:HD11	2.09	0.51
1:2:436:ALA:HB2	1:2:486:PHE:CZ	2.45	0.51
1:1:164:LEU:HD21	1:1:313:ARG:HA	1.93	0.51
1:1:139:ILE:HG22	1:1:240:ILE:HD12	1.92	0.51
1:1:169:THR:O	1:1:170:LEU:HD23	2.11	0.51
1:1:166:LYS:HB2	1:1:166:LYS:HZ2	1.75	0.51
1:2:497:SER:HA	1:2:500:LYS:HZ2	1.73	0.51
1:2:545:LYS:NZ	1:2:550:LEU:O	2.39	0.50
1:2:474:MET:HE2	1:2:482:ILE:CG1	2.41	0.50
1:2:487:LYS:HD2	1:2:526:THR:O	2.11	0.50
1:1:216:ARG:NH2	1:1:250:LEU:HD21	2.27	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:461:MET:HE3	1:2:471:PHE:CB	2.42	0.50
1:2:569:ILE:HD12	1:2:608:ILE:HD12	1.94	0.50
1:1:251:GLY:HA2	4:1:962:HOH:O	2.11	0.50
1:1:194:ASN:HB3	1:1:197:SER:OG	2.12	0.49
1:2:518:VAL:HA	1:2:522:LEU:HD12	1.95	0.49
1:1:161:MET:HE3	1:1:171:PHE:HB2	1.93	0.49
1:2:606:LYS:HD2	1:2:609:GLN:HE22	1.77	0.49
1:1:159:THR:HG23	4:1:4:HOH:O	2.12	0.49
1:1:243:GLY:HA3	4:1:907:HOH:O	2.12	0.49
1:2:448:HIS:O	1:2:451:ARG:HB3	2.13	0.49
1:2:442:SER:C	1:2:444:SER:H	2.20	0.49
1:1:320:GLU:CG	4:1:1:HOH:O	2.52	0.48
1:2:449:ASP:OD2	1:2:602:PHE:HD2	1.96	0.48
1:2:589:SER:CB	4:2:23:HOH:O	2.58	0.48
1:1:314:GLU:O	1:1:315:LYS:C	2.57	0.48
1:2:464:LEU:HD21	1:2:613:ARG:HA	1.94	0.48
1:2:500:LYS:HG3	1:2:501:PRO:CD	2.42	0.48
1:2:516:ARG:HB2	1:2:555:VAL:HG11	1.95	0.48
1:1:176:TYR:HB2	1:1:180:PHE:CD1	2.48	0.48
1:1:281:ARG:O	1:1:284:LEU:HB2	2.14	0.48
1:2:433:SER:HB3	1:2:435:ILE:HG13	1.96	0.48
1:2:468:LYS:O	1:2:530:ARG:NH1	2.43	0.48
1:2:487:LYS:HB2	1:2:528:GLY:N	2.29	0.47
1:2:558:GLU:HB2	1:2:561:ARG:NH2	2.29	0.47
1:1:187:LYS:HA	1:1:190:GLN:HG2	1.96	0.47
1:2:464:LEU:HA	1:2:617:PHE:CE1	2.48	0.47
1:2:521:GLU:O	1:2:527:ASN:ND2	2.38	0.47
1:2:617:PHE:O	1:2:621:GLY:N	2.48	0.47
1:1:174:MET:HA	1:1:181:ARG:O	2.14	0.47
1:1:242:ASP:HA	1:1:271:VAL:O	2.15	0.47
1:1:210:HIS:HD2	4:1:812:HOH:O	1.96	0.47
1:2:528:GLY:O	1:2:529:ALA:C	2.57	0.47
1:1:192:ASN:C	1:1:194:ASN:H	2.23	0.46
1:1:194:ASN:O	1:1:195:PRO:C	2.57	0.46
1:2:481:ARG:CZ	4:2:37:HOH:O	2.62	0.46
1:1:163:GLN:NE2	1:1:309:GLN:NE2	2.63	0.46
1:1:153:MET:O	1:1:156:PHE:HB3	2.15	0.46
1:2:589:SER:HB3	4:2:23:HOH:O	2.14	0.46
1:1:177:SER:OG	1:1:207:GLY:HA3	2.16	0.46
1:1:183:HIS:HB3	1:1:202:ILE:HD11	1.98	0.46
1:2:500:LYS:N	1:2:501:PRO:CD	2.79	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:483:HIS:O	1:2:484:PHE:HB3	2.17	0.45
1:1:250:LEU:CD1	1:2:549:PRO:HB2	2.46	0.45
1:2:438:LEU:HD13	1:2:518:VAL:HG21	1.99	0.45
1:2:500:LYS:N	1:2:501:PRO:HD3	2.32	0.45
1:2:578:GLU:HG3	1:2:579:LYS:HD2	1.99	0.45
1:2:481:ARG:HD3	1:2:483:HIS:CE1	2.51	0.45
1:1:161:MET:HE2	1:1:161:MET:HB3	1.76	0.45
1:2:437:PHE:HB2	1:2:473:LEU:HD13	1.99	0.45
1:2:510:HIS:O	1:2:511:THR:C	2.60	0.45
1:2:483:HIS:CA	4:2:37:HOH:O	2.57	0.44
1:2:459:THR:CG2	1:2:463:GLN:NE2	2.72	0.44
1:1:139:ILE:O	1:1:175:GLN:HB2	2.17	0.44
1:2:491:ASN:O	1:2:492:ASN:HB2	2.18	0.44
1:1:152:ARG:O	1:1:155:GLU:HB3	2.17	0.44
1:2:511:THR:HG21	1:2:587:ILE:CD1	2.48	0.44
1:2:544:GLU:HA	1:2:583:GLU:OE1	2.17	0.44
1:1:150:PHE:O	1:1:154:LYS:HG3	2.18	0.44
1:2:445:ILE:CG2	1:2:450:PHE:HB2	2.45	0.44
1:1:187:LYS:HE2	1:1:187:LYS:HB2	1.61	0.43
1:1:200:LYS:N	1:1:201:PRO:CD	2.77	0.43
1:1:222:LEU:C	1:1:224:ASN:H	2.25	0.43
1:1:245:LYS:HE3	1:1:252:TYR:CE2	2.53	0.43
1:1:248:ASP:HA	1:1:249:PRO:HD2	1.74	0.43
1:2:518:VAL:CG1	1:2:537:LEU:HD13	2.43	0.43
1:2:606:LYS:HD2	1:2:609:GLN:NE2	2.34	0.43
1:1:221:GLU:O	1:1:224:ASN:HB3	2.18	0.43
1:2:448:HIS:HD2	1:2:452:ARG:CZ	2.32	0.43
1:2:435:ILE:O	1:2:486:PHE:HE1	2.01	0.43
1:2:443:GLY:N	1:2:506:LEU:HA	2.33	0.43
1:1:249:PRO:HG3	1:2:549:PRO:HG2	2.00	0.43
1:1:311:GLN:H	1:1:311:GLN:HE21	1.66	0.43
1:1:213:THR:O	1:1:216:ARG:HB3	2.17	0.43
1:2:446:ILE:HA	1:2:447:PRO:HD2	1.61	0.43
1:2:513:THR:OG1	1:2:550:LEU:HD13	2.19	0.43
1:1:276:ARG:HD3	1:1:276:ARG:N	2.29	0.43
1:2:511:THR:HG21	1:2:587:ILE:HD13	2.01	0.43
1:2:602:PHE:O	1:2:603:GLU:C	2.62	0.43
1:1:192:ASN:O	1:1:194:ASN:N	2.46	0.42
1:2:488:GLU:O	1:2:489:PHE:C	2.62	0.42
1:2:571:VAL:HG11	1:2:602:PHE:CZ	2.53	0.42
1:2:579:LYS:O	1:2:582:GLN:HB3	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:437:PHE:HB2	1:2:473:LEU:CD1	2.49	0.42
1:1:189:PHE:C	1:1:191:ASN:N	2.77	0.42
1:2:591:PRO:HA	1:2:592:PRO:HD3	1.65	0.42
1:2:558:GLU:O	1:2:562:GLU:OE1	2.37	0.42
1:2:513:THR:OG1	1:2:548:ASP:OD1	2.27	0.42
1:2:611:GLN:O	1:2:613:ARG:N	2.52	0.42
1:2:610:ASN:CB	1:2:613:ARG:HH21	2.32	0.42
1:2:480:PHE:CZ	1:2:513:THR:HG22	2.55	0.42
1:2:491:ASN:O	1:2:492:ASN:CB	2.67	0.42
1:2:613:ARG:HE	1:2:613:ARG:HB3	1.61	0.42
1:1:311:GLN:O	1:1:315:LYS:HD3	2.20	0.42
1:2:446:ILE:HG12	4:2:35:HOH:O	2.18	0.42
1:2:470:LEU:HG	1:2:530:ARG:NH2	2.35	0.42
1:2:535:LYS:HG2	4:2:45:HOH:O	2.20	0.41
1:1:139:ILE:O	1:1:175:GLN:HA	2.20	0.41
1:2:560:ASP:C	1:2:563:GLY:H	2.28	0.41
1:2:550:LEU:HD23	1:2:555:VAL:HG13	2.01	0.41
1:1:256:ILE:N	1:1:257:PRO:CD	2.83	0.41
1:2:509:THR:O	1:2:546:PHE:N	2.54	0.41
1:1:260:ASP:O	1:1:261:ARG:C	2.63	0.41
1:2:437:PHE:O	1:2:473:LEU:HD12	2.21	0.41
1:2:570:GLY:HA3	1:2:584:LEU:HD11	2.02	0.41
1:1:187:LYS:HB3	1:1:228:GLY:CA	2.39	0.41
1:2:610:ASN:OD1	1:2:613:ARG:NH2	2.53	0.41
1:1:176:TYR:HB2	1:1:180:PHE:CE1	2.56	0.41
1:2:481:ARG:NH2	4:2:37:HOH:O	2.54	0.41
1:1:209:THR:HG22	1:1:245:LYS:HA	2.03	0.40
1:1:266:ARG:HE	1:1:266:ARG:HB2	1.62	0.40
1:2:471:PHE:O	1:2:486:PHE:HA	2.20	0.40
1:2:474:MET:HA	1:2:481:ARG:O	2.21	0.40
1:2:446:ILE:O	1:2:449:ASP:N	2.53	0.40
1:2:611:GLN:C	1:2:613:ARG:N	2.79	0.40
1:1:236:ILE:HD11	1:1:319:ILE:HG21	2.03	0.40
1:1:268:VAL:HG12	1:1:284:LEU:HD22	2.04	0.40
1:1:148:HIS:O	1:1:152:ARG:HG3	2.21	0.40
1:1:160:VAL:HG12	1:1:164:LEU:HD12	2.04	0.40
1:2:435:ILE:O	1:2:486:PHE:CE1	2.75	0.40
1:2:522:LEU:C	1:2:524:ASN:H	2.29	0.40
1:2:578:GLU:O	1:2:579:LYS:HD2	2.22	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:1:25:HOH:O	4:1:826:HOH:O[4_555]	0.96	1.24

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	1	187/189 (99%)	162 (87%)	22 (12%)	3 (2%)	7	20
1	2	187/189 (99%)	158 (84%)	20 (11%)	9 (5%)	2	3
All	All	374/378 (99%)	320 (86%)	42 (11%)	12 (3%)	3	7

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	1	278	GLU
1	2	492	ASN
1	2	507	GLY
1	2	604	ALA
1	2	466	LYS
1	2	620	GLU
1	2	447	PRO
1	2	477	SER
1	2	611	GLN
1	1	177	SER
1	2	612	LEU
1	1	195	PRO

5.3.2 Protein sidechains [i](#)

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

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

analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	1	152/168 (90%)	148 (97%)	4 (3%)	40	70
1	2	168/168 (100%)	164 (98%)	4 (2%)	43	72
All	All	320/336 (95%)	312 (98%)	8 (2%)	42	71

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	1	166	LYS
1	1	173	LEU
1	1	187	LYS
1	1	311	GLN
1	2	481	ARG
1	2	521	GLU
1	2	553	GLU
1	2	590	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	1	191	ASN
1	1	194	ASN
1	1	285	ASN
1	1	309	GLN
1	1	311	GLN
1	2	463	GLN
1	2	491	ASN
1	2	510	HIS
1	2	532	ASN
1	2	609	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 5 ligands modelled in this entry, 3 are monoatomic - leaving 2 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	$\# Z > 2$
3	ACE	1	132	1	1,2,2	1.31	0	0,1,1	-	-
3	ACE	2	432	1	1,2,2	1.17	0	0,1,1	-	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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.