



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 28, 2018 – 06:13 AM EST

PDB ID : 1BHO
Title : MAC-1 I DOMAIN MAGNESIUM 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

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20030736

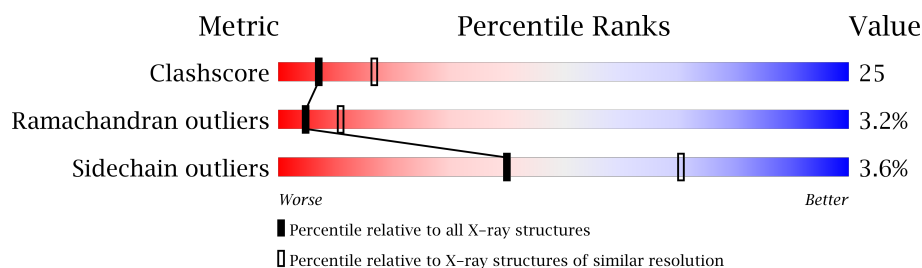
1 Overall quality at a glance

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	112137	2590 (2.70-2.70)
Ramachandran outliers	110173	2550 (2.70-2.70)
Sidechain outliers	110143	2550 (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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	1	190	
1	2	190	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 3187 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	190	Total	C	N	O	S	0	0	0
			1530	975	271	281	3			
1	2	190	Total	C	N	O	S	0	0	0
			1530	975	271	281	3			

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 3 is water.

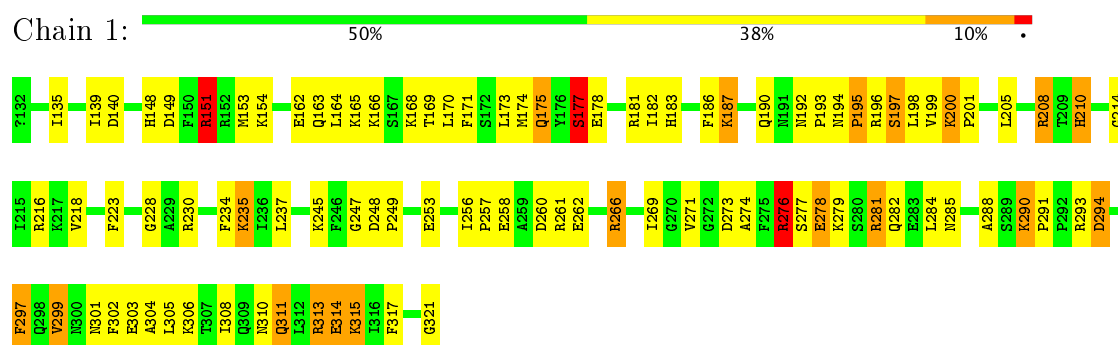
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	1	90	Total	O	0	0
			90	90		
3	2	35	Total	O	0	0
			35	35		

3 Residue-property plots

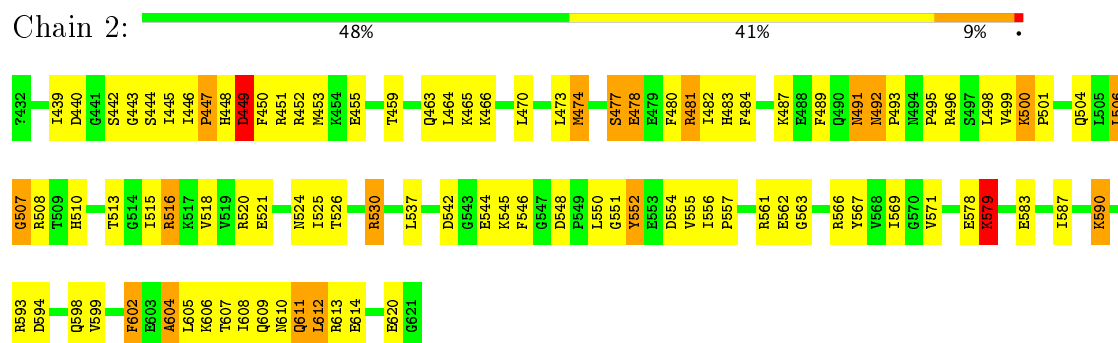
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are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

Note EDS was not executed.

• Molecule 1: CD11B



• 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	48.59 Å 123.27 Å 75.65 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	10.00 – 2.70	Depositor
% Data completeness (in resolution range)	60.4 (10.00-2.70)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.10	Depositor
Refinement program	PROLSQ	Depositor
R, R_{free}	0.181 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	3187	wwPDB-VP
Average B, all atoms (Å ²)	14.0	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: MG, 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	1.06	0/1557	1.92	42/2095 (2.0%)
1	2	1.06	0/1557	1.92	38/2095 (1.8%)
All	All	1.06	0/3114	1.92	80/4190 (1.9%)

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	1	0	2

There are no bond length outliers.

All (80) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	2	593	ARG	CD-NE-CZ	16.04	146.06	123.60
1	1	216	ARG	NE-CZ-NH1	15.96	128.28	120.30
1	2	521	GLU	CA-CB-CG	13.52	143.14	113.40
1	2	554	ASP	CB-CG-OD1	12.68	129.71	118.30
1	1	293	ARG	NE-CZ-NH1	11.70	126.15	120.30
1	1	293	ARG	CD-NE-CZ	11.61	139.86	123.60
1	1	216	ARG	CD-NE-CZ	10.73	138.62	123.60
1	2	566	ARG	NE-CZ-NH2	9.39	124.99	120.30
1	2	593	ARG	NE-CZ-NH2	9.25	124.92	120.30
1	1	276	ARG	NE-CZ-NH1	9.20	124.90	120.30
1	2	474	MET	N-CA-CB	9.14	127.06	110.60
1	1	315	LYS	CB-CG-CD	9.07	135.19	111.60
1	2	566	ARG	CD-NE-CZ	8.89	136.05	123.60
1	2	590	LYS	CB-CG-CD	8.71	134.25	111.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2	590	LYS	CA-CB-CG	8.68	132.50	113.40
1	2	508	ARG	NE-CZ-NH1	8.61	124.61	120.30
1	1	151	ARG	NE-CZ-NH1	-8.59	116.00	120.30
1	1	216	ARG	NE-CZ-NH2	-8.05	116.28	120.30
1	1	175	GLN	N-CA-CB	8.04	125.07	110.60
1	2	478	GLU	CA-CB-CG	8.04	131.08	113.40
1	2	500	LYS	CA-CB-CG	7.96	130.90	113.40
1	1	281	ARG	NE-CZ-NH1	7.89	124.25	120.30
1	1	299	VAL	CB-CA-C	7.85	126.31	111.40
1	1	140	ASP	CB-CG-OD1	7.83	125.35	118.30
1	2	530	ARG	NE-CZ-NH2	-7.66	116.47	120.30
1	2	477	SER	N-CA-CB	7.59	121.89	110.50
1	1	177	SER	N-CA-CB	7.59	121.88	110.50
1	2	562	GLU	CA-CB-CG	7.36	129.59	113.40
1	2	561	ARG	NE-CZ-NH1	7.34	123.97	120.30
1	2	449	ASP	CB-CG-OD1	7.25	124.83	118.30
1	1	317	PHE	N-CA-CB	7.17	123.51	110.60
1	2	516	ARG	CD-NE-CZ	7.16	133.63	123.60
1	1	315	LYS	CA-CB-CG	7.02	128.85	113.40
1	2	561	ARG	NE-CZ-NH2	-6.98	116.81	120.30
1	1	208	ARG	CA-CB-CG	6.95	128.70	113.40
1	1	253	GLU	CA-CB-CG	6.90	128.57	113.40
1	1	294	ASP	CB-CG-OD2	-6.88	112.11	118.30
1	2	491	ASN	CA-CB-CG	6.86	128.48	113.40
1	2	521	GLU	N-CA-CB	6.66	122.59	110.60
1	2	544	GLU	OE1-CD-OE2	-6.64	115.33	123.30
1	1	261	ARG	N-CA-CB	6.60	122.48	110.60
1	2	508	ARG	NE-CZ-NH2	-6.53	117.03	120.30
1	1	148	HIS	CA-CB-CG	6.34	124.38	113.60
1	2	520	ARG	NE-CZ-NH2	6.25	123.42	120.30
1	1	200	LYS	CA-CB-CG	6.19	127.03	113.40
1	2	544	GLU	CG-CD-OE1	6.16	130.62	118.30
1	1	293	ARG	CG-CD-NE	6.14	124.70	111.80
1	2	602	PHE	CB-CA-C	6.10	122.59	110.40
1	1	208	ARG	CB-CA-C	6.08	122.55	110.40
1	1	208	ARG	CD-NE-CZ	-6.07	115.10	123.60
1	1	321	GLY	CA-C-O	-6.05	109.71	120.60
1	1	301	ASN	CB-CA-C	6.00	122.41	110.40
1	2	594	ASP	CB-CG-OD2	5.96	123.67	118.30
1	1	276	ARG	CD-NE-CZ	5.93	131.91	123.60
1	1	175	GLN	O-C-N	5.88	132.10	122.70
1	1	313	ARG	CD-NE-CZ	5.78	131.70	123.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	314	GLU	OE1-CD-OE2	-5.74	116.41	123.30
1	2	554	ASP	CB-CG-OD2	-5.69	113.18	118.30
1	2	491	ASN	CB-CA-C	5.67	121.74	110.40
1	1	197	SER	CB-CA-C	5.53	120.60	110.10
1	1	186	PHE	CB-CG-CD1	-5.49	116.96	120.80
1	1	234	PHE	N-CA-CB	5.45	120.42	110.60
1	1	165	LYS	C-N-CA	5.42	135.26	121.70
1	1	230	ARG	NE-CZ-NH1	-5.42	117.59	120.30
1	2	506	LEU	CA-C-N	5.41	127.02	116.20
1	1	290	LYS	CB-CG-CD	5.36	125.53	111.60
1	1	262	GLU	OE1-CD-OE2	-5.34	116.89	123.30
1	2	474	MET	CA-CB-CG	5.34	122.38	113.30
1	2	593	ARG	NH1-CZ-NH2	-5.32	113.55	119.40
1	2	466	LYS	CD-CE-NZ	5.28	123.84	111.70
1	1	297	PHE	N-CA-CB	5.24	120.02	110.60
1	1	258	GLU	N-CA-CB	5.12	119.81	110.60
1	1	235	LYS	CA-CB-CG	5.11	124.64	113.40
1	2	579	LYS	CB-CG-CD	5.10	124.85	111.60
1	2	546	PHE	CA-CB-CG	5.09	126.12	113.90
1	1	175	GLN	CA-CB-CG	5.09	124.59	113.40
1	2	524	ASN	CB-CA-C	5.07	120.54	110.40
1	2	552	TYR	CB-CA-C	5.07	120.53	110.40
1	2	567	TYR	CA-CB-CG	5.06	123.02	113.40
1	1	195	PRO	C-N-CA	5.05	134.34	121.70

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	1	151	ARG	Sidechain
1	1	266	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	1530	0	1548	74	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	2	1530	0	1548	82	0
2	1	1	0	0	0	0
2	2	1	0	0	0	0
3	1	90	0	0	5	0
3	2	35	0	0	6	0
All	All	3187	0	3096	155	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 25.

All (155) 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)
1:2:609:GLN:HB2	3:2:42:HOH:O	1.69	0.92
1:2:500:LYS:HG3	1:2:501:PRO:HD3	1.53	0.91
1:1:311:GLN:HE21	1:1:311:GLN:H	1.18	0.91
1:2:569:ILE:HD11	1:2:612:LEU:HD22	1.55	0.87
1:2:542:ASP:OD1	3:2:18:HOH:O	1.96	0.82
1:1:294:ASP:O	1:1:315:LYS:NZ	2.16	0.79
1:2:518:VAL:HG11	1:2:537:LEU:HD13	1.66	0.78
1:2:474:MET:HE2	1:2:482:ILE:HG12	1.66	0.78
1:1:306:LYS:HD2	1:1:306:LYS:H	1.49	0.77
1:2:445:ILE:HG22	1:2:450:PHE:HB2	1.65	0.77
1:1:277:SER:C	1:1:279:LYS:H	1.90	0.74
1:1:294:ASP:HB3	3:1:15:HOH:O	1.86	0.73
1:2:449:ASP:HB3	1:2:602:PHE:CD2	2.23	0.72
1:1:168:LYS:HA	1:1:168:LYS:HE2	1.72	0.71
1:1:173:LEU:HD23	1:1:174:MET:N	2.07	0.69
1:1:311:GLN:NE2	1:1:311:GLN:H	1.90	0.69
1:2:473:LEU:HG	1:2:474:MET:N	2.08	0.68
1:2:563:GLY:HA2	3:2:48:HOH:O	1.94	0.68
1:1:260:ASP:HB2	3:1:848:HOH:O	1.94	0.68
1:2:500:LYS:CG	1:2:501:PRO:HD3	2.24	0.68
1:1:288:ALA:O	3:1:858:HOH:O	2.11	0.67
1:1:299:VAL:HG22	1:1:304:ALA:HB3	1.77	0.67
1:2:515:ILE:HD11	1:2:587:ILE:HG23	1.76	0.67
1:1:135:ILE:O	1:1:171:PHE:HA	1.95	0.66
1:2:439:ILE:HD11	1:2:473:LEU:HD21	1.76	0.66
1:2:459:THR:CG2	1:2:463:GLN:HE21	2.09	0.66
1:1:181:ARG:HG2	1:1:205:LEU:HD11	1.76	0.65
1:1:306:LYS:CD	1:1:306:LYS:H	2.09	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:153:MET:HE3	1:1:302:PHE:HE2	1.60	0.65
1:1:306:LYS:N	1:1:306:LYS:HD2	2.12	0.65
1:1:178:GLU:HG3	1:1:208:ARG:H	1.62	0.65
1:2:483:HIS:O	1:2:484:PHE:HB3	1.98	0.64
1:2:606:LYS:HD3	1:2:606:LYS:N	2.14	0.63
1:1:218:VAL:HG11	1:1:237:LEU:HD13	1.79	0.63
1:2:610:ASN:HA	1:2:613:ARG:HH21	1.64	0.63
1:1:214:GLY:O	1:1:218:VAL:HG23	1.98	0.62
1:2:474:MET:CE	1:2:482:ILE:HG12	2.28	0.62
1:1:299:VAL:CG1	1:1:305:LEU:HD23	2.30	0.61
1:2:480:PHE:CZ	1:2:513:THR:HG22	2.35	0.61
1:2:552:TYR:O	1:2:556:ILE:HB	2.00	0.61
1:2:449:ASP:HB3	1:2:602:PHE:CG	2.36	0.61
1:1:277:SER:O	1:1:281:ARG:HG2	2.00	0.61
1:2:459:THR:HG22	1:2:463:GLN:HE21	1.66	0.60
1:1:178:GLU:HG2	1:1:208:ARG:HG2	1.83	0.59
1:1:271:VAL:CG2	1:1:305:LEU:HD21	2.33	0.58
1:1:164:LEU:HD21	1:1:313:ARG:HA	1.85	0.58
1:2:515:ILE:HD11	1:2:587:ILE:CG2	2.33	0.58
1:1:153:MET:CE	1:1:302:PHE:HE2	2.15	0.58
1:1:266:ARG:NH2	3:1:858:HOH:O	2.38	0.56
1:1:299:VAL:HG11	1:1:305:LEU:HD23	1.87	0.56
1:2:492:ASN:ND2	1:2:498:LEU:HD21	2.21	0.56
1:2:515:ILE:CD1	1:2:587:ILE:HG23	2.35	0.56
1:2:545:LYS:HE2	1:2:548:ASP:HB3	1.88	0.55
1:1:276:ARG:H	1:1:276:ARG:CD	2.20	0.55
1:2:604:ALA:O	1:2:607:THR:OG1	2.25	0.55
1:1:162:GLU:OE2	1:1:196:ARG:HG2	2.07	0.55
1:1:281:ARG:O	1:1:284:LEU:HB2	2.07	0.54
1:2:446:ILE:HD12	1:2:448:HIS:CE1	2.43	0.54
1:1:192:ASN:O	1:1:194:ASN:N	2.35	0.54
1:1:200:LYS:HB3	1:1:201:PRO:HD3	1.88	0.53
1:1:169:THR:O	1:1:170:LEU:HD23	2.09	0.53
1:2:464:LEU:HD23	1:2:613:ARG:HG3	1.89	0.53
1:1:314:GLU:O	1:1:315:LYS:C	2.47	0.53
1:2:578:GLU:O	1:2:579:LYS:HD2	2.10	0.52
1:1:245:LYS:HD2	1:1:248:ASP:HB3	1.90	0.52
1:1:279:LYS:O	1:1:282:GLN:HB3	2.10	0.52
1:1:299:VAL:HG22	1:1:304:ALA:CB	2.40	0.52
1:2:443:GLY:HA2	1:2:506:LEU:HD23	1.92	0.52
1:2:552:TYR:O	1:2:556:ILE:N	2.38	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:492:ASN:N	1:2:493:PRO:HD3	2.25	0.51
1:2:480:PHE:CZ	1:2:513:THR:CG2	2.93	0.51
1:1:277:SER:O	1:1:279:LYS:N	2.44	0.51
1:2:439:ILE:CD1	1:2:473:LEU:HD11	2.41	0.51
1:2:451:ARG:HH12	1:2:455:GLU:HB2	1.76	0.50
1:1:277:SER:C	1:1:279:LYS:N	2.60	0.50
1:1:276:ARG:H	1:1:276:ARG:HD3	1.77	0.50
1:2:610:ASN:CB	1:2:613:ARG:HH21	2.25	0.49
1:2:448:HIS:O	1:2:451:ARG:HB3	2.12	0.49
1:2:610:ASN:OD1	1:2:613:ARG:NH2	2.45	0.49
1:1:256:ILE:N	1:1:257:PRO:CD	2.76	0.49
1:1:154:LYS:HE3	1:1:199:VAL:O	2.12	0.49
1:2:506:LEU:O	1:2:507:GLY:O	2.31	0.49
1:2:545:LYS:NZ	1:2:551:GLY:HA2	2.27	0.48
1:2:442:SER:OG	3:2:18:HOH:O	2.20	0.48
1:1:178:GLU:CG	1:1:208:ARG:HG2	2.43	0.48
1:2:452:ARG:O	1:2:453:MET:C	2.50	0.48
1:2:513:THR:OG1	1:2:550:LEU:HD13	2.13	0.48
1:2:516:ARG:HB2	1:2:555:VAL:HG12	1.94	0.48
1:2:571:VAL:HG11	1:2:602:PHE:CZ	2.48	0.48
1:1:187:LYS:HA	1:1:190:GLN:HG2	1.95	0.47
1:1:303:GLU:O	1:1:306:LYS:HD3	2.14	0.47
1:1:271:VAL:HG22	1:1:305:LEU:HD21	1.95	0.47
1:2:478:GLU:HG2	1:2:507:GLY:HA3	1.95	0.47
1:1:187:LYS:HB3	1:1:228:GLY:HA3	1.97	0.47
1:1:282:GLN:HA	1:1:285:ASN:HD22	1.80	0.47
1:1:308:ILE:C	1:1:308:ILE:HD12	2.34	0.47
1:1:183:HIS:HB3	3:1:824:HOH:O	2.15	0.46
1:2:474:MET:HE2	1:2:482:ILE:CG1	2.43	0.46
1:2:487:LYS:HD2	1:2:526:THR:O	2.16	0.46
1:1:290:LYS:HA	1:1:291:PRO:C	2.36	0.46
1:2:481:ARG:HD3	1:2:483:HIS:CE1	2.50	0.46
1:2:442:SER:C	1:2:444:SER:H	2.19	0.46
1:1:269:ILE:HA	1:1:297:PHE:O	2.16	0.45
1:2:569:ILE:HD12	1:2:608:ILE:CD1	2.46	0.45
1:2:440:ASP:C	1:2:440:ASP:OD1	2.54	0.45
1:2:443:GLY:HA2	1:2:506:LEU:CD2	2.46	0.45
1:1:139:ILE:O	1:1:139:ILE:HG13	2.17	0.45
1:2:583:GLU:O	1:2:587:ILE:HG13	2.17	0.45
1:2:496:ARG:O	1:2:500:LYS:HG2	2.17	0.45
1:1:139:ILE:O	1:1:175:GLN:HB2	2.17	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:599:VAL:HG13	1:2:604:ALA:O	2.18	0.44
1:1:313:ARG:NE	1:1:314:GLU:OE2	2.51	0.44
1:2:492:ASN:H	1:2:493:PRO:HD3	1.82	0.44
1:2:556:ILE:HB	1:2:557:PRO:HD3	2.00	0.44
1:2:599:VAL:HG11	1:2:605:LEU:HD23	1.99	0.44
1:2:504:GLN:HB3	3:2:22:HOH:O	2.17	0.44
1:2:610:ASN:O	1:2:614:GLU:HG2	2.17	0.44
1:1:274:ALA:O	1:1:276:ARG:NH1	2.43	0.44
1:2:552:TYR:O	1:2:556:ILE:CB	2.65	0.43
1:1:174:MET:HE3	1:1:182:ILE:HG12	2.00	0.43
1:1:149:ASP:HB3	1:1:302:PHE:CG	2.53	0.43
1:1:310:ASN:O	1:1:314:GLU:HG2	2.18	0.43
1:2:525:ILE:HG23	1:2:526:THR:N	2.33	0.43
1:1:192:ASN:O	1:1:198:LEU:HD11	2.19	0.43
1:2:516:ARG:HB2	1:2:555:VAL:CG1	2.48	0.43
1:2:439:ILE:HD13	1:2:473:LEU:HD11	1.99	0.43
1:2:495:PRO:O	1:2:499:VAL:HG23	2.19	0.43
1:1:278:GLU:HG2	1:1:278:GLU:O	2.18	0.42
1:1:168:LYS:HA	1:1:168:LYS:CE	2.47	0.42
1:1:256:ILE:HB	1:1:257:PRO:HD3	2.01	0.42
1:1:271:VAL:HG21	1:1:305:LEU:HD21	2.00	0.42
1:2:613:ARG:HB3	1:2:613:ARG:HE	1.53	0.42
1:1:177:SER:O	1:1:210:HIS:HB2	2.20	0.42
1:2:571:VAL:HG11	1:2:602:PHE:CE1	2.55	0.42
1:2:446:ILE:HA	1:2:447:PRO:HD2	1.78	0.42
1:2:470:LEU:HD12	1:2:530:ARG:NE	2.34	0.42
1:2:491:ASN:O	1:2:492:ASN:HB2	2.20	0.42
1:2:556:ILE:HD13	1:2:556:ILE:HA	1.69	0.42
1:1:174:MET:CE	1:1:182:ILE:HG12	2.50	0.42
1:1:163:GLN:OE1	1:1:313:ARG:HD3	2.20	0.41
1:2:599:VAL:CG1	1:2:604:ALA:O	2.69	0.41
1:2:474:MET:HB2	1:2:481:ARG:O	2.21	0.41
1:1:194:ASN:HD22	1:1:197:SER:CB	2.34	0.41
1:1:308:ILE:HA	1:1:311:GLN:CD	2.41	0.41
1:2:611:GLN:C	1:2:613:ARG:N	2.74	0.41
1:2:610:ASN:CA	1:2:613:ARG:HH21	2.33	0.41
1:1:273:ASP:O	1:1:276:ARG:HD2	2.21	0.41
1:1:223:PHE:CD1	1:1:235:LYS:HD2	2.56	0.41
1:2:443:GLY:CA	1:2:506:LEU:CD2	2.98	0.41
1:1:210:HIS:CE1	1:1:247:GLY:O	2.75	0.40
1:2:446:ILE:HG12	3:2:35:HOH:O	2.21	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:465:LYS:HE2	1:2:489:PHE:HE1	1.85	0.40
1:1:299:VAL:CG2	1:1:304:ALA:CB	2.99	0.40
1:1:249:PRO:HB2	1:2:550:LEU:HD11	2.02	0.40
1:2:611:GLN:O	1:2:613:ARG:N	2.54	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	1	188/190 (99%)	169 (90%)	15 (8%)	4 (2%)	8	21
1	2	188/190 (99%)	161 (86%)	19 (10%)	8 (4%)	3	6
All	All	376/380 (99%)	330 (88%)	34 (9%)	12 (3%)	5	11

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	2	492	ASN
1	2	507	GLY
1	2	604	ALA
1	2	620	GLU
1	1	278	GLU
1	1	177	SER
1	2	477	SER
1	2	611	GLN
1	2	447	PRO
1	2	612	LEU
1	1	193	PRO
1	1	195	PRO

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	1	168/168 (100%)	162 (96%)	6 (4%)	40	70
1	2	168/168 (100%)	162 (96%)	6 (4%)	40	70
All	All	336/336 (100%)	324 (96%)	12 (4%)	40	70

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	1	151	ARG
1	1	166	LYS
1	1	187	LYS
1	1	210	HIS
1	1	276	ARG
1	1	311	GLN
1	2	449	ASP
1	2	481	ARG
1	2	510	HIS
1	2	579	LYS
1	2	590	LYS
1	2	598	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	1	190	GLN
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	492	ASN
1	2	510	HIS

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 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

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.