



# wwPDB X-ray Structure Validation Summary Report

Jun 22, 2024 – 05:59 PM EDT

PDB ID : 5L5L  
Title : Plexin A4 full extracellular region, domains 1 to 8 modeled, data to 8 angstrom, spacegroup P2(1)  
Authors : Janssen, B.J.C.; Kong, Y.; Malinauskas, T.; Vangoor, V.R.; Coles, C.H.; Kaufmann, R.; Ni, T.; Gilbert, R.J.C.; Padilla-Parra, S.; Pasterkamp, R.J.; Jones, E.Y.  
Deposited on : 2016-05-28  
Resolution : 8.00 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto: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>.

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

MolProbity : 4.02b-467  
Xtriage (Phenix) : 1.13  
EDS : 2.37.1  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.37.1

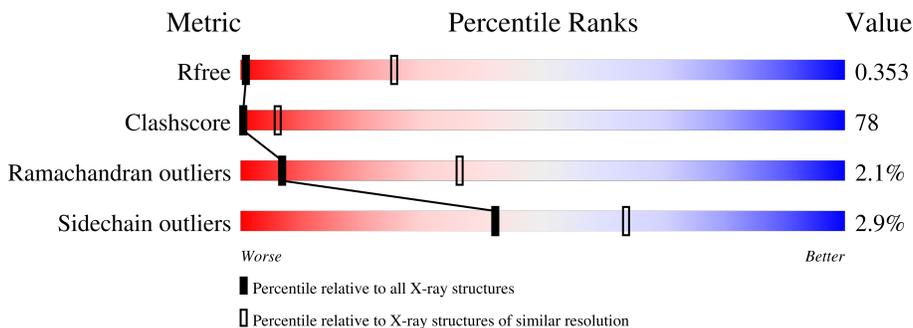
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 8.00 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))
$R_{free}$	130704	1005 (11.50-3.90)
Clashscore	141614	1070 (11.50-3.90)
Ramachandran outliers	138981	1003 (11.50-3.90)
Sidechain outliers	138945	1003 (11.50-3.86)

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  $\geq 3$ , 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  $\leq 5\%$ .

Mol	Chain	Length	Quality of chain
1	A	1207	 27% 52% 17%
1	B	1207	 25% 47% 24%

## 2 Entry composition i

There is only 1 type of molecule in this entry. The entry contains 15030 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 Plexin-A4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	1000	7841	4938	1356	1482	65	0	0	0
1	B	915	7189	4533	1239	1357	60	0	0	0

There are 26 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	33	GLU	-	expression tag	UNP Q80UG2
A	34	THR	-	expression tag	UNP Q80UG2
A	35	GLY	-	expression tag	UNP Q80UG2
A	1230	GLY	-	expression tag	UNP Q80UG2
A	1231	ARG	-	expression tag	UNP Q80UG2
A	1232	THR	-	expression tag	UNP Q80UG2
A	1233	LYS	-	expression tag	UNP Q80UG2
A	1234	HIS	-	expression tag	UNP Q80UG2
A	1235	HIS	-	expression tag	UNP Q80UG2
A	1236	HIS	-	expression tag	UNP Q80UG2
A	1237	HIS	-	expression tag	UNP Q80UG2
A	1238	HIS	-	expression tag	UNP Q80UG2
A	1239	HIS	-	expression tag	UNP Q80UG2
B	33	GLU	-	expression tag	UNP Q80UG2
B	34	THR	-	expression tag	UNP Q80UG2
B	35	GLY	-	expression tag	UNP Q80UG2
B	1230	GLY	-	expression tag	UNP Q80UG2
B	1231	ARG	-	expression tag	UNP Q80UG2
B	1232	THR	-	expression tag	UNP Q80UG2
B	1233	LYS	-	expression tag	UNP Q80UG2
B	1234	HIS	-	expression tag	UNP Q80UG2
B	1235	HIS	-	expression tag	UNP Q80UG2
B	1236	HIS	-	expression tag	UNP Q80UG2
B	1237	HIS	-	expression tag	UNP Q80UG2
B	1238	HIS	-	expression tag	UNP Q80UG2

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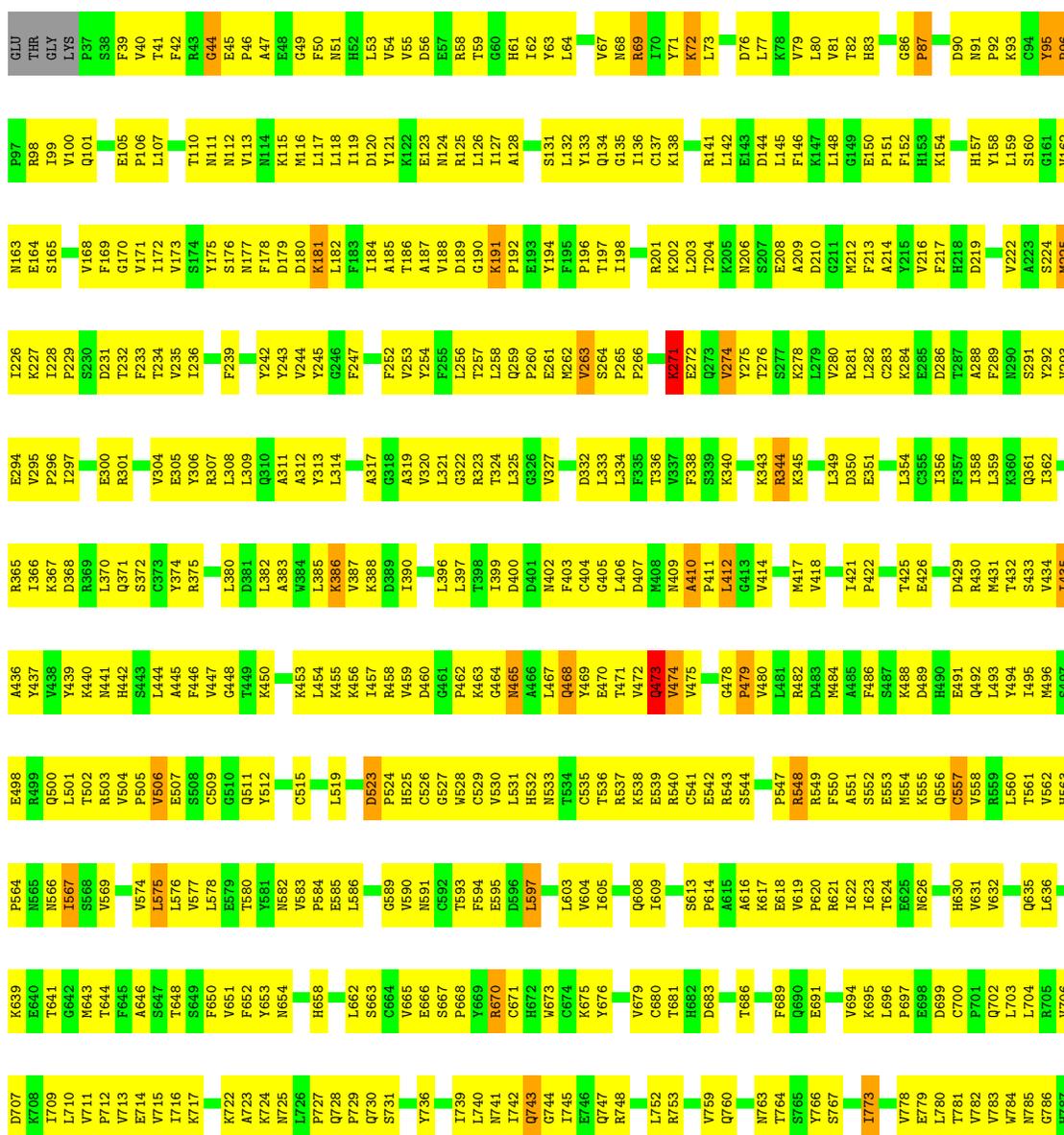
Chain	Residue	Modelled	Actual	Comment	Reference
B	1239	HIS	-	expression tag	UNP Q80UG2

### 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.

- Molecule 1: Plexin-A4

Chain A:  27% 52% 17%



F788	M866	H925	L994	ILE	PHE	LYS	HIS
M789	P857	A926	F995	ALA	GLY	LEU	HIS
I790	E861	E930	H996	VAL	PHE	ASN	HIS
D791	I862	I931	R997	TRP	ILE	TYR	
N792	I863	C932	R998	THR	LEU	THR	
M796	P864	W933	Y1002	THR	ASP	VAL	
K797	V865	A934	I1003	HIS	ASN	LEU	
V798	T866	V935	I1004	LEU	VAL	VAL	
Y799	G867	G936	C1005	ASP	GLY	GLY	
L800	P868	R937	M1006	ILE	LEU	GLU	
Y801	R869	R938	T1007	LEU	LEU	LYS	
K802	E870	F939	T1008	ASN	ILE	PRO	
C803	G871	F940	S1009	PRO	LEU	THR	
G804	G872	M941	S1010	GLN	ASN	VAL	
A805	T873	A942	V1013	ILE	THR	THR	
M806	K874	R943	L1014	ARG	THR	VAL	
R807	V875	L947	L1015	ALA	ASN	SER	
L812	T876	L948	K1016	LYS	PHE	ASP	
C813	I877	Y949	K1017	HIS	THR	VAL	
L814	L882	F950	V1018	GLY	TYR	GLN	
D817	E855	M951	T1019	LYS	TRP	LEU	
F820	R856	T952	V1020	GLU	ASN	LEU	
E821	R857	L953	Q1021	HIS	PRO	GLY	
C822	D888	T954	V1022	ILE	VAL	SER	
G823	I889	A956	D1023	ASN	PHE	PRO	
W824	A890	R956	R1024	ILE	GLY	ASN	
C825	A891	D957	A1025	ALA	ALA	LYS	
G826	R882	L958	R1026	GLU	PHE	ILE	
S827	E883	K959	R1027	VAL	SER	GLY	
P828	K894	M961	Q1029	LEU	PRO	ARG	
G829	V895	R962	R1030	ALA	GLY	HIS	
Q830	A896	G963	L1031	THR	ILE	LYS	
C831	E889	G964	V1032	ALA	LEU	VAL	
T832	E889	M965	F1033	MET	GLU	ALA	
L833	E889	V971	Q1034	THR	LEU	ARG	
H836	P902	T972	Y1036	CYS	LYS	VAL	
C837	L903	I973	V1036	GLN	PRO	GLY	
D838	V904	T974	ASP	ALA	GLY	GLY	
E841	D905	T974	PRO	PRO	THR	THR	
S842	P909	L978	THR	LEU	PRO	GLU	
W844	A910	G975	ILE	ALA	ILE	SER	
L845	I913	M977	THR	LEU	ILE	TYR	
E846	V914	N979	ALA	GLY	LEU	SER	
L847	C915	A980	PRO	ASP	LEU	ALA	
S848	E916	G981	GLU	PRO	GLN	ILE	
G849	M917	V982	THR	THR	THR	ALA	
A850	G918	V986	ILE	ASP	PRO	PRO	
Y851	I919	M987	LEU	LEU	PRO	GLY	
S852	A920	F988	THR	THR	VAL	THR	
K853	K921	G989	VAL	ARG	ALA	LYS	
C854	P922	S990	GLY	PRO	GLY	GLY	
T855	Q924	Q991	THR	GLU	ASN	HIS	
			PRO	GLU	THR	HIS	

• Molecule 1: Plexin-A4



GLU	P87	M163	I226	V295	I366	Y439
THR	R88	E164	K227	P296	K367	K440
GLY	I99	S165	I228	I297	D368	M441
LYS	V100		P229		R369	H442
ASP	Q101	V168	D231	E300	L370	S443
THR	S38	F169	S230	R301	Q371	L444
LEU	F39	G170	T232	V304	S372	A445
VAL	V40	V171	T233	E305	C373	F446
GLN	T41	I172	F234	E306	Y374	V447
ASP	F42	V173	V235	R307	R375	G448
LEU	R43	S174	I236	Y307	R376	T449
VAL	G44	Y175	F239	L308	L380	K450
GLY	E45	S176		L309	D381	
PRO	P46	M177		Q310	L382	
THR	A47	M114	Y242	A311	A383	K453
ASN	E48	K115	Y243	A312	W384	L454
GLN	G49	M116	V253	A313	W384	K455
LEU	F50	L117	V254	Y313	L385	K456
ALA	N51	L118	Y245	L314	K386	I457
LYS	H52	L119	G246	L314	V387	R458
THR	L53	I119	F247	A317	K388	V459
TYR	L54	D120		G318	D389	D460
TRP	V54	Y121	F252	A319	I390	G461
PRO	V55	K122	V253	V320	I390	P462
ASN	D56	E123	Y254	L321	L396	K463
GLY	E57	M124	F255	G322	L397	G464
VAL	R58	R125	L256	R323	L397	G464
PRO	T59	L126	T257	R323	T398	M465
THR	G60	I127	Q259	T324	I399	A466
GLY	H61	A128	G326	L325	D401	Q468
LEU	I62	E131	E193	L325	L401	Y469
ARG	V63	Y194	Y194	L325	F403	E470
ASN	L64	F195	F195	V327	C404	A471
GLY	V67	P196	M263	D332	G405	V472
LEU	N68	T197	P265	L333	L406	Q473
THR	R69	I198	P266	L334	L406	V474
ALA	I70	K201	P266	F335	M409	V475
LEU	W71	K202		T336	A410	
LEU	K72	L203	K273	L336	P411	
LYS	L73	T204	V274	L336	L412	
GLY	D76	K205	Y275	F337	G413	
PRO	L77	N206		V337	V414	
ALA	K78	A209	K278	R344	M417	
THR	V79	D210	L279	K345	V418	
SER	L80	G211	R280	L349	I421	
PRO	V81	M212	R281	D350	I425	
GLY	T82	F213	L282	E351	T425	
LEU	H83	A214	C283	E351	K488	
ASP	P151	Y215	K284	L354	D489	
HIS	F152	V216	E285	C355	H490	
GLN	H53	F217	D286	I356	D429	E491
LEU	K154	H218	T287	F357	R430	Q492
THR	D90	D219	A288	L358	M431	L493
PRO	N91	E220	F289	R359	T432	Y494
ASP	P92	F221	V290	K360	S433	I495
LEU	H158	V222	N291	Q361	V434	M496
THR	L159	V222	S291	I362	I435	S497
GLY	S160	A223	Y292	V293	A436	E498
ARG	G94	S224	E293	E294	R437	R499
PRO	C94	G161	E294		V438	Q500
ASN	Y95	G161				
THR	S96	V162				
HIS	P96					



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	142.18Å 241.00Å 144.07Å 90.00° 99.83° 90.00°	Depositor
Resolution (Å)	47.74 – 8.00 47.74 – 8.00	Depositor EDS
% Data completeness (in resolution range)	99.1 (47.74-8.00) 99.5 (47.74-8.00)	Depositor EDS
$R_{merge}$	0.16	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.18 (at 8.32Å)	Xtrriage
Refinement program	PHENIX 1.8.2_1309	Depositor
R, $R_{free}$	0.349 , 0.349 0.348 , 0.353	Depositor DCC
$R_{free}$ test set	488 reflections (4.85%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	450.9	Xtrriage
Anisotropy	0.543	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.40 , 550.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.43$ , $\langle L^2 \rangle = 0.25$	Xtrriage
Estimated twinning fraction	0.043 for l,-k,h	Xtrriage
$F_o, F_c$ correlation	0.70	EDS
Total number of atoms	15030	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	264.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.04% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 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	1.01	5/8007 (0.1%)	1.36	27/10846 (0.2%)
1	B	1.00	5/7344 (0.1%)	1.32	24/9943 (0.2%)
All	All	1.01	10/15351 (0.1%)	1.34	51/20789 (0.2%)

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	3
1	B	0	4
All	All	0	7

The worst 5 of 10 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	506	VAL	C-N	23.13	1.87	1.34
1	B	506	VAL	C-N	21.10	1.82	1.34
1	A	557	CYS	C-N	-20.82	0.86	1.34
1	B	557	CYS	C-N	-17.13	0.94	1.34
1	A	700	CYS	C-N	-15.63	1.04	1.34

The worst 5 of 51 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	747	GLN	CG-CD-OE1	-38.83	43.94	121.60
1	A	747	GLN	CG-CD-OE1	-38.81	43.98	121.60
1	A	653	TYR	O-C-N	-33.42	69.23	122.70
1	B	557	CYS	O-C-N	-31.89	71.68	122.70
1	A	653	TYR	CA-C-N	23.37	168.61	117.20

There are no chirality outliers.

5 of 7 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	854	CYS	Mainchain
1	A	863	ILE	Peptide
1	A	95	TYR	Peptide
1	B	557	CYS	Mainchain
1	B	95	TYR	Peptide

## 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	A	7841	0	7710	1244	34
1	B	7189	0	7050	1075	67
All	All	15030	0	14760	2319	69

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 78.

The worst 5 of 2319 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:A:868:PRO:HD2	1:A:981:GLY:CA	1.32	1.52
1:A:868:PRO:CD	1:A:981:GLY:CA	1.87	1.50
1:A:873:THR:CA	1:A:982:SER:HB2	1.46	1.43
1:A:873:THR:HA	1:A:982:SER:CB	1.48	1.40
1:B:506:VAL:HG22	1:B:525:HIS:NE2	1.33	1.38

The worst 5 of 69 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:A:146:PHE:CE1	1:B:730:GLN:CD[1_655]	0.64	1.56
1:B:287:THR:OG1	1:B:840:HIS:CG[1_655]	0.67	1.53
1:A:146:PHE:CE1	1:B:730:GLN:OE1[1_655]	0.77	1.43
1:A:146:PHE:CD1	1:B:730:GLN:OE1[1_655]	0.78	1.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:287:THR:CA	1:B:840:HIS:NE2[1_655]	0.79	1.41

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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	994/1207 (82%)	923 (93%)	51 (5%)	20 (2%)	7	38
1	B	907/1207 (75%)	845 (93%)	43 (5%)	19 (2%)	7	36
All	All	1901/2414 (79%)	1768 (93%)	94 (5%)	39 (2%)	7	36

5 of 39 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	96	PRO
1	A	181	LYS
1	A	191	LYS
1	A	410	ALA
1	A	465	ASN

### 5.3.2 Protein sidechains [i](#)

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	888/1067 (83%)	861 (97%)	27 (3%)	41	63
1	B	812/1067 (76%)	789 (97%)	23 (3%)	43	65

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	1700/2134 (80%)	1650 (97%)	50 (3%)	42 64

5 of 50 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	72	LYS
1	B	523	ASP
1	B	892	HIS
1	B	271	LYS
1	B	435	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 53 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	101	GLN
1	B	473	GLN
1	B	792	ASN
1	B	157	HIS
1	B	361	GLN

### 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 monosaccharides in this entry.

### 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	B	6
1	A	5

The worst 5 of 11 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	854:CYS	C	855:THR	N	2.49
1	A	802:LYS	C	803:CYS	N	2.46
1	A	951:MET	C	952:THR	N	2.32
1	B	653:TYR	C	654:ASN	N	2.31
1	B	802:LYS	C	803:CYS	N	2.01

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

Unable to reproduce the depositors R factor - this section is therefore empty.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

### 6.3 Carbohydrates

Unable to reproduce the depositors R factor - this section is therefore empty.

### 6.4 Ligands

Unable to reproduce the depositors R factor - this section is therefore empty.

### 6.5 Other polymers

Unable to reproduce the depositors R factor - this section is therefore empty.