



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 08:30 PM GMT

PDB ID : 1KLI  
Title : Cofactor-and substrate-assisted activation of factor VIIa  
Authors : Sichler, K.; Banner, D.W.; D'Arcy, A.; Hopfner, K.P.; Huber, R.; Bode, W.;  
Kresse, G.B.; Kopetzki, E.; Brandstetter, H.  
Deposited on : 2001-12-12  
Resolution : 1.69 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.

---

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

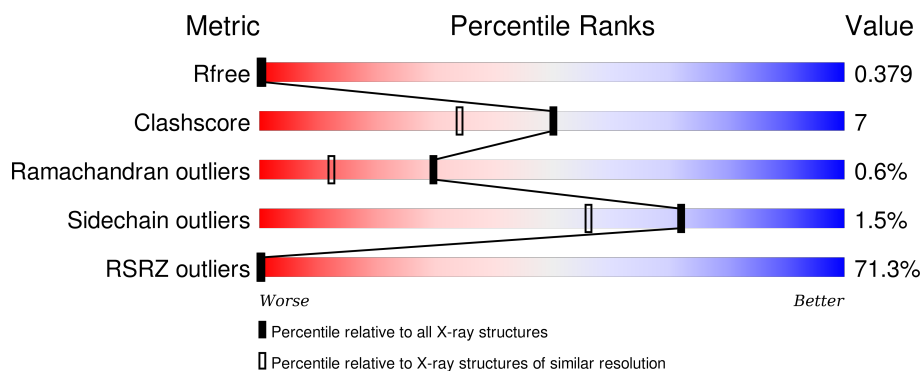
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.69 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	3190 (1.70-1.70)
Clashscore	102246	3585 (1.70-1.70)
Ramachandran outliers	100387	3527 (1.70-1.70)
Sidechain outliers	100360	3527 (1.70-1.70)
RSRZ outliers	91569	3200 (1.70-1.70)

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	L	69	
2	H	254	

## 2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 2796 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.

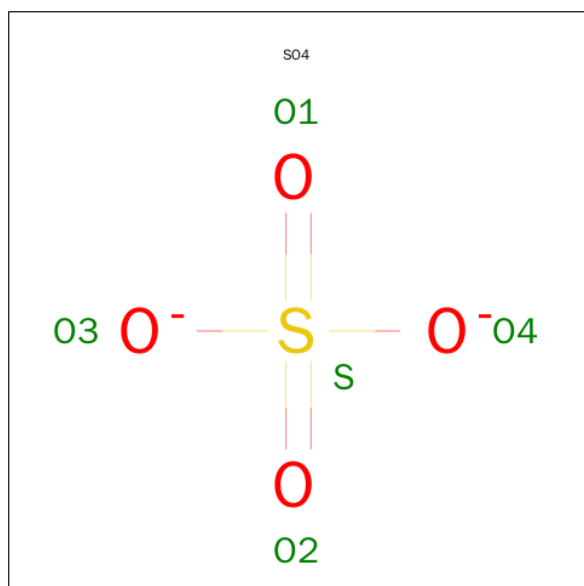
- Molecule 1 is a protein called factor VIIa.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	L	61	Total	C	N	O	S	18	1	0
			469	283	84	95	7			

- Molecule 2 is a protein called factor VIIa.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	254	Total	C	N	O	S	16	5	0
			1992	1266	353	360	13			

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	H	1	Total	O	S	0	0
			5	4	1		
3	H	1	Total	O	S	0	0
			5	4	1		

*Continued on next page...*

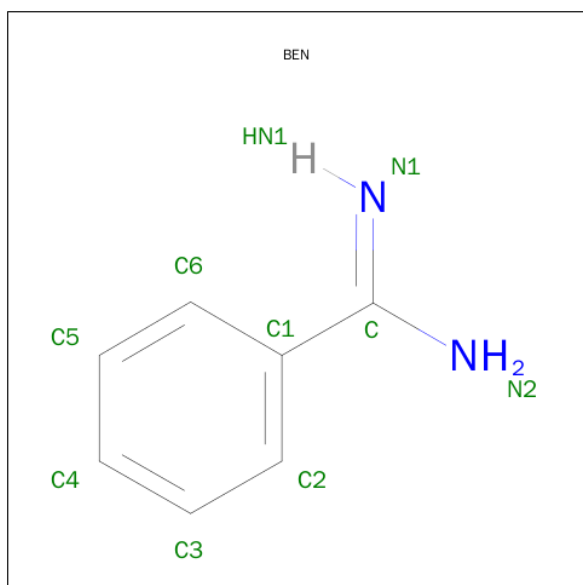
*Continued from previous page...*

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	H	1	Total	O	S	0	0
			5	4	1		
3	H	1	Total	O	S	0	0
			5	4	1		

- Molecule 4 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	H	1	Total	Ca	0	0
			1	1		

- Molecule 5 is BENZAMIDINE (three-letter code: BEN) (formula: C<sub>7</sub>H<sub>8</sub>N<sub>2</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	H	1	Total	C	N	0	0
			9	7	2		

- Molecule 6 is GLYCEROL (three-letter code: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	H	1	Total	C	O	0	0
			6	3	3		

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	H	237	Total	O	0	0
			237	237		
7	L	62	Total	O	0	0
			62	62		



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	94.44Å 94.44Å 114.31Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 1.69 24.45 – 1.66	Depositor EDS
% Data completeness (in resolution range)	(Not available) (20.00-1.69) 96.9 (24.45-1.66)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.13 (at 1.66Å)	Xtriage
Refinement program	CNS	Depositor
R, $R_{free}$	0.209 , 0.225 0.379 , 0.379	Depositor DCC
$R_{free}$ test set	5882 reflections (10.13%)	DCC
Wilson B-factor (Å <sup>2</sup> )	18.0	Xtriage
Anisotropy	0.278	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.41 , 37.9	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	1 of 59659 reflections (0.002%)	Xtriage
$F_o, F_c$ correlation	0.83	EDS
Total number of atoms	2796	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.60% 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: GOL, CA, BEN, SO4

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	L	0.27	0/482	0.53	0/651
2	H	0.30	0/2062	0.59	1/2807 (0.0%)
All	All	0.29	0/2544	0.58	1/3458 (0.0%)

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
2	H	0	1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
2	H	199	HIS	N-CA-C	-5.78	95.39	111.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	H	107	ARG	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	L	469	0	439	9	0
2	H	1992	0	1977	28	4
3	H	20	0	0	0	0
4	H	1	0	0	0	0
5	H	9	0	8	0	0
6	H	6	0	7	0	0
7	H	237	0	0	5	4
7	L	62	0	0	0	3
All	All	2796	0	2431	34	8

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 7.

All (34) 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)
2:H:50[B]:ILE:HG22	2:H:111:PRO:HB3	1.50	0.94
1:L:88:GLN:HE22	1:L:94:GLU:HB2	1.47	0.79
2:H:127:THR:O	2:H:129(B):ARG:HG2	1.84	0.76
2:H:50[B]:ILE:CG2	2:H:111:PRO:HB3	2.18	0.73
2:H:45:THR:OG1	2:H:198:PRO:HB3	1.97	0.64
2:H:35[A]:VAL:HG22	2:H:64[A]:LEU:HD23	1.81	0.62
2:H:62:ARG:NH2	2:H:250:VAL:HG23	2.14	0.62
2:H:50[B]:ILE:HG22	2:H:111:PRO:CB	2.28	0.62
2:H:60(B):ILE:HD12	2:H:64[A]:LEU:HD21	1.81	0.61
2:H:64[B]:LEU:HG	2:H:85:VAL:HG21	1.84	0.60
1:L:140:ILE:HD11	2:H:26:GLU:HG3	1.86	0.57
2:H:48:ASN:HD21	2:H:51:TRP:HB2	1.69	0.55
1:L:115:HIS:HE1	7:H:516:HOH:O	1.89	0.55
2:H:48:ASN:ND2	2:H:51:TRP:HB2	2.24	0.52
2:H:144:LEU:HD21	2:H:152:ALA:HB2	1.92	0.51
2:H:27:CYS:HB3	7:H:568:HOH:O	2.10	0.50
1:L:140:ILE:HD11	2:H:26:GLU:CG	2.42	0.49
2:H:48:ASN:HB2	7:H:627:HOH:O	2.13	0.48
2:H:235:ILE:O	2:H:239[A]:GLN:HG3	2.13	0.48
1:L:89:LEU:HG	1:L:108:THR:HG23	1.95	0.48
1:L:110:ARG:HD2	1:L:110:ARG:C	2.34	0.47
2:H:256:PHE:HA	2:H:257:PRO:C	2.35	0.47
2:H:51:TRP:CZ3	2:H:107:ARG:HB2	2.51	0.45
1:L:99:GLU:HA	2:H:204:ARG:HD2	1.99	0.45

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:98:THR:HB	7:H:710:HOH:O	2.16	0.44
2:H:35[A]:VAL:CG2	2:H:41:LEU:HD22	2.48	0.44
1:L:101:TYR:OH	1:L:115:HIS:HD2	2.01	0.44
2:H:90:ILE:HG23	2:H:91:PRO:HD2	2.01	0.43
1:L:105:HIS:HB2	1:L:109:LYS:HB2	2.01	0.43
2:H:176:ILE:HD13	2:H:182:CYS:SG	2.59	0.42
2:H:100:ASN:HA	2:H:100:ASN:HD22	1.66	0.41
2:H:135:PHE:HB3	2:H:159:ASN:ND2	2.36	0.41
2:H:135:PHE:HB3	2:H:159:ASN:HD21	1.86	0.40
2:H:37:ASN:HB2	7:H:740:HOH:O	2.21	0.40

All (8) 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)
2:H:77:ASP:O	7:L:748:HOH:O[5_555]	2.03	0.17
7:H:677:HOH:O	7:H:774:HOH:O[4_454]	2.05	0.15
7:H:673:HOH:O	7:H:769:HOH:O[4_454]	2.06	0.14
2:H:40:GLN:N	7:L:530:HOH:O[5_555]	2.09	0.11
2:H:74:SER:O	7:L:604:HOH:O[5_555]	2.09	0.11
2:H:147:ARG:O	2:H:253:ARG:N[3_555]	2.10	0.10
7:H:779:HOH:O	7:H:788:HOH:O[4_454]	2.14	0.06
7:H:598:HOH:O	7:H:657:HOH:O[4_454]	2.16	0.04

## 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	L	60/69 (87%)	54 (90%)	4 (7%)	2 (3%)	5	0
2	H	257/254 (101%)	246 (96%)	11 (4%)	0	100	100
All	All	317/323 (98%)	300 (95%)	15 (5%)	2 (1%)	30	12

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	L	86	ASP
1	L	88	GLN

### 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	L	55/60 (92%)	55 (100%)	0	100	100
2	H	221/216 (102%)	217 (98%)	4 (2%)	66	49
All	All	276/276 (100%)	272 (99%)	4 (1%)	72	59

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	H	29	TRP
2	H	100	ASN
2	H	159	ASN
2	H	217	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	L	88	GLN
1	L	93	ASN
1	L	115	HIS
2	H	60(D)	ASN
2	H	63	ASN
2	H	100	ASN
2	H	109	HIS
2	H	159	ASN
2	H	170(A)	GLN
2	H	217	GLN

### 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 ⓘ

Of 7 ligands modelled in this entry, 1 is monoatomic - leaving 6 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$
6	GOL	H	1000	-	5,5,5	0.42	0	5,5,5	1.90	3 (60%)
5	BEN	H	300	-	9,9,9	2.14	4 (44%)	9,11,11	1.22	1 (11%)
3	SO4	H	400	-	4,4,4	0.67	0	6,6,6	0.50	0
3	SO4	H	401	-	4,4,4	1.03	0	6,6,6	0.30	0
3	SO4	H	402	-	4,4,4	0.84	0	6,6,6	0.36	0
3	SO4	H	403	-	4,4,4	0.55	0	6,6,6	0.17	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
6	GOL	H	1000	-	-	0/4/4/4	0/0/0/0
5	BEN	H	300	-	-	0/4/4/4	0/1/1/1
3	SO4	H	400	-	-	0/0/0/0	0/0/0/0
3	SO4	H	401	-	-	0/0/0/0	0/0/0/0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	SO4	H	402	-	-	0/0/0/0	0/0/0/0
3	SO4	H	403	-	-	0/0/0/0	0/0/0/0

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	H	300	BEN	C5-C4	2.48	1.44	1.38
5	H	300	BEN	C-N1	2.67	1.38	1.28
5	H	300	BEN	C5-C6	3.05	1.45	1.38
5	H	300	BEN	C6-C1	3.27	1.44	1.39

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	H	1000	GOL	O2-C2-C3	2.23	118.89	108.65
6	H	1000	GOL	C3-C2-C1	2.24	119.89	111.12
5	H	300	BEN	C1-C-N2	2.24	121.69	118.11
6	H	1000	GOL	O2-C2-C1	2.70	121.02	108.65

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 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	L	60/69 (86%)	3.17	32 (53%)  	15, 21, 82, 90	2 (3%)
2	H	254/254 (100%)	3.08	192 (75%)  	12, 20, 46, 79	5 (1%)
All	All	314/323 (97%)	3.09	224 (71%)  	12, 20, 59, 90	7 (2%)

All (224) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	L	90	ILE	14.8
2	H	170(E)	VAL	14.3
1	L	89	LEU	14.2
2	H	170(H)	SER	13.8
1	L	87	ASP	11.3
2	H	170(F)	GLY	11.0
1	L	86	ASP	10.5
1	L	88	GLN	9.5
2	H	222	VAL	8.4
2	H	184	TYR	8.2
2	H	168	CYS	8.0
2	H	170(C)	ARG	7.6
2	H	145	LEU	7.4
1	L	108	THR	7.4
2	H	223	GLY	7.1
2	H	170(D)	LYS	7.1
1	L	85	LYS	7.0
2	H	225	PHE	7.0
2	H	169	LEU	6.9
2	H	220	CYS	6.7
2	H	60(D)	ASN	6.5
2	H	144	LEU	6.4
2	H	221	THR	6.4
2	H	135	PHE	6.2

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
2	H	163	LEU	6.1
2	H	175	ASN	5.6
1	L	92	VAL	5.6
2	H	170(A)	GLN	5.4
2	H	17	VAL	5.4
2	H	176	ILE	5.3
1	L	144	ARG	5.3
2	H	170(G)	ASP	5.3
1	L	107	GLY	5.3
2	H	21	VAL	5.2
2	H	217	GLN	5.2
2	H	170(B)	SER	5.1
2	H	188(A)	SER	5.1
1	L	105	HIS	5.0
2	H	19	GLY	4.9
2	H	221(A)	ALA	4.9
2	H	18	GLY	4.7
2	H	170(I)	PRO	4.7
2	H	191	CYS	4.7
2	H	62	ARG	4.7
2	H	183	ALA	4.7
2	H	215	TRP	4.6
2	H	170	GLN	4.6
2	H	16	ILE	4.4
2	H	227	VAL	4.4
2	H	212	ILE	4.3
2	H	155	LEU	4.3
2	H	182	CYS	4.3
2	H	150	ALA	4.3
2	H	27	CYS	4.3
2	H	73	LEU	4.2
1	L	93	ASN	4.1
2	H	149	GLY	4.1
2	H	129(F)	PHE	4.0
2	H	211	GLY	4.0
1	L	106	THR	4.0
2	H	181	PHE	3.9
2	H	185	SER	3.9
2	H	58	CYS	3.9
2	H	129(D)	LEU	3.9
2	H	35[A]	VAL	3.9
2	H	147	ARG	3.9

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
2	H	251	LEU	3.8
1	L	140	ILE	3.8
2	H	90	ILE	3.8
2	H	164	MET	3.8
2	H	190	SER	3.8
2	H	29	TRP	3.8
2	H	193	GLY	3.7
2	H	141	TRP	3.7
2	H	33	LEU	3.7
2	H	186	ASP	3.7
2	H	68	LEU	3.7
2	H	167	ASP	3.7
2	H	74	SER	3.7
2	H	138	VAL	3.6
2	H	156	MET	3.6
2	H	192	LYS	3.5
2	H	105	LEU	3.5
2	H	98	THR	3.5
2	H	158	LEU	3.5
2	H	204	ARG	3.5
2	H	59	PHE	3.5
2	H	153	LEU	3.5
2	H	213	VAL	3.4
2	H	197	GLY	3.4
1	L	98	CYS	3.4
2	H	55	ALA	3.4
2	H	121	LEU	3.4
2	H	137	LEU	3.4
2	H	61	TRP	3.4
2	H	85	VAL	3.4
1	L	141	LEU	3.3
2	H	224	HIS	3.3
2	H	66	ALA	3.3
2	H	42	CYS	3.3
2	H	37	ASN	3.3
2	H	67	VAL	3.3
2	H	63	ASN	3.3
2	H	31	VAL	3.2
2	H	207	TRP	3.2
1	L	143	LYS	3.2
2	H	187	GLY	3.2
2	H	157	VAL	3.2

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
2	H	228	TYR	3.2
2	H	128	PHE	3.1
2	H	152	ALA	3.1
2	H	161	PRO	3.1
2	H	198	PRO	3.1
2	H	134	ARG	3.1
2	H	209	LEU	3.1
2	H	151	THR	3.1
2	H	195	SER	3.1
2	H	101	HIS	3.1
2	H	84	ARG	3.0
2	H	208	TYR	3.0
2	H	103	ILE	3.0
2	H	219	GLY	3.0
2	H	47	ILE	3.0
2	H	139	SER	3.0
2	H	231	VAL	3.0
2	H	146	ASP	2.9
2	H	56	ALA	2.9
2	H	38	GLY	2.9
2	H	129	SER	2.9
2	H	237	TRP	2.9
2	H	104	ALA	2.9
2	H	50[A]	ILE	2.9
2	H	229	THR	2.9
2	H	166	GLN	2.8
2	H	64[A]	LEU	2.8
1	L	125	VAL	2.8
2	H	188	LYS	2.8
2	H	39	ALA	2.8
2	H	203	TYR	2.8
2	H	52	VAL	2.8
2	H	160	VAL	2.8
2	H	159	ASN	2.8
2	H	143	GLN	2.7
2	H	53	VAL	2.7
2	H	41	LEU	2.7
2	H	210	THR	2.7
1	L	101	TYR	2.7
2	H	46	LEU	2.7
1	L	94	GLU	2.7
2	H	28	PRO	2.7

*Continued on next page...*

*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
2	H	118	VAL	2.7
2	H	60(B)	ILE	2.7
2	H	34	LEU	2.7
2	H	97	GLY	2.6
1	L	122	ALA	2.6
2	H	76	HIS	2.6
2	H	136	SER	2.6
1	L	95	ASN	2.6
2	H	60(A)	LYS	2.6
2	H	75	GLU	2.5
2	H	65	ILE	2.5
2	H	82[A]	SER	2.5
2	H	57	HIS	2.5
2	H	45	THR	2.5
2	H	106	LEU	2.5
2	H	129(B)	ARG	2.5
1	L	138	ILE	2.5
2	H	123	LEU	2.5
2	H	30	GLN	2.5
2	H	189	ASP	2.5
2	H	124	PRO	2.5
2	H	32	LEU	2.5
2	H	214	SER	2.5
2	H	60(C)	LYS	2.4
2	H	23	PRO	2.4
2	H	99	THR	2.4
1	L	103	SER	2.4
2	H	88	VAL	2.4
2	H	200	ALA	2.4
2	H	202	HIS	2.4
2	H	199	HIS	2.4
2	H	184(A)	GLY	2.3
2	H	94	TYR	2.3
2	H	22	CYS	2.3
2	H	93	THR	2.3
2	H	77	ASP	2.3
1	L	111	SER	2.3
1	L	91	CYS	2.3
2	H	109	HIS	2.3
2	H	226	GLY	2.3
2	H	238	LEU	2.3
2	H	140	GLY	2.3

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	L	102	CYS	2.3
2	H	48	ASN	2.2
2	H	51	TRP	2.2
2	H	165	THR	2.2
2	H	180	MET	2.2
1	L	120	LEU	2.2
1	L	139	PRO	2.2
2	H	235	ILE	2.2
2	H	119	VAL	2.2
2	H	256	PHE	2.2
1	L	134	PRO	2.2
1	L	136	GLY	2.2
2	H	26	GLU	2.2
2	H	196	GLY	2.2
2	H	96	PRO	2.1
2	H	108	LEU	2.1
2	H	142	GLY	2.1
2	H	129(E)	ALA	2.1
2	H	120	PRO	2.1
2	H	177	THR	2.1
1	L	112	CYS	2.1
2	H	89	ILE	2.1
2	H	111	PRO	2.1
2	H	194	ASP	2.1
2	H	205	GLY	2.1
2	H	178	GLU	2.1
2	H	179	TYR	2.0
2	H	234	TYR	2.0
2	H	43	GLY	2.0
2	H	122	CYS	2.0
2	H	230	ARG	2.0
2	H	129(C)	THR	2.0

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

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

## 6.3 Carbohydrates [i](#)

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( $\text{\AA}^2$ )	Q<0.9
6	GOL	H	1000	6/6	0.78	0.22	0.15	29,44,52,54	0
3	SO4	H	402	5/5	0.59	0.32	-0.04	45,46,55,56	5
5	BEN	H	300	9/9	0.57	0.24	-0.32	22,26,28,30	0
3	SO4	H	401	5/5	0.81	0.21	-0.72	33,38,44,44	5
4	CA	H	900	1/1	0.53	0.19	-1.38	20,20,20,20	0
3	SO4	H	400	5/5	0.77	0.20	-	41,42,42,45	5
3	SO4	H	403	5/5	0.90	0.15	-	41,44,47,49	5

## 6.5 Other polymers [i](#)

There are no such residues in this entry.