



wwPDB X-ray Structure Validation Summary Report

Feb 28, 2014 – 08:01 PM GMT

PDB ID : 2A5Y
Title : Structure of a CED-4/CED-9 complex
Authors : Yan, N.; Liu, Q.; Hao, Q.; Gu, L.; Shi, Y.
Deposited on : 2005-07-01
Resolution : 2.60 Å(reported)

This is a wwPDB validation summary 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>

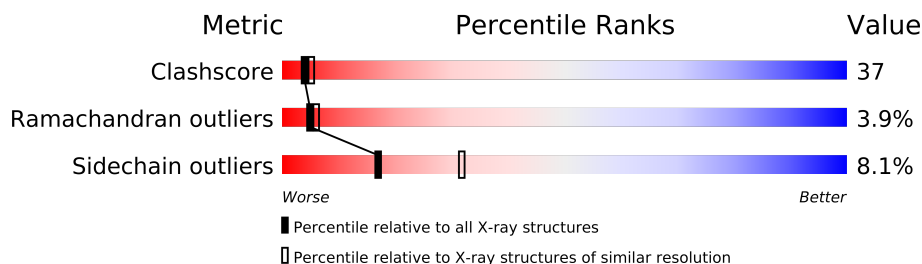
The following versions of software and data (see [references](#)) were used in the production of this report:

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	A	204	
2	B	549	
2	C	549	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 8730 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 Apoptosis regulator ced-9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	173	Total	C	N	O	S	0	0	0
			1417	900	246	262	9			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	107	SER	CYS	ENGINEERED	UNP P41958
A	135	SER	CYS	ENGINEERED	UNP P41958
A	164	SER	CYS	ENGINEERED	UNP P41958

- Molecule 2 is a protein called ced-4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	501	Total	C	N	O	S	0	0	0
			4028	2568	674	757	29			
2	C	373	Total	C	N	O	S	0	0	0
			2961	1885	493	558	25			

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	Mg	0	0
			1	1		
3	C	1	Total	Mg	0	0
			1	1		

- Molecule 4 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: C₁₀H₁₆N₅O₁₃P₃).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	B	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
4	C	1	Total	C	N	O	P	0	0
			31	10	5	13	3		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	32	Total	O	0	0
			32	32		
5	B	145	Total	O	0	0
			145	145		
5	C	83	Total	O	0	0
			83	83		

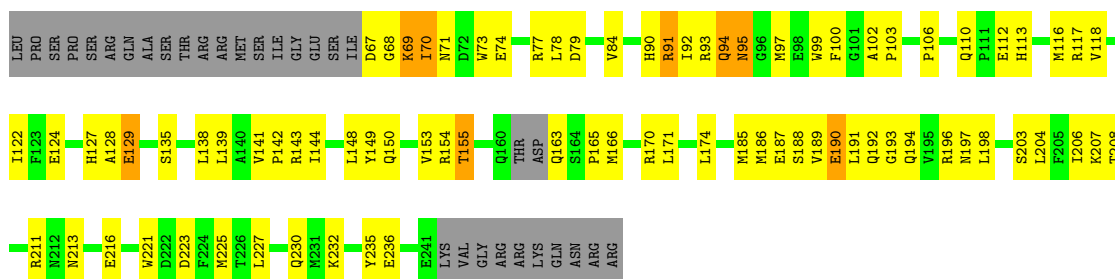
3 Residue-property plots

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.

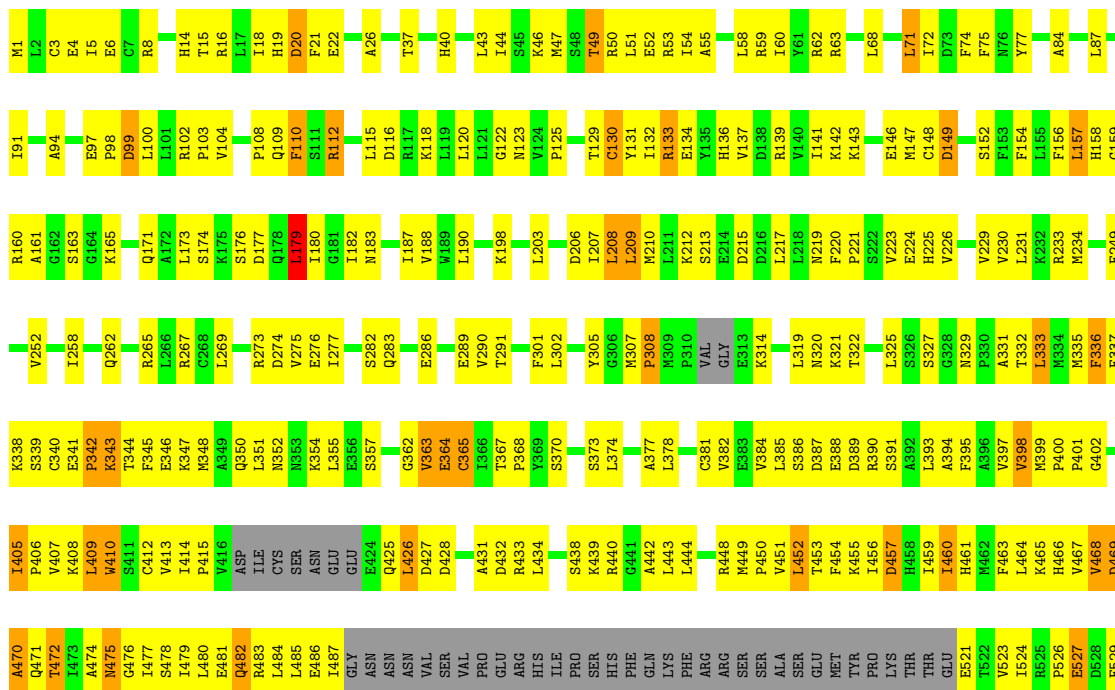
- Molecule 1: Apoptosis regulator ced-9

Chain A:



- Molecule 2: ced-4

Chain B:



PE30	K631	PE32	Q534	L535	H536	Q637	K638	F539	Y540	D541	S542	L543	LYS	ASN	PHE	ALA	CYS
------	------	------	------	------	------	------	------	------	------	------	------	------	-----	-----	-----	-----	-----

● Molecule 2: ced-4

Chain C: 

PHE	ARG	ARG	SER	SER	ALA	SER	GLU	MET	TYR	PRO	LYS	THR	THR	GLU	GLU	VAL	ILE	ARG	PRO	PRO	GLU	ASP	PHE	PRO	LYS	PHE	M533	Q534	L535	H536	Q537	Y540	D541	S542	L543	LYS	ASN	PHE	ALA	CYS	CYS																
L443	V382	E383	V384	L385	S386	D387	E388	D389	R390	S391	A392	L393	A394	F395	A396	V397	V398	M399	P400	P401	V403	D404	I405	P406	V407	K408	L409	W410	S411	C412	V413	I414	PRO	VAL	ASP	ILE	CYS	SER	ASN	GLU	GLU	GLY	ASN	ASN	VAL	SER	PRO	GLU	ARG	HIS	ILE	PRO	SER	HIS	PHE	GLN	LYS
L444	V383	E384	L386	S387	D388	E389	R391	S392	A393	L394	F396	V399	V400	D401	F402	V404	G405	P407	A408	L410	W411	S412	C413	V414	I415	K416	L417	S418	C419	V420	I421	PRO	VAL	ASP	ILE	CYS	SER	ASN	GLU	GLU	GLY	ASN	ASN	VAL	SER	PRO	GLU	ARG	HIS	ILE	PRO	SER	HIS	PHE	GLN	LYS	
K447	L302	Y305	R306	K307	P308	M309	P310	L319	I323	S327	G328	N329	P330	A331	T332	L333	K334	K335	F336	F337	K338	C339	C340	E341	R342	K343	F344	F345	K348	K349	Q350	N353	K354	L355	E356	V361	G362	E363	E364	C365	I366	T367	P368	Y369	L374	Q379	R380	C381									
R448	V223	E224	T227	S228	V229	K232	I235	C236	N237	A238	L239	I240	D241	R242	P243	N244	L245	L246	F249	D250	V253	Q254	E255	I258	R259	W260	A261	Q262	L266	R267	C268	L269	T272	R273	D274	V275	E276	I277	S278	A280	Q283	V290	T291	S292	L293												
M449	C130	R133	E134	Y135	H136	V140	I141	K142	E146	M147	F154	L155	F156	L157	H158	G159	R160	G164	K165	I168	L173	L179	D185	S186	I187	V188	W189	L190	K191	T195	A196	P197	L203	F204	T205	D206	L207	M208	L209	M210	R211	K212	L216														
P450	C131	R134	E135	Y136	H137	V141	I142	K143	E147	M148	F155	L156	F157	H159	G160	R161	G165	K166	I169	L174	L180	D186	S187	I188	V189	W190	L191	K192	T196	A197	P198	L204	F205	T206	D207	M209	L210	M211	R212	K213	L217																
V451	T227	S228	V229	K232	I235	C236	N237	A238	L239	I240	D241	R242	P243	N244	L245	L246	F249	D250	V253	Q254	E255	I258	R259	W260	A261	Q262	L266	R267	C268	L269	T272	R273	D274	V275	E276	I277	S278	A280	Q283	V290	T291	S292	L293														
L452	T228	S229	K233	I236	C237	N238	A239	L240	I241	D242	R243	P244	N245	L246	F249	D250	V253	Q254	E255	I258	R259	W260	A261	Q262	L266	R267	C268	L269	T272	R273	D274	V275	E276	I277	S278	A280	Q283	V290	T291	S292	L293																
T453	T229	K234	I237	C238	N239	A240	L241	I242	D243	R244	P245	N246	L247	F249	D250	V253	Q254	E255	I258	R259	W260	A261	Q262	L266	R267	C268	L269	T272	R273	D274	V275	E276	I277	S278	A280	Q283	V290	T291	S292	L293																	
F454	T230	K235	I238	C239	N240	A241	L242	I243	D244	R245	P246	N247	L248	F249	D250	V253	Q254	E255	I258	R259	W260	A261	Q262	L266	R267	C268	L269	T272	R273	D274	V275	E276	I277	S278	A280	Q283	V290	T291	S292	L293																	
K455	T231	K236	I239	C240	N241	A242	L243	I244	D245	R246	P247	N248	L249	F249	D250	V253	Q254	E255	I258	R259	W260	A261	Q262	L266	R267	C268	L269	T272	R273	D274	V275	E276	I277	S278	A280	Q283	V290	T291	S292	L293																	
I456	T232	K237	I240	C241	N242	A243	L244	I245	D246	R247	P248	N249	L250	F249	D250	V253	Q254	E255	I258	R259	W260	A261	Q262	L266	R267	C268	L269	T272	R273	D274	V275	E276	I277	S278	A280	Q283	V290	T291	S292	L293																	
I459	T233	K238	I241	C242	N243	A244	L245	I246	D247	R248	P249	N250	L251	F249	D250	V253	Q254	E255	I258	R259	W260	A261	Q262	L266	R267	C268	L269	T272	R273	D274	V275	E276	I277	S278	A280	Q283	V290	T291	S292	L293																	
I460	T234	K239	I242	C243	N244	A245	L246	I247	D248	R249	P250	N251	L252	F249	D250	V253	Q254	E255	I258	R259	W260	A261	Q262	L266	R267	C268	L269	T272	R273	D274	V275	E276	I277	S278	A280	Q283	V290	T291	S292	L293																	
H461	T235	K240	I243	C244	N245	A246	L247	I248	D249	R250	P251	N252	L253	F249	D250	V253	Q254	E255	I258	R259	W260	A261	Q262	L266	R267	C268	L269	T272	R273	D274	V275	E276	I277	S278	A280	Q283	V290	T291	S292	L293																	
M462	T236	K241	I244	C245	N246	A247	L248	I249	D250	R251	P252	N253	L254	F249	D250	V253	Q254	E255	I258	R259	W260	A261	Q262	L266	R267	C268	L269	T272	R273	D274	V275	E276	I277	S278	A280	Q283	V290	T291	S292	L293																	
F463	T237	K242	I245	C246	N247	A248	L249	I250	D251	R252	P253	N254	L255	F249	D250	V253	Q254	E255	I258	R259	W260	A261	Q262	L266	R267	C268	L269	T272	R273	D274	V275	E276	I277	S278	A280	Q283	V290	T291	S292	L293																	
L464	T238	K243	I246	C247	N248	A249	L250	I251	D252	R253	P254	N255	L256	F249	D250	V253	Q254	E255	I258	R259	W260	A261	Q262	L266	R267	C268	L269	T272	R273	D274	V275	E276	I277	S278	A280	Q283	V290	T291	S292	L293																	
V467	T239	K244	I247	C248	N249	A250	L251	I252	D253	R254	P255	N256	L257	F249	D250	V253	Q254	E255	I258	R259	W260	A261	Q262	L266	R267	C268	L269	T272	R273	D274	V275	E276	I277	S278	A280	Q283	V290	T291	S292	L293																	
V468	T240	K245	I248	C249	N250	A251	L252	I253	D254	R255	P256	N257	L258	F249	D250	V253	Q254	E255	I258	R259	W260	A261	Q262	L266	R267	C268	L269	T272	R273	D274	V275	E276	I277	S278	A280	Q283	V290	T291	S292	L293																	
D469	T241	K246	I249	C250	N251	A252	L253	I254	D255	R256	P257	N258	L259	F249	D250	V253	Q254	E255	I258	R259	W260	A261	Q262	L266	R267	C268	L269	T272	R273	D274	V275	E276	I277	S278	A280	Q283	V290	T291	S292	L293																	
A470	T242	K247	I250	C251	N252	A253	L254	I255	D256	R257	P258	N259	L260	F249	D250	V253	Q254	E255	I258	R259	W260	A261	Q262	L266	R267	C268	L269	T272	R273	D274	V275	E276	I277	S278	A280	Q283	V290	T291	S292	L293																	
Q471	T243	K248	I251	C252	N253	A254	L255	I256	D257	R258	P259	N260	L261	F249	D250	V253	Q254	E255	I258	R259	W260	A261	Q262	L266	R267	C268	L269	T272	R273	D274	V275	E276	I277	S278	A280	Q283	V290	T291	S292	L293																	
T472	T244	K249	I252	C253	N254	A255	L256	I257	D258	R259	P260	N261	L262	F249	D250	V253	Q254	E255	I258	R259	W260	A261	Q262	L266	R267	C268	L269	T272	R273	D274	V275	E276	I277	S278	A280	Q283	V290	T291	S292	L293																	
L473	T245	K250	I253	C254	N255	A256	L257	I258	D259	R260	P261	N262	L263	F249	D250	V253	Q254	E255	I258	R259	W260	A261	Q262	L266	R267	C268	L269	T272	R273	D274	V275	E276	I277	S278	A280	Q283	V290	T291	S292	L293																	
A474	T246	K251	I254	C255	N256	A257	L258	I259	D260	R261	P262	N263	L264	F249	D250	V253	Q254	E255	I258	R259	W260	A261	Q262	L266	R267	C268	L269	T272	R273	D274	V275	E276	I277	S278	A280	Q283	V290	T291	S292	L293																	
M475	T247	K252	I255	C256	N257	A258	L259	I260	D261	R262	P263	N264	L265	F249	D250	V253	Q254	E255	I258	R259	W260	A261	Q262	L266	R267	C268	L269	T272	R273	D274	V275	E276	I277	S278	A280	Q283	V290	T291	S292	L293																	
G476	T248	K253	I256	C257	N258	A259	L260	I261	D262	R263	P264	N265	L266	F249	D250	V253	Q254	E255	I258	R259	W260	A261	Q262	L266	R267	C268	L269	T272	R273	D274	V275	E276	I277	S278	A280	Q283	V290	T291	S292	L293																	
N477	T249	K254	I257	C258	N259	A260	L261	I262	D263	R264	P265	N266	L267	F249	D250	V253	Q254	E255	I258	R259	W260	A261	Q262	L266	R267	C268	L269	T272	R273	D274	V275	E276	I277	S278	A280	Q283	V290	T291	S292	L293																	
S478	T250	K255	I258	C259	N260	A261	L262	I263	D264	R265	P266	N267	L268	F249	D250	V253	Q254	E255	I258	R259	W260	A261	Q262	L266	R267	C268	L269	T272	R273	D274	V275	E276	I277	S278	A280	Q283	V290	T291	S292	L293																	
L479	T251	K256	I259	C260	N261	A262	L263	I264	D265	R266	P267	N268	L269	F249	D250	V253	Q254	E255	I258	R259	W260	A261	Q262	L266	R267	C268	L269	T272	R273	D274	V275	E276	I277	S278	A280	Q283	V290	T291	S292	L293																	
D480	T252	K257	I260	C261	N262	A263	L264	I265	D266	R267	P268	N269	L270	F249	D250	V253	Q254	E255	I258	R259	W260	A261	Q262	L266	R267	C268	L269	T272	R273	D274	V275	E276	I277	S278	A280	Q283	V290	T291	S292	L293																	
E481	T253	K258	I261	C262	N263	A264	L265	I266	D267	R268	P269	N270	L271	F249	D250	V253	Q254	E255	I258	R259	W260	A261	Q262	L266	R267	C268	L269	T272	R273	D274	V275	E276	I277	S278	A280	Q283	V290	T291	S292	L293																	
Q482	T254	K259	I262	C263	N264	A265	L266	I267	D268	R269	P270	N271	L272	F249	D250	V253	Q254	E255	I258	R259	W260	A261	Q262	L266	R267	C268	L269	T272	R273	D274	V275	E276	I277	S278	A280	Q283	V290	T291	S292	L293																	
ARG	T255	K260	I263	C264	N265	A266	L267	I268	D269	R270	P271	N272	L273	F249	D250	V253	Q254	E255	I258	R259	W260	A261	Q262	L266	R267	C268	L269	T272	R273	D274	V275	E276	I277	S278	A280	Q283	V290	T291	S292	L293																	

4 Data and refinement statistics

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

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α , β , γ	128.90Å 128.90Å 209.93Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.00 – 2.60	Depositor
% Data completeness (in resolution range)	(Not available) (40.00-2.60)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS	Depositor
R, R_{free}	0.249 , 0.277	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	8730	wwPDB-VP
Average B, all atoms (Å ²)	82.0	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, ATP

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	A	0.42	0/1450	0.75	3/1950 (0.2%)
2	B	0.37	0/4101	0.66	0/5540
2	C	0.35	0/3010	0.65	1/4061 (0.0%)
All	All	0.37	0/8561	0.67	4/11551 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	68	GLY	N-CA-C	11.40	141.59	113.10
1	A	69	LYS	N-CA-C	6.55	128.70	111.00
1	A	68	GLY	CA-C-N	-5.44	105.24	117.20
2	C	134	GLU	CB-CA-C	5.31	121.03	110.40

There are no chirality outliers.

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	A	1417	0	1365	85	0
2	B	4028	0	4052	335	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	2961	0	2998	241	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
4	B	31	0	12	4	0
4	C	31	0	12	3	0
5	A	32	0	0	7	0
5	B	145	0	0	22	0
5	C	83	0	0	16	0
All	All	8730	0	8439	633	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 37.

The worst 5 of 633 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:302:LEU:HA	2:B:337:PHE:HZ	1.05	1.11
2:C:332:THR:HA	2:C:335:MET:HE3	1.15	1.07
2:C:433:ARG:HH11	2:C:433:ARG:HB2	1.17	1.05
2:C:307:MET:HG3	2:C:308:PRO:HD2	1.36	1.04
2:B:49:THR:HG22	2:B:52:GLU:H	1.22	1.01

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	A	169/204 (83%)	144 (85%)	18 (11%)	7 (4%)	4	5
2	B	493/549 (90%)	430 (87%)	46 (9%)	17 (3%)	6	8
2	C	367/549 (67%)	315 (86%)	36 (10%)	16 (4%)	4	5
All	All	1029/1302 (79%)	889 (86%)	100 (10%)	40 (4%)	5	6

5 of 40 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	470	ALA
2	C	342	PRO
2	C	343	LYS
2	C	450	PRO
2	C	470	ALA

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	A	151/179 (84%)	142 (94%)	9 (6%)	27	51
2	B	457/501 (91%)	415 (91%)	42 (9%)	13	24
2	C	338/501 (68%)	312 (92%)	26 (8%)	18	35
All	All	946/1181 (80%)	869 (92%)	77 (8%)	17	32

5 of 77 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	365	CYS
2	B	457	ASP
2	C	433	ARG
2	B	391	SER
2	B	426	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 35 such sidechains are listed below:

Mol	Chain	Res	Type
2	B	237	ASN
2	B	352	ASN
2	C	482	GLN
2	B	244	ASN
2	B	262	GLN

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 4 ligands modelled in this entry, 2 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	$\# Z > 2$
4	ATP	B	551	3	33,33,33	2.34	11 (33%)	52,52,52	1.93	15 (28%)
4	ATP	C	551	3	33,33,33	1.79	8 (24%)	52,52,52	1.70	11 (21%)

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	ATP	B	551	3	-	0/22/38/38	0/1/3/3
4	ATP	C	551	3	-	0/22/38/38	0/1/3/3

The worst 5 of 19 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	551	ATP	O4'-C1'	8.81	1.54	1.41
4	C	551	ATP	C8-N9	5.54	1.44	1.36
4	B	551	ATP	C8-N9	4.59	1.43	1.36
4	C	551	ATP	O4'-C1'	4.09	1.47	1.41
4	B	551	ATP	C4-N3	3.95	1.41	1.35

The worst 5 of 26 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	551	ATP	PA-O3A-PB	-6.55	112.46	131.68
4	B	551	ATP	PB-O3B-PG	-5.14	116.60	131.68
4	C	551	ATP	O4'-C1'-C2'	-4.75	99.50	106.77
4	C	551	ATP	C8-N9-C4	-4.06	103.80	106.90
4	C	551	ATP	PB-O3B-PG	-3.99	120.00	131.68

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.