



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 10:15 PM UTC

PDB ID : 1KSF / pdb_00001ksf
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 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
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
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

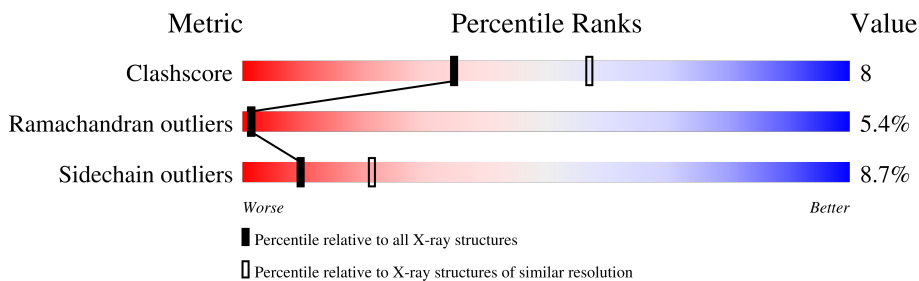
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (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 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	X	758	 68% 20% • • 6%

2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 5929 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 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			

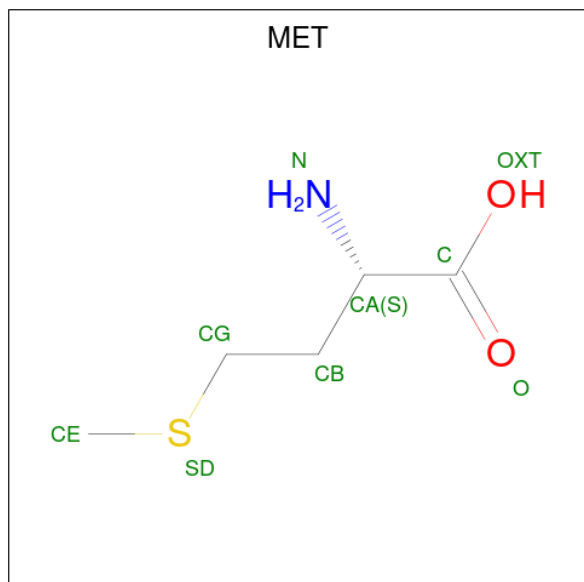
There is a discrepancy between the modelled and reference sequences:

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

- Molecule 2 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

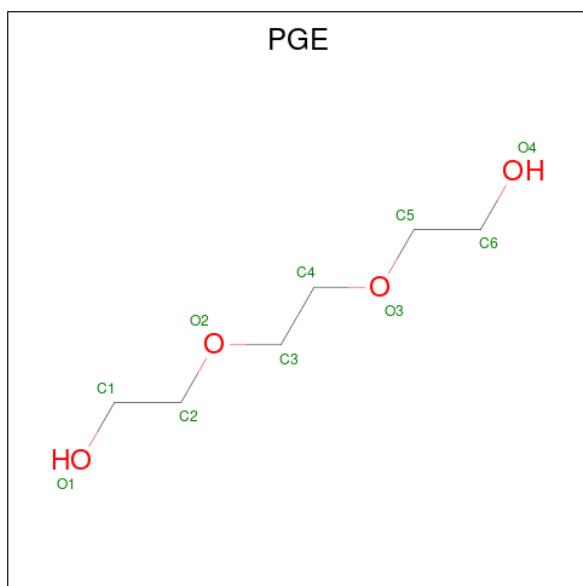
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	X	2	Total	Mg	0	0
			2	2		

- Molecule 3 is METHIONINE (CCD ID: MET) (formula: C₅H₁₁NO₂S).



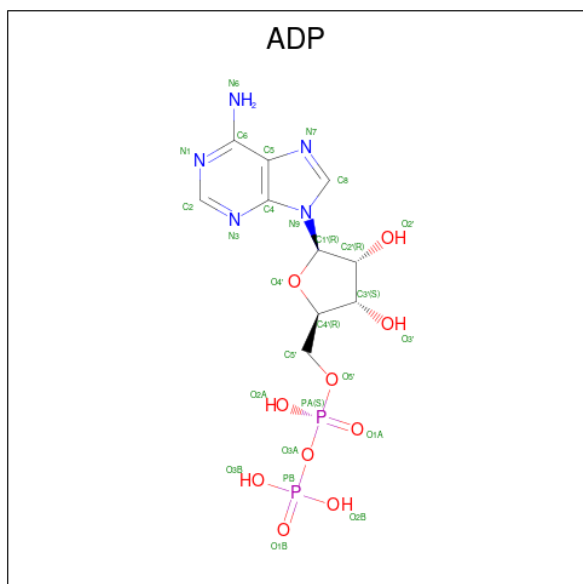
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	X	1	Total	C	N	O	S	0	0
			8	5	1	1	1		

- Molecule 4 is TRIETHYLENE GLYCOL (CCD ID: PGE) (formula: $C_6H_{14}O_4$).



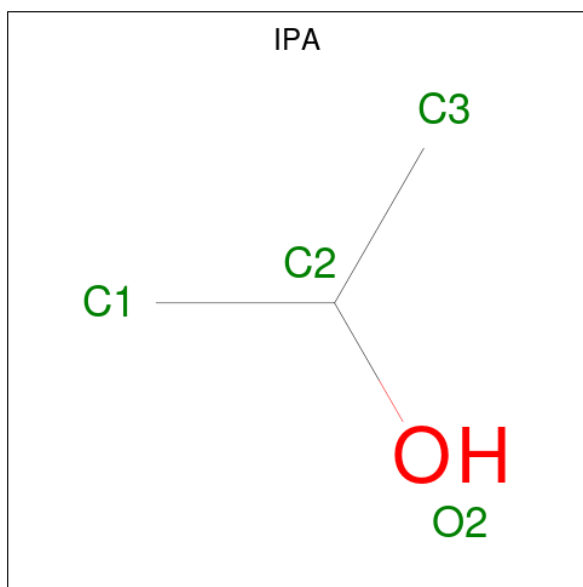
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	X	1	Total	C	O	0	0
			10	6	4		
4	X	1	Total	C	O	0	0
			10	6	4		

- Molecule 5 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: 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 (CCD ID: IPA) (formula: C_3H_8O).



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		
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		

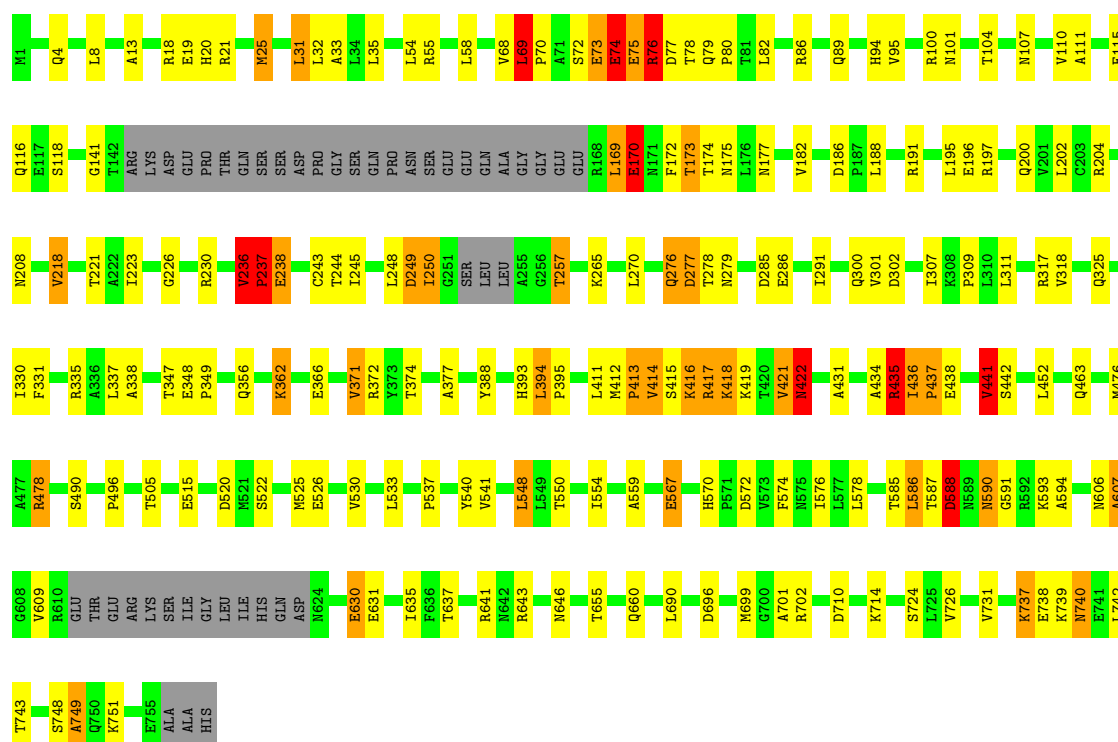
3 Residue-property plots

These plots are drawn for all protein, RNA, 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: ATP-DEPENDENT CLP PROTEASE ATP-BINDING SUBUNIT CLPA

Chain X: 



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore 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 5.0	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: ADP, IPA, PGE, MG

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	1.16	18/5664 (0.3%)	1.05	36/7645 (0.5%)

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 (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	X	436	ILE	CA-C	8.69	1.62	1.52
1	X	394	LEU	CA-C	-8.52	1.42	1.52
1	X	371	VAL	CA-CB	7.40	1.63	1.55
1	X	537	PRO	CA-C	7.30	1.58	1.52
1	X	362	LYS	C-O	-7.20	1.17	1.24
1	X	318	VAL	CA-CB	6.93	1.63	1.54
1	X	726	VAL	CA-CB	6.53	1.62	1.54
1	X	637	THR	CA-CB	6.43	1.62	1.53
1	X	362	LYS	CA-C	6.21	1.59	1.52
1	X	173	THR	CA-CB	5.98	1.59	1.53
1	X	422	ASN	CB-CG	-5.79	1.37	1.52
1	X	75	GLU	N-CA	5.51	1.53	1.46
1	X	526	GLU	CA-C	5.47	1.59	1.52
1	X	111	ALA	CA-C	5.29	1.60	1.52
1	X	236	VAL	CA-CB	5.28	1.60	1.54
1	X	25	MET	SD-CE	-5.23	1.66	1.79
1	X	490	SER	CA-C	-5.20	1.46	1.52
1	X	702	ARG	C-O	-5.12	1.19	1.24

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	590	ASN	N-CA-C	9.99	125.08	110.59
1	X	76	ARG	N-CA-C	9.79	125.71	109.46
1	X	737	LYS	N-CA-C	9.55	121.38	110.97
1	X	526	GLU	N-CA-C	9.33	121.53	111.36
1	X	74	GLU	N-CA-C	8.62	129.16	110.80
1	X	609	VAL	N-CA-C	8.45	119.99	108.84
1	X	394	LEU	N-CA-C	8.37	128.30	109.81
1	X	537	PRO	N-CA-C	8.18	120.68	110.70
1	X	591	GLY	N-CA-C	-8.13	103.51	115.63
1	X	525	MET	N-CA-C	-8.08	98.52	110.48
1	X	20	HIS	N-CA-C	-7.57	104.02	113.18
1	X	75	GLU	N-CA-C	7.52	126.82	110.80
1	X	442	SER	N-CA-C	7.27	121.01	112.72
1	X	276	GLN	N-CA-C	-7.25	102.21	113.02
1	X	436	ILE	N-CA-C	7.18	124.39	108.88
1	X	587	THR	N-CA-C	6.95	120.18	108.02
1	X	69	LEU	N-CA-C	6.61	124.41	109.81
1	X	238	GLU	N-CA-C	6.60	124.86	110.80
1	X	435	ARG	N-CA-C	6.49	115.95	108.49
1	X	541	VAL	N-CA-C	-6.30	104.35	110.72
1	X	237	PRO	N-CA-C	6.26	125.37	112.47
1	X	630	GLU	N-CA-C	5.89	123.35	110.80
1	X	19	GLU	N-CA-C	-5.85	106.06	113.43
1	X	169	LEU	N-CA-C	5.77	116.70	108.74
1	X	631	GLU	N-CA-C	5.70	117.95	111.11
1	X	588	ASP	N-CA-C	-5.48	98.42	108.02
1	X	73	GLU	N-CA-C	5.46	122.44	110.80
1	X	116	GLN	N-CA-C	5.29	117.80	111.71
1	X	548	LEU	N-CA-C	5.26	122.00	110.80
1	X	393	HIS	N-CA-C	5.19	117.69	109.50
1	X	441	VAL	N-CA-C	5.10	119.96	109.34
1	X	4	GLN	N-CA-C	-5.07	105.46	111.69
1	X	257	THR	N-CA-C	5.07	117.65	107.41
1	X	751	LYS	N-CA-C	-5.07	100.01	110.80
1	X	559	ALA	N-CA-C	5.05	115.98	108.60
1	X	388	TYR	N-CA-C	5.05	120.43	113.97

All (3) chirality outliers are listed below:

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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atom
1	X	421	VAL	CA

There are no planarity outliers.

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	X	5583	0	5667	86	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	86	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 8.

All (86) 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: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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:554:ILE:HD11	1:X:593:LYS:HB3	1.85	0.58
1:X:570:HIS:HD2	1:X:572:ASP:HB2	1.68	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
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: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:94:HIS:HB3	4:X:785:PGE:H5	1.92	0.50
1:X:169:LEU:HG	1:X:170:GLU:HG2	1.94	0.50
1:X:748:SER:O	1:X:749:ALA:HB2	2.11	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:31:LEU:HD13	1:X:58:LEU:HD11	1.96	0.46
1:X:191:ARG:NH2	1:X:347:THR:O	2.48	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:86:ARG:NH1	1:X:115:GLU:OE2	2.50	0.45
1:X:476:MET:HE3	1:X:476:MET:HB2	1.52	0.45
1:X:550:THR:HG23	1:X:594:ALA:HB2	1.98	0.45
1:X:567:GLU:H	1:X:567:GLU:HG3	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:520:ASP:OD1	1:X:522:SER:OG	2.30	0.43
1:X:737:LYS:C	1:X:739:LYS:H	2.27	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:HD23	1:X:411:LEU:HA	1.94	0.42
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:HA	1:X:76:ARG:HD3	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%)	1 1

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
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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
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%)	548 (91%)	52 (9%)	9 21

All (52) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	X	8	LEU
1	X	18	ARG
1	X	31	LEU
1	X	35	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	197	ARG
1	X	218	VAL
1	X	244	THR
1	X	249	ASP
1	X	257	THR
1	X	265	LYS
1	X	278	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	X	302	ASP
1	X	307	ILE
1	X	311	LEU
1	X	330	ILE
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	567	GLU
1	X	585	THR
1	X	586	LEU
1	X	588	ASP
1	X	606	ASN
1	X	646	ASN
1	X	655	THR
1	X	660	GLN
1	X	690	LEU
1	X	731	VAL
1	X	738	GLU
1	X	740	ASN
1	X	742	LEU
1	X	743	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	X	22	HIS
1	X	56	GLN
1	X	64	GLN
1	X	116	GLN
1	X	140	HIS
1	X	177	ASN
1	X	200	GLN
1	X	329	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	X	356	GLN
1	X	393	HIS
1	X	422	ASN
1	X	556	HIS
1	X	570	HIS
1	X	575	ASN
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	740	ASN
1	X	747	GLN
1	X	750	GLN
1	X	752	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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
6	IPA	X	796	-	3,3,3	0.49	0	3,3,3	0.37	0
6	IPA	X	794	-	3,3,3	0.51	0	3,3,3	0.31	0
4	PGE	X	785	-	9,9,9	1.96	4 (44%)	8,8,8	0.76	0
5	ADP	X	780	-	28,29,29	1.26	4 (14%)	43,45,45	1.70	10 (23%)
4	PGE	X	786	-	9,9,9	1.74	3 (33%)	8,8,8	0.37	0
6	IPA	X	795	-	3,3,3	0.68	0	3,3,3	0.20	0
5	ADP	X	781	-	28,29,29	1.00	1 (3%)	43,45,45	1.74	6 (13%)
6	IPA	X	792	-	3,3,3	0.57	0	3,3,3	0.36	0
6	IPA	X	791	-	3,3,3	0.60	0	3,3,3	0.41	0
3	MET	X	784	-	6,7,8	1.08	1 (16%)	2,7,9	0.23	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
4	PGE	X	785	-	-	5/7/7/7	-
5	ADP	X	780	-	-	1/16/32/32	0/3/3/3
4	PGE	X	786	-	-	2/7/7/7	-
5	ADP	X	781	-	-	2/16/32/32	0/3/3/3
3	MET	X	784	-	-	1/5/6/8	-

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	X	780	ADP	C5-N7	-3.12	1.33	1.39
4	X	785	PGE	O3-C4	2.98	1.55	1.42
5	X	781	ADP	C5-N7	-2.85	1.33	1.39
5	X	780	ADP	C8-N7	2.45	1.36	1.31
5	X	780	ADP	C4-N9	-2.45	1.32	1.37
5	X	780	ADP	O3'-C3'	-2.27	1.37	1.43
3	X	784	MET	CE-SD	2.18	1.92	1.78
4	X	786	PGE	O3-C4	2.14	1.51	1.42
4	X	786	PGE	O2-C2	2.12	1.51	1.42
4	X	786	PGE	O2-C3	2.08	1.51	1.42
4	X	785	PGE	O2-C2	2.03	1.50	1.42
4	X	785	PGE	O4-C6	2.03	1.52	1.42
4	X	785	PGE	O1-C1	2.01	1.52	1.42

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	X	781	ADP	N3-C2-N1	-5.45	120.33	128.58
5	X	780	ADP	N3-C2-N1	-5.07	120.90	128.58
5	X	781	ADP	C5-C4-N3	-4.94	119.92	126.72
5	X	780	ADP	N9-C8-N7	-4.15	108.06	113.94
5	X	780	ADP	C5-C4-N3	-3.94	121.30	126.72
5	X	781	ADP	C2-N3-C4	3.71	120.88	111.83
5	X	781	ADP	N3-C4-N9	3.65	133.38	127.17
5	X	781	ADP	C5-N7-C8	3.43	108.83	103.45
5	X	781	ADP	N9-C8-N7	-3.39	109.13	113.94
5	X	780	ADP	C2-N3-C4	3.20	119.64	111.83
5	X	780	ADP	C5-N7-C8	2.72	107.72	103.45
5	X	780	ADP	C4-N9-C8	2.30	108.16	105.74
5	X	780	ADP	C4-C5-N7	-2.24	108.02	110.58
5	X	780	ADP	O3'-C3'-C2'	-2.21	104.73	111.82
5	X	780	ADP	N3-C4-N9	2.06	130.66	127.17
5	X	780	ADP	C5-C4-N9	2.04	108.04	105.81

There are no chirality outliers.

All (11) torsion outliers are listed below:

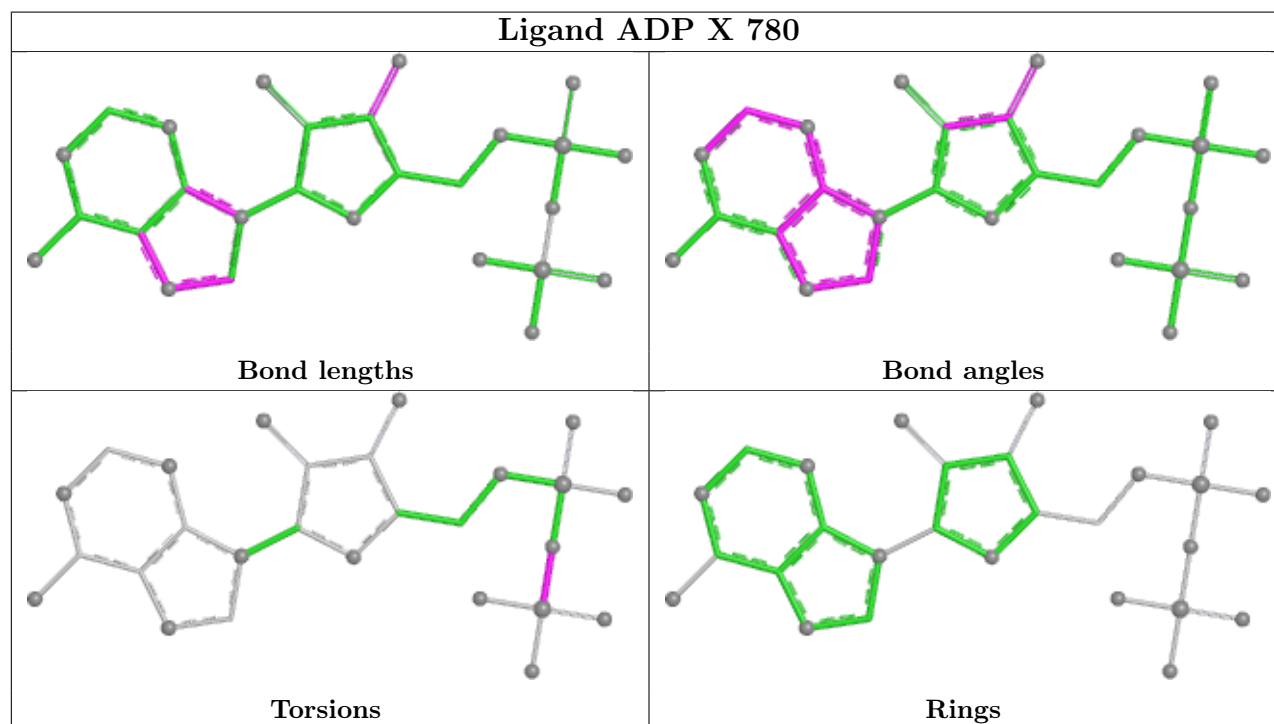
Mol	Chain	Res	Type	Atoms
4	X	785	PGE	O2-C3-C4-O3
4	X	786	PGE	O3-C5-C6-O4
4	X	786	PGE	O1-C1-C2-O2
4	X	785	PGE	C1-C2-O2-C3
4	X	785	PGE	C3-C4-O3-C5
4	X	785	PGE	C4-C3-O2-C2
4	X	785	PGE	C6-C5-O3-C4
5	X	780	ADP	PA-O3A-PB-O2B
3	X	784	MET	CA-CB-CG-SD
5	X	781	ADP	C3'-C4'-C5'-O5'
5	X	781	ADP	O4'-C4'-C5'-O5'

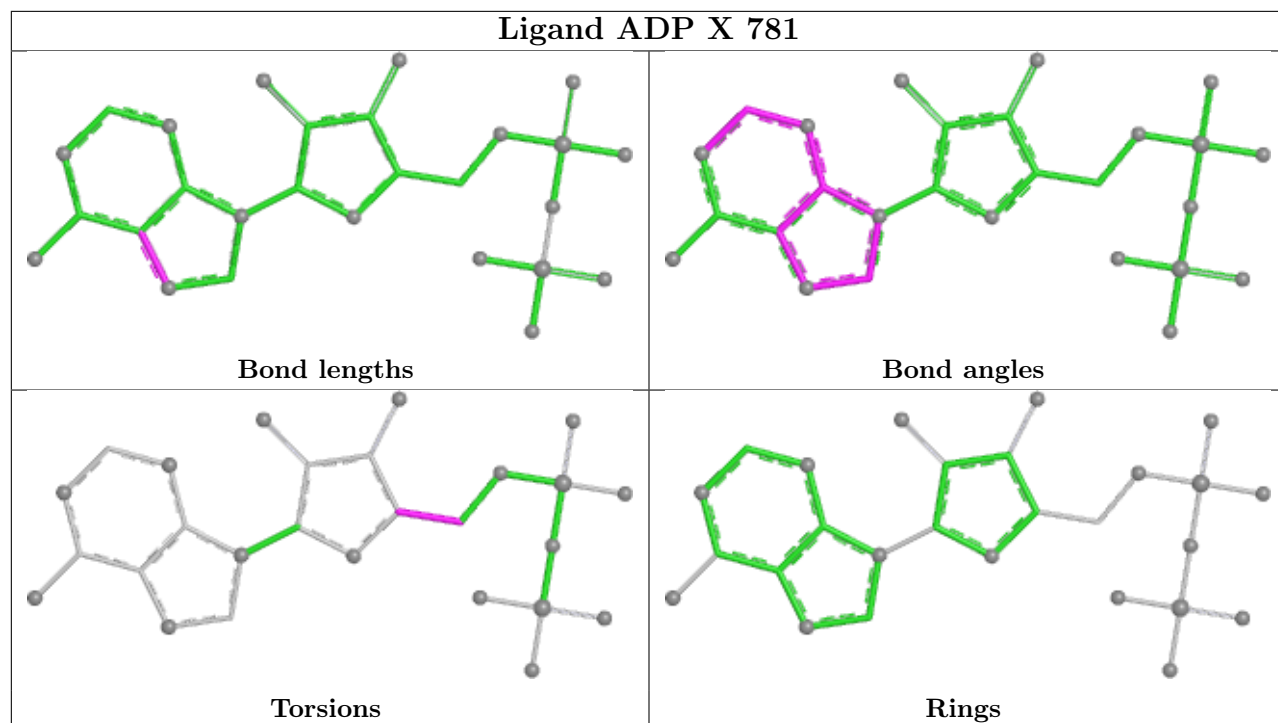
There are no ring outliers.

3 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	X	785	PGE	4	0
4	X	786	PGE	1	0
5	X	781	ADP	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





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.