



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 06:34 PM GMT

PDB ID : 1BHQ
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
<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
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

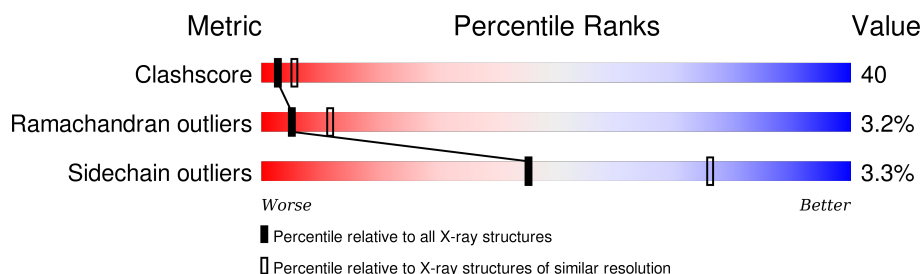
1 Overall quality at a glance

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	102246	2422 (2.70-2.70)
Ramachandran outliers	100387	2382 (2.70-2.70)
Sidechain outliers	100360	2382 (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	189	
1	2	189	

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.

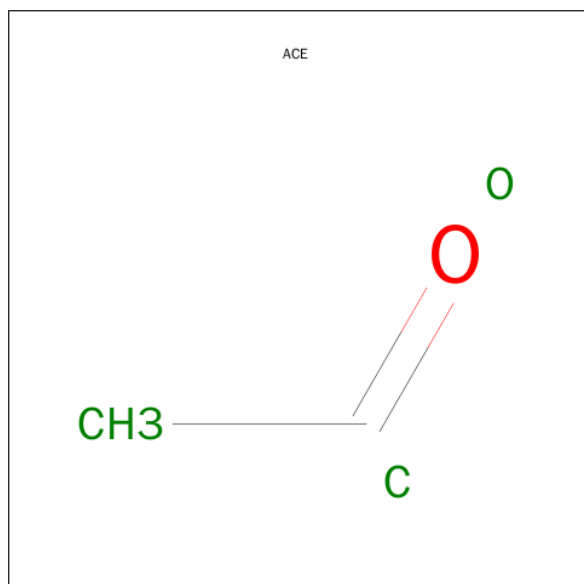
- Molecule 1 is a protein called CD11B.

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 (three-letter code: CD) (formula: Cd).

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

- Molecule 3 is ACETYL GROUP (three-letter code: 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.

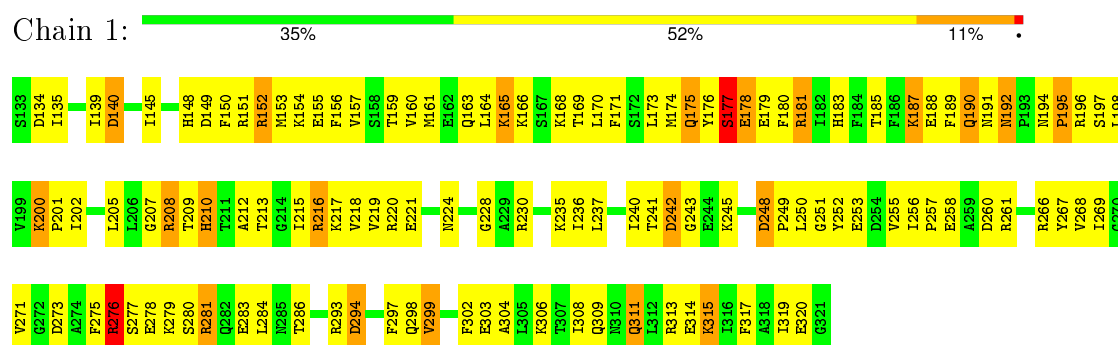
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	1	97	Total	O	0	0
			97	97		
4	2	40	Total	O	0	0
			40	40		

3 Residue-property plots

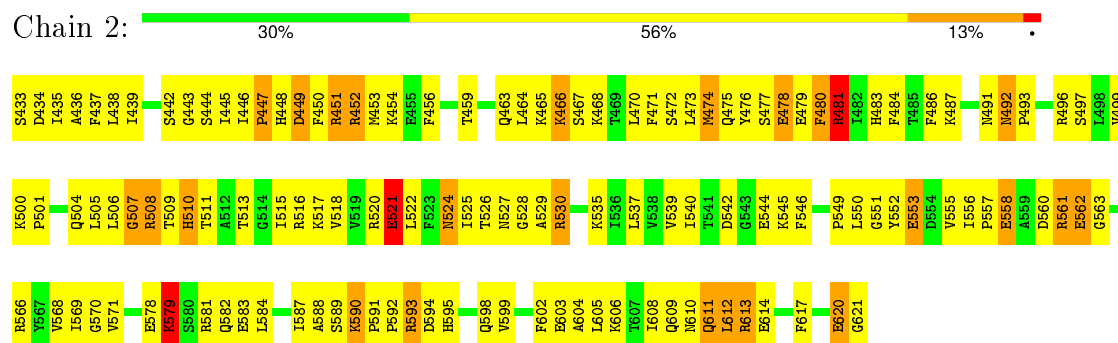
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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 ($\text{RSRZ} > 2$). 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 will therefore be incomplete.

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	48.42 Å 122.39 Å 75.36 Å 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: ACE, CD

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	1.09	1/1556 (0.1%)	2.09	52/2093 (2.5%)
1	2	1.07	0/1556	1.94	44/2093 (2.1%)
All	All	1.08	1/3112 (0.0%)	2.01	96/4186 (2.3%)

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 (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1	208	ARG	CA-CB	-5.01	1.43	1.53

All (96) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2	593	ARG	CD-NE-CZ	25.49	159.28	123.60
1	1	276	ARG	NE-CZ-NH1	19.04	129.82	120.30
1	1	216	ARG	NE-CZ-NH1	17.32	128.96	120.30
1	1	276	ARG	NE-CZ-NH2	-13.82	113.39	120.30
1	1	276	ARG	CD-NE-CZ	13.50	142.50	123.60
1	2	521	GLU	CA-CB-CG	13.50	143.10	113.40
1	1	216	ARG	NE-CZ-NH2	-12.45	114.08	120.30
1	1	208	ARG	CA-CB-CG	11.45	138.59	113.40
1	2	593	ARG	NE-CZ-NH2	11.15	125.88	120.30
1	1	293	ARG	CD-NE-CZ	10.88	138.83	123.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	216	ARG	CD-NE-CZ	10.67	138.53	123.60
1	1	281	ARG	NE-CZ-NH1	10.53	125.56	120.30
1	1	315	LYS	CB-CG-CD	9.84	137.18	111.60
1	2	562	GLU	CA-CB-CG	9.34	133.94	113.40
1	1	293	ARG	NE-CZ-NH1	9.28	124.94	120.30
1	1	253	GLU	CA-CB-CG	9.11	133.44	113.40
1	1	315	LYS	CA-CB-CG	8.81	132.78	113.40
1	1	267	TYR	CB-CG-CD2	-8.51	115.89	121.00
1	1	179	GLU	CA-CB-CG	8.45	131.98	113.40
1	2	590	LYS	CA-CB-CG	8.43	131.95	113.40
1	1	175	GLN	N-CA-CB	8.42	125.75	110.60
1	2	593	ARG	NH1-CZ-NH2	-8.27	110.31	119.40
1	1	235	LYS	CA-CB-CG	8.12	131.27	113.40
1	1	242	ASP	CB-CG-OD1	8.10	125.59	118.30
1	1	299	VAL	CB-CA-C	7.88	126.38	111.40
1	2	474	MET	N-CA-CB	7.76	124.57	110.60
1	1	151	ARG	NE-CZ-NH2	-7.69	116.45	120.30
1	2	449	ASP	CB-CG-OD1	7.68	125.21	118.30
1	1	134	ASP	CB-CG-OD1	7.44	125.00	118.30
1	2	590	LYS	CB-CG-CD	7.44	130.95	111.60
1	2	478	GLU	CA-CB-CG	7.41	129.69	113.40
1	2	553	GLU	CA-CB-CG	7.30	129.45	113.40
1	1	179	GLU	N-CA-CB	7.07	123.33	110.60
1	1	200	LYS	CA-CB-CG	7.03	128.86	113.40
1	2	508	ARG	NE-CZ-NH1	7.02	123.81	120.30
1	2	561	ARG	NE-CZ-NH2	-6.95	116.83	120.30
1	1	248	ASP	CB-CG-OD1	6.91	124.52	118.30
1	2	613	ARG	CD-NE-CZ	6.88	133.23	123.60
1	1	235	LYS	CB-CG-CD	6.87	129.47	111.60
1	1	293	ARG	CA-CB-CG	6.85	128.48	113.40
1	1	293	ARG	CG-CD-NE	6.80	126.07	111.80
1	1	261	ARG	N-CA-CB	6.78	122.81	110.60
1	1	267	TYR	CB-CG-CD1	6.77	125.06	121.00
1	2	520	ARG	CD-NE-CZ	6.76	133.06	123.60
1	1	293	ARG	NE-CZ-NH2	-6.67	116.97	120.30
1	2	451	ARG	NE-CZ-NH1	6.58	123.59	120.30
1	2	558	GLU	CA-CB-CG	6.55	127.82	113.40
1	2	521	GLU	N-CA-CB	6.52	122.34	110.60
1	2	465	LYS	CB-CG-CD	6.49	128.48	111.60
1	2	520	ARG	NE-CZ-NH2	6.44	123.52	120.30
1	1	152	ARG	NE-CZ-NH1	6.28	123.44	120.30
1	1	220	ARG	NE-CZ-NH1	6.28	123.44	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2	496	ARG	NE-CZ-NH1	6.21	123.41	120.30
1	2	480	PHE	C-N-CA	6.21	137.21	121.70
1	2	479	GLU	CG-CD-OE1	6.17	130.65	118.30
1	2	542	ASP	CB-CG-OD1	6.17	123.85	118.30
1	1	317	PHE	N-CA-CB	6.13	121.64	110.60
1	1	151	ARG	NH1-CZ-NH2	6.12	126.14	119.40
1	1	192	ASN	CB-CA-C	6.12	122.65	110.40
1	1	151	ARG	NE-CZ-NH1	-6.11	117.25	120.30
1	2	566	ARG	NE-CZ-NH1	-6.06	117.27	120.30
1	2	552	TYR	CB-CG-CD1	-5.98	117.41	121.00
1	2	530	ARG	CD-NE-CZ	-5.96	115.26	123.60
1	1	261	ARG	NE-CZ-NH1	5.95	123.27	120.30
1	2	593	ARG	CG-CD-NE	5.92	124.24	111.80
1	1	165	LYS	N-CA-CB	5.91	121.24	110.60
1	1	177	SER	N-CA-CB	5.91	119.37	110.50
1	2	552	TYR	CB-CG-CD2	5.89	124.53	121.00
1	2	614	GLU	CG-CD-OE1	5.87	130.04	118.30
1	2	614	GLU	CG-CD-OE2	-5.80	106.70	118.30
1	1	281	ARG	NE-CZ-NH2	-5.79	117.41	120.30
1	2	496	ARG	NE-CZ-NH2	-5.77	117.42	120.30
1	2	593	ARG	CA-CB-CG	5.74	126.02	113.40
1	2	594	ASP	CB-CG-OD2	5.72	123.45	118.30
1	1	294	ASP	CB-CG-OD2	-5.68	113.19	118.30
1	1	212	ALA	CB-CA-C	5.64	118.56	110.10
1	1	200	LYS	CB-CA-C	5.63	121.65	110.40
1	1	134	ASP	CB-CG-OD2	-5.54	113.32	118.30
1	2	481	ARG	NE-CZ-NH1	5.50	123.05	120.30
1	1	317	PHE	CA-CB-CG	5.50	127.10	113.90
1	2	579	LYS	N-CA-CB	5.50	120.50	110.60
1	2	581	ARG	CD-NE-CZ	5.50	131.29	123.60
1	1	230	ARG	NE-CZ-NH1	-5.46	117.57	120.30
1	2	434	ASP	CB-CG-OD1	-5.39	113.44	118.30
1	2	476	TYR	CB-CG-CD1	5.36	124.22	121.00
1	1	298	GLN	N-CA-CB	5.23	120.01	110.60
1	2	603	GLU	CA-CB-CG	5.21	124.86	113.40
1	2	476	TYR	CB-CG-CD2	-5.17	117.90	121.00
1	1	181	ARG	CB-CA-C	-5.14	100.13	110.40
1	1	190	GLN	CA-CB-CG	5.13	124.69	113.40
1	2	524	ASN	CB-CA-C	5.08	120.55	110.40
1	1	178	GLU	CA-CB-CG	5.07	124.56	113.40
1	1	140	ASP	CB-CG-OD1	5.07	122.86	118.30
1	2	452	ARG	CD-NE-CZ	-5.05	116.53	123.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2	562	GLU	N-CA-CB	5.05	119.69	110.60
1	1	258	GLU	OE1-CD-OE2	5.00	129.31	123.30

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	115	0
1	2	1527	0	1544	133	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	246	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 40.

All (246) 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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:2:439: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
1:1:277:SER:C	1:1:279:LYS:H	1.81	0.82
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
1:1:306: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
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
1:1:266: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
1:1:153:MET:HE3	1:1:302:PHE:HE2	1.55	0.71
1:1:273:ASP:O	1:1:276:ARG:HD2	1.90	0.71
1:2:545:LYS:HZ2	1:2:551:GLY:HA2	1.55	0.71
1:2:445:ILE:HG22	1:2:450:PHE:HB2	1.71	0.71
1:1:276:ARG:CD	1:1:276:ARG:H	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:O	1:1:165:LYS:HG3	1.92	0.69
1:2:439:ILE:CD1	1:2:473:LEU:HD21	2.23	0.69
1:1:277:SER:O	1:1:279:LYS:N	2.25	0.69
1:2:483:HIS:HA	4:2:37:HOH:O	1.94	0.68
1:2:449:ASP:HB3	1:2:602:PHE:CD2	2.28	0.68
1:2:459:THR:HG22	1:2:463:GLN:NE2	2.09	0.68
1:1:320:GLU:CD	4:1:1:HOH:O	2.26	0.67
1:2:516:ARG:HB2	1:2:555:VAL:CG1	2.25	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:200:LYS:N	1:1:201:PRO:HD2	2.10	0.66
1:2:497:SER:HA	1:2:500:LYS:HZ2	1.58	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
1:1:303: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
1:2:516: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
1:2:439: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
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
1:2:439: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
1:1:299: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
1:2:610:ASN:CG	4:2:42:HOH:O	2.40	0.58
1:2:472:SER:OG	1:2:522:LEU:HD22	2.04	0.58
1:2:500:LYS:HG3	1:2:501:PRO:HD3	1.86	0.58
1:2:478:GLU:HG2	1:2:507:GLY:HA3	1.86	0.58
1:1:308:ILE:HA	1:1:311:GLN:NE2	2.19	0.58
1:1:252:TYR:HA	1:1:255:VAL:HG22	1.85	0.58
1:1:166:LYS:HB2	1:1:166:LYS:NZ	2.19	0.57
1:1:306:LYS:CD	1:1:306:LYS:H	2.07	0.57
1:1:275:PHE:HA	1:1:280:SER:OG	2.03	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:2:500:LYS:CG	1:2:501:PRO:HD3	2.35	0.55
1:2:492:ASN:H	1:2:493:PRO:HD3	1.69	0.55
1:1:148:HIS:CD2	1:1:152:ARG:HH21	2.24	0.55
1:2:436:ALA:O	1:2:537:LEU:HA	2.07	0.55
1:2:481:ARG:HG3	1:2:505:LEU:HD21	1.90	0.54
1:2:487:LYS:HB2	1:2:527:ASN:C	2.28	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
1:2:453: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
1:1:286:THR:HG21	4:1:845:HOH:O	2.07	0.54
1:2:513:THR:O	1:2:517:LYS:HG3	2.08	0.53
1:2:524:ASN:OD1	1:2:525:ILE:N	2.41	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
1:2:556:ILE:CB	1:2:557:PRO:HD3	2.29	0.53
1:1:163:GLN:HE22	1:1:309:GLN:NE2	2.07	0.53
1:2:606:LYS:HA	1:2:609:GLN:NE2	2.24	0.53
1:2:545:LYS:NZ	1:2:550:LEU:O	2.39	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
1:2:464:LEU:HA	1:2:617:PHE:CZ	2.45	0.52
1:1:148:HIS:HD2	1:1:152:ARG:HE	1.57	0.52
1:2:439:ILE:CG2	1:2:540:ILE:HD12	2.40	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
1:1:185:THR:HG23	1:1:188:GLU:OE1	2.10	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
1:1:269:ILE:HA	1:1:297:PHE:O	2.09	0.51
1:2:436:ALA:HB2	1:2:486:PHE:CZ	2.45	0.51
1:1:192:ASN:O	1:1:198:LEU:HD11	2.09	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
1:1:161:MET:HE3	1:1:171:PHE:CG	2.46	0.51
1:1:189:PHE:C	1:1:191:ASN:H	2.13	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:452:ARG:O	1:2:453:MET:C	2.49	0.50
1:2:487:LYS:HD2	1:2:526:THR:O	2.11	0.50
1:2:569:ILE:HD12	1:2:608:ILE:HD12	1.94	0.50
1:1:216:ARG:NH2	1:1:250:LEU:HD21	2.27	0.50
1:1:251:GLY:HA2	4:1:962:HOH:O	2.11	0.50
1:2:518:VAL:HA	1:2:522:LEU:HD12	1.95	0.49
1:1:194:ASN:HB3	1:1:197:SER:OG	2.12	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
1:2:589:SER:CB	4:2:23:HOH:O	2.58	0.49
1:1:308:ILE:HA	1:1:311:GLN:CD	2.33	0.48
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
1:2:464: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
1:1:281: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
1:1:176:TYR:HB2	1:1:180:PHE:CD1	2.48	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
1:2:617:PHE:O	1:2:621:GLY:N	2.48	0.47
1:2:521:GLU:O	1:2:527:ASN:ND2	2.38	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
1:1:153:MET:HE3	1:1:302:PHE:CE2	2.45	0.47
1:1:308:ILE:C	1:1:308:ILE:HD12	2.35	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
1:1:252:TYR:OH	1:1:283:GLU:OE2	2.18	0.46
1:2:589:SER:HB3	4:2:23:HOH:O	2.14	0.46
1:2:500:LYS:N	1:2:501:PRO:CD	2.79	0.46
1:1:183:HIS:HB3	1:1:202:ILE:HD11	1.98	0.46
1:1:177:SER:OG	1:1:207:GLY:HA3	2.16	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
1:2:497:SER:HA	1:2:500:LYS:HZ3	1.76	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
1:2:437:PHE:HB2	1:2:473:LEU:HD13	1.99	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
1:2:545:LYS:HZ1	1:2:551:GLY:HA2	1.79	0.44
1:2:445:ILE:CG2	1:2:450:PHE:HB2	2.45	0.44
1:1:150:PHE:O	1:1:154:LYS:HG3	2.18	0.44
1:1:314:GLU:O	1:1:315:LYS:C	2.57	0.44
1:2:442:SER:C	1:2:444:SER:H	2.20	0.44
1:1:187:LYS:HE2	1:1:187:LYS:HB2	1.61	0.43
1:2:518:VAL:CG1	1:2:537:LEU:HD13	2.43	0.43
1:1:200:LYS:N	1:1:201:PRO:CD	2.77	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
1:2:606:LYS:HD2	1:2:609:GLN:NE2	2.34	0.43
1:2:448:HIS:HD2	1:2:452:ARG:CZ	2.32	0.43
1:1:221:GLU:O	1:1:224:ASN:HB3	2.18	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
1:1:311:GLN:HE21	1:1:311:GLN:H	1.66	0.43
1:1:249:PRO:HG3	1:2:549:PRO:HG2	2.00	0.43
1:2:513:THR:OG1	1:2:550:LEU:HD13	2.19	0.43
1:2:446:ILE:HA	1:2:447:PRO:HD2	1.61	0.43
1:1:213:THR:O	1:1:216:ARG:HB3	2.17	0.43
1:1:276:ARG:N	1:1:276:ARG:HD3	2.29	0.43
1:2:511:THR:HG21	1:2:587:ILE:HD13	2.01	0.43
1:2:571:VAL:HG11	1:2:602:PHE:CZ	2.53	0.42
1:1:192:ASN:O	1:1:194:ASN:N	2.46	0.42
1:2:579:LYS:O	1:2:582:GLN:HB3	2.19	0.42
1:2:437:PHE:HB2	1:2:473:LEU:CD1	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:528:GLY:O	1:2:529:ALA:C	2.57	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
1:2:611: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
1:2:613:ARG:HB3	1:2:613:ARG:HE	1.61	0.42
1:2:491:ASN:O	1:2:492:ASN:CB	2.67	0.42
1:1:192:ASN:C	1:1:194:ASN:H	2.23	0.42
1:1:194:ASN:O	1:1:195:PRO:C	2.57	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
1:2:550:LEU:HD23	1:2:555:VAL:HG13	2.01	0.41
1:2:509:THR:O	1:2:546:PHE:N	2.54	0.41
1:1:256:ILE:N	1:1:257:PRO:CD	2.83	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
1:2:481:ARG:NH2	4:2:37:HOH:O	2.54	0.41
1:1:176:TYR:HB2	1:1:180:PHE:CE1	2.56	0.41
1:2:471:PHE:O	1:2:486:PHE:HA	2.20	0.40
1:1:266:ARG:HE	1:1:266:ARG:HB2	1.62	0.40
1:2:474:MET:HA	1:2:481:ARG:O	2.21	0.40
1:1:209:THR:HG22	1:1:245:LYS:HA	2.03	0.40
1:2:446:ILE:O	1:2:449:ASP:N	2.53	0.40
1:1:268:VAL:HG12	1:1:284:LEU:HD22	2.04	0.40
1:1:236:ILE:HD11	1:1:319:ILE:HG21	2.03	0.40
1:2:435:ILE:O	1:2:486:PHE:CE1	2.75	0.40
1:1:160:VAL:HG12	1:1:164:LEU:HD12	2.04	0.40
1:1:148:HIS:O	1:1:152:ARG:HG3	2.21	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

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	187/189 (99%)	162 (87%)	22 (12%)	3 (2%)	12	30
1	2	187/189 (99%)	158 (84%)	20 (11%)	9 (5%)	3	5
All	All	374/378 (99%)	320 (86%)	42 (11%)	12 (3%)	5	12

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

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%)	164 (98%)	4 (2%)	57	85

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	2	168/168 (100%)	161 (96%)	7 (4%)	36	68
All	All	336/336 (100%)	325 (97%)	11 (3%)	45	76

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	1	187	LYS
1	1	210	HIS
1	1	276	ARG
1	1	311	GLN
1	2	481	ARG
1	2	510	HIS
1	2	521	GLU
1	2	553	GLU
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 (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	1	148	HIS
1	1	191	ASN
1	1	194	ASN
1	1	210	HIS
1	1	285	ASN
1	1	309	GLN
1	1	311	GLN
1	2	448	HIS
1	2	463	GLN
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 [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 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	2,2,2	0.80	0	0,1,1	0.00	-
3	ACE	2	432	1	2,2,2	0.77	0	0,1,1	0.00	-

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
3	ACE	1	132	1	-	0/0/0/0	0/0/0/0
3	ACE	2	432	1	-	0/0/0/0	0/0/0/0

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

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates [i](#)

EDS was not executed - this section will therefore be empty.

6.4 Ligands [i](#)

EDS was not executed - this section will therefore be empty.

6.5 Other polymers [i](#)

EDS was not executed - this section will therefore be empty.