



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 07:50 AM GMT

PDB ID : 3CD3  
Title : Crystal structure of phosphorylated human feline sarcoma viral oncogene homologue (v-FES) in complex with staurosporine and a consensus peptide  
Authors : Filippakopoulos, P.; Salah, E.; Cooper, C.; Picaud, S.S.; Elkins, J.M.; von Delft, F.; Arrowsmith, C.H.; Edwards, A.M.; Weigelt, J.; Bountra, C.; Knapp, S.; Structural Genomics Consortium (SGC)  
Deposited on : 2008-02-26  
Resolution : 1.98 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](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 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

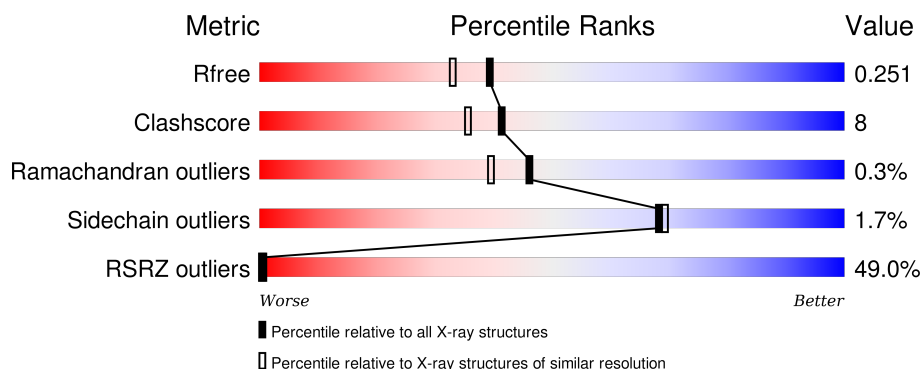
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.98 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))
$R_{free}$	91344	8664 (2.00-1.96)
Clashscore	102246	9905 (2.00-1.96)
Ramachandran outliers	100387	9792 (2.00-1.96)
Sidechain outliers	100360	9791 (2.00-1.96)
RSRZ outliers	91569	8679 (2.00-1.96)

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.

Mol	Chain	Length	Quality of chain
1	A	377	
2	B	6	

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 3232 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 Proto-oncogene tyrosine-protein kinase Fes/Fps.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	P	S			
1	A	353	2771	1777	477	502	1	14	0	9	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	446	SER	-	EXPRESSION TAG	UNP P07332
A	447	MET	-	EXPRESSION TAG	UNP P07332

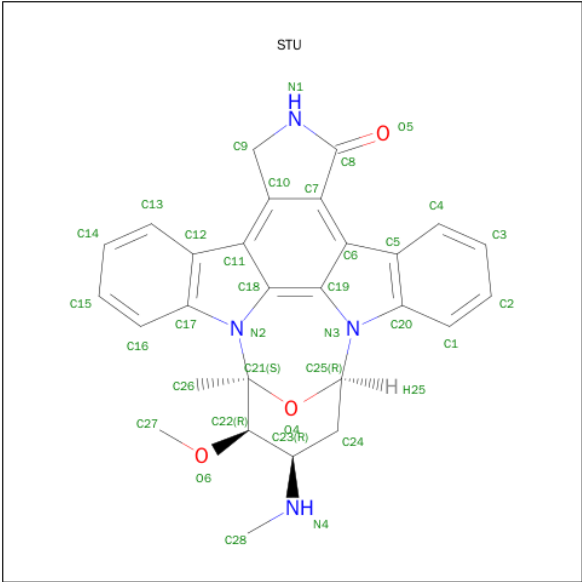
- Molecule 2 is a protein called Synthetic peptide.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
2	B	6	47	31	5	11	0	0	0

- Molecule 3 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	2	Total	Cl	0	0
			2	2		

- Molecule 4 is STAUROSPORINE (three-letter code: STU) (formula: C<sub>28</sub>H<sub>26</sub>N<sub>4</sub>O<sub>3</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			35	28	4	3		
4	A	1	Total	C	N	O	0	0
			35	28	4	3		
4	A	1	Total	C	N	O	0	0
			35	28	4	3		

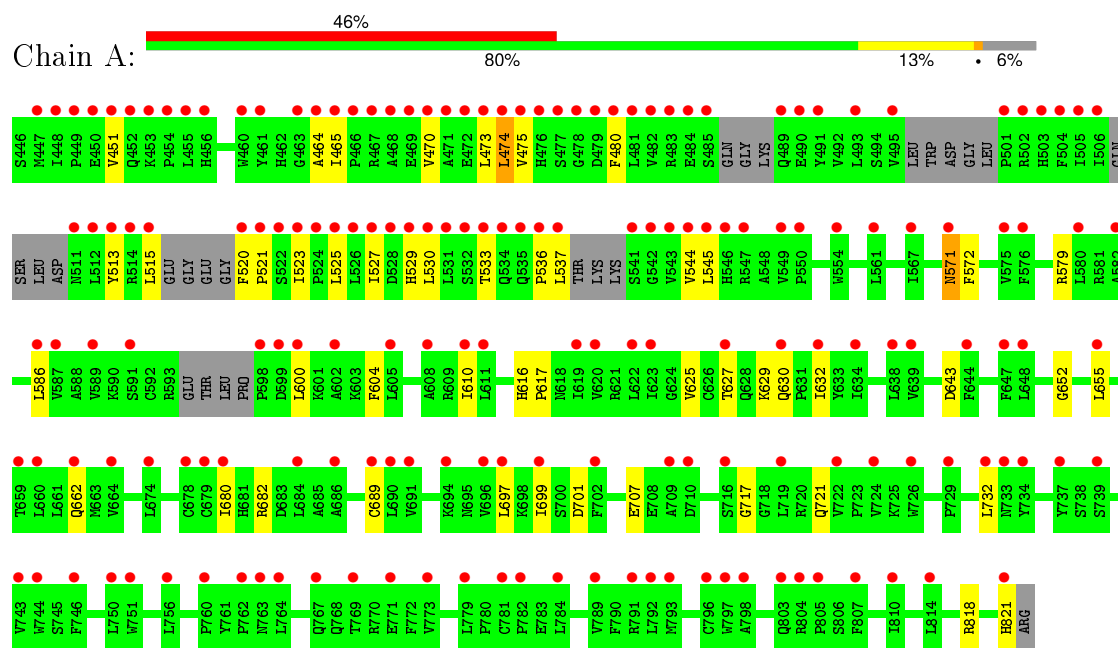
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	299	Total	O	0	0
			299	299		
5	B	8	Total	O	0	0
			8	8		

### 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: Proto-oncogene tyrosine-protein kinase Fes/Fps



- Molecule 2: Synthetic peptide



There are no outlier residues recorded for this chain.

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	35.45Å 76.91Å 150.63Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	15.35 – 1.98 14.95 – 1.98	Depositor EDS
% Data completeness (in resolution range)	97.3 (15.35-1.98) 97.6 (14.95-1.98)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	0.08	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.95 (at 1.98Å)	Xtriage
Refinement program	REFMAC 5.4.0066	Depositor
R, $R_{free}$	0.185 , 0.247 0.199 , 0.251	Depositor DCC
$R_{free}$ test set	1447 reflections (5.28%)	DCC
Wilson B-factor (Å <sup>2</sup> )	26.7	Xtriage
Anisotropy	0.253	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 60.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.45$ , $\langle L^2 \rangle = 0.28$	Xtriage
Outliers	0 of 28827 reflections	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	3232	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	49.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.88% 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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

## 5 Model quality

### 5.1 Standard geometry

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

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	0.68	0/2854	0.74	0/3863
2	B	0.81	0/45	0.89	0/59
All	All	0.68	0/2899	0.74	0/3922

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

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	A	2771	0	2699	40	0
2	B	47	0	45	0	0
3	A	2	0	0	0	0
4	A	105	0	78	9	0
5	A	299	0	0	2	0
5	B	8	0	0	1	0
All	All	3232	0	2822	49	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 (49) 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:627:THR:HA	1:A:632:ILE:HD12	1.56	0.86
4:A:903:STU:H16	4:A:903:STU:H261	1.57	0.85
4:A:902:STU:H261	4:A:902:STU:H16	1.65	0.77
4:A:901:STU:H16	4:A:901:STU:H261	1.69	0.74
1:A:717:GLY:O	5:A:310:HOH:O	2.05	0.73
1:A:610:ILE:CD1	1:A:707[B]:GLU:HG3	2.29	0.63
1:A:625:VAL:HG12	1:A:627:THR:HG23	1.81	0.62
1:A:721:GLN:HG3	5:B:165:HOH:O	1.99	0.62
1:A:465:ILE:HD11	1:A:473:LEU:CD1	2.30	0.61
4:A:903:STU:H16	4:A:903:STU:C26	2.31	0.59
1:A:689:CYS:SG	1:A:699[A]:ILE:HD12	2.44	0.58
1:A:610:ILE:HD13	1:A:707[B]:GLU:HG3	1.86	0.57
1:A:465:ILE:HD11	1:A:473:LEU:HD12	1.87	0.56
1:A:530:LEU:HD13	1:A:537:LEU:CD2	2.35	0.56
1:A:610:ILE:HD13	1:A:707[B]:GLU:CG	2.36	0.55
1:A:610:ILE:HD13	1:A:707[B]:GLU:OE1	2.07	0.55
1:A:465:ILE:O	1:A:465:ILE:HG23	2.07	0.54
4:A:903:STU:C16	4:A:903:STU:H261	2.35	0.54
1:A:627:THR:HA	1:A:632:ILE:CD1	2.36	0.52
1:A:464:ALA:HB1	1:A:630:GLN:HE21	1.75	0.51
1:A:579:ARG:HG2	1:A:586:LEU:HD23	1.94	0.50
4:A:901:STU:H273	4:A:901:STU:C17	2.42	0.49
1:A:697:LEU:HD21	1:A:699[A]:ILE:CD1	2.42	0.49
1:A:652:GLY:HA2	1:A:655:LEU:HD12	1.95	0.48
1:A:662:GLN:HB2	1:A:818:ARG:NE	2.29	0.48
1:A:604:PHE:HE2	1:A:632:ILE:HG22	1.78	0.47
1:A:523:ILE:O	1:A:527:ILE:HG12	2.13	0.47
1:A:480:PHE:CG	1:A:545:LEU:HD22	2.49	0.47
4:A:903:STU:C16	4:A:903:STU:C26	2.91	0.47
1:A:465:ILE:HD11	1:A:473:LEU:HD11	1.96	0.47
1:A:697:LEU:HD23	1:A:697:LEU:C	2.36	0.46
1:A:470:VAL:HG12	1:A:474:LEU:HD22	1.96	0.46
1:A:529:HIS:CE1	1:A:533:THR:HG21	2.50	0.46
1:A:515:LEU:CD1	1:A:537:LEU:HD22	2.46	0.46
1:A:572:PHE:CE1	1:A:600:LEU:HG	2.51	0.46
1:A:629:LYS:HD2	5:A:332:HOH:O	2.17	0.45
1:A:536:PRO:HA	1:A:544:VAL:HG22	1.99	0.45
1:A:513:TYR:O	1:A:520:PHE:N	2.51	0.44
1:A:451:VAL:O	1:A:451:VAL:HG12	2.18	0.43
1:A:616:HIS:CG	1:A:617:PRO:HD2	2.53	0.43
1:A:521:PRO:HD2	1:A:525:LEU:HD13	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:465:ILE:O	1:A:465:ILE:CG2	2.67	0.42
1:A:732:LEU:HD23	1:A:732:LEU:C	2.41	0.41
4:A:902:STU:H261	4:A:902:STU:C16	2.42	0.41
1:A:464:ALA:HB3	1:A:632:ILE:HD11	2.03	0.41
4:A:901:STU:H16	4:A:901:STU:C26	2.43	0.40
1:A:680:ILE:HG22	1:A:682:ARG:HG3	2.04	0.40

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	347/377 (92%)	338 (97%)	8 (2%)	1 (0%)	46	39
2	B	4/6 (67%)	4 (100%)	0	0	100	100
All	All	351/383 (92%)	342 (97%)	8 (2%)	1 (0%)	46	39

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	701	ASP

### 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	293/326 (90%)	287 (98%)	6 (2%)	63	63
2	B	5/5 (100%)	5 (100%)	0	100	100
All	All	298/331 (90%)	292 (98%)	6 (2%)	68	63

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	474	LEU
1	A	475	VAL
1	A	571[A]	ASN
1	A	571[B]	ASN
1	A	643	ASP
1	A	821	HIS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	529	HIS
1	A	630	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

1 non-standard protein/DNA/RNA residue is 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$
1	PTR	A	713	1	14,16,17	2.05	1 (7%)	18,22,24	1.13	2 (11%)

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
1	PTR	A	713	1	-	0/9/11/13	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	713	PTR	OH-CZ	-7.27	1.23	1.40

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	713	PTR	O-C-CA	-2.40	119.24	125.49
1	A	713	PTR	OH-CZ-CE2	2.16	125.86	119.22

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 5 ligands modelled in this entry, 2 are monoatomic - leaving 3 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	STU	A	901	-	27,42,42	1.48	4 (14%)	23,68,68	0.95	1 (4%)
4	STU	A	902	-	27,42,42	1.63	6 (22%)	23,68,68	1.14	2 (8%)
4	STU	A	903	-	27,42,42	1.59	5 (18%)	23,68,68	0.81	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	STU	A	901	-	-	0/4/42/42	0/0/8/8
4	STU	A	902	-	-	0/4/42/42	0/0/8/8
4	STU	A	903	-	-	0/4/42/42	0/0/8/8

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	903	STU	C11-C18	-3.13	1.38	1.42
4	A	902	STU	C11-C18	-3.07	1.38	1.42
4	A	901	STU	C7-C8	-2.34	1.40	1.49
4	A	902	STU	C7-C8	-2.08	1.41	1.49
4	A	903	STU	C10-C11	-2.06	1.39	1.42
4	A	903	STU	C7-C8	-2.03	1.41	1.49
4	A	902	STU	C24-C25	2.07	1.54	1.51
4	A	901	STU	C15-C16	2.22	1.41	1.36
4	A	902	STU	C26-C21	3.05	1.55	1.51
4	A	902	STU	C22-C23	3.13	1.56	1.52
4	A	901	STU	C24-C25	3.28	1.57	1.51
4	A	902	STU	O6-C22	3.39	1.49	1.42
4	A	903	STU	O6-C22	3.76	1.49	1.42
4	A	903	STU	C24-C25	4.02	1.58	1.51
4	A	901	STU	O6-C22	4.07	1.50	1.42

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	902	STU	C1-C20-N3	-2.54	129.13	132.18
4	A	901	STU	O5-C8-C7	-2.38	124.65	128.62
4	A	902	STU	C16-C17-C12	-2.21	117.54	120.73

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	901	STU	3	0
4	A	902	STU	2	0
4	A	903	STU	4	0

## 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

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	352/377 (93%)	2.43	175 (49%)  	35, 47, 61, 74	0
2	B	5/6 (83%)	0.96	0  	42, 42, 45, 49	0
All	All	357/383 (93%)	2.41	175 (49%)  	35, 46, 61, 74	0

All (175) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	512	LEU	10.6
1	A	489	GLN	9.2
1	A	468	ALA	9.0
1	A	533	THR	8.2
1	A	471	ALA	7.8
1	A	543	VAL	7.6
1	A	513	TYR	7.1
1	A	515	LEU	7.1
1	A	541	SER	6.9
1	A	530	LEU	6.6
1	A	473	LEU	6.4
1	A	495	VAL	6.4
1	A	545	LEU	6.4
1	A	532	SER	6.3
1	A	600	LEU	6.3
1	A	531	LEU	6.3
1	A	466	PRO	6.3
1	A	598	PRO	6.2
1	A	503	HIS	5.9
1	A	475	VAL	5.9
1	A	527	ILE	5.8
1	A	476	HIS	5.7
1	A	523	ILE	5.7
1	A	536	PRO	5.7

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Mol	Chain	Res	Type	RSRZ
1	A	474	LEU	5.5
1	A	504	PHE	5.3
1	A	549	VAL	5.3
1	A	470	VAL	5.0
1	A	599	ASP	5.0
1	A	542	GLY	5.0
1	A	511	ASN	4.9
1	A	524	PRO	4.9
1	A	467	ARG	4.9
1	A	716	SER	4.8
1	A	482	VAL	4.7
1	A	763	ASN	4.7
1	A	544	VAL	4.6
1	A	479	ASP	4.6
1	A	537	LEU	4.6
1	A	501	PRO	4.6
1	A	454	PRO	4.6
1	A	455	LEU	4.6
1	A	449	PRO	4.5
1	A	506	ILE	4.5
1	A	719	LEU	4.5
1	A	764	LEU	4.5
1	A	534	GLN	4.4
1	A	521	PRO	4.4
1	A	485	SER	4.3
1	A	792	LEU	4.3
1	A	477	SER	4.2
1	A	505	ILE	4.2
1	A	526	LEU	4.2
1	A	529	HIS	4.2
1	A	490	GLU	4.2
1	A	691	VAL	4.1
1	A	514	ARG	4.1
1	A	480	PHE	4.1
1	A	567	ILE	4.0
1	A	769	THR	4.0
1	A	623[A]	ILE	4.0
1	A	680	ILE	4.0
1	A	502	ARG	4.0
1	A	478	GLY	3.9
1	A	546	HIS	3.9
1	A	448	ILE	3.9

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Mol	Chain	Res	Type	RSRZ
1	A	810	ILE	3.9
1	A	464	ALA	3.8
1	A	630	GLN	3.8
1	A	690	LEU	3.8
1	A	756	LEU	3.8
1	A	571[A]	ASN	3.8
1	A	679	CYS	3.7
1	A	469	GLU	3.7
1	A	493	LEU	3.7
1	A	814	LEU	3.7
1	A	743	VAL	3.7
1	A	674	LEU	3.6
1	A	484	GLU	3.6
1	A	602	ALA	3.6
1	A	807	PHE	3.6
1	A	465	ILE	3.5
1	A	528	ASP	3.5
1	A	535	GLN	3.5
1	A	451	VAL	3.4
1	A	619	ILE	3.4
1	A	481	LEU	3.4
1	A	734	TYR	3.4
1	A	472	GLU	3.4
1	A	550	PRO	3.3
1	A	452	GLN	3.2
1	A	610	ILE	3.2
1	A	611	LEU	3.2
1	A	575	VAL	3.2
1	A	580	LEU	3.2
1	A	710	ASP	3.1
1	A	781	CYS	3.1
1	A	461	TYR	3.1
1	A	726	TRP	3.1
1	A	796	CYS	3.1
1	A	729	PRO	3.0
1	A	460	TRP	3.0
1	A	644	PHE	3.0
1	A	767	GLN	2.9
1	A	744	TRP	2.9
1	A	547	ARG	2.9
1	A	697	LEU	2.9
1	A	773	VAL	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	522	SER	2.8
1	A	686	ALA	2.8
1	A	587	VAL	2.8
1	A	660	LEU	2.7
1	A	699[A]	ILE	2.7
1	A	771	GLU	2.7
1	A	789	VAL	2.7
1	A	447	MET	2.7
1	A	694	LYS	2.7
1	A	762	PRO	2.7
1	A	620	VAL	2.7
1	A	648	LEU	2.7
1	A	655	LEU	2.6
1	A	639	VAL	2.6
1	A	463	GLY	2.6
1	A	483	ARG	2.6
1	A	804	ARG	2.6
1	A	627	THR	2.6
1	A	678	CYS	2.5
1	A	491	TYR	2.5
1	A	821	HIS	2.5
1	A	589	VAL	2.5
1	A	732	LEU	2.5
1	A	664	VAL	2.5
1	A	779	LEU	2.5
1	A	525	LEU	2.4
1	A	689	CYS	2.4
1	A	791	ARG	2.4
1	A	622	LEU	2.4
1	A	659	THR	2.4
1	A	634	ILE	2.3
1	A	576	PHE	2.3
1	A	751	TRP	2.3
1	A	684	LEU	2.3
1	A	722	VAL	2.3
1	A	647	PHE	2.3
1	A	739[A]	SER	2.3
1	A	582	ALA	2.3
1	A	709	ALA	2.3
1	A	456	HIS	2.3
1	A	453	LYS	2.2
1	A	733	ASN	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	737	TYR	2.2
1	A	702	PHE	2.2
1	A	746	PHE	2.2
1	A	608	ALA	2.2
1	A	797	TRP	2.2
1	A	638	LEU	2.2
1	A	450	GLU	2.1
1	A	805	PRO	2.1
1	A	662	GLN	2.1
1	A	724	VAL	2.1
1	A	586	LEU	2.1
1	A	605	LEU	2.1
1	A	784	LEU	2.1
1	A	760	PRO	2.1
1	A	554	TRP	2.1
1	A	798	ALA	2.1
1	A	793	MET	2.1
1	A	520	PHE	2.0
1	A	632	ILE	2.0
1	A	561	LEU	2.0
1	A	591	SER	2.0
1	A	782	PRO	2.0
1	A	803	GLN	2.0
1	A	750	LEU	2.0
1	A	696	VAL	2.0

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
1	PTR	A	713	16/17	0.77	0.23	-	40,47,77,79	0

## 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
4	STU	A	903	35/35	0.80	0.23	0.32	36,45,63,73	0
4	STU	A	902	35/35	0.86	0.20	-0.55	33,43,50,61	0
4	STU	A	901	35/35	0.87	0.16	-0.73	28,33,40,49	0
3	CL	A	904	1/1	0.97	0.09	-2.27	39,39,39,39	0
3	CL	A	905	1/1	0.97	0.12	-	47,47,47,47	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.