



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 07:49 AM GMT

PDB ID : 3CBL  
Title : Crystal structure of 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 : 2008-02-22  
Resolution : 1.75 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

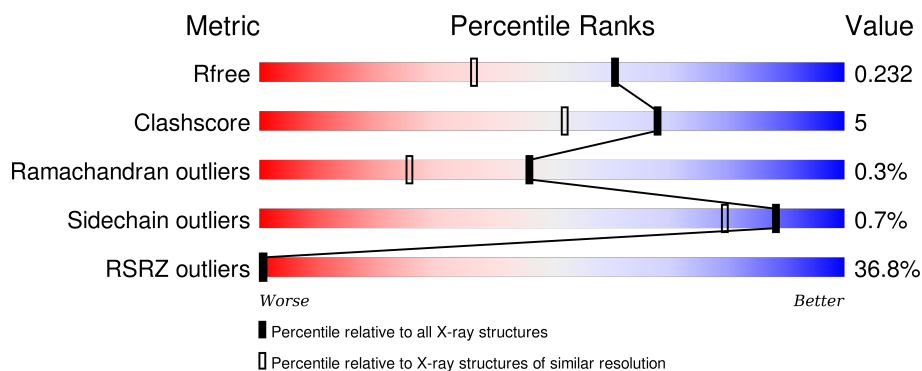
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.75 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	1609 (1.76-1.76)
Clashscore	102246	1730 (1.76-1.76)
Ramachandran outliers	100387	1711 (1.76-1.76)
Sidechain outliers	100360	1711 (1.76-1.76)
RSRZ outliers	91569	1610 (1.76-1.76)

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 [i](#)

There are 4 unique types of molecules in this entry. The entry contains 3304 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	S			
1	A	356	2824	1815	479	515	15	0	13	0

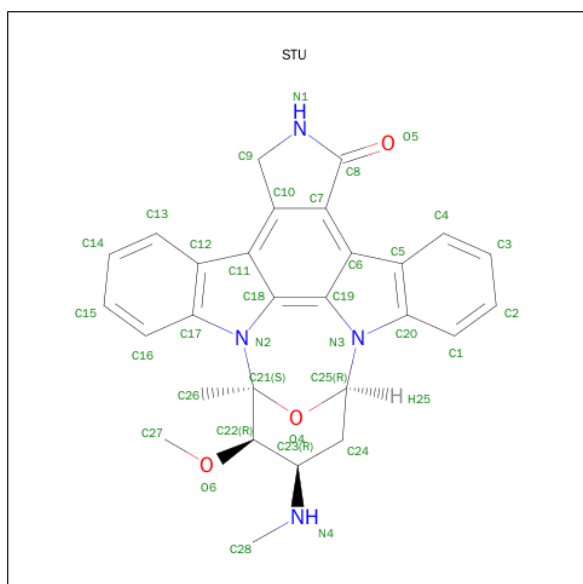
There are 2 discrepancies between the modelled and reference sequences:

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 STAUROSPORINE (three-letter code: STU) (formula:  $C_{28}H_{26}N_4O_3$ ).



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

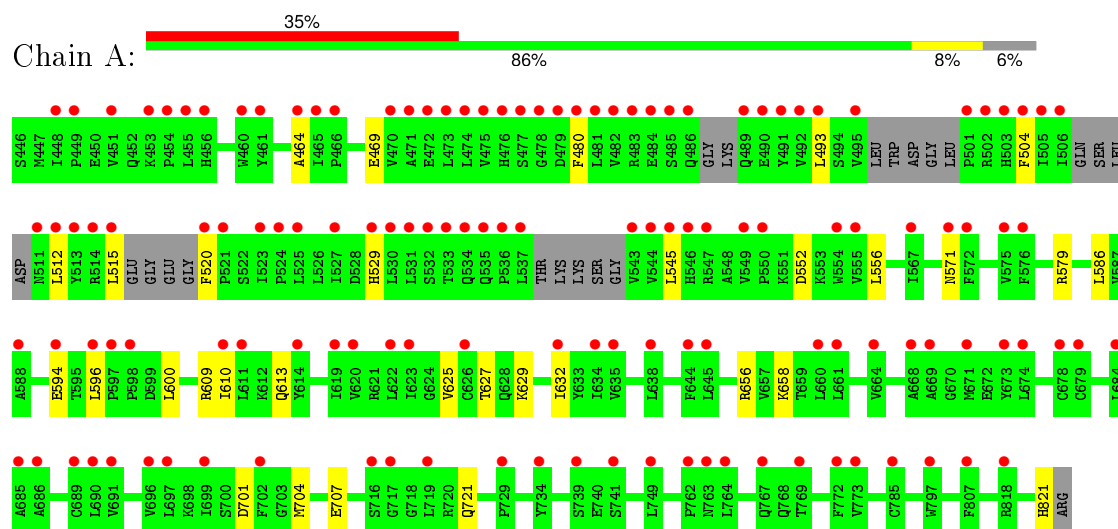
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	320	Total	O	0	0
			320	320		
4	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, $\alpha$ , $\beta$ , $\gamma$	35.68 Å 77.18 Å 149.49 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	38.58 – 1.75 38.59 – 1.75	Depositor EDS
% Data completeness (in resolution range)	99.1 (38.58-1.75) 99.1 (38.59-1.75)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	0.07	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.80 (at 1.75 Å)	Xtriage
Refinement program	REFMAC 5.4.0066	Depositor
R, $R_{free}$	0.180 , 0.227 0.187 , 0.232	Depositor DCC
$R_{free}$ test set	2141 reflections (5.33%)	DCC
Wilson B-factor (Å <sup>2</sup> )	21.1	Xtriage
Anisotropy	0.040	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 51.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 42304 reflections	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	3304	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.21% 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 [i](#)

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

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

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	0/2935	0.73	2/3977 (0.1%)
2	B	0.78	0/45	0.81	0/59
All	All	0.68	0/2980	0.73	2/4036 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	556	LEU	CA-CB-CG	6.17	129.49	115.30
1	A	552	ASP	CB-CG-OD1	5.30	123.07	118.30

There are no chirality outliers.

There are no planarity outliers.

### 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	2824	0	2778	22	0
2	B	47	0	45	0	0
3	A	105	0	78	6	0
4	A	320	0	0	2	0
4	B	8	0	0	1	0
All	All	3304	0	2901	28	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 5.

All (28) 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)
3:A:902:STU:H261	3:A:902:STU:H16	1.63	0.81
1:A:627:THR:HA	1:A:632:ILE:HD12	1.62	0.80
1:A:704[A]:MET:HE2	4:A:321:HOH:O	1.87	0.74
3:A:903:STU:H16	3:A:903:STU:H261	1.74	0.68
1:A:704[A]:MET:CE	4:A:321:HOH:O	2.44	0.63
3:A:901:STU:H16	3:A:901:STU:H261	1.80	0.63
1:A:480:PHE:CG	1:A:545:LEU:HD22	2.34	0.63
1:A:625:VAL:HG12	1:A:627:THR:HG23	1.81	0.62
1:A:721:GLN:HG2	4:B:169:HOH:O	2.03	0.59
1:A:493:LEU:HD23	1:A:515:LEU:HD11	1.84	0.59
1:A:629:LYS:O	1:A:632:ILE:HD13	2.03	0.58
1:A:464:ALA:HB3	1:A:632:ILE:HD11	1.88	0.55
1:A:469:GLU:OE1	1:A:609:ARG:NH2	2.40	0.54
3:A:902:STU:C26	3:A:902:STU:H16	2.38	0.53
1:A:493:LEU:CD2	1:A:515:LEU:HD11	2.40	0.51
1:A:504:PHE:HB3	1:A:515:LEU:HD22	1.92	0.50
1:A:480:PHE:CD1	1:A:545:LEU:HD22	2.47	0.49
1:A:579:ARG:HG2	1:A:586:LEU:HD23	1.95	0.49
1:A:571[B]:ASN:ND2	1:A:721:GLN:HE22	2.13	0.46
1:A:613:GLN:NE2	1:A:707[B]:GLU:OE2	2.38	0.46
1:A:512:LEU:HD23	1:A:520:PHE:C	2.36	0.46
1:A:520:PHE:CZ	1:A:529:HIS:CB	2.99	0.45
1:A:656:ARG:HD3	1:A:658:LYS:HZ3	1.83	0.44
3:A:903:STU:H16	3:A:903:STU:C26	2.45	0.42
3:A:902:STU:C26	3:A:902:STU:C16	2.98	0.41
1:A:610:ILE:CD1	1:A:707[B]:GLU:HG3	2.51	0.41
1:A:596:LEU:HD22	1:A:600:LEU:HD23	2.02	0.41
1:A:464:ALA:CB	1:A:632:ILE:HD11	2.51	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	357/377 (95%)	349 (98%)	7 (2%)	1 (0%)	46	25
2	B	4/6 (67%)	4 (100%)	0	0	100	100
All	All	361/383 (94%)	353 (98%)	7 (2%)	1 (0%)	46	25

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	701	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	305/327 (93%)	303 (99%)	2 (1%)	88	79
2	B	5/5 (100%)	5 (100%)	0	100	100
All	All	310/332 (93%)	308 (99%)	2 (1%)	88	83

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	594	GLU
1	A	821	HIS

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 molecules 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 ⓘ

3 ligands 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$
3	STU	A	901	-	27,42,42	1.46	6 (22%)	23,68,68	0.95	1 (4%)
3	STU	A	902	-	27,42,42	1.22	3 (11%)	23,68,68	1.10	1 (4%)
3	STU	A	903	-	27,42,42	1.48	4 (14%)	23,68,68	1.09	2 (8%)

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
3	STU	A	901	-	-	0/4/42/42	0/0/8/8
3	STU	A	902	-	-	0/4/42/42	0/0/8/8
3	STU	A	903	-	-	0/4/42/42	0/0/8/8

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	902	STU	C11-C18	-2.46	1.39	1.42
3	A	901	STU	C6-C19	-2.38	1.39	1.42
3	A	901	STU	C7-C6	-2.32	1.39	1.43
3	A	903	STU	C11-C18	-2.20	1.39	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	903	STU	C7-C8	-2.16	1.40	1.49
3	A	901	STU	C7-C8	-2.02	1.41	1.49
3	A	901	STU	C26-C21	2.03	1.54	1.51
3	A	902	STU	C3-C4	2.06	1.41	1.36
3	A	902	STU	C22-C23	2.22	1.55	1.52
3	A	901	STU	C3-C4	2.41	1.42	1.36
3	A	901	STU	C24-C25	2.88	1.56	1.51
3	A	903	STU	C26-C21	3.19	1.55	1.51
3	A	903	STU	C24-C25	4.33	1.58	1.51

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	903	STU	C1-C20-N3	-2.14	129.61	132.18
3	A	903	STU	C16-C17-C12	-2.11	117.69	120.73
3	A	901	STU	C16-C17-C12	-2.08	117.73	120.73
3	A	902	STU	C16-C17-C12	-2.00	117.84	120.73

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	901	STU	1	0
3	A	902	STU	3	0
3	A	903	STU	2	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	356/377 (94%)	2.16	133 (37%)  	24, 37, 52, 63	0
2	B	5/6 (83%)	0.20	0  	31, 32, 38, 51	0
All	All	361/383 (94%)	2.14	133 (36%)  	24, 37, 52, 63	0

All (133) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	512	LEU	11.1
1	A	536	PRO	10.3
1	A	513	TYR	9.0
1	A	471	ALA	8.5
1	A	473	LEU	8.5
1	A	495	VAL	8.2
1	A	478	GLY	7.7
1	A	544	VAL	7.7
1	A	480	PHE	7.4
1	A	537	LEU	7.3
1	A	474	LEU	7.1
1	A	515	LEU	6.8
1	A	546	HIS	6.7
1	A	477	SER	6.5
1	A	543	VAL	6.4
1	A	506	ILE	6.4
1	A	470	VAL	6.4
1	A	460	TRP	6.4
1	A	533	THR	6.4
1	A	530	LEU	6.3
1	A	520	PHE	6.0
1	A	549	VAL	6.0
1	A	531	LEU	5.8
1	A	511	ASN	5.8

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Mol	Chain	Res	Type	RSRZ
1	A	529	HIS	5.4
1	A	493	LEU	5.4
1	A	504	PHE	5.3
1	A	535	GLN	5.2
1	A	489	GLN	5.2
1	A	523	ILE	5.0
1	A	532	SER	5.0
1	A	521	PRO	4.9
1	A	454	PRO	4.9
1	A	475	VAL	4.9
1	A	545	LEU	4.8
1	A	479	ASP	4.7
1	A	482	VAL	4.6
1	A	503	HIS	4.4
1	A	716	SER	4.2
1	A	505	ILE	4.2
1	A	501	PRO	3.9
1	A	485	SER	3.9
1	A	527	ILE	3.8
1	A	764	LEU	3.8
1	A	456	HIS	3.8
1	A	717	GLY	3.8
1	A	465	ILE	3.8
1	A	491	TYR	3.7
1	A	678	CYS	3.6
1	A	476	HIS	3.6
1	A	767	GLN	3.6
1	A	534	GLN	3.6
1	A	679	CYS	3.6
1	A	525	LEU	3.4
1	A	492	VAL	3.3
1	A	455	LEU	3.3
1	A	620	VAL	3.3
1	A	514	ARG	3.3
1	A	524	PRO	3.3
1	A	571[A]	ASN	3.2
1	A	699[A]	ILE	3.2
1	A	486	GLN	3.2
1	A	483	ARG	3.1
1	A	702	PHE	3.1
1	A	684	LEU	3.1
1	A	691	VAL	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	596	LEU	3.1
1	A	690	LEU	3.0
1	A	773	VAL	3.0
1	A	611	LEU	3.0
1	A	461	TYR	3.0
1	A	547	ARG	3.0
1	A	490	GLU	2.9
1	A	674	LEU	2.9
1	A	686	ALA	2.9
1	A	597	PRO	2.8
1	A	772	PHE	2.8
1	A	689	CYS	2.8
1	A	634	ILE	2.7
1	A	449	PRO	2.7
1	A	661	LEU	2.7
1	A	466	PRO	2.7
1	A	719	LEU	2.7
1	A	623[A]	ILE	2.7
1	A	763	ASN	2.7
1	A	567	ILE	2.6
1	A	619	ILE	2.6
1	A	448	ILE	2.5
1	A	484	GLU	2.5
1	A	575	VAL	2.5
1	A	554	TRP	2.5
1	A	638	LEU	2.5
1	A	739[A]	SER	2.4
1	A	588	ALA	2.4
1	A	610	ILE	2.4
1	A	572	PHE	2.4
1	A	576	PHE	2.4
1	A	635	VAL	2.4
1	A	594	GLU	2.4
1	A	451[A]	VAL	2.4
1	A	769	THR	2.4
1	A	818[A]	ARG	2.3
1	A	696	VAL	2.3
1	A	472	GLU	2.3
1	A	632	ILE	2.3
1	A	453	LYS	2.3
1	A	622	LEU	2.3
1	A	749	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	671	MET	2.3
1	A	741[A]	SER	2.3
1	A	785	CYS	2.3
1	A	660	LEU	2.2
1	A	797	TRP	2.2
1	A	807	PHE	2.2
1	A	626	CYS	2.2
1	A	464	ALA	2.2
1	A	669	ALA	2.2
1	A	481	LEU	2.2
1	A	645	LEU	2.2
1	A	644	PHE	2.1
1	A	502	ARG	2.1
1	A	550	PRO	2.1
1	A	673	TYR	2.1
1	A	555	VAL	2.1
1	A	729	PRO	2.1
1	A	697	LEU	2.1
1	A	664	VAL	2.0
1	A	762	PRO	2.0
1	A	614	TYR	2.0
1	A	734	TYR	2.0
1	A	668	ALA	2.0
1	A	598	PRO	2.0
1	A	685	ALA	2.0

## 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 ⓘ

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( $\text{\AA}^2$ )	Q<0.9
3	STU	A	903	35/35	0.82	0.19	0.19	30,35,43,47	0
3	STU	A	902	35/35	0.89	0.16	-0.44	24,30,34,38	0
3	STU	A	901	35/35	0.93	0.11	-3.81	18,22,27,36	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.