Full wwPDB X-ray Structure Validation Report (i)

Jan 31, 2016 – 08:01 PM GMT

PDB ID	:	1IDN
Title	:	MAC-1 I DOMAIN METAL FREE
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 (i) symbol.

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

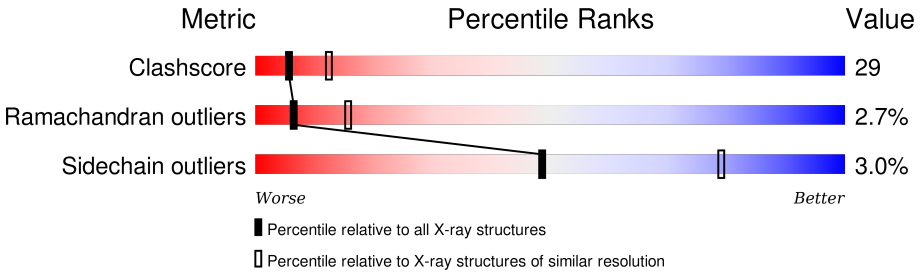
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
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 <=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	49% 39% 9% •
1	2	190	41% 45% 12% •

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 3238 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 water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	1	129	Total	O	0	0
			129	129		
2	2	49	Total	O	0	0
			49	49		

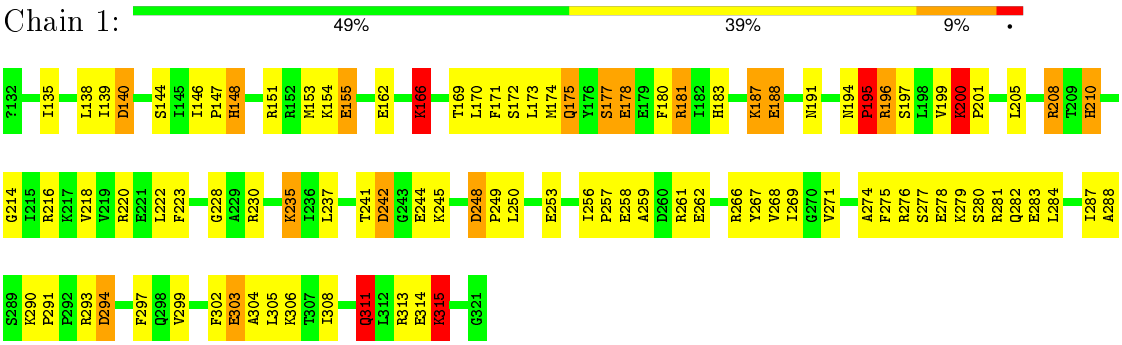
3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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 (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.

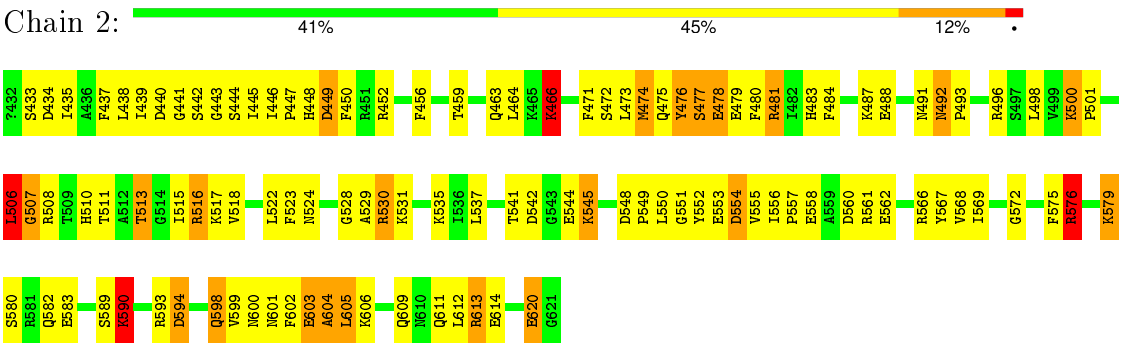
- Molecule 1: CD11B

Chain 1:



- Molecule 1: CD11B

Chain 2:



4 Data and refinement statistics (i)

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	49.32Å 124.05Å 76.38Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	10.00 – 2.70	Depositor
% Data completeness (in resolution range)	68.0 (10.00-2.70)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.10	Depositor
Refinement program	PROLSQ	Depositor
R, R_{free}	0.174 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	3238	wwPDB-VP
Average B, all atoms (Å^2)	12.0	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

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	1.11	1/1557 (0.1%)	1.98	41/2095 (2.0%)
1	2	1.06	1/1557 (0.1%)	1.97	46/2095 (2.2%)
All	All	1.08	2/3114 (0.1%)	1.97	87/4190 (2.1%)

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 (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	2	593	ARG	CD-NE	-5.84	1.36	1.46
1	1	177	SER	CA-CB	-5.25	1.45	1.52

All (87) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	1	216	ARG	NE-CZ-NH2	19.24	129.92	120.30
1	2	613	ARG	CD-NE-CZ	18.58	149.61	123.60
1	1	216	ARG	CD-NE-CZ	17.87	148.62	123.60
1	2	593	ARG	CD-NE-CZ	17.23	147.72	123.60
1	1	151	ARG	CD-NE-CZ	15.35	145.08	123.60
1	2	613	ARG	NE-CZ-NH2	11.53	126.07	120.30
1	2	508	ARG	NE-CZ-NH1	11.43	126.01	120.30
1	1	216	ARG	NE-CZ-NH1	-10.97	114.82	120.30
1	1	315	LYS	CA-CB-CG	10.88	137.34	113.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	2	506	LEU	CA-CB-CG	10.46	139.36	115.30
1	2	566	ARG	CD-NE-CZ	10.46	138.25	123.60
1	1	200	LYS	CB-CG-CD	10.22	138.18	111.60
1	2	593	ARG	CG-CD-NE	9.38	131.49	111.80
1	1	200	LYS	CA-CB-CG	9.37	134.02	113.40
1	1	181	ARG	CA-CB-CG	9.23	133.71	113.40
1	2	590	LYS	CA-CB-CG	8.81	132.78	113.40
1	2	500	LYS	CA-CB-CG	8.75	132.65	113.40
1	1	200	LYS	CG-CD-CE	8.64	137.81	111.90
1	2	554	ASP	CB-CG-OD1	8.33	125.79	118.30
1	2	562	GLU	CA-CB-CG	8.32	131.71	113.40
1	1	230	ARG	NE-CZ-NH1	-8.27	116.16	120.30
1	1	294	ASP	CB-CG-OD2	-8.06	111.05	118.30
1	1	148	HIS	CA-CB-CG	7.81	126.88	113.60
1	2	434	ASP	CB-CA-C	7.77	125.94	110.40
1	2	474	MET	N-CA-CB	7.71	124.48	110.60
1	1	196	ARG	NE-CZ-NH2	7.67	124.14	120.30
1	1	177	SER	N-CA-CB	7.62	121.94	110.50
1	2	576	ARG	CG-CD-NE	7.34	127.22	111.80
1	2	553	GLU	CA-CB-CG	7.31	129.48	113.40
1	2	548	ASP	CB-CG-OD1	7.29	124.86	118.30
1	1	261	ARG	N-CA-CB	6.98	123.16	110.60
1	1	248	ASP	CB-CG-OD2	6.86	124.47	118.30
1	1	155	GLU	CG-CD-OE1	6.86	132.01	118.30
1	2	516	ARG	CD-NE-CZ	6.75	133.04	123.60
1	1	175	GLN	N-CA-CB	6.63	122.54	110.60
1	1	303	GLU	CA-CB-CG	6.42	127.53	113.40
1	1	235	LYS	CA-CB-CG	6.41	127.49	113.40
1	1	175	GLN	CA-CB-CG	6.39	127.46	113.40
1	2	474	MET	CA-CB-CG	6.36	124.11	113.30
1	2	508	ARG	CD-NE-CZ	6.28	132.39	123.60
1	1	288	ALA	CB-CA-C	-6.27	100.70	110.10
1	1	177	SER	CA-CB-OG	6.26	128.10	111.20
1	1	178	GLU	OE1-CD-OE2	6.18	130.71	123.30
1	1	276	ARG	NE-CZ-NH1	6.15	123.38	120.30
1	2	567	TYR	CA-CB-CG	6.11	125.00	113.40
1	2	481	ARG	CA-CB-CG	6.10	126.81	113.40
1	1	293	ARG	NE-CZ-NH1	5.99	123.30	120.30
1	2	598	GLN	CA-CB-CG	5.99	126.58	113.40
1	1	253	GLU	CA-CB-CG	5.96	126.51	113.40
1	2	605	LEU	CA-CB-CG	5.95	128.98	115.30
1	1	311	GLN	CA-CB-CG	5.94	126.47	113.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	2	561	ARG	NE-CZ-NH1	5.91	123.25	120.30
1	2	481	ARG	NE-CZ-NH1	-5.88	117.36	120.30
1	2	560	ASP	CB-CG-OD2	5.84	123.56	118.30
1	2	479	GLU	CG-CD-OE1	5.81	129.91	118.30
1	2	449	ASP	CB-CG-OD1	5.80	123.52	118.30
1	1	166	LYS	CB-CA-C	5.77	121.95	110.40
1	2	568	VAL	CA-CB-CG1	5.76	119.55	110.90
1	2	594	ASP	CA-CB-CG	5.75	126.06	113.40
1	1	155	GLU	OE1-CD-OE2	-5.74	116.42	123.30
1	2	566	ARG	NE-CZ-NH1	5.67	123.14	120.30
1	1	242	ASP	CB-CG-OD1	5.61	123.35	118.30
1	1	195	PRO	C-N-CA	5.61	135.72	121.70
1	2	558	GLU	CG-CD-OE1	-5.55	107.20	118.30
1	1	258	GLU	N-CA-CB	5.48	120.46	110.60
1	1	315	LYS	CB-CG-CD	5.46	125.79	111.60
1	2	572	GLY	C-N-CA	5.43	135.28	121.70
1	1	188	GLU	CG-CD-OE1	5.40	129.11	118.30
1	2	508	ARG	NE-CZ-NH2	-5.39	117.61	120.30
1	2	476	TYR	CB-CG-CD2	5.37	124.22	121.00
1	2	478	GLU	CA-CB-CG	5.32	125.10	113.40
1	1	267	TYR	CB-CG-CD2	-5.30	117.82	121.00
1	2	530	ARG	NE-CZ-NH2	-5.29	117.65	120.30
1	1	208	ARG	CD-NE-CZ	-5.26	116.24	123.60
1	2	542	ASP	CB-CG-OD1	5.25	123.03	118.30
1	2	590	LYS	CB-CG-CD	5.22	125.17	111.60
1	1	140	ASP	CB-CG-OD2	-5.18	113.64	118.30
1	2	553	GLU	CB-CA-C	-5.17	100.05	110.40
1	2	545	LYS	N-CA-CB	-5.17	101.30	110.60
1	1	196	ARG	NE-CZ-NH1	-5.15	117.72	120.30
1	2	513	THR	N-CA-CB	5.14	120.07	110.30
1	2	603	GLU	CA-CB-CG	5.12	124.66	113.40
1	1	181	ARG	CD-NE-CZ	5.11	130.75	123.60
1	2	558	GLU	O-C-N	5.11	130.87	122.70
1	2	466	LYS	CA-CB-CG	5.07	124.56	113.40
1	2	491	ASN	CA-CB-CG	5.03	124.47	113.40
1	1	315	LYS	N-CA-CB	5.03	119.64	110.60

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	2	576	ARG	Sidechain

5.2 Too-close contacts (i)

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	1550	90	0
1	2	1530	0	1550	93	1
2	1	129	0	0	13	0
2	2	49	0	0	6	1
All	All	3238	0	3100	180	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 29.

All (180) 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)
1:1:181:ARG:HG2	1:1:205:LEU:HD11	1.29	1.11
1:2:439:ILE:HD11	1:2:473:LEU:HD21	1.29	1.10
1:2:518:VAL:HG13	1:2:522:LEU:HD12	1.45	0.98
1:1:183:HIS:HB3	2:1:824:HOH:O	1.62	0.98
1:2:609:GLN:HB2	2:2:42:HOH:O	1.68	0.93
1:1:311:GLN:H	1:1:311:GLN:HE21	1.11	0.91
1:1:294:ASP:O	1:1:315:LYS:NZ	2.06	0.88
1:1:218:VAL:HG11	1:1:237:LEU:HD13	1.56	0.86
1:2:472:SER:OG	1:2:522:LEU:HD22	1.80	0.80
1:1:311:GLN:NE2	1:1:311:GLN:H	1.79	0.80
1:1:242:ASP:OD1	2:1:61:HOH:O	1.98	0.79
1:2:445:ILE:HG22	1:2:450:PHE:HB2	1.63	0.79
1:1:277:SER:C	1:1:279:LYS:H	1.85	0.77
1:1:194:ASN:HD22	1:1:197:SER:H	1.33	0.75
1:1:306:LYS:HD2	1:1:306:LYS:H	1.52	0.74
1:2:599:VAL:HG11	1:2:605:LEU:HD23	1.71	0.73
1:2:449:ASP:HB3	1:2:602:PHE:CD2	2.25	0.72
1:2:478:GLU:HG2	1:2:507:GLY:HA3	1.71	0.71
1:1:306:LYS:CD	1:1:306:LYS:H	2.03	0.71
1:2:466:LYS:HE3	1:2:620:GLU:HG2	1.72	0.71
1:1:306:LYS:N	1:1:306:LYS:HD2	2.05	0.71
1:2:518:VAL:HG11	1:2:537:LEU:HD13	1.72	0.71
1:2:513:THR:OG1	1:2:550:LEU:HD13	1.91	0.70

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:162:GLU:HA	2:1:53:HOH:O	1.90	0.70
1:2:609:GLN:CG	2:2:42:HOH:O	2.39	0.69
1:2:500:LYS:HG3	1:2:501:PRO:HD3	1.75	0.68
1:1:155:GLU:OE2	2:1:915:HOH:O	2.11	0.68
1:2:609:GLN:CB	2:2:42:HOH:O	2.36	0.68
1:1:195:PRO:O	1:1:199:VAL:HG23	1.95	0.67
1:1:178:GLU:HG3	1:1:208:ARG:H	1.59	0.67
1:2:545:LYS:NZ	1:2:551:GLY:HA2	2.10	0.67
1:1:166:LYS:NZ	1:1:166:LYS:HB2	2.12	0.65
1:1:178:GLU:OE2	1:1:208:ARG:HG3	1.96	0.65
1:1:144:SER:O	2:1:810:HOH:O	2.15	0.65
1:1:277:SER:O	1:1:281:ARG:HG2	1.97	0.64
1:1:155:GLU:OE1	1:1:196:ARG:NH1	2.31	0.64
1:2:466:LYS:HE3	1:2:620:GLU:CG	2.28	0.63
1:2:449:ASP:OD2	1:2:602:PHE:HD2	1.82	0.63
1:1:244:GLU:OE2	1:1:280:SER:HB3	1.98	0.63
1:2:442:SER:C	1:2:444:SER:H	2.03	0.62
1:1:194:ASN:HD22	1:1:197:SER:N	1.98	0.62
1:1:181:ARG:HG2	1:1:205:LEU:CD1	2.20	0.62
1:1:162:GLU:CA	2:1:53:HOH:O	2.47	0.61
1:1:173:LEU:HD23	1:1:174:MET:N	2.15	0.61
1:2:603:GLU:O	1:2:606:LYS:HG2	2.01	0.61
1:1:269:ILE:HA	1:1:297:PHE:O	2.00	0.61
1:1:308:ILE:HA	1:1:311:GLN:NE2	2.14	0.61
1:2:437:PHE:HB2	1:2:473:LEU:HD12	1.83	0.60
1:2:545:LYS:HZ1	1:2:551:GLY:HA2	1.68	0.59
1:1:220:ARG:NH1	2:1:59:HOH:O	2.35	0.58
1:2:439:ILE:HD11	1:2:473:LEU:CD2	2.18	0.58
1:2:477:SER:OG	1:2:478:GLU:N	2.36	0.57
1:2:444:SER:HA	2:2:36:HOH:O	2.04	0.57
1:2:459:THR:HG22	1:2:463:GLN:HE21	1.70	0.57
1:1:181:ARG:NE	1:1:205:LEU:HD21	2.21	0.56
1:1:266:ARG:NH2	2:1:858:HOH:O	2.38	0.56
1:1:277:SER:C	1:1:279:LYS:N	2.57	0.56
1:2:513:THR:O	1:2:517:LYS:HG3	2.06	0.56
1:2:609:GLN:CD	2:2:42:HOH:O	2.43	0.55
1:2:473:LEU:HG	1:2:474:MET:N	2.20	0.55
1:2:443:GLY:N	1:2:506:LEU:HA	2.21	0.55
1:1:187:LYS:HB3	1:1:228:GLY:HA3	1.88	0.55
1:1:148:HIS:HB2	2:1:816:HOH:O	2.06	0.55
1:1:138:LEU:HA	1:1:174:MET:O	2.07	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:180:PHE:N	2:1:837:HOH:O	2.32	0.55
1:2:531:LYS:HA	2:2:47:HOH:O	2.06	0.55
1:2:511:THR:O	1:2:515:ILE:HG13	2.07	0.55
1:2:448:HIS:HD2	1:2:452:ARG:CZ	2.20	0.54
1:1:274:ALA:O	1:1:280:SER:OG	2.19	0.54
1:2:445:ILE:CG2	1:2:450:PHE:HB2	2.33	0.53
1:2:440:ASP:C	1:2:440:ASP:OD1	2.47	0.53
1:2:459:THR:HG22	1:2:463:GLN:HG3	1.92	0.52
1:2:556:ILE:HB	1:2:557:PRO:HD3	1.90	0.52
1:1:172:SER:OG	1:1:222:LEU:HD22	2.10	0.52
1:2:524:ASN:O	1:2:529:ALA:HB3	2.10	0.52
1:2:544:GLU:HA	1:2:583:GLU:OE1	2.09	0.52
1:1:279:LYS:O	1:1:282:GLN:HB3	2.10	0.51
1:1:166:LYS:HZ1	1:1:166:LYS:HB2	1.75	0.51
1:2:550:LEU:HA	1:2:554:ASP:OD2	2.10	0.51
1:2:443:GLY:HA2	1:2:506:LEU:CD2	2.41	0.51
1:1:177:SER:O	1:1:210:HIS:HB2	2.11	0.51
1:2:516:ARG:HB2	1:2:555:VAL:CG1	2.41	0.51
1:1:178:GLU:CD	1:1:208:ARG:HG3	2.31	0.51
1:1:169:THR:HG22	1:1:170:LEU:N	2.26	0.50
1:1:299:VAL:CG2	1:1:304:ALA:HB3	2.42	0.50
1:2:456:PHE:HE2	1:2:605:LEU:O	1.94	0.50
1:1:135:ILE:O	1:1:171:PHE:HA	2.11	0.50
1:1:294:ASP:HB3	2:1:15:HOH:O	2.12	0.50
1:1:277:SER:O	1:1:279:LYS:N	2.44	0.50
1:2:506:LEU:O	1:2:507:GLY:O	2.30	0.49
1:2:552:TYR:O	1:2:556:ILE:HG12	2.12	0.49
1:1:256:ILE:O	1:1:259:ALA:HB3	2.12	0.49
1:1:244:GLU:HA	1:1:283:GLU:OE1	2.12	0.49
1:1:313:ARG:NE	1:1:314:GLU:OE2	2.46	0.49
1:1:166:LYS:NZ	1:1:166:LYS:CB	2.75	0.49
1:1:146:ILE:HB	1:1:147:PRO:HD2	1.94	0.49
1:2:556:ILE:N	1:2:557:PRO:CD	2.76	0.49
1:1:153:MET:CE	1:1:302:PHE:HE2	2.26	0.49
1:2:443:GLY:HA2	1:2:506:LEU:HD23	1.94	0.48
1:2:516:ARG:NH1	1:2:550:LEU:HD21	2.28	0.48
1:2:498:LEU:O	1:2:501:PRO:HD2	2.14	0.48
1:1:256:ILE:HB	1:1:257:PRO:HD3	1.96	0.48
1:1:275:PHE:HA	1:1:280:SER:OG	2.14	0.48
1:2:496:ARG:O	1:2:500:LYS:HG2	2.14	0.48
1:2:511:THR:HG22	1:2:515:ILE:HD11	1.96	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:194:ASN:O	1:1:195:PRO:C	2.52	0.47
1:2:456:PHE:CE2	1:2:605:LEU:O	2.68	0.47
1:1:214:GLY:O	1:1:218:VAL:HG23	2.13	0.47
1:1:144:SER:HB2	2:1:810:HOH:O	2.15	0.47
1:2:611:GLN:OE1	1:2:611:GLN:N	2.44	0.47
1:2:530:ARG:O	1:2:535:LYS:NZ	2.42	0.47
1:2:599:VAL:HG13	1:2:604:ALA:O	2.14	0.47
1:1:290:LYS:HA	1:1:291:PRO:C	2.36	0.46
1:1:303:GLU:O	1:1:306:LYS:HD3	2.15	0.46
1:2:516:ARG:HB2	1:2:555:VAL:HG11	1.97	0.46
1:2:477:SER:O	1:2:510:HIS:HB2	2.15	0.46
1:1:245:LYS:HD2	1:1:248:ASP:HB3	1.98	0.46
1:1:299:VAL:HG11	1:1:305:LEU:HD23	1.96	0.46
1:1:302:PHE:HE1	2:1:808:HOH:O	1.99	0.45
1:1:223:PHE:CD1	1:1:235:LYS:HD2	2.51	0.45
1:1:194:ASN:ND2	1:1:197:SER:H	2.09	0.45
1:2:464:LEU:HD21	1:2:613:ARG:HA	1.97	0.45
1:2:480:PHE:CZ	1:2:513:THR:HG22	2.51	0.45
1:1:268:VAL:HG12	1:1:284:LEU:HD22	1.99	0.45
1:2:439:ILE:HG12	1:2:473:LEU:HD11	1.98	0.45
1:1:308:ILE:C	1:1:308:ILE:HD12	2.37	0.45
1:1:139:ILE:HG13	1:1:175:GLN:CB	2.46	0.45
1:2:611:GLN:HA	1:2:614:GLU:HG2	1.98	0.45
1:1:249:PRO:HB2	1:2:550:LEU:HD11	1.98	0.45
1:2:459:THR:CG2	1:2:463:GLN:HE21	2.28	0.45
1:2:600:ASN:O	1:2:601:ASN:HB3	2.17	0.44
1:1:169:THR:O	1:1:170:LEU:HD23	2.17	0.44
1:2:464:LEU:HD23	1:2:613:ARG:HG3	2.00	0.44
1:2:446:ILE:HD11	1:2:449:ASP:OD1	2.18	0.44
1:1:311:GLN:N	1:1:311:GLN:HE21	1.95	0.44
1:2:576:ARG:O	1:2:576:ARG:HG2	2.18	0.44
1:1:138:LEU:HD22	1:1:218:VAL:HG21	2.00	0.44
1:2:575:PHE:HA	1:2:580:SER:OG	2.18	0.44
1:2:439:ILE:CD1	1:2:473:LEU:HD11	2.47	0.44
1:2:439:ILE:CD1	1:2:473:LEU:HD21	2.21	0.44
1:2:579:LYS:O	1:2:582:GLN:HB3	2.18	0.43
1:2:484:PHE:HA	1:2:488:GLU:OE2	2.18	0.43
1:2:443:GLY:CA	1:2:506:LEU:HD22	2.48	0.43
1:1:256:ILE:N	1:1:257:PRO:CD	2.81	0.43
1:1:299:VAL:CG1	1:1:305:LEU:HD23	2.48	0.43
1:2:541:THR:HG23	1:2:575:PHE:CZ	2.54	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:250:LEU:CD1	1:2:549:PRO:HB2	2.48	0.43
1:2:487:LYS:HB2	1:2:528:GLY:N	2.33	0.43
1:1:262:GLU:OE1	1:1:262:GLU:HA	2.19	0.43
1:1:249:PRO:CB	1:2:550:LEU:HD11	2.49	0.42
1:2:550:LEU:H	1:2:550:LEU:HD12	1.84	0.42
1:2:483:HIS:O	1:2:484:PHE:HB3	2.19	0.42
1:1:287:ILE:HD13	1:1:287:ILE:HG21	1.85	0.42
1:1:139:ILE:HG13	1:1:175:GLN:HB3	2.01	0.42
1:2:492:ASN:H	1:2:493:PRO:HD3	1.84	0.42
1:1:188:GLU:HA	1:1:191:ASN:HD22	1.83	0.42
1:2:435:ILE:O	1:2:471:PHE:HA	2.19	0.42
1:2:545:LYS:HZ2	1:2:551:GLY:HA2	1.82	0.42
1:2:438:LEU:HD12	1:2:474:MET:HG3	2.02	0.42
1:1:139:ILE:O	1:1:175:GLN:HB2	2.20	0.41
1:1:140:ASP:CB	1:1:241:THR:HA	2.50	0.41
1:2:449:ASP:OD2	1:2:602:PHE:CD2	2.68	0.41
1:1:271:VAL:CG2	1:1:305:LEU:HD21	2.50	0.41
1:2:441:GLY:HA3	1:2:475:GLN:OE1	2.21	0.41
1:1:248:ASP:OD1	1:1:249:PRO:HD2	2.20	0.41
1:1:154:LYS:HE3	1:1:199:VAL:O	2.21	0.41
1:1:169:THR:CG2	1:1:170:LEU:N	2.84	0.41
1:2:442:SER:C	1:2:444:SER:N	2.73	0.41
1:2:474:MET:HB2	1:2:481:ARG:O	2.21	0.41
1:1:218:VAL:CG1	1:1:237:LEU:HD13	2.40	0.41
1:1:281:ARG:C	1:1:283:GLU:N	2.73	0.41
1:2:476:TYR:HB2	1:2:480:PHE:CD1	2.56	0.41
1:1:153:MET:HE2	1:1:302:PHE:HE2	1.84	0.41
1:2:492:ASN:ND2	1:2:498:LEU:HD21	2.36	0.40
1:2:433:SER:HB3	1:2:435:ILE:HG13	2.03	0.40
1:1:200:LYS:HB3	1:1:201:PRO:HD3	2.03	0.40
1:2:437:PHE:HB2	1:2:473:LEU:CD1	2.48	0.40
1:2:446:ILE:HA	1:2:447:PRO:HD2	1.62	0.40
1:2:569:ILE:HD11	1:2:612:LEU:HD22	2.04	0.40
1:2:589:SER:C	1:2:590:LYS:HE3	2.42	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)
1:2:590:LYS:O	2:2:34:HOH:O[2_555]	2.13	0.07

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%)	164 (87%)	22 (12%)	2 (1%)	17 42
1	2	188/190 (99%)	156 (83%)	24 (13%)	8 (4%)	3 7
All	All	376/380 (99%)	320 (85%)	46 (12%)	10 (3%)	6 16

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	2	492	ASN
1	2	506	LEU
1	2	507	GLY
1	2	466	LYS
1	2	604	ALA
1	1	278	GLU
1	2	620	GLU
1	2	477	SER
1	2	523	PHE
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%)	42 73
1	2	168/168 (100%)	164 (98%)	4 (2%)	57 85
All	All	336/336 (100%)	326 (97%)	10 (3%)	48 79

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	1	166	LYS
1	1	187	LYS
1	1	200	LYS
1	1	210	HIS
1	1	311	GLN
1	1	315	LYS
1	2	579	LYS
1	2	590	LYS
1	2	594	ASP
1	2	598	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	1	191	ASN
1	1	194	ASN
1	1	210	HIS
1	1	285	ASN
1	1	298	GLN
1	1	300	ASN
1	1	309	GLN
1	1	311	GLN
1	2	448	HIS
1	2	463	GLN
1	2	492	ASN

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 carbohydrates in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

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

6.1 Protein, DNA and RNA chains

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

6.2 Non-standard residues in protein, DNA, RNA chains

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

6.3 Carbohydrates

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

6.4 Ligands

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

6.5 Other polymers

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