



# wwPDB X-ray Structure Validation Summary Report ⓘ

May 18, 2016 – 08:08 PM EDT

PDB ID : 1A81  
Title : CRYSTAL STRUCTURE OF THE TANDEM SH2 DOMAIN OF THE SYK KINASE BOUND TO A DUALY TYROSINE-PHOSPHORYLATED ITAM  
Authors : Fuetterer, K.; Waksman, G.  
Deposited on : 1998-03-31  
Resolution : 3.00 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  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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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  
Mogul : 1.7.1 (RC1), CSD as537be (2016)  
Xtriage (Phenix) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : rb-20027457

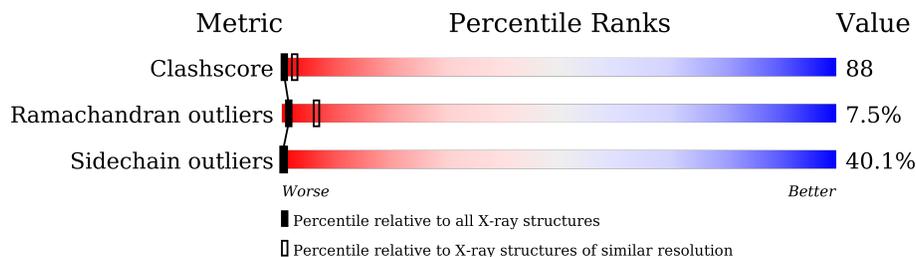
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.00 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))
Clashscore	102246	1912 (3.00-3.00)
Ramachandran outliers	100387	1853 (3.00-3.00)
Sidechain outliers	100360	1856 (3.00-3.00)

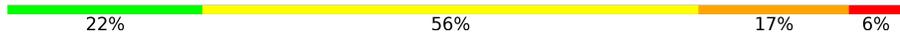
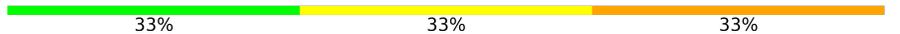
The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	254	
1	C	254	
1	E	254	
1	G	254	
1	I	254	
1	K	254	
2	B	18	

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Mol	Chain	Length	Quality of chain
2	D	18	
2	F	18	
2	H	18	
2	J	18	
2	L	18	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	PTR	J	181	-	-	X	-

## 2 Entry composition i

There are 2 unique types of molecules in this entry. The entry contains 12201 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 SYK KINASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	254	Total 2015	C 1279	N 360	O 370	S 6	0	0	0
1	C	254	Total 2015	C 1279	N 360	O 370	S 6	0	0	0
1	E	220	Total 1742	C 1106	N 314	O 316	S 6	0	0	0
1	G	220	Total 1738	C 1103	N 313	O 316	S 6	0	0	0
1	I	254	Total 2011	C 1276	N 359	O 370	S 6	0	0	0
1	K	220	Total 1738	C 1103	N 313	O 316	S 6	0	0	0

- Molecule 2 is a protein called T-CELL SURFACE GLYCOPROTEIN CD3 EPSILON CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
2	B	18	Total 157	C 93	N 27	O 35	P 2	0	0	0
2	D	18	Total 157	C 93	N 27	O 35	P 2	0	0	0
2	F	18	Total 157	C 93	N 27	O 35	P 2	0	0	0
2	H	18	Total 157	C 93	N 27	O 35	P 2	0	0	0
2	J	18	Total 157	C 93	N 27	O 35	P 2	0	0	0
2	L	18	Total 157	C 93	N 27	O 35	P 2	0	0	0

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	170	PTR	TYR	CONFLICT	UNP P07766

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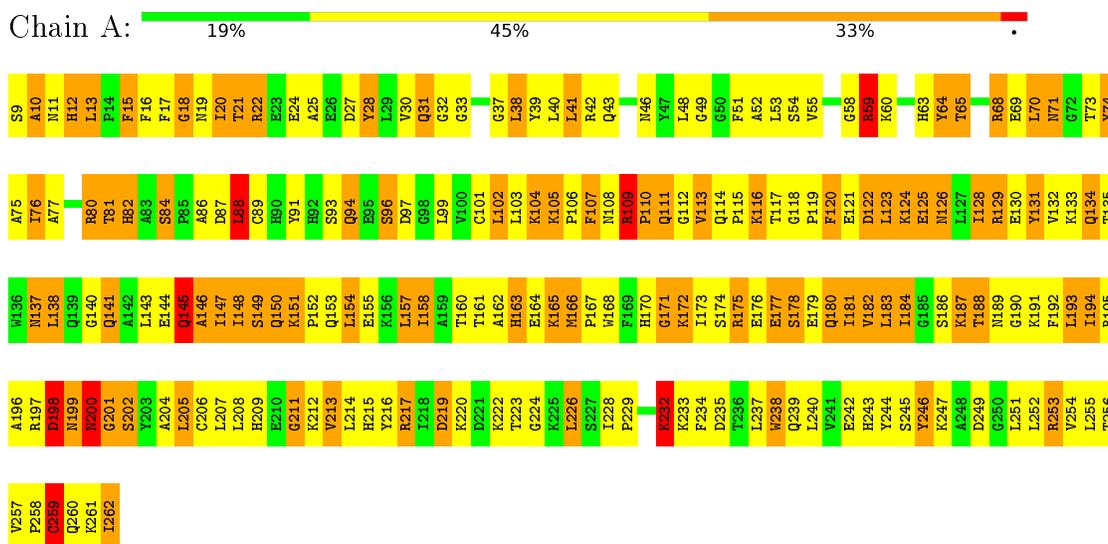
<b>Chain</b>	<b>Residue</b>	<b>Modelled</b>	<b>Actual</b>	<b>Comment</b>	<b>Reference</b>
B	181	PTR	TYR	CONFLICT	UNP P07766
D	170	PTR	TYR	MODIFIED RESIDUE	UNP P07766
D	181	PTR	TYR	MODIFIED RESIDUE	UNP P07766
F	170	PTR	TYR	MODIFIED RESIDUE	UNP P07766
F	181	PTR	TYR	MODIFIED RESIDUE	UNP P07766
H	170	PTR	TYR	MODIFIED RESIDUE	UNP P07766
H	181	PTR	TYR	MODIFIED RESIDUE	UNP P07766
J	170	PTR	TYR	MODIFIED RESIDUE	UNP P07766
J	181	PTR	TYR	MODIFIED RESIDUE	UNP P07766
L	170	PTR	TYR	MODIFIED RESIDUE	UNP P07766
L	181	PTR	TYR	MODIFIED RESIDUE	UNP P07766

### 3 Residue-property plots

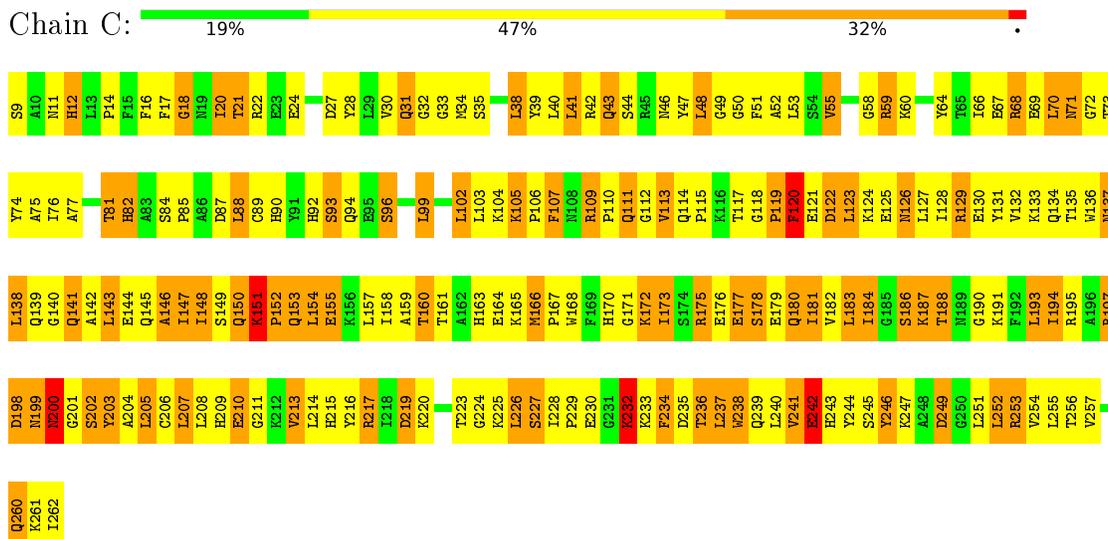
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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: SYK KINASE

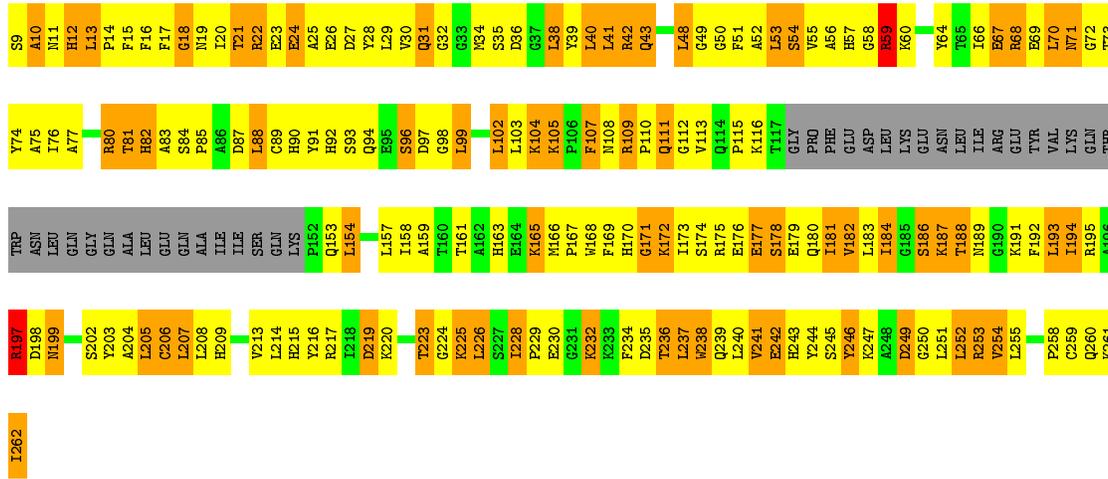


- Molecule 1: SYK KINASE



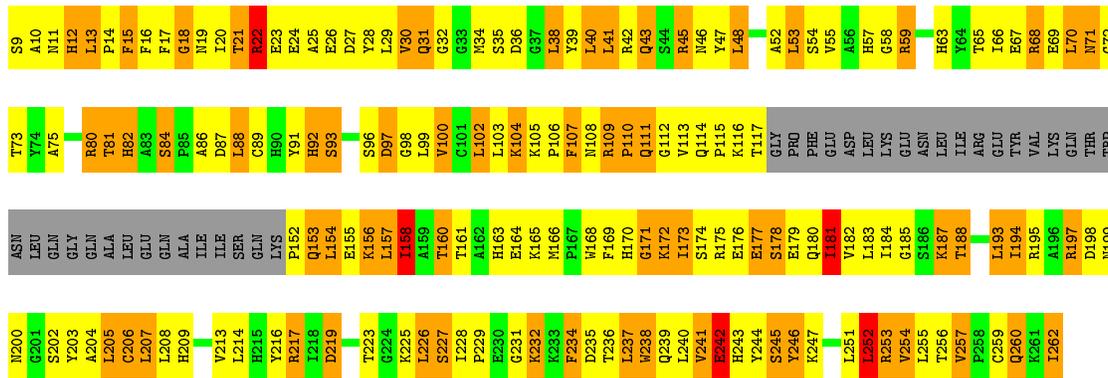
- Molecule 1: SYK KINASE

Chain E: 



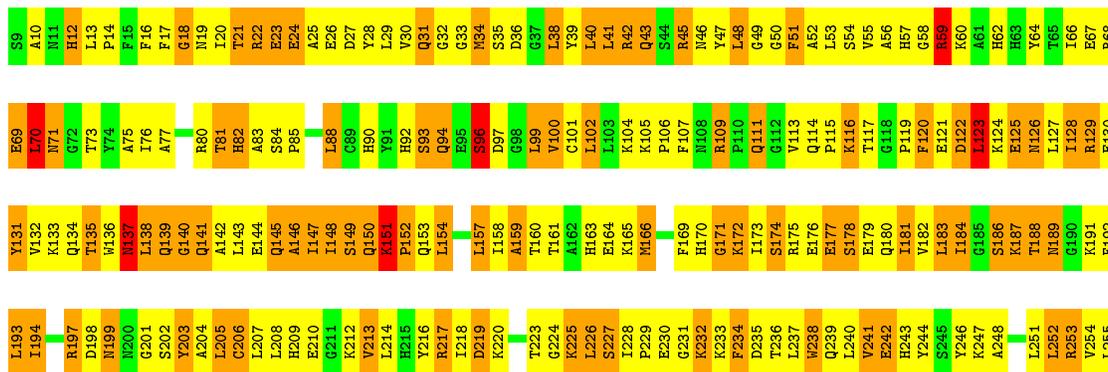
- Molecule 1: SYK KINASE

Chain G: 



- Molecule 1: SYK KINASE

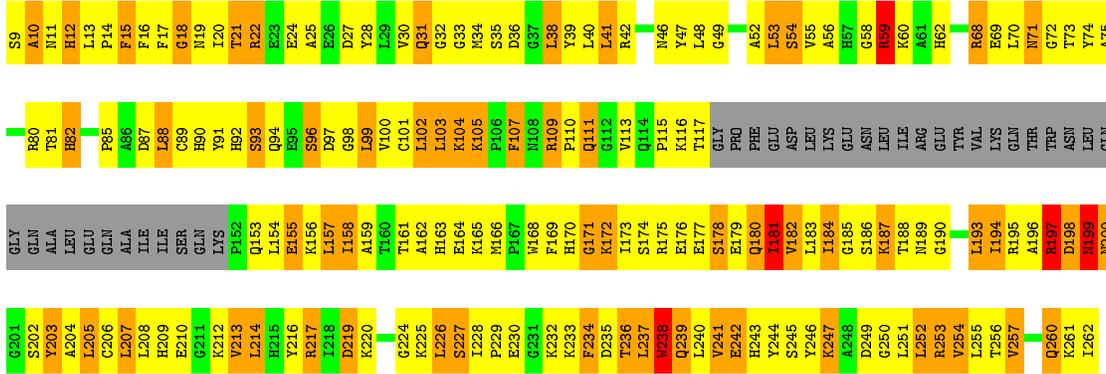
Chain I: 





- Molecule 1: SYK KINASE

Chain K: 17% 44% 24% 13%



- Molecule 2: T-CELL SURFACE GLYCOPROTEIN CD3 EPSILON CHAIN

Chain B: 22% 44% 22% 11%



- Molecule 2: T-CELL SURFACE GLYCOPROTEIN CD3 EPSILON CHAIN

Chain D: 17% 56% 22% 6%



- Molecule 2: T-CELL SURFACE GLYCOPROTEIN CD3 EPSILON CHAIN

Chain F: 11% 61% 28%



- Molecule 2: T-CELL SURFACE GLYCOPROTEIN CD3 EPSILON CHAIN

Chain H: 17% 44% 39%



- Molecule 2: T-CELL SURFACE GLYCOPROTEIN CD3 EPSILON CHAIN

Chain J: 22% 56% 17% 6%



- Molecule 2: T-CELL SURFACE GLYCOPROTEIN CD3 EPSILON CHAIN

Chain L:   
33% 33% 33%

A horizontal bar chart for Chain L showing the percentage of residues in different validation categories. The bar is divided into three equal segments of 33% each, colored green, yellow, and orange from left to right.



## 4 Data and refinement statistics

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

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	85.50 Å 146.90 Å 91.50 Å 90.00° 97.60° 90.00°	Depositor
Resolution (Å)	30.00 – 3.00	Depositor
% Data completeness (in resolution range)	89.8 (30.00-3.00)	Depositor
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.05	Depositor
Refinement program	X-PLOR 3.85	Depositor
R, $R_{free}$	0.226 , 0.317	Depositor
Estimated twinning fraction	No twinning to report.	Xtrriage
Total number of atoms	12201	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	46.0	wwPDB-VP

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: PTR

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	0.85	2/2062 (0.1%)	0.96	2/2787 (0.1%)
1	C	0.80	0/2062	0.93	2/2787 (0.1%)
1	E	0.62	0/1783	0.80	2/2405 (0.1%)
1	G	0.84	0/1779	0.98	3/2401 (0.1%)
1	I	0.74	0/2058	0.87	1/2783 (0.0%)
1	K	0.64	1/1779 (0.1%)	0.79	2/2401 (0.1%)
2	B	0.62	0/124	1.09	0/161
2	D	0.87	0/124	1.04	0/161
2	F	0.58	0/124	0.91	0/161
2	H	0.79	0/124	1.19	1/161 (0.6%)
2	J	0.55	0/124	0.91	0/161
2	L	0.53	0/124	0.98	0/161
All	All	0.75	3/12267 (0.0%)	0.90	13/16530 (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	2

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	259	CYS	CB-SG	-5.32	1.73	1.81
1	K	89	CYS	CB-SG	5.20	1.91	1.82
1	A	46	ASN	CG-ND2	-5.05	1.20	1.32

The worst 5 of 13 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	184	LEU	CA-CB-CG	-6.91	99.41	115.30
1	G	100	VAL	CB-CA-C	-6.28	99.48	111.40
1	K	199	ASN	N-CA-C	-6.14	94.43	111.00
1	G	198	ASP	N-CA-C	5.89	126.89	111.00
1	A	109	ARG	NE-CZ-NH1	-5.79	117.40	120.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	28	TYR	Sidechain
1	A	64	TYR	Sidechain

## 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	2015	0	1977	387	0
1	C	2015	0	1977	403	0
1	E	1742	0	1718	277	0
1	G	1738	0	1707	293	0
1	I	2011	0	1966	383	0
1	K	1738	0	1707	301	0
2	B	157	0	139	25	0
2	D	157	0	139	30	0
2	F	157	0	139	33	0
2	H	157	0	139	33	0
2	J	157	0	139	30	0
2	L	157	0	139	27	0
All	All	12201	0	11886	2118	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 88.

The worst 5 of 2118 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:I:21:THR:HG23	1:I:24:GLU:OE1	1.45	1.16
1:I:128:ILE:HG22	1:I:158:ILE:HG12	1.26	1.15
1:C:128:ILE:HG22	1:C:158:ILE:HG12	1.23	1.14
1:E:21:THR:HG23	1:E:24:GLU:HB2	1.22	1.13
1:A:70:LEU:HD12	1:A:70:LEU:H	1.04	1.12

There are no symmetry-related clashes.

## 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	252/254 (99%)	190 (75%)	39 (16%)	23 (9%)	1	4
1	C	252/254 (99%)	184 (73%)	51 (20%)	17 (7%)	1	8
1	E	216/254 (85%)	164 (76%)	41 (19%)	11 (5%)	2	15
1	G	216/254 (85%)	167 (77%)	36 (17%)	13 (6%)	2	11
1	I	252/254 (99%)	179 (71%)	47 (19%)	26 (10%)	1	3
1	K	216/254 (85%)	158 (73%)	44 (20%)	14 (6%)	1	8
2	B	14/18 (78%)	9 (64%)	3 (21%)	2 (14%)	0	1
2	D	14/18 (78%)	11 (79%)	1 (7%)	2 (14%)	0	1
2	F	14/18 (78%)	8 (57%)	6 (43%)	0	100	100
2	H	14/18 (78%)	10 (71%)	3 (21%)	1 (7%)	1	7
2	J	14/18 (78%)	9 (64%)	4 (29%)	1 (7%)	1	7
2	L	14/18 (78%)	9 (64%)	4 (29%)	1 (7%)	1	7
All	All	1488/1632 (91%)	1098 (74%)	279 (19%)	111 (8%)	1	6

5 of 111 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	18	GLY

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Mol	Chain	Res	Type
1	A	137	ASN
1	A	140	GLY
1	A	171	GLY
1	A	177	GLU

### 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	211/216 (98%)	124 (59%)	87 (41%)	0	0
1	C	211/216 (98%)	125 (59%)	86 (41%)	0	0
1	E	183/216 (85%)	118 (64%)	65 (36%)	0	1
1	G	182/216 (84%)	105 (58%)	77 (42%)	0	0
1	I	210/216 (97%)	123 (59%)	87 (41%)	0	0
1	K	182/216 (84%)	116 (64%)	66 (36%)	0	1
2	B	14/14 (100%)	6 (43%)	8 (57%)	0	0
2	D	14/14 (100%)	8 (57%)	6 (43%)	0	0
2	F	14/14 (100%)	8 (57%)	6 (43%)	0	0
2	H	14/14 (100%)	8 (57%)	6 (43%)	0	0
2	J	14/14 (100%)	8 (57%)	6 (43%)	0	0
2	L	14/14 (100%)	8 (57%)	6 (43%)	0	0
All	All	1263/1380 (92%)	757 (60%)	506 (40%)	0	0

5 of 506 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	186	SER
1	G	84	SER
1	K	178	SER
1	E	199	ASN
2	F	179	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 47 such sidechains are listed below:

Mol	Chain	Res	Type
1	E	170	HIS
1	G	57	HIS
1	K	153	GLN
1	E	243	HIS
1	G	108	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

12 non-standard protein/DNA/RNA residues are modelled in this entry.

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
2	PTR	B	170	2	13,16,17	0.63	0	19,22,24	1.13	3 (15%)
2	PTR	B	181	2	13,16,17	0.89	0	19,22,24	2.12	4 (21%)
2	PTR	D	170	2	13,16,17	0.75	0	19,22,24	0.81	1 (5%)
2	PTR	D	181	2	13,16,17	0.93	1 (7%)	19,22,24	1.53	5 (26%)
2	PTR	F	170	2	13,16,17	0.73	0	19,22,24	0.89	1 (5%)
2	PTR	F	181	2	13,16,17	0.78	0	19,22,24	1.19	2 (10%)
2	PTR	H	170	2	13,16,17	0.96	1 (7%)	19,22,24	1.00	1 (5%)
2	PTR	H	181	2	13,16,17	0.93	0	19,22,24	1.78	6 (31%)
2	PTR	J	170	2	13,16,17	0.83	0	19,22,24	0.88	1 (5%)
2	PTR	J	181	2	13,16,17	0.94	0	19,22,24	1.08	2 (10%)
2	PTR	L	170	2	13,16,17	1.03	1 (7%)	19,22,24	1.20	1 (5%)
2	PTR	L	181	2	13,16,17	0.97	0	19,22,24	0.99	2 (10%)

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
2	PTR	B	170	2	-	0/9/11/13	0/1/1/1
2	PTR	B	181	2	-	0/9/11/13	0/1/1/1
2	PTR	D	170	2	-	0/9/11/13	0/1/1/1
2	PTR	D	181	2	-	0/9/11/13	0/1/1/1
2	PTR	F	170	2	-	0/9/11/13	0/1/1/1
2	PTR	F	181	2	-	0/9/11/13	0/1/1/1
2	PTR	H	170	2	-	0/9/11/13	0/1/1/1
2	PTR	H	181	2	-	0/9/11/13	0/1/1/1
2	PTR	J	170	2	-	0/9/11/13	0/1/1/1
2	PTR	J	181	2	-	0/9/11/13	0/1/1/1
2	PTR	L	170	2	-	0/9/11/13	0/1/1/1
2	PTR	L	181	2	-	0/9/11/13	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	181	PTR	OH-CZ	-2.27	1.35	1.40
2	H	170	PTR	CB-CA	-2.25	1.49	1.53
2	L	170	PTR	P-O3P	-2.19	1.47	1.54

The worst 5 of 29 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
2	B	181	PTR	O2P-P-OH	-5.29	88.61	105.47
2	H	181	PTR	O2P-P-OH	-3.08	95.67	105.47
2	H	181	PTR	O3P-P-O1P	-3.00	100.83	110.63
2	D	181	PTR	O3P-P-O1P	-2.99	100.87	110.63
2	F	181	PTR	O2P-P-O1P	-2.81	101.46	110.63

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

9 monomers are involved in 27 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	170	PTR	2	0
2	B	181	PTR	4	0
2	D	170	PTR	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	181	PTR	2	0
2	F	170	PTR	1	0
2	F	181	PTR	1	0
2	H	170	PTR	4	0
2	H	181	PTR	2	0
2	J	181	PTR	8	0

## 5.5 Carbohydrates [i](#)

There are no carbohydrates 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](#)

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.