



Full wwPDB X-ray Structure Validation Report i

Feb 27, 2014 – 08:35 PM GMT

PDB ID : 1KSF
Title : Crystal Structure of ClpA, an HSP100 chaperone and regulator of ClpAP protease: Structural basis of differences in Function of the Two AAA+ ATPase domains
Authors : Guo, F.; Maurizi, M.R.; Esser, L.; Xia, D.
Deposited on : 2002-01-12
Resolution : 2.60 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

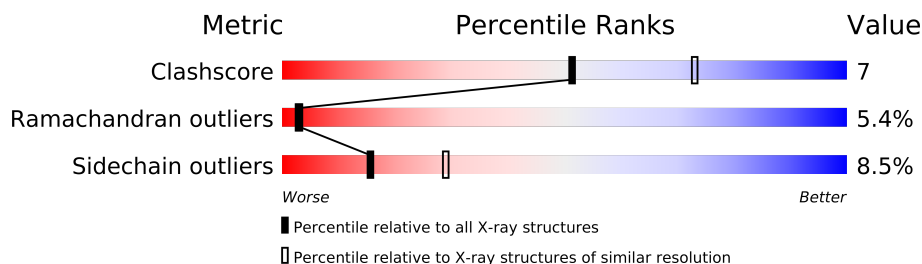
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 21963
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

The reported resolution of this entry is 2.60 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	79885	2154 (2.60-2.60)
Ramachandran outliers	78287	2113 (2.60-2.60)
Sidechain outliers	78261	2113 (2.60-2.60)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	X	758	

2 Entry composition i

There are 7 unique types of molecules in this entry. The entry contains 5929 atoms, of which 0 are hydrogen and 0 are deuterium.

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 ATP-DEPENDENT CLP PROTEASE ATP-BINDING SUB-UNIT CLPA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	X	714	Total	C	N	O	S	0	0	0
			5583	3510	1002	1054	17			

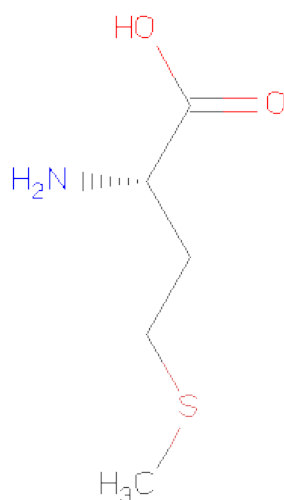
There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
X	169	LEU	MET	ENGINEERED	UNP P0ABH9

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

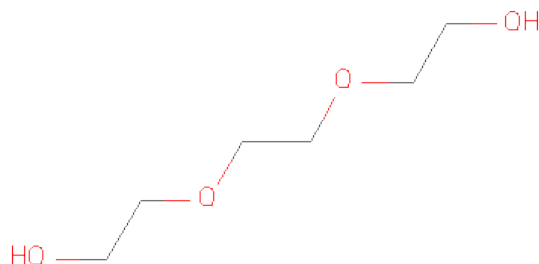
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	X	2	Total	Mg	0	0
			2	2		

- Molecule 3 is METHIONINE (three-letter code: MET) (formula: C₅H₁₁NO₂S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	X	1	Total	C	N	O	S	0	0
			8	5	1	1	1		

- Molecule 4 is TRIETHYLENE GLYCOL (three-letter code: PGE) (formula: $C_6H_{14}O_4$).



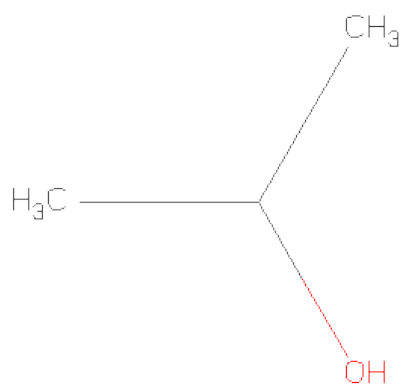
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	X	1	Total	C	O	0	0
			10	6	4		
4	X	1	Total	C	O	0	0
			10	6	4		

- Molecule 5 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	X	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
5	X	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

- Molecule 6 is ISOPROPYL ALCOHOL (three-letter code: IPA) (formula: C₃H₈O).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	X	1	Total	C	O	0	0
			4	3	1		
6	X	1	Total	C	O	0	0
			4	3	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	X	1	Total	C	O	0	0
			4	3	1		
6	X	1	Total	C	O	0	0
			4	3	1		
6	X	1	Total	C	O	0	0
			4	3	1		

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	X	242	Total	O	0	0
			242	242		

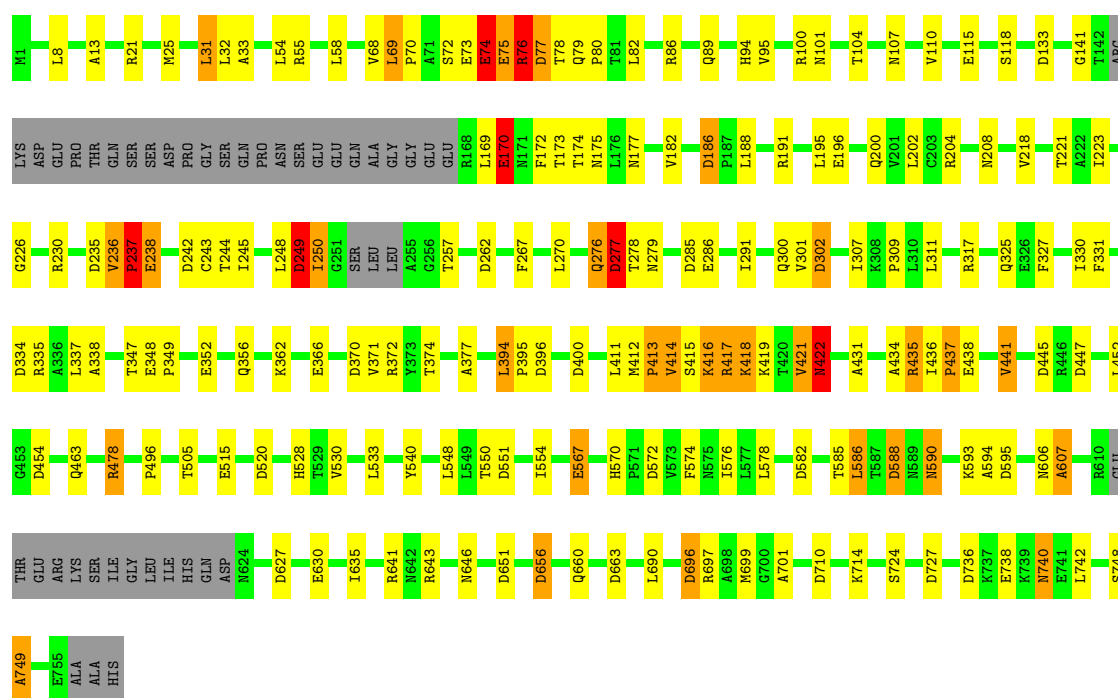
3 Residue-property plots

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 ($RSRZ > 2$). 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: ATP-DEPENDENT CLP PROTEASE ATP-BINDING SUBUNIT CLPA

Chain X: 



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section will therefore be incomplete.

Property	Value	Source
Space group	P 65	Depositor
Cell constants a, b, c, α , β , γ	124.11Å 124.11Å 97.04Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	20.00 – 2.60	Depositor
% Data completeness (in resolution range)	100.0 (20.00-2.60)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	REFMAC 5	Depositor
R, R_{free}	0.216 , 0.304	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	5929	wwPDB-VP
Average B, all atoms (Å ²)	49.0	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, PGE, IPA, ADP

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	X	0.82	1/5664 (0.0%)	0.78	34/7645 (0.4%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	X	3	0

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	X	422	ASN	CB-CG	-5.86	1.37	1.51

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	74	GLU	N-CA-C	6.73	129.16	111.00
1	X	394	LEU	N-CA-C	6.41	128.30	111.00
1	X	133	ASP	CB-CG-OD2	6.15	123.84	118.30
1	X	186	ASP	CB-CG-OD2	5.88	123.59	118.30
1	X	75	GLU	N-CA-C	5.86	126.82	111.00
1	X	77	ASP	CB-CG-OD2	5.74	123.47	118.30
1	X	235	ASP	CB-CG-OD2	5.63	123.37	118.30
1	X	302	ASP	CB-CG-OD2	5.61	123.35	118.30
1	X	663	ASP	CB-CG-OD2	5.55	123.30	118.30
1	X	445	ASP	CB-CG-OD2	5.45	123.21	118.30
1	X	76	ARG	N-CA-C	5.45	125.71	111.00
1	X	520	ASP	CB-CG-OD2	5.42	123.18	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	249	ASP	CB-CG-OD2	5.39	123.15	118.30
1	X	727	ASP	CB-CG-OD2	5.38	123.14	118.30
1	X	696	ASP	CB-CG-OD2	5.38	123.14	118.30
1	X	651	ASP	CB-CG-OD2	5.37	123.13	118.30
1	X	454	ASP	CB-CG-OD2	5.30	123.07	118.30
1	X	447	ASP	CB-CG-OD2	5.26	123.03	118.30
1	X	590	ASN	N-CA-C	5.21	125.08	111.00
1	X	400	ASP	CB-CG-OD2	5.18	122.96	118.30
1	X	595	ASP	CB-CG-OD2	5.17	122.96	118.30
1	X	370	ASP	CB-CG-OD2	5.16	122.95	118.30
1	X	238	GLU	N-CA-C	5.13	124.86	111.00
1	X	656	ASP	CB-CG-OD2	5.13	122.92	118.30
1	X	736	ASP	CB-CG-OD2	5.12	122.91	118.30
1	X	237	PRO	N-CA-C	5.11	125.37	112.10
1	X	262	ASP	CB-CG-OD2	5.11	122.90	118.30
1	X	551	ASP	CB-CG-OD2	5.10	122.89	118.30
1	X	334	ASP	CB-CG-OD2	5.09	122.88	118.30
1	X	396	ASP	CB-CG-OD2	5.09	122.88	118.30
1	X	582	ASP	CB-CG-OD2	5.08	122.88	118.30
1	X	242	ASP	CB-CG-OD2	5.05	122.85	118.30
1	X	277	ASP	CB-CG-OD2	5.04	122.83	118.30
1	X	627	ASP	CB-CG-OD2	5.04	122.83	118.30

All (3) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	X	74	GLU	CA
1	X	394	LEU	CA
1	X	421	VAL	CA

There are no planarity outliers.

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	X	5583	0	5667	83	0
2	X	2	0	0	0	0
3	X	8	0	8	0	0
4	X	20	0	28	5	0
5	X	54	0	24	1	0
6	X	20	0	40	0	0
7	X	242	0	0	6	0
All	All	5929	0	5767	83	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 7.

All (83) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:X:421:VAL:HG22	1:X:422:ASN:H	1.10	1.07
1:X:421:VAL:HG22	1:X:422:ASN:N	1.89	0.86
1:X:421:VAL:CG2	1:X:422:ASN:H	1.93	0.80
1:X:276:GLN:O	1:X:277:ASP:HB2	1.95	0.65
1:X:250:ILE:HG21	1:X:286:GLU:O	1.97	0.65
1:X:435:ARG:O	1:X:437:PRO:HD3	1.97	0.65
1:X:236:VAL:N	1:X:237:PRO:HD3	2.13	0.64
1:X:248:LEU:HG	1:X:249:ASP:H	1.62	0.63
1:X:191:ARG:NH1	7:X:901:HOH:O	2.30	0.62
1:X:418:LYS:HG2	1:X:422:ASN:HD21	1.64	0.62
1:X:434:ALA:HB1	4:X:786:PGE:H62	1.82	0.62
1:X:169:LEU:HD13	1:X:270:LEU:HD13	1.83	0.61
1:X:243:CYS:SG	1:X:279:ASN:ND2	2.74	0.61
1:X:576:ILE:HG23	1:X:586:LEU:HD11	1.83	0.61
1:X:374:THR:HG21	1:X:421:VAL:N	2.17	0.60
1:X:174:THR:HG22	1:X:175:ASN:H	1.67	0.59
1:X:724:SER:O	1:X:748:SER:HB3	2.03	0.58
1:X:570:HIS:HD2	1:X:572:ASP:HB2	1.68	0.58
1:X:554:ILE:HD11	1:X:593:LYS:HB3	1.85	0.58
1:X:202:LEU:HB3	1:X:317:ARG:HH21	1.68	0.58
1:X:362:LYS:HD3	1:X:366:GLU:OE2	2.04	0.57
1:X:13:ALA:HB2	1:X:33:ALA:HB2	1.88	0.56
1:X:349:PRO:HG2	1:X:395:PRO:HG3	1.88	0.55
1:X:374:THR:HG21	1:X:421:VAL:H	1.69	0.55
1:X:110:VAL:HG21	4:X:785:PGE:H32	1.89	0.55
1:X:417:ARG:O	1:X:418:LYS:HB2	2.07	0.55
1:X:21:ARG:HD3	1:X:70:PRO:HG3	1.89	0.55
1:X:550:THR:HG21	1:X:588:ASP:HB3	1.88	0.54
1:X:195:LEU:HD13	1:X:230:ARG:HD2	1.89	0.54

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:X:204:ARG:O	1:X:208:ASN:ND2	2.39	0.54
1:X:412:MET:O	1:X:414:VAL:N	2.41	0.54
1:X:107:ASN:OD1	4:X:785:PGE:H4	2.08	0.54
1:X:191:ARG:HD3	1:X:223:ILE:HD11	1.91	0.53
1:X:177:ASN:ND2	1:X:245:ILE:H	2.06	0.52
1:X:701:ALA:HB3	5:X:781:ADP:C8	2.45	0.52
1:X:748:SER:O	1:X:749:ALA:HB2	2.11	0.51
1:X:104:THR:H	1:X:107:ASN:HD22	1.58	0.51
1:X:416:LYS:O	1:X:418:LYS:N	2.44	0.50
1:X:200:GLN:NE2	7:X:1104:HOH:O	2.45	0.50
1:X:607:ALA:HB1	1:X:635:ILE:HD13	1.94	0.50
1:X:169:LEU:HG	1:X:170:GLU:HG2	1.94	0.50
1:X:94:HIS:HB3	4:X:785:PGE:H5	1.92	0.50
1:X:236:VAL:O	1:X:236:VAL:HG13	2.09	0.49
1:X:248:LEU:HG	1:X:249:ASP:N	2.27	0.49
1:X:279:ASN:OD1	1:X:317:ARG:NH1	2.45	0.49
1:X:69:LEU:N	1:X:70:PRO:HD3	2.27	0.49
1:X:95:VAL:HG13	1:X:100:ARG:HB2	1.93	0.48
1:X:188:LEU:HD22	1:X:226:GLY:HA3	1.95	0.48
1:X:421:VAL:CG2	1:X:422:ASN:N	2.60	0.47
1:X:291:ILE:HA	1:X:301:VAL:HG22	1.97	0.47
1:X:377:ALA:HB2	1:X:422:ASN:CB	2.45	0.47
1:X:72:SER:O	1:X:74:GLU:N	2.48	0.46
1:X:191:ARG:NH2	1:X:347:THR:O	2.48	0.46
1:X:31:LEU:HD13	1:X:58:LEU:HD11	1.96	0.46
1:X:607:ALA:HB1	1:X:635:ILE:CD1	2.46	0.46
1:X:578:LEU:HD22	1:X:643:ARG:HD2	1.97	0.46
1:X:236:VAL:N	1:X:237:PRO:CD	2.75	0.46
1:X:94:HIS:CD2	4:X:785:PGE:H42	2.51	0.45
1:X:550:THR:HG23	1:X:594:ALA:HB2	1.98	0.45
1:X:86:ARG:NH1	1:X:115:GLU:OE2	2.50	0.45
1:X:567:GLU:HG3	1:X:567:GLU:H	1.53	0.44
1:X:221:THR:OG1	1:X:285:ASP:OD2	2.37	0.43
1:X:325:GLN:OE1	1:X:590:ASN:ND2	2.52	0.43
1:X:101:ASN:ND2	7:X:955:HOH:O	2.51	0.43
1:X:25:MET:HB3	1:X:80:PRO:HA	2.01	0.43
1:X:418:LYS:HD3	1:X:422:ASN:OD1	2.19	0.43
1:X:89:GLN:HG2	7:X:899:HOH:O	2.18	0.42
1:X:574:PHE:O	1:X:578:LEU:HG	2.19	0.42
1:X:218:VAL:HG22	1:X:348:GLU:HA	2.01	0.42
1:X:188:LEU:HD23	1:X:195:LEU:HD11	2.02	0.42
1:X:411:LEU:HA	1:X:411:LEU:HD23	1.94	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:X:431:ALA:O	1:X:435:ARG:HG3	2.20	0.41
1:X:570:HIS:CD2	1:X:572:ASP:H	2.37	0.41
1:X:641:ARG:HD2	7:X:988:HOH:O	2.19	0.41
1:X:696:ASP:HB3	1:X:699:MET:H	1.85	0.41
1:X:291:ILE:HD11	1:X:331:PHE:CZ	2.56	0.41
1:X:76:ARG:HD3	1:X:76:ARG:HA	1.84	0.41
1:X:496:PRO:HB3	7:X:976:HOH:O	2.21	0.41
1:X:710:ASP:HA	1:X:714:LYS:HG3	2.02	0.41
1:X:79:GLN:HA	1:X:80:PRO:HD3	1.95	0.40
1:X:740:ASN:HD22	1:X:740:ASN:HA	1.68	0.40
1:X:32:LEU:HD11	1:X:55:ARG:HD2	2.04	0.40
1:X:478:ARG:HA	1:X:478:ARG:HD3	1.90	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	X	706/758 (93%)	611 (86%)	57 (8%)	38 (5%)	3 3

All (38) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	X	73	GLU
1	X	75	GLU
1	X	170	GLU
1	X	237	PRO
1	X	238	GLU
1	X	300	GLN
1	X	309	PRO
1	X	394	LEU
1	X	413	PRO
1	X	415	SER
1	X	417	ARG

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Mol	Chain	Res	Type
1	X	419	LYS
1	X	421	VAL
1	X	436	ILE
1	X	548	LEU
1	X	607	ALA
1	X	630	GLU
1	X	172	PHE
1	X	277	ASP
1	X	416	LYS
1	X	74	GLU
1	X	141	GLY
1	X	335	ARG
1	X	337	LEU
1	X	338	ALA
1	X	414	VAL
1	X	441	VAL
1	X	540	TYR
1	X	182	VAL
1	X	236	VAL
1	X	250	ILE
1	X	438	GLU
1	X	533	LEU
1	X	749	ALA
1	X	418	LYS
1	X	69	LEU
1	X	437	PRO
1	X	530	VAL

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	X	600/639 (94%)	549 (92%)	51 (8%)	15	29

All (51) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	X	8	LEU

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Mol	Chain	Res	Type
1	X	31	LEU
1	X	54	LEU
1	X	68	VAL
1	X	76	ARG
1	X	77	ASP
1	X	78	THR
1	X	82	LEU
1	X	118	SER
1	X	170	GLU
1	X	173	THR
1	X	186	ASP
1	X	196	GLU
1	X	244	THR
1	X	249	ASP
1	X	257	THR
1	X	267	PHE
1	X	276	GLN
1	X	278	THR
1	X	302	ASP
1	X	307	ILE
1	X	311	LEU
1	X	327	PHE
1	X	330	ILE
1	X	352	GLU
1	X	356	GLN
1	X	371	VAL
1	X	372	ARG
1	X	413	PRO
1	X	422	ASN
1	X	435	ARG
1	X	441	VAL
1	X	452	LEU
1	X	463	GLN
1	X	478	ARG
1	X	505	THR
1	X	515	GLU
1	X	528	HIS
1	X	567	GLU
1	X	585	THR
1	X	586	LEU
1	X	588	ASP
1	X	606	ASN

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Mol	Chain	Res	Type
1	X	646	ASN
1	X	656	ASP
1	X	660	GLN
1	X	690	LEU
1	X	697	ARG
1	X	738	GLU
1	X	740	ASN
1	X	742	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	X	177	ASN
1	X	200	GLN
1	X	233	GLN
1	X	356	GLN
1	X	422	ASN
1	X	463	GLN
1	X	545	GLN
1	X	570	HIS
1	X	589	ASN
1	X	590	ASN
1	X	606	ASN
1	X	659	HIS
1	X	660	GLN
1	X	688	ASN
1	X	711	ASN
1	X	740	ASN
1	X	752	HIS

5.3.3 RNA ⓘ

There are no RNA chains 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

Of 12 ligands modelled in this entry, 2 are monoatomic - leaving 10 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	$\# Z > 2$
5	ADP	X	780	-	29,29,29	1.23	2 (6%)	45,45,45	1.85	7 (15%)
5	ADP	X	781	-	29,29,29	1.00	0	45,45,45	1.91	5 (11%)
3	MET	X	784	-	7,7,8	7.56	3 (42%)	5,7,9	0.98	1 (20%)
4	PGE	X	785	-	9,9,9	1.96	4 (44%)	8,8,8	0.74	0
4	PGE	X	786	-	9,9,9	1.74	3 (33%)	8,8,8	0.32	0
6	IPA	X	791	-	3,3,3	0.61	0	3,3,3	0.43	0
6	IPA	X	792	-	3,3,3	0.58	0	3,3,3	0.38	0
6	IPA	X	794	-	3,3,3	0.54	0	3,3,3	0.34	0
6	IPA	X	795	-	3,3,3	0.68	0	3,3,3	0.24	0
6	IPA	X	796	-	3,3,3	0.52	0	3,3,3	0.40	0

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
5	ADP	X	780	-	-	0/16/32/32	0/1/3/3
5	ADP	X	781	-	-	0/16/32/32	0/1/3/3
3	MET	X	784	-	-	0/4/6/8	0/0/0/0
4	PGE	X	785	-	-	0/7/7/7	0/0/0/0
4	PGE	X	786	-	-	0/7/7/7	0/0/0/0
6	IPA	X	791	-	-	0/0/0/0	0/0/0/0
6	IPA	X	792	-	-	0/0/0/0	0/0/0/0
6	IPA	X	794	-	-	0/0/0/0	0/0/0/0
6	IPA	X	795	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	IPA	X	796	-	-	0/0/0/0	0/0/0/0

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	X	784	MET	O-C	19.49	1.24	1.11
3	X	784	MET	CA-C	3.74	1.55	1.48
5	X	780	ADP	C4-N9	-3.53	1.32	1.37
4	X	785	PGE	O3-C4	3.02	1.55	1.42
5	X	780	ADP	O3'-C3'	-2.33	1.37	1.43
4	X	786	PGE	O3-C4	2.18	1.51	1.42
3	X	784	MET	CE-SD	2.17	1.92	1.78
4	X	786	PGE	O2-C2	2.16	1.51	1.42
4	X	786	PGE	O2-C3	2.11	1.51	1.42
4	X	785	PGE	O2-C2	2.07	1.50	1.42
4	X	785	PGE	O3-C5	2.03	1.50	1.42
4	X	785	PGE	O2-C3	2.00	1.50	1.42

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	X	781	ADP	N3-C2-N1	-10.02	120.33	128.71
5	X	780	ADP	N3-C2-N1	-9.34	120.90	128.71
5	X	781	ADP	N3-C4-N9	4.40	133.38	125.43
5	X	780	ADP	PA-O3A-PB	-3.33	121.90	131.68
5	X	780	ADP	N3-C4-N9	2.90	130.66	125.43
5	X	781	ADP	C5-C4-N3	-2.65	119.92	125.70
5	X	781	ADP	C2-N3-C4	2.41	120.88	114.01
5	X	780	ADP	C3'-C2'-C1'	2.24	104.41	100.91
5	X	780	ADP	N7-C8-N9	-2.23	108.06	114.36
5	X	780	ADP	O3'-C3'-C2'	-2.18	104.73	111.83
3	X	784	MET	C-CA-N	-2.11	111.72	113.83
5	X	781	ADP	C3'-C2'-C1'	2.11	104.20	100.91
5	X	780	ADP	C5-C4-N3	-2.02	121.30	125.70

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

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.