



wwPDB X-ray Structure Validation Summary Report

Feb 27, 2014 – 03:01 AM GMT

PDB ID : 3QA8
Title : Crystal Structure of inhibitor of kappa B kinase beta
Authors : Xu, G.; Lo, Y.C.; Li, Q.; Napolitano, G.; Wu, X.; Jiang, X.; Dreano, M.;
Karin, M.; Wu, H.
Deposited on : 2011-01-10
Resolution : 3.60 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>

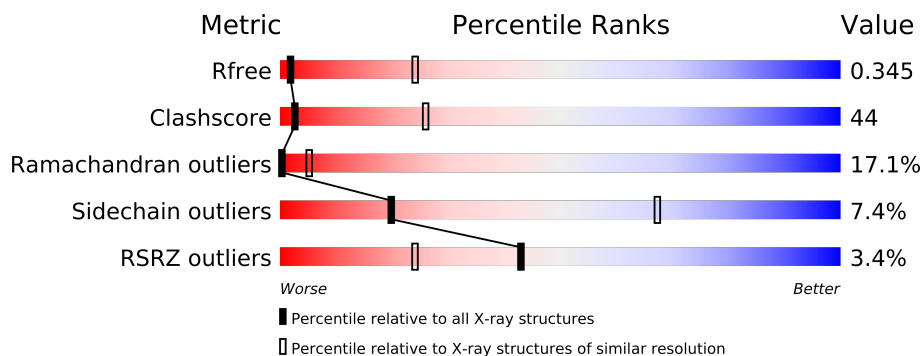
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.15 2013
Xtriage (Phenix)	:	dev-1323
EDS	:	stable22639
Percentile statistics	:	21963
Refmac	:	5.8.0049
CCP4	:	6.3.0 (Settle)
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 3.60 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))
R_{free}	66092	1020 (3.86-3.34)
Clashscore	79885	1155 (3.80-3.40)
Ramachandran outliers	78287	1109 (3.80-3.40)
Sidechain outliers	78261	1108 (3.80-3.40)
RSRZ outliers	66119	1000 (3.84-3.36)

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.

Mol	Chain	Length	Quality of chain
1	A	676	
1	B	676	
1	C	676	
1	D	676	
1	E	676	
1	F	676	
1	G	676	
1	H	676	

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 39026 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 MGC80376 protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	622	Total	C	N	O	S	0	0	0
			5048	3189	899	929	31			
1	B	622	Total	C	N	O	S	0	0	0
			5048	3189	899	929	31			
1	C	622	Total	C	N	O	S	0	0	0
			5048	3189	899	929	31			
1	D	622	Total	C	N	O	S	0	0	0
			5048	3189	899	929	31			
1	E	622	Total	C	N	O	S	0	0	0
			5048	3189	899	929	31			
1	F	622	Total	C	N	O	S	0	0	0
			5048	3189	899	929	31			
1	G	541	Total	C	N	O	S	0	0	0
			4369	2764	779	800	26			
1	H	541	Total	C	N	O	S	0	0	0
			4369	2764	779	800	26			

There are 152 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	GLY	-	EXPRESSION TAG	UNP Q6INT1
A	1	GLY	-	EXPRESSION TAG	UNP Q6INT1
A	2	GLY	-	EXPRESSION TAG	UNP Q6INT1
A	3	ARG	-	EXPRESSION TAG	UNP Q6INT1
A	4	SER	-	EXPRESSION TAG	UNP Q6INT1
A	5	PRO	-	EXPRESSION TAG	UNP Q6INT1
A	6	SER	-	EXPRESSION TAG	UNP Q6INT1
A	7	LEU	-	EXPRESSION TAG	UNP Q6INT1
A	8	PRO	-	EXPRESSION TAG	UNP Q6INT1
A	9	THR	-	EXPRESSION TAG	UNP Q6INT1
A	10	GLN	-	EXPRESSION TAG	UNP Q6INT1
A	11	THR	-	EXPRESSION TAG	UNP Q6INT1
A	12	CYS	-	EXPRESSION TAG	UNP Q6INT1

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Chain	Residue	Modelled	Actual	Comment	Reference
A	13	GLY	-	EXPRESSION TAG	UNP Q6INT1
A	14	PRO	-	EXPRESSION TAG	UNP Q6INT1
A	15	TRP	-	EXPRESSION TAG	UNP Q6INT1
A	16	GLU	-	EXPRESSION TAG	UNP Q6INT1
A	177	GLU	SER	ENGINEERED MUTATION	UNP Q6INT1
A	181	GLU	SER	ENGINEERED MUTATION	UNP Q6INT1
B	0	GLY	-	EXPRESSION TAG	UNP Q6INT1
B	1	GLY	-	EXPRESSION TAG	UNP Q6INT1
B	2	GLY	-	EXPRESSION TAG	UNP Q6INT1
B	3	ARG	-	EXPRESSION TAG	UNP Q6INT1
B	4	SER	-	EXPRESSION TAG	UNP Q6INT1
B	5	PRO	-	EXPRESSION TAG	UNP Q6INT1
B	6	SER	-	EXPRESSION TAG	UNP Q6INT1
B	7	LEU	-	EXPRESSION TAG	UNP Q6INT1
B	8	PRO	-	EXPRESSION TAG	UNP Q6INT1
B	9	THR	-	EXPRESSION TAG	UNP Q6INT1
B	10	GLN	-	EXPRESSION TAG	UNP Q6INT1
B	11	THR	-	EXPRESSION TAG	UNP Q6INT1
B	12	CYS	-	EXPRESSION TAG	UNP Q6INT1
B	13	GLY	-	EXPRESSION TAG	UNP Q6INT1
B	14	PRO	-	EXPRESSION TAG	UNP Q6INT1
B	15	TRP	-	EXPRESSION TAG	UNP Q6INT1
B	16	GLU	-	EXPRESSION TAG	UNP Q6INT1
B	177	GLU	SER	ENGINEERED MUTATION	UNP Q6INT1
B	181	GLU	SER	ENGINEERED MUTATION	UNP Q6INT1
C	0	GLY	-	EXPRESSION TAG	UNP Q6INT1
C	1	GLY	-	EXPRESSION TAG	UNP Q6INT1
C	2	GLY	-	EXPRESSION TAG	UNP Q6INT1
C	3	ARG	-	EXPRESSION TAG	UNP Q6INT1
C	4	SER	-	EXPRESSION TAG	UNP Q6INT1
C	5	PRO	-	EXPRESSION TAG	UNP Q6INT1
C	6	SER	-	EXPRESSION TAG	UNP Q6INT1
C	7	LEU	-	EXPRESSION TAG	UNP Q6INT1
C	8	PRO	-	EXPRESSION TAG	UNP Q6INT1
C	9	THR	-	EXPRESSION TAG	UNP Q6INT1
C	10	GLN	-	EXPRESSION TAG	UNP Q6INT1
C	11	THR	-	EXPRESSION TAG	UNP Q6INT1
C	12	CYS	-	EXPRESSION TAG	UNP Q6INT1
C	13	GLY	-	EXPRESSION TAG	UNP Q6INT1
C	14	PRO	-	EXPRESSION TAG	UNP Q6INT1
C	15	TRP	-	EXPRESSION TAG	UNP Q6INT1
C	16	GLU	-	EXPRESSION TAG	UNP Q6INT1

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Chain	Residue	Modelled	Actual	Comment	Reference
C	177	GLU	SER	ENGINEERED MUTATION	UNP Q6INT1
C	181	GLU	SER	ENGINEERED MUTATION	UNP Q6INT1
D	0	GLY	-	EXPRESSION TAG	UNP Q6INT1
D	1	GLY	-	EXPRESSION TAG	UNP Q6INT1
D	2	GLY	-	EXPRESSION TAG	UNP Q6INT1
D	3	ARG	-	EXPRESSION TAG	UNP Q6INT1
D	4	SER	-	EXPRESSION TAG	UNP Q6INT1
D	5	PRO	-	EXPRESSION TAG	UNP Q6INT1
D	6	SER	-	EXPRESSION TAG	UNP Q6INT1
D	7	LEU	-	EXPRESSION TAG	UNP Q6INT1
D	8	PRO	-	EXPRESSION TAG	UNP Q6INT1
D	9	THR	-	EXPRESSION TAG	UNP Q6INT1
D	10	GLN	-	EXPRESSION TAG	UNP Q6INT1
D	11	THR	-	EXPRESSION TAG	UNP Q6INT1
D	12	CYS	-	EXPRESSION TAG	UNP Q6INT1
D	13	GLY	-	EXPRESSION TAG	UNP Q6INT1
D	14	PRO	-	EXPRESSION TAG	UNP Q6INT1
D	15	TRP	-	EXPRESSION TAG	UNP Q6INT1
D	16	GLU	-	EXPRESSION TAG	UNP Q6INT1
D	177	GLU	SER	ENGINEERED MUTATION	UNP Q6INT1
D	181	GLU	SER	ENGINEERED MUTATION	UNP Q6INT1
E	0	GLY	-	EXPRESSION TAG	UNP Q6INT1
E	1	GLY	-	EXPRESSION TAG	UNP Q6INT1
E	2	GLY	-	EXPRESSION TAG	UNP Q6INT1
E	3	ARG	-	EXPRESSION TAG	UNP Q6INT1
E	4	SER	-	EXPRESSION TAG	UNP Q6INT1
E	5	PRO	-	EXPRESSION TAG	UNP Q6INT1
E	6	SER	-	EXPRESSION TAG	UNP Q6INT1
E	7	LEU	-	EXPRESSION TAG	UNP Q6INT1
E	8	PRO	-	EXPRESSION TAG	UNP Q6INT1
E	9	THR	-	EXPRESSION TAG	UNP Q6INT1
E	10	GLN	-	EXPRESSION TAG	UNP Q6INT1
E	11	THR	-	EXPRESSION TAG	UNP Q6INT1
E	12	CYS	-	EXPRESSION TAG	UNP Q6INT1
E	13	GLY	-	EXPRESSION TAG	UNP Q6INT1
E	14	PRO	-	EXPRESSION TAG	UNP Q6INT1
E	15	TRP	-	EXPRESSION TAG	UNP Q6INT1
E	16	GLU	-	EXPRESSION TAG	UNP Q6INT1
E	177	GLU	SER	ENGINEERED MUTATION	UNP Q6INT1
E	181	GLU	SER	ENGINEERED MUTATION	UNP Q6INT1
F	0	GLY	-	EXPRESSION TAG	UNP Q6INT1
F	1	GLY	-	EXPRESSION TAG	UNP Q6INT1

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Chain	Residue	Modelled	Actual	Comment	Reference
F	2	GLY	-	EXPRESSION TAG	UNP Q6INT1
F	3	ARG	-	EXPRESSION TAG	UNP Q6INT1
F	4	SER	-	EXPRESSION TAG	UNP Q6INT1
F	5	PRO	-	EXPRESSION TAG	UNP Q6INT1
F	6	SER	-	EXPRESSION TAG	UNP Q6INT1
F	7	LEU	-	EXPRESSION TAG	UNP Q6INT1
F	8	PRO	-	EXPRESSION TAG	UNP Q6INT1
F	9	THR	-	EXPRESSION TAG	UNP Q6INT1
F	10	GLN	-	EXPRESSION TAG	UNP Q6INT1
F	11	THR	-	EXPRESSION TAG	UNP Q6INT1
F	12	CYS	-	EXPRESSION TAG	UNP Q6INT1
F	13	GLY	-	EXPRESSION TAG	UNP Q6INT1
F	14	PRO	-	EXPRESSION TAG	UNP Q6INT1
F	15	TRP	-	EXPRESSION TAG	UNP Q6INT1
F	16	GLU	-	EXPRESSION TAG	UNP Q6INT1
F	177	GLU	SER	ENGINEERED MUTATION	UNP Q6INT1
F	181	GLU	SER	ENGINEERED MUTATION	UNP Q6INT1
G	0	GLY	-	EXPRESSION TAG	UNP Q6INT1
G	1	GLY	-	EXPRESSION TAG	UNP Q6INT1
G	2	GLY	-	EXPRESSION TAG	UNP Q6INT1
G	3	ARG	-	EXPRESSION TAG	UNP Q6INT1
G	4	SER	-	EXPRESSION TAG	UNP Q6INT1
G	5	PRO	-	EXPRESSION TAG	UNP Q6INT1
G	6	SER	-	EXPRESSION TAG	UNP Q6INT1
G	7	LEU	-	EXPRESSION TAG	UNP Q6INT1
G	8	PRO	-	EXPRESSION TAG	UNP Q6INT1
G	9	THR	-	EXPRESSION TAG	UNP Q6INT1
G	10	GLN	-	EXPRESSION TAG	UNP Q6INT1
G	11	THR	-	EXPRESSION TAG	UNP Q6INT1
G	12	CYS	-	EXPRESSION TAG	UNP Q6INT1
G	13	GLY	-	EXPRESSION TAG	UNP Q6INT1
G	14	PRO	-	EXPRESSION TAG	UNP Q6INT1
G	15	TRP	-	EXPRESSION TAG	UNP Q6INT1
G	16	GLU	-	EXPRESSION TAG	UNP Q6INT1
G	177	GLU	SER	ENGINEERED MUTATION	UNP Q6INT1
G	181	GLU	SER	ENGINEERED MUTATION	UNP Q6INT1
H	0	GLY	-	EXPRESSION TAG	UNP Q6INT1
H	1	GLY	-	EXPRESSION TAG	UNP Q6INT1
H	2	GLY	-	EXPRESSION TAG	UNP Q6INT1
H	3	ARG	-	EXPRESSION TAG	UNP Q6INT1
H	4	SER	-	EXPRESSION TAG	UNP Q6INT1
H	5	PRO	-	EXPRESSION TAG	UNP Q6INT1

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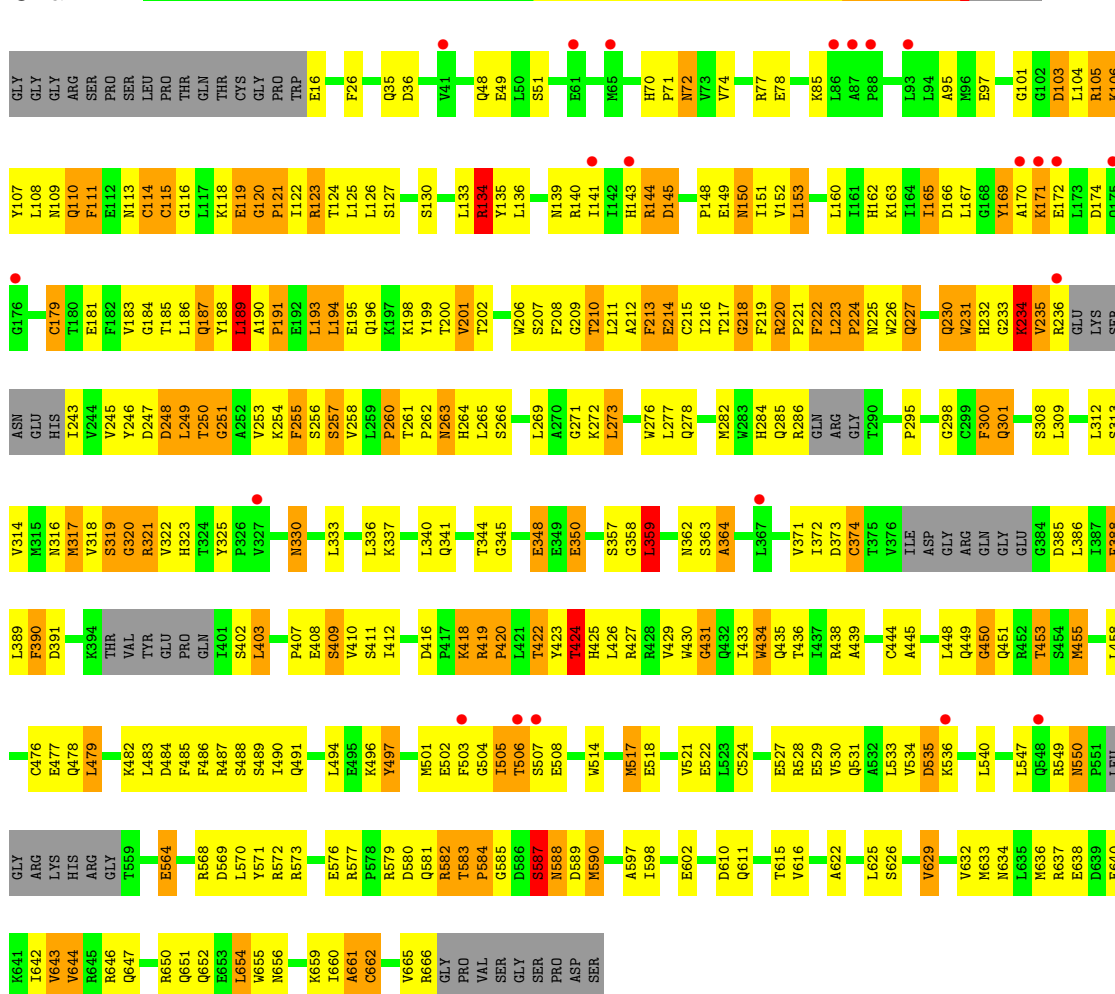
Chain	Residue	Modelled	Actual	Comment	Reference
H	6	SER	-	EXPRESSION TAG	UNP Q6INT1
H	7	LEU	-	EXPRESSION TAG	UNP Q6INT1
H	8	PRO	-	EXPRESSION TAG	UNP Q6INT1
H	9	THR	-	EXPRESSION TAG	UNP Q6INT1
H	10	GLN	-	EXPRESSION TAG	UNP Q6INT1
H	11	THR	-	EXPRESSION TAG	UNP Q6INT1
H	12	CYS	-	EXPRESSION TAG	UNP Q6INT1
H	13	GLY	-	EXPRESSION TAG	UNP Q6INT1
H	14	PRO	-	EXPRESSION TAG	UNP Q6INT1
H	15	TRP	-	EXPRESSION TAG	UNP Q6INT1
H	16	GLU	-	EXPRESSION TAG	UNP Q6INT1
H	177	GLU	SER	ENGINEERED MUTATION	UNP Q6INT1
H	181	GLU	SER	ENGINEERED MUTATION	UNP Q6INT1

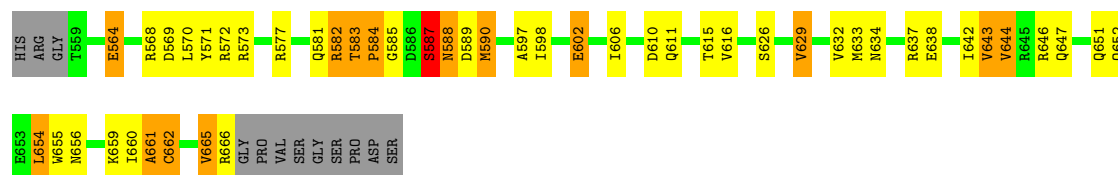
3 Residue-property plots

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.

• Molecule 1: MGC80376 protein

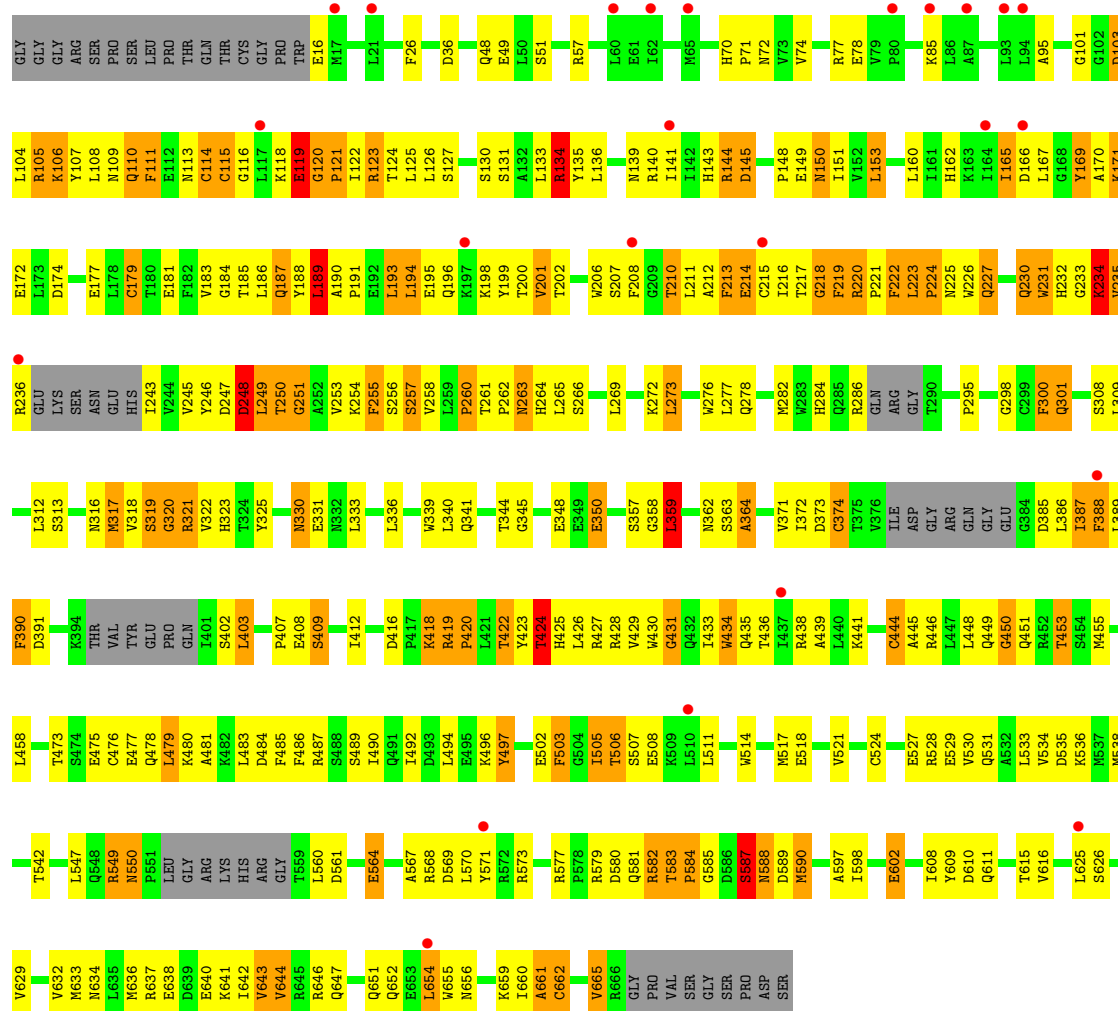
Chain A:





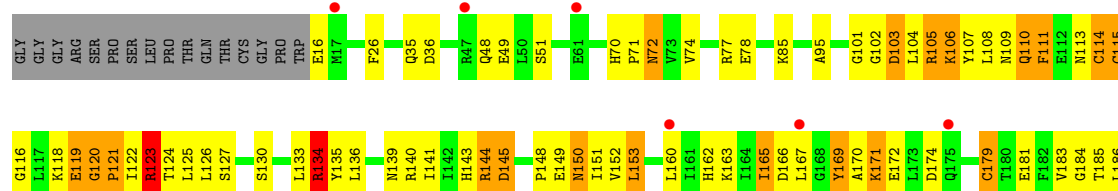
• Molecule 1: MGC80376 protein

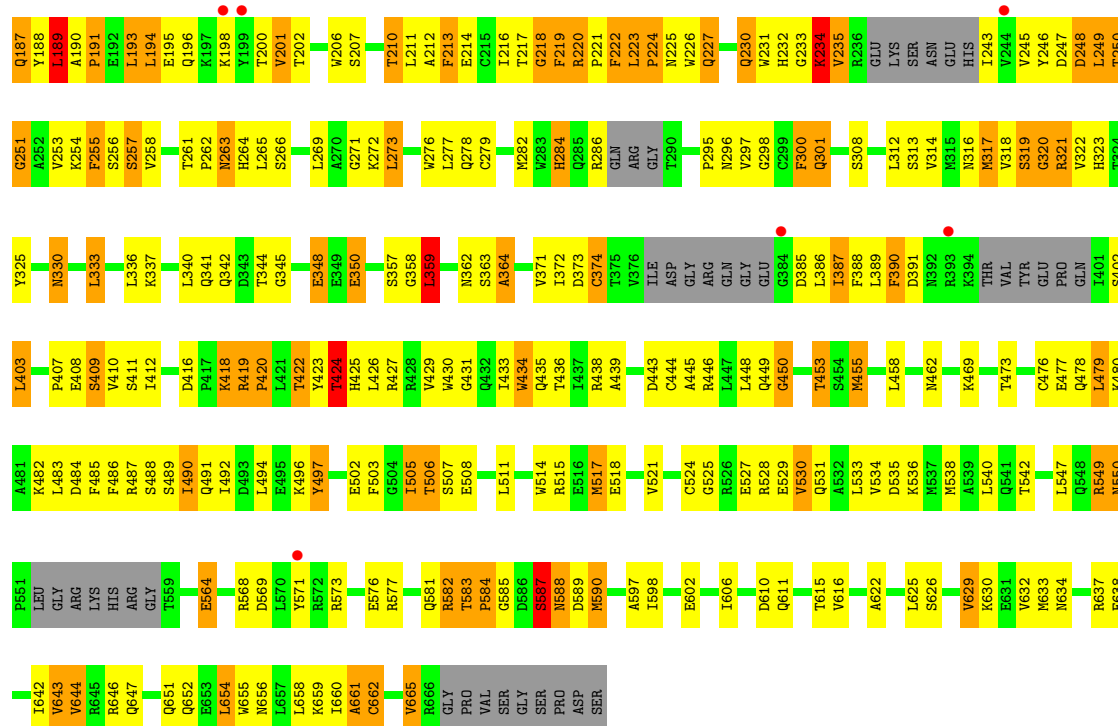
Chain D:



• Molecule 1: MGC80376 protein

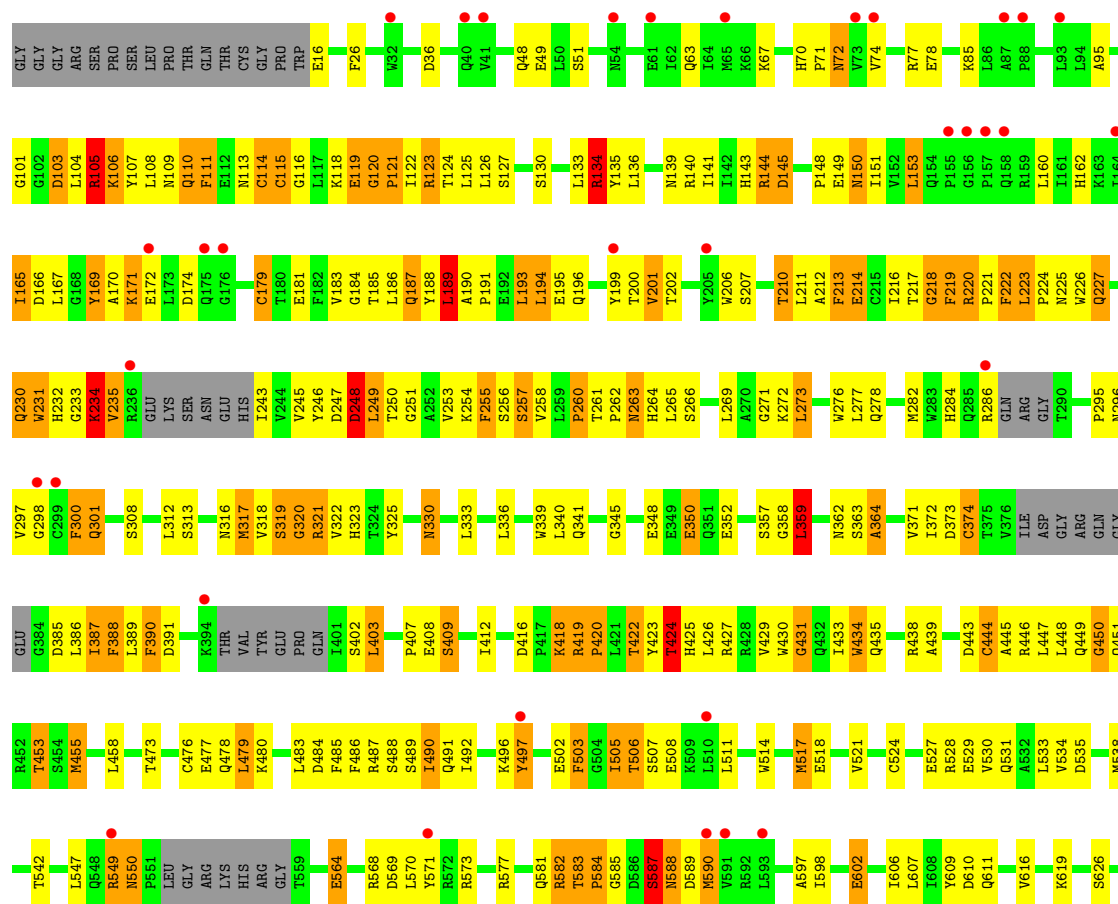
Chain E:

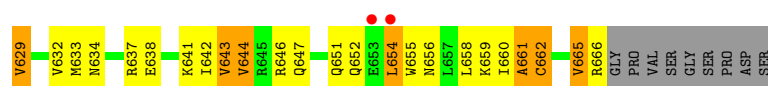




• Molecule 1: MGC80376 protein

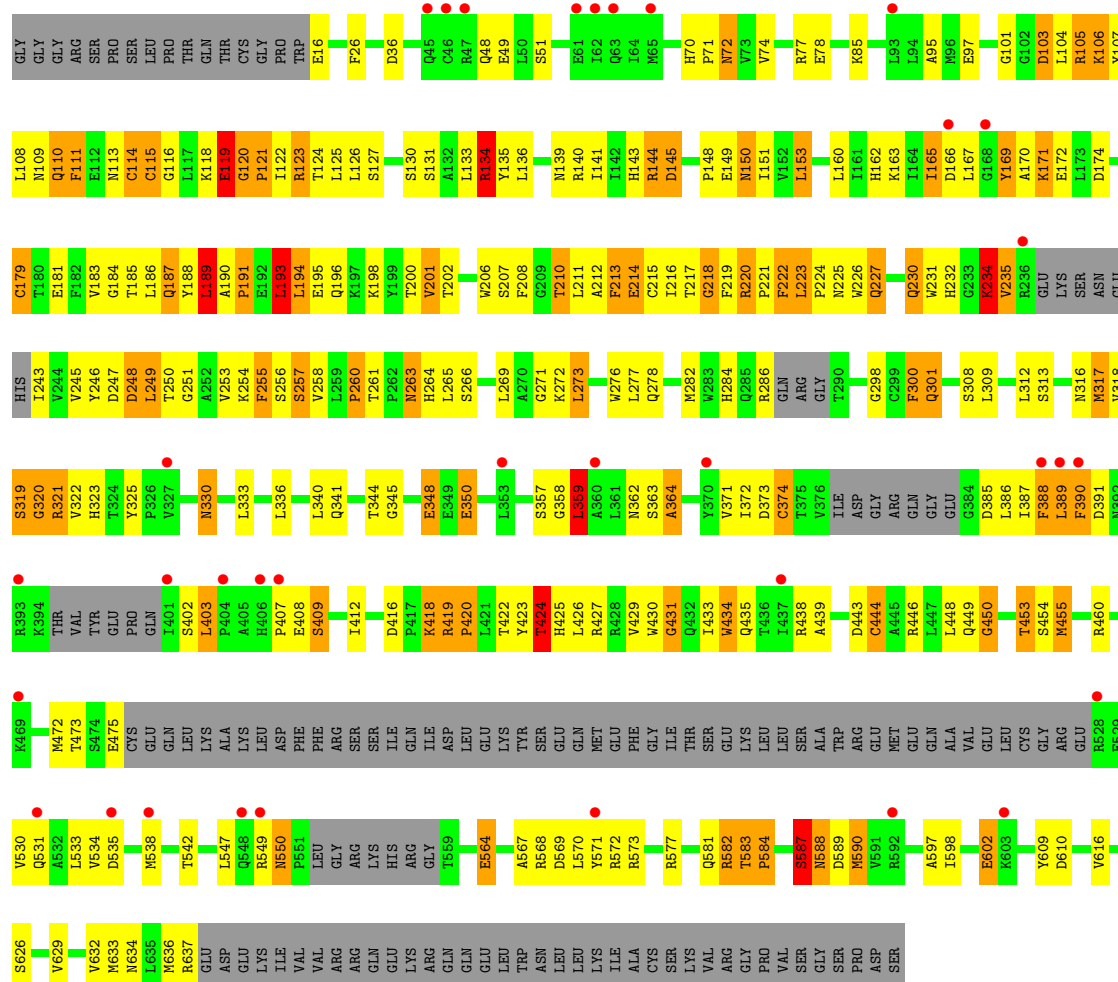
Chain F:





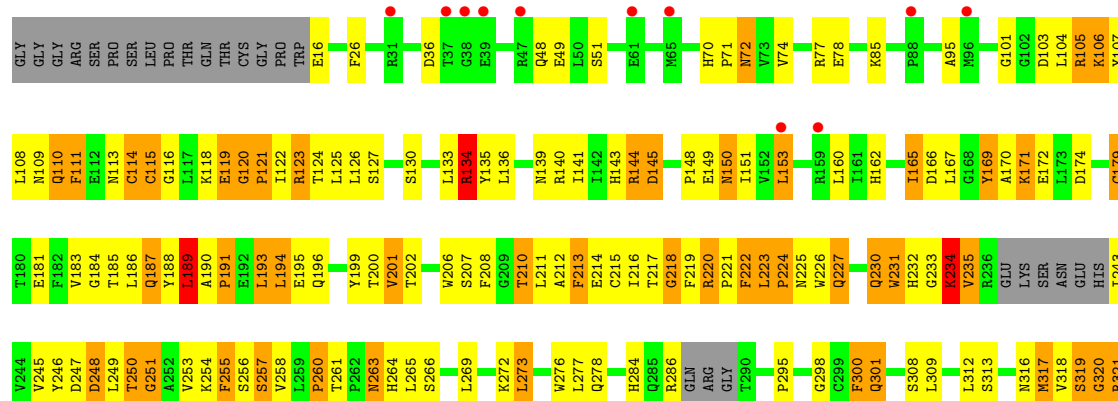
• Molecule 1: MGC80376 protein

Chain G:



• Molecule 1: MGC80376 protein

Chain H:



V322	V323	H323	T324	Y325	N330	L333	L336	K337	S338	H339	L340	Q341	T344	G345	E348	E349	E350	S357	G358	L359	N362	S363	A364	V371	I372	C374	T375	V376	ILE	ASP	GLY	ARG	GLN	GLY	GLU	G384	D385	L386	I387	F388	L389	F390	D391	K394	THR	VAL	TYR	GLU	PRO	GLN							
I401	S402	I403	P407	E408	S409	I412	D416	P417	K418	R419	P420	I421	T422	Y423	T424	H425	I426	R427	R428	Y429	W430	G431	I432	I433	W434	Q435	T436	I437	R438	D443	C444	A445	R446	I447	I448	Q449	Q450	Q451	R452	T453	S454	M455	I458	Y461	S466	M472	E475	CYS	GLU	PRO	GLN						
LEU	LYS	ALA	LYS	LEU	ASP	PHE	ARG	SER	ILE	GLN	ILE	ASP	LEU	GLU	LYS	TYR	SER	GLU	GLN	MET	GLU	PHE	GLY	ILE	THR	SER	GLU	LYS	LEU	LEU	SER	ALA	TRP	ARG	GLU	MET	GLU	GLN	ALA	VAL	GLU	LEU	CYS	GLY	ARG	GLU	R528	E529	V530	Q531	A532	I533	V534	D535	K536	M537	M538
Q541	T542	D543	S544	L547	Q548	R549	N550	P551	LEU	GLY	ARG	ARG	LYS	HIS	ARG	GLY	T559	L563	E564	R568	D569	L570	Y571	R572	R573	R577	Q581	R582	T583	P584	G585	D586	S587	N588	D589	M590	L596	A597	I598	E602	Y609	D610	Q611	V616	S626	V629	V632										
M633	M634	R637	ASP	GLU	GLU	LYS	ILE	VAL	VAL	ARG	ARG	GLN	GLU	LYS	ARG	GLN	GLN	GLU	LEU	TRP	ASN	LEU	LYS	ILE	ALA	CYS	SER	LYS	VAL	ARG	GLY	PRO	VAL	SER	GLY	SER	PRO	ASP	SER	L596	A597	I598	E602	Y609	D610	Q611	V616	S626	V629	V632							

4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	103.17Å 140.34Å 161.17Å 71.28° 79.56° 86.04°	Depositor
Resolution (Å)	15.00 – 3.60 48.67 – 3.50	Depositor EDS
% Data completeness (in resolution range)	78.7 (15.00-3.60) 76.9 (48.67-3.50)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	0.04	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.18 (at 3.48Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.6.4_486)	Depositor
R, R_{free}	0.308 , 0.344 0.308 , 0.345	Depositor DCC
R_{free} test set	4124 reflections (5.07%)	DCC
Wilson B-factor (Å ²)	84.5	Xtriage
Anisotropy	0.749	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.24 , 97.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Outliers	0 of 96343 reflections	Xtriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	39026	wwPDB-VP
Average B, all atoms (Å ²)	199.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.42% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality i

5.1 Standard geometry i

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	0.74	0/5136	0.97	9/6931 (0.1%)
1	B	0.76	0/5136	0.97	10/6931 (0.1%)
1	C	0.78	1/5136 (0.0%)	0.98	11/6931 (0.2%)
1	D	0.74	2/5136 (0.0%)	0.96	10/6931 (0.1%)
1	E	0.77	1/5136 (0.0%)	0.98	10/6931 (0.1%)
1	F	0.75	0/5136	0.96	10/6931 (0.1%)
1	G	0.74	1/4448 (0.0%)	0.96	7/6012 (0.1%)
1	H	0.75	0/4448	0.97	8/6012 (0.1%)
All	All	0.75	5/39712 (0.0%)	0.97	75/53610 (0.1%)

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	A	0	11
1	B	0	11
1	C	0	10
1	D	0	11
1	E	0	10
1	F	0	11
1	G	0	11
1	H	0	11
All	All	0	86

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	279	CYS	CB-SG	-6.95	1.70	1.82
1	C	279	CYS	CB-SG	-5.47	1.73	1.81
1	G	119	GLU	CG-CD	5.22	1.59	1.51
1	D	119	GLU	CG-CD	5.14	1.59	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	331	GLU	CG-CD	5.14	1.59	1.51

The worst 5 of 75 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	123	ARG	NE-CZ-NH1	6.50	123.55	120.30
1	E	153	LEU	CA-CB-CG	6.42	130.08	115.30
1	A	153	LEU	CA-CB-CG	6.28	129.73	115.30
1	C	153	LEU	CA-CB-CG	6.27	129.72	115.30
1	D	153	LEU	CA-CB-CG	6.27	129.71	115.30

There are no chirality outliers.

5 of 86 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	119	GLU	Peptide
1	A	120	GLY	Peptide
1	A	169	TYR	Peptide
1	A	221	PRO	Peptide
1	A	223	LEU	Peptide

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	5048	0	0	226	3
1	B	5048	0	0	239	2
1	C	5048	0	0	255	4
1	D	5048	0	0	256	0
1	E	5048	0	0	241	2
1	F	5048	0	0	219	0
1	G	4369	0	0	182	0
1	H	4369	0	0	180	1
All	All	39026	0	0	1733	6

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 44.

The worst 5 of 1733 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:E:547:LEU:CD1	1:E:615:THR:CG2	1.86	1.51
1:A:230:GLN:O	1:A:232:HIS:N	1.66	1.28
1:D:230:GLN:O	1:D:232:HIS:N	1.67	1.27
1:G:230:GLN:O	1:G:232:HIS:N	1.68	1.26
1:B:230:GLN:O	1:B:232:HIS:N	1.67	1.26

The worst 5 of 6 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	Distance(Å)	Clash(Å)
1:A:501:MET:SD	1:E:364:ALA:O[1_565]	1.61	0.59
1:E:515:ARG:NH1	1:H:394:LYS:NZ[1_465]	1.76	0.44
1:B:617:VAL:CG2	1:C:519:GLN:OE1[1_465]	1.96	0.24
1:A:522:GLU:OE1	1:C:295:PRO:CB[1_565]	2.01	0.19
1:A:522:GLU:OE1	1:C:295:PRO:CG[1_565]	2.04	0.16

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	610/676 (90%)	360 (59%)	145 (24%)	105 (17%)	0	5
1	B	610/676 (90%)	362 (59%)	143 (23%)	105 (17%)	0	5
1	C	610/676 (90%)	359 (59%)	147 (24%)	104 (17%)	0	5
1	D	610/676 (90%)	363 (60%)	143 (23%)	104 (17%)	0	5
1	E	610/676 (90%)	361 (59%)	147 (24%)	102 (17%)	0	6
1	F	610/676 (90%)	362 (59%)	144 (24%)	104 (17%)	0	5
1	G	527/676 (78%)	310 (59%)	126 (24%)	91 (17%)	0	5
1	H	527/676 (78%)	313 (59%)	121 (23%)	93 (18%)	0	4
All	All	4714/5408 (87%)	2790 (59%)	1116 (24%)	808 (17%)	0	5

5 of 808 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	101	GLY
1	A	106	LYS
1	A	110	GLN
1	A	111	PHE
1	A	166	ASP

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	563/609 (92%)	520 (92%)	43 (8%)	19	66
1	B	563/609 (92%)	521 (92%)	42 (8%)	19	67
1	C	563/609 (92%)	520 (92%)	43 (8%)	19	66
1	D	563/609 (92%)	519 (92%)	44 (8%)	18	65
1	E	563/609 (92%)	520 (92%)	43 (8%)	19	66
1	F	563/609 (92%)	521 (92%)	42 (8%)	19	67
1	G	488/609 (80%)	456 (93%)	32 (7%)	24	73
1	H	488/609 (80%)	455 (93%)	33 (7%)	22	71
All	All	4354/4872 (89%)	4032 (93%)	322 (7%)	20	67

5 of 322 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	339	TRP
1	E	219	PHE
1	H	234	LYS
1	D	422	THR
1	D	517	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 ⓘ

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 ⓘ

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ > 2			OWAB(Å ²)	Q < 0.9
1	A	622/676 (92%)	0.24	22 (3%)	42	23	76, 189, 275, 337	0
1	B	622/676 (92%)	0.14	11 (1%)	65	39	71, 191, 274, 336	0
1	C	622/676 (92%)	0.22	6 (0%)	79	53	58, 188, 275, 327	0
1	D	622/676 (92%)	0.14	24 (3%)	37	21	85, 194, 278, 327	0
1	E	622/676 (92%)	0.21	12 (1%)	64	37	74, 190, 274, 330	0
1	F	622/676 (92%)	0.26	35 (5%)	24	13	93, 200, 283, 331	0
1	G	541/676 (80%)	0.36	34 (6%)	19	11	96, 214, 302, 387	0
1	H	541/676 (80%)	0.27	19 (3%)	42	23	79, 194, 293, 423	0
All	All	4814/5408 (89%)	0.23	163 (3%)	43	24	58, 195, 283, 423	0

The worst 5 of 163 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	537	MET	7.8
1	A	65	MET	7.0
1	A	93	LEU	6.9
1	F	155	PRO	6.4
1	G	571	TYR	6.3

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

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

There are no ligands in this entry.

6.5 Other polymers ⓘ

There are no such residues in this entry.