



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 07:00 PM GMT

PDB ID : 1DKI  
Title : CRYSTAL STRUCTURE OF THE ZYMOGEN FORM OF STREPTOCOCCAL PYROGENIC EXOTOXIN B ACTIVE SITE (C47S) MUTANT  
Authors : Kagawa, T.F.; Cooney, J.C.; Baker, H.M.; McSweeney, S.; Liu, M.; Gubba, S.; Musser, J.M.; Baker, E.N.  
Deposited on : 1999-12-07  
Resolution : 1.60 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

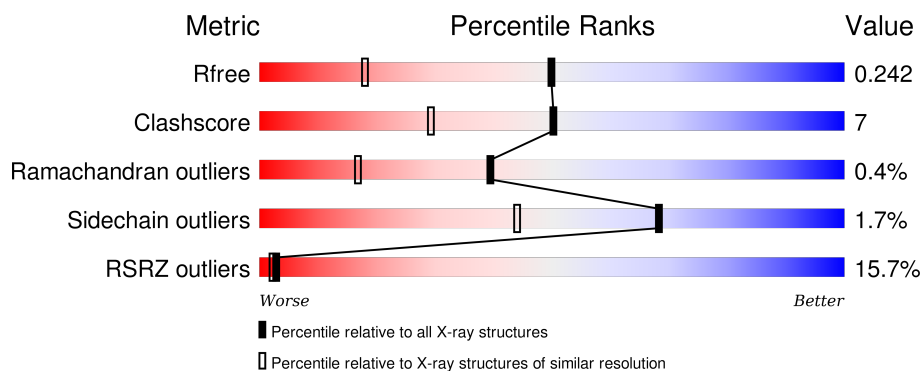
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.60 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	2475 (1.60-1.60)
Clashscore	102246	2732 (1.60-1.60)
Ramachandran outliers	100387	2654 (1.60-1.60)
Sidechain outliers	100360	2653 (1.60-1.60)
RSRZ outliers	91569	2479 (1.60-1.60)

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	371	<div> <div>17%</div> <div>68%</div> <div>13%</div> <div>•</div> <div>18%</div> </div>
1	B	371	<div> <div>16%</div> <div>67%</div> <div>17%</div> <div>•</div> <div>14%</div> </div>
1	C	371	<div> <div>11%</div> <div>81%</div> <div>11%</div> <div>9%</div> </div>
1	D	371	<div> <div>11%</div> <div>80%</div> <div>10%</div> <div>•</div> <div>10%</div> </div>

## 2 Entry composition [i](#)

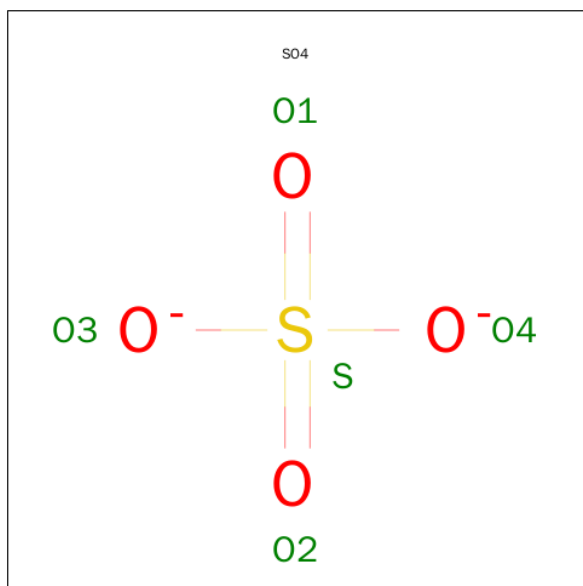
There are 3 unique types of molecules in this entry. The entry contains 10562 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 PYROGENIC EXOTOXIN B ZYMOGEN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	303	Total	C	N	O	S	0	0	0
			2312	1463	400	443	6			
1	B	320	Total	C	N	O	S	0	0	2
			2426	1529	425	466	6			
1	C	339	Total	C	N	O	S	0	0	1
			2590	1638	446	500	6			
1	D	334	Total	C	N	O	S	0	0	0
			2575	1624	444	501	6			

- Molecule 2 is SULFATE ION (three-letter code: SO<sub>4</sub>) (formula: O<sub>4</sub>S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	C	1	Total	O	S	0	0
			5	4	1		
2	D	1	Total	O	S	0	0
			5	4	1		

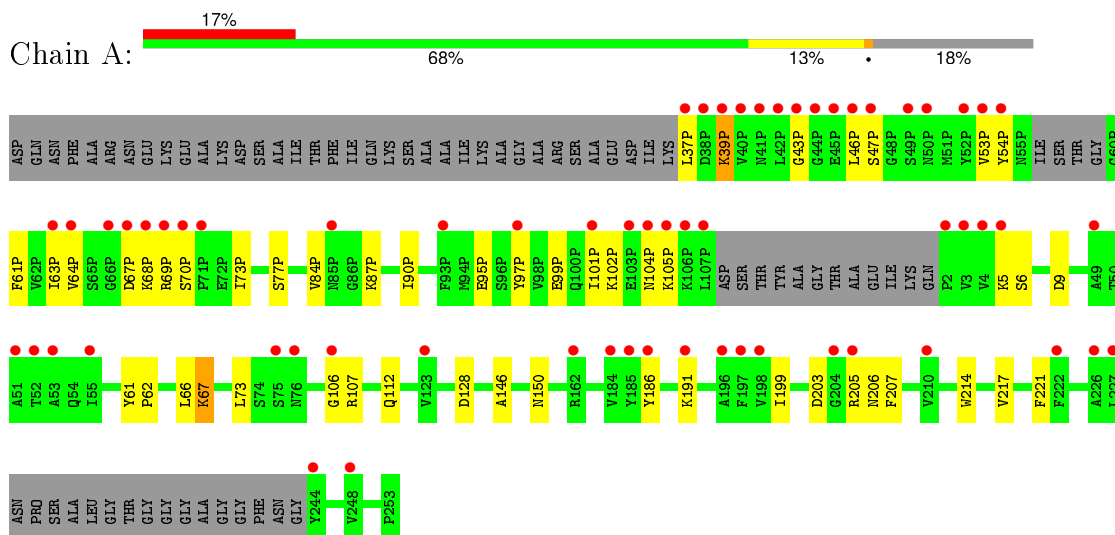
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	120	Total	O	0	0
			120	120		
3	B	98	Total	O	0	0
			98	98		
3	C	188	Total	O	0	0
			188	188		
3	D	233	Total	O	0	0
			233	233		

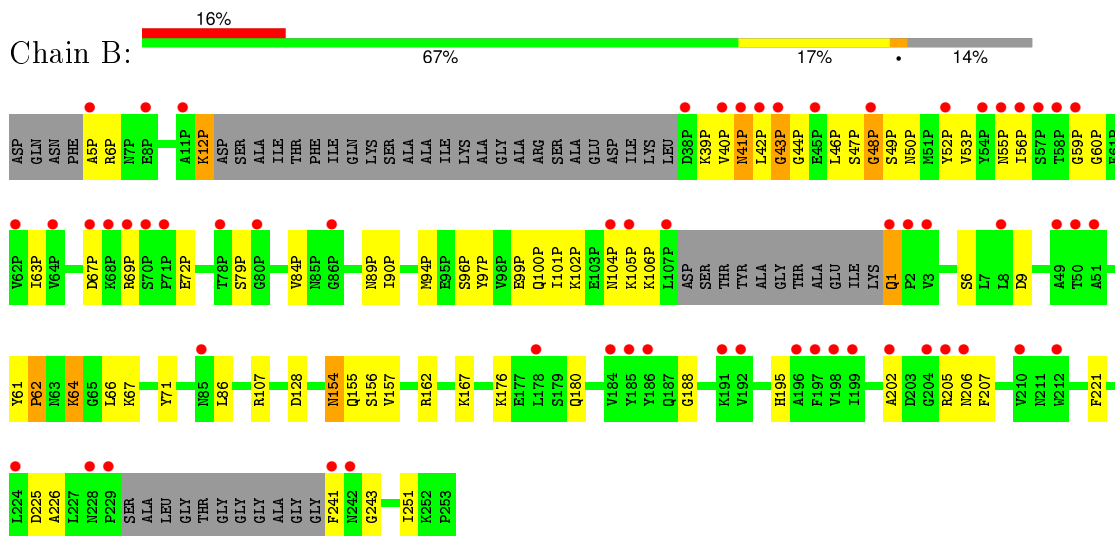
### 3 Residue-property plots

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.

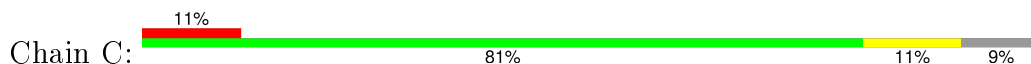
- Molecule 1: PYROGENIC EXOTOXIN B ZYMOGEN

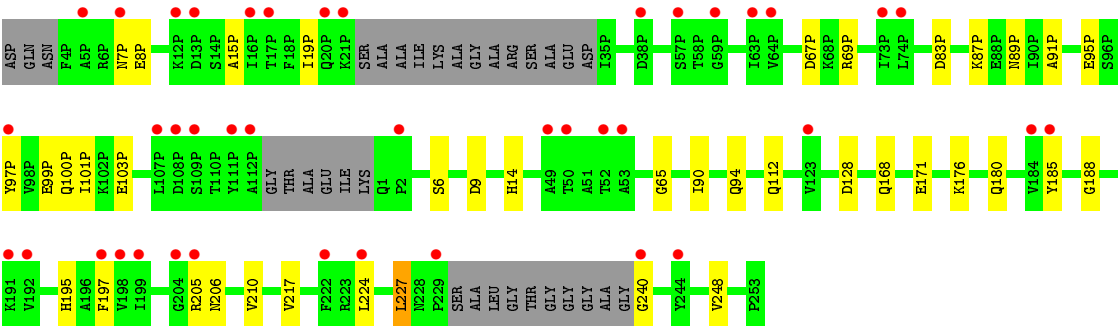


- Molecule 1: PYROGENIC EXOTOXIN B ZYMOGEN

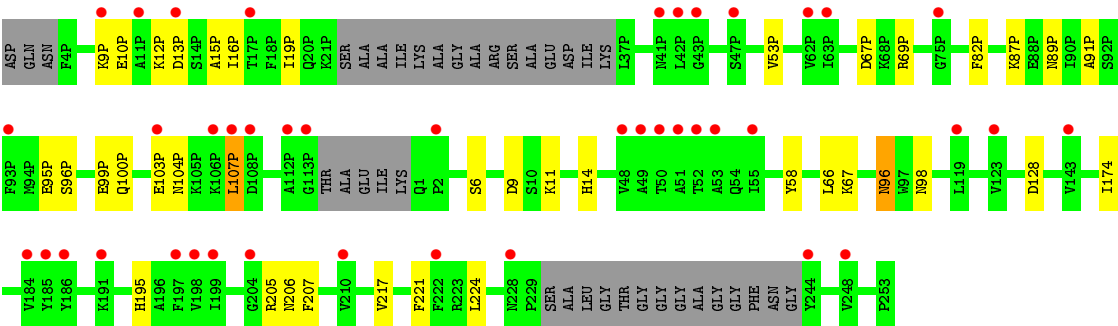
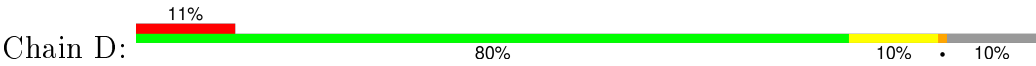


- Molecule 1: PYROGENIC EXOTOXIN B ZYMOGEN





● Molecule 1: PYROGENIC EXOTOXIN B ZYMOGEN



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	46.66Å 116.56Å 144.73Å 90.00° 94.17° 90.00°	Depositor
Resolution (Å)	30.00 – 1.60 28.94 – 1.60	Depositor EDS
% Data completeness (in resolution range)	83.1 (30.00-1.60) 83.1 (28.94-1.60)	Depositor EDS
$R_{merge}$	0.04	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.48 (at 1.60Å)	Xtriage
Refinement program	CNS 0.9	Depositor
R, $R_{free}$	0.218 , 0.245 0.216 , 0.242	Depositor DCC
$R_{free}$ test set	16726 reflections (11.03%)	DCC
Wilson B-factor (Å <sup>2</sup> )	29.6	Xtriage
Anisotropy	0.036	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 48.7	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 168400 reflections	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	10562	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.47% 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: 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	A	0.45	0/2365	0.66	0/3195
1	B	0.40	0/2480	0.63	1/3350 (0.0%)
1	C	0.46	0/2647	0.66	1/3576 (0.0%)
1	D	0.50	0/2632	0.68	0/3556
All	All	0.46	0/10124	0.66	2/13677 (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	C	188	GLY	N-CA-C	-5.41	99.57	113.10
1	B	188	GLY	N-CA-C	-5.12	100.31	113.10

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	2312	0	2196	38	0
1	B	2426	0	2287	48	0
1	C	2590	0	2455	25	0
1	D	2575	0	2457	25	0
2	A	5	0	0	0	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	5	0	0	0	0
2	C	5	0	0	0	0
2	D	5	0	0	0	0
3	A	120	0	0	2	0
3	B	98	0	0	0	0
3	C	188	0	0	3	0
3	D	233	0	0	2	0
All	All	10562	0	9395	135	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 7.

All (135) 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:C:7(P):ASN:CA	1:C:8(P):GLU:N	1.79	1.44
1:B:6(P):ARG:HH12	1:B:72(P):GLU:HA	1.02	1.08
1:B:225:ASP:CA	1:B:226:ALA:N	2.21	1.04
1:B:99(P):GLU:CA	1:B:100(P):GLN:N	2.28	0.96
1:B:6(P):ARG:NH1	1:B:72(P):GLU:HA	1.84	0.90
1:B:154:ASN:HD22	1:B:156:SER:H	1.12	0.89
1:B:53(P):VAL:HG22	1:B:63(P):ILE:HD12	1.58	0.83
1:C:99(P):GLU:CA	1:C:100(P):GLN:N	2.45	0.79
1:A:39(P):LYS:HB2	1:A:39(P):LYS:NZ	1.97	0.78
1:A:66:LEU:O	1:A:67:LYS:HD2	1.84	0.77
1:B:102(P):LYS:HA	1:B:105(P):LYS:HD3	1.68	0.75
1:A:64(P):VAL:HG12	1:A:73(P):ILE:HD13	1.69	0.74
1:C:176:LYS:HE2	1:C:180:GLN:NE2	2.03	0.73
1:C:14:HIS:HD2	3:C:1149:HOH:O	1.74	0.71
1:B:12(P):LYS:NZ	1:B:12(P):LYS:HB2	2.06	0.70
1:A:101(P):ILE:HA	1:A:104(P):ASN:HD22	1.56	0.70
1:D:96:ASN:HD22	1:D:96:ASN:C	1.96	0.69
1:C:87(P):LYS:HE2	1:C:217:VAL:HG11	1.74	0.69
1:B:5(P):ALA:N	1:B:67(P):ASP:HA	2.09	0.68
1:B:66:LEU:O	1:B:67:LYS:HD2	1.94	0.66
1:A:106:GLY:HA2	3:A:1059:HOH:O	1.96	0.65
1:B:56(P):ILE:HB	1:B:59(P):GLY:O	1.96	0.64
1:A:39(P):LYS:HB2	1:A:39(P):LYS:HZ2	1.63	0.64
1:A:146:ALA:HA	1:A:150:ASN:HD22	1.64	0.62
1:C:176:LYS:HE2	1:C:180:GLN:HE22	1.64	0.61
1:B:205:ARG:O	1:B:206:ASN:HB2	1.99	0.61

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:241:PHE:CZ	1:B:243:GLY:HA2	2.35	0.61
1:A:73:LEU:HD12	3:A:1058:HOH:O	2.00	0.61
1:A:46(P):LEU:HD21	1:A:95(P):GLU:HG3	1.82	0.60
1:D:14:HIS:HD2	3:D:1052:HOH:O	1.85	0.59
1:B:154:ASN:ND2	1:B:156:SER:H	1.94	0.58
1:D:10(P):GLU:O	1:D:13(P):ASP:HB3	2.04	0.58
1:A:203:ASP:OD2	1:A:207:PHE:HB2	2.03	0.58
1:A:70(P):SER:HB3	1:A:104(P):ASN:ND2	2.19	0.58
1:B:61:TYR:CG	1:B:62:PRO:HA	2.39	0.58
1:D:87(P):LYS:HE2	1:D:217:VAL:HG11	1.86	0.57
1:B:12(P):LYS:HZ2	1:B:12(P):LYS:HB2	1.69	0.56
1:B:1:GLN:HE22	1:B:202:ALA:CB	2.18	0.56
1:B:89(P):ASN:HA	1:B:195:HIS:HB3	1.87	0.56
1:B:67(P):ASP:OD2	1:B:69(P):ARG:HB2	2.05	0.56
1:B:61:TYR:CD1	1:B:62:PRO:HA	2.40	0.56
1:B:162:ARG:NH2	1:B:167:LYS:HG2	2.21	0.56
1:D:96(P):SER:O	1:D:100(P):GLN:HG3	2.05	0.56
1:B:154:ASN:HD22	1:B:156:SER:N	1.93	0.55
1:A:207:PHE:HB3	1:A:221:PHE:HB3	1.89	0.55
1:B:49(P):SER:HB2	1:B:52(P):TYR:OH	2.06	0.55
1:B:86:LEU:N	1:B:86:LEU:HD12	2.22	0.54
1:D:205:ARG:O	1:D:206:ASN:HB2	2.07	0.54
1:C:89(P):ASN:HA	1:C:195:HIS:HB3	1.89	0.54
1:A:101(P):ILE:HA	1:A:104(P):ASN:ND2	2.23	0.54
1:B:96(P):SER:O	1:B:100(P):GLN:HG3	2.08	0.54
1:B:1:GLN:HE22	1:B:202:ALA:HB1	1.72	0.53
1:D:89(P):ASN:HA	1:D:195:HIS:HB3	1.91	0.53
1:A:205:ARG:O	1:A:206:ASN:HB2	2.09	0.52
1:C:100(P):GLN:HB3	1:C:227:LEU:HD13	1.91	0.52
1:A:37(P):LEU:HB3	1:A:54(P):TYR:HB3	1.91	0.52
1:C:14:HIS:HE1	3:C:1105:HOH:O	1.92	0.52
1:D:207:PHE:HB3	1:D:221:PHE:HB3	1.92	0.51
1:B:207:PHE:HB3	1:B:221:PHE:HB3	1.92	0.51
1:B:94(P):MET:O	1:B:97(P):TYR:HB2	2.11	0.50
1:D:96:ASN:HD22	1:D:98:ASN:H	1.60	0.49
1:C:205:ARG:O	1:C:206:ASN:HB2	2.10	0.49
1:A:53(P):VAL:HG22	1:A:63(P):ILE:HG23	1.94	0.49
1:C:97(P):TYR:O	1:C:101(P):ILE:HG13	2.12	0.49
1:A:61:TYR:CG	1:A:62:PRO:HA	2.48	0.49
1:A:43(P):GLY:HA2	1:A:47(P):SER:HB3	1.95	0.48
1:B:47(P):SER:O	1:B:48(P):GLY:O	2.31	0.48

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:6:SER:HB3	1:C:9:ASP:HB2	1.95	0.48
1:D:174:ILE:HD12	1:D:224:LEU:HD11	1.96	0.47
1:B:71:TYR:OH	1:B:86:LEU:HD22	2.14	0.47
1:A:102(P):LYS:O	1:A:105(P):LYS:HB2	2.14	0.47
1:D:14:HIS:HE1	3:D:1113:HOH:O	1.97	0.47
1:A:66:LEU:C	1:A:67:LYS:HD2	2.34	0.47
1:B:42(P):LEU:HD11	1:B:53(P):VAL:HG23	1.95	0.47
1:B:157:VAL:HG22	1:B:251:ILE:HA	1.97	0.47
1:D:91(P):ALA:O	1:D:95(P):GLU:HG3	2.14	0.46
1:C:168:GLN:CD	1:C:168:GLN:H	2.18	0.46
1:D:6:SER:HB3	1:D:9:ASP:HB2	1.98	0.46
1:A:186:TYR:CD1	1:A:199:ILE:HD12	2.51	0.46
1:C:15(P):ALA:O	1:C:19(P):ILE:HG13	2.15	0.46
1:D:11:LYS:HD2	1:D:58:TYR:CD1	2.51	0.46
1:A:64(P):VAL:HG12	1:A:73(P):ILE:CD1	2.44	0.45
1:D:96:ASN:HD21	1:D:98:ASN:HB2	1.81	0.45
1:D:96:ASN:ND2	1:D:98:ASN:H	2.15	0.45
1:B:40(P):VAL:HG22	1:B:55(P):ASN:ND2	2.32	0.45
1:D:15(P):ALA:O	1:D:19(P):ILE:HG13	2.17	0.45
1:A:214:TRP:CZ3	1:B:107:ARG:HD3	2.52	0.45
1:D:99(P):GLU:O	1:D:103(P):GLU:HB2	2.16	0.45
1:A:6:SER:HB3	1:A:9:ASP:HB2	1.98	0.45
1:B:104(P):ASN:C	1:B:106(P):LYS:H	2.20	0.45
1:B:64:LYS:HB3	1:B:64:LYS:HE3	1.79	0.45
1:A:70(P):SER:HB3	1:A:104(P):ASN:HD22	1.82	0.44
1:A:39(P):LYS:HB2	1:A:39(P):LYS:HZ3	1.82	0.44
1:B:41(P):ASN:HD22	1:B:41(P):ASN:C	2.21	0.44
1:C:91(P):ALA:O	1:C:95(P):GLU:HG3	2.18	0.44
1:C:100(P):GLN:HG2	1:C:227:LEU:HD22	2.00	0.44
1:C:112:GLN:CD	3:C:1094:HOH:O	2.56	0.44
1:B:176:LYS:HG2	1:B:180:GLN:NE2	2.33	0.43
1:B:50(P):ASN:O	1:B:101(P):ILE:HD13	2.18	0.43
1:B:162:ARG:HH21	1:B:167:LYS:HG2	1.82	0.43
1:C:83(P):ASP:OD1	1:C:87(P):LYS:NZ	2.52	0.43
1:A:87(P):LYS:HZ2	1:A:217:VAL:HG13	1.83	0.43
1:B:84(P):VAL:HG12	1:B:90(P):ILE:CG2	2.49	0.43
1:B:42(P):LEU:HB3	1:B:46(P):LEU:HB2	2.01	0.42
1:B:60(P):GLY:HA2	1:B:79(P):SER:O	2.18	0.42
1:C:103(P):GLU:OE1	1:C:240:GLY:HA2	2.19	0.42
1:D:67(P):ASP:OD2	1:D:69(P):ARG:HB2	2.19	0.42
1:B:154:ASN:ND2	1:B:155:GLN:N	2.68	0.42

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:65:GLY:HA3	1:C:90:ILE:O	2.19	0.42
1:A:46(P):LEU:CD2	1:A:95(P):GLU:HG3	2.48	0.42
1:A:84(P):VAL:HG12	1:A:90(P):ILE:CG2	2.50	0.42
1:B:41(P):ASN:HD22	1:B:43(P):GLY:H	1.68	0.42
1:A:69(P):ARG:HD2	1:A:104(P):ASN:O	2.19	0.42
1:D:9(P):LYS:O	1:D:13(P):ASP:HB2	2.20	0.41
1:A:203:ASP:CG	1:A:207:PHE:HB2	2.39	0.41
1:D:96:ASN:ND2	1:D:96:ASN:C	2.71	0.41
1:B:97(P):TYR:O	1:B:101(P):ILE:HG13	2.20	0.41
1:D:53(P):VAL:HG11	1:D:82(P):PHE:CD2	2.55	0.41
1:D:66:LEU:O	1:D:67:LYS:HD3	2.20	0.41
1:D:12(P):LYS:O	1:D:16(P):ILE:HG13	2.21	0.41
1:A:97(P):TYR:O	1:A:101(P):ILE:HG13	2.21	0.41
1:A:61(P):PHE:CE2	1:A:77(P):SER:HB3	2.56	0.41
1:C:171:GLU:HG2	1:C:224:LEU:HD12	2.02	0.41
1:A:5:LYS:O	1:A:6:SER:C	2.59	0.41
1:B:6:SER:HB3	1:B:9:ASP:HB2	2.03	0.41
1:D:104(P):ASN:O	1:D:107(P):LEU:HB2	2.21	0.41
1:C:197:PHE:CD1	1:C:210:VAL:HG13	2.56	0.41
1:A:107:ARG:HD2	1:A:107:ARG:HH11	1.74	0.41
1:A:95(P):GLU:O	1:A:99(P):GLU:HG3	2.21	0.41
1:C:67(P):ASP:OD1	1:C:69(P):ARG:HB2	2.20	0.41
1:C:185:TYR:HB3	1:C:248:VAL:HB	2.03	0.41
1:A:39(P):LYS:HB3	1:A:54(P):TYR:CE2	2.56	0.40
1:A:67(P):ASP:OD1	1:A:69(P):ARG:HB2	2.21	0.40
1:B:154:ASN:HD22	1:B:155:GLN:N	2.19	0.40
1:C:168:GLN:CD	1:C:168:GLN:N	2.75	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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	295/371 (80%)	281 (95%)	13 (4%)	1 (0%)	46	23
1	B	308/371 (83%)	293 (95%)	11 (4%)	4 (1%)	15	2
1	C	327/371 (88%)	323 (99%)	4 (1%)	0	100	100
1	D	326/371 (88%)	319 (98%)	7 (2%)	0	100	100
All	All	1256/1484 (85%)	1216 (97%)	35 (3%)	5 (0%)	39	17

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	39(P)	LYS
1	B	43(P)	GLY
1	B	44(P)	GLY
1	B	48(P)	GLY
1	A	68(P)	LYS

### 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	241/300 (80%)	236 (98%)	5 (2%)	61	33
1	B	251/300 (84%)	244 (97%)	7 (3%)	51	22
1	C	270/300 (90%)	267 (99%)	3 (1%)	80	63
1	D	272/300 (91%)	269 (99%)	3 (1%)	80	63
All	All	1034/1200 (86%)	1016 (98%)	18 (2%)	68	44

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	39(P)	LYS
1	A	67	LYS
1	A	112	GLN
1	A	128	ASP
1	A	191	LYS
1	B	12(P)	LYS

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	B	41(P)	ASN
1	B	1	GLN
1	B	62	PRO
1	B	64	LYS
1	B	128	ASP
1	B	154	ASN
1	C	94	GLN
1	C	128	ASP
1	C	227	LEU
1	D	107(P)	LEU
1	D	96	ASN
1	D	128	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	104(P)	ASN
1	A	112	GLN
1	A	150	ASN
1	B	41(P)	ASN
1	B	50(P)	ASN
1	B	1	GLN
1	B	36	GLN
1	B	76	ASN
1	B	85	ASN
1	B	94	GLN
1	B	154	ASN
1	B	180	GLN
1	C	14	HIS
1	C	159	GLN
1	C	161	ASN
1	C	180	GLN
1	D	20(P)	GLN
1	D	50(P)	ASN
1	D	85(P)	ASN
1	D	14	HIS
1	D	63	ASN
1	D	94	GLN
1	D	96	ASN
1	D	173	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 ⓘ

4 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	$\# Z  > 2$
2	SO4	A	1001	-	4,4,4	0.53	0	6,6,6	0.25	0
2	SO4	B	1002	-	4,4,4	0.35	0	6,6,6	0.15	0
2	SO4	C	1003	-	4,4,4	0.62	0	6,6,6	0.32	0
2	SO4	D	1004	-	4,4,4	0.35	0	6,6,6	0.31	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
2	SO4	A	1001	-	-	0/0/0/0	0/0/0/0
2	SO4	B	1002	-	-	0/0/0/0	0/0/0/0
2	SO4	C	1003	-	-	0/0/0/0	0/0/0/0
2	SO4	D	1004	-	-	0/0/0/0	0/0/0/0

There are no bond length outliers.

There are no bond angle outliers.

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

There are no such residues in this entry.

## 5.8 Polymer linkage issues

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	303/371 (81%)	0.92	62 (20%) <b>1</b> <b>1</b>	21, 36, 70, 73	0
1	B	320/371 (86%)	0.99	59 (18%) <b>2</b> <b>1</b>	21, 40, 68, 76	0
1	C	339/371 (91%)	0.54	41 (12%) <b>6</b> <b>5</b>	20, 34, 63, 72	0
1	D	334/371 (90%)	0.51	42 (12%) <b>5</b> <b>4</b>	18, 29, 62, 74	0
All	All	1296/1484 (87%)	0.73	204 (15%) <b>3</b> <b>2</b>	18, 35, 67, 76	0

All (204) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	107(P)	LEU	8.2
1	B	59(P)	GLY	7.8
1	B	107(P)	LEU	7.5
1	B	58(P)	THR	7.4
1	A	42(P)	LEU	7.3
1	A	37(P)	LEU	6.9
1	B	5(P)	ALA	6.7
1	B	204	GLY	6.3
1	B	56(P)	ILE	6.3
1	A	52(P)	TYR	6.3
1	B	57(P)	SER	6.2
1	A	46(P)	LEU	6.1
1	A	3	VAL	6.1
1	A	70(P)	SER	6.0
1	C	112(P)	ALA	5.8
1	A	66(P)	GLY	5.8
1	A	68(P)	LYS	5.7
1	B	78(P)	THR	5.5
1	A	244	TYR	5.5
1	A	104(P)	ASN	5.4
1	B	69(P)	ARG	4.9

*Continued on next page...*

*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	A	64(P)	VAL	4.9
1	B	1	GLN	4.9
1	D	107(P)	LEU	4.8
1	A	69(P)	ARG	4.7
1	B	43(P)	GLY	4.7
1	A	103(P)	GLU	4.7
1	B	2	PRO	4.6
1	A	101(P)	ILE	4.6
1	D	103(P)	GLU	4.5
1	A	204	GLY	4.4
1	B	241	PHE	4.4
1	D	198	VAL	4.3
1	C	16(P)	ILE	4.3
1	A	197	PHE	4.3
1	B	205	ARG	4.3
1	B	67(P)	ASP	4.3
1	A	44(P)	GLY	4.2
1	A	54(P)	TYR	4.1
1	B	198	VAL	4.1
1	B	197	PHE	4.1
1	A	47(P)	SER	4.1
1	B	199	ILE	4.0
1	C	74(P)	LEU	4.0
1	B	229	PRO	4.0
1	A	222	PHE	4.0
1	D	55	ILE	3.9
1	C	63(P)	ILE	3.8
1	A	67(P)	ASP	3.8
1	D	185	TYR	3.8
1	D	63(P)	ILE	3.7
1	B	41(P)	ASN	3.7
1	C	7(P)	ASN	3.7
1	A	43(P)	GLY	3.6
1	D	52	THR	3.6
1	B	40(P)	VAL	3.6
1	B	8(P)	GLU	3.6
1	D	108(P)	ASP	3.6
1	B	86(P)	GLY	3.6
1	D	42(P)	LEU	3.5
1	A	205	ARG	3.5
1	A	40(P)	VAL	3.5
1	B	3	VAL	3.5

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	D	184	VAL	3.5
1	C	123	VAL	3.4
1	D	48	VAL	3.4
1	D	197	PHE	3.4
1	A	2	PRO	3.4
1	A	106(P)	LYS	3.3
1	B	70(P)	SER	3.3
1	B	55(P)	ASN	3.3
1	D	112(P)	ALA	3.3
1	C	198	VAL	3.3
1	C	20(P)	GLN	3.3
1	B	11(P)	ALA	3.3
1	A	38(P)	ASP	3.3
1	D	43(P)	GLY	3.3
1	D	143	VAL	3.2
1	D	222	PHE	3.2
1	B	202	ALA	3.2
1	D	49	ALA	3.2
1	C	107(P)	LEU	3.2
1	C	108(P)	ASP	3.2
1	D	13(P)	ASP	3.2
1	A	198	VAL	3.1
1	A	4	VAL	3.1
1	A	184	VAL	3.1
1	A	39(P)	LYS	3.0
1	C	222	PHE	3.0
1	C	224	LEU	3.0
1	A	105(P)	LYS	3.0
1	D	2	PRO	3.0
1	A	51	ALA	3.0
1	A	191	LYS	3.0
1	B	80(P)	GLY	3.0
1	C	12(P)	LYS	3.0
1	C	199	ILE	3.0
1	A	52	THR	2.9
1	C	52	THR	2.9
1	A	186	TYR	2.9
1	D	210	VAL	2.9
1	C	13(P)	ASP	2.9
1	C	197	PHE	2.9
1	D	51	ALA	2.9
1	B	38(P)	ASP	2.8

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	B	104(P)	ASN	2.8
1	D	106(P)	LYS	2.8
1	A	185	TYR	2.8
1	D	244	TYR	2.8
1	B	48(P)	GLY	2.8
1	A	93(P)	PHE	2.8
1	B	242	ASN	2.8
1	C	5(P)	ALA	2.8
1	A	41(P)	ASN	2.8
1	C	191	LYS	2.7
1	C	184	VAL	2.7
1	C	192	VAL	2.7
1	B	49	ALA	2.7
1	A	97(P)	TYR	2.7
1	C	17(P)	THR	2.7
1	D	186	TYR	2.7
1	D	53	ALA	2.7
1	A	53(P)	VAL	2.7
1	D	113(P)	GLY	2.7
1	B	186	TYR	2.7
1	D	248	VAL	2.6
1	A	49(P)	SER	2.6
1	A	55	ILE	2.6
1	D	9(P)	LYS	2.6
1	C	49	ALA	2.6
1	D	93(P)	PHE	2.6
1	B	51	ALA	2.6
1	C	97(P)	TYR	2.6
1	C	109(P)	SER	2.6
1	B	228	ASN	2.6
1	A	63(P)	ILE	2.6
1	A	226	ALA	2.5
1	A	227	LEU	2.5
1	B	45(P)	GLU	2.5
1	B	212	TRP	2.5
1	A	45(P)	GLU	2.5
1	C	38(P)	ASP	2.5
1	B	42(P)	LEU	2.5
1	B	105(P)	LYS	2.5
1	D	199	ILE	2.5
1	B	71(P)	PRO	2.5
1	C	21(P)	LYS	2.5

*Continued on next page...*

*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	A	75	SER	2.4
1	A	49	ALA	2.4
1	B	64(P)	VAL	2.4
1	C	205	ARG	2.4
1	D	17(P)	THR	2.4
1	D	204	GLY	2.4
1	D	191	LYS	2.4
1	A	76	ASN	2.4
1	B	52(P)	TYR	2.4
1	B	206	ASN	2.4
1	A	53	ALA	2.4
1	D	123	VAL	2.4
1	C	204	GLY	2.4
1	C	240	GLY	2.4
1	D	47(P)	SER	2.4
1	A	5	LYS	2.3
1	B	68(P)	LYS	2.3
1	D	62(P)	VAL	2.3
1	C	185	TYR	2.3
1	B	184	VAL	2.3
1	D	228	ASN	2.3
1	C	57(P)	SER	2.3
1	A	71(P)	PRO	2.3
1	A	85(P)	ASN	2.3
1	B	192	VAL	2.3
1	B	50	THR	2.2
1	B	185	TYR	2.2
1	C	59(P)	GLY	2.2
1	A	210	VAL	2.2
1	D	75(P)	GLY	2.2
1	A	123	VAL	2.2
1	B	54(P)	TYR	2.2
1	B	210	VAL	2.2
1	C	111(P)	TYR	2.2
1	A	106	GLY	2.1
1	D	119	LEU	2.1
1	A	50(P)	ASN	2.1
1	D	50	THR	2.1
1	C	53	ALA	2.1
1	B	62(P)	VAL	2.1
1	B	191	LYS	2.1
1	B	178	LEU	2.1

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	C	73(P)	ILE	2.1
1	A	248	VAL	2.1
1	C	229	PRO	2.1
1	B	85	ASN	2.1
1	D	11(P)	ALA	2.1
1	C	50	THR	2.0
1	A	162	ARG	2.0
1	B	224	LEU	2.0
1	D	41(P)	ASN	2.0
1	C	64(P)	VAL	2.0
1	A	196	ALA	2.0
1	B	196	ALA	2.0
1	C	244	TYR	2.0
1	B	8	LEU	2.0
1	C	2	PRO	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
2	SO4	C	1003	5/5	0.97	0.08	-1.09	28,29,31,31	0
2	SO4	D	1004	5/5	0.99	0.06	-1.50	25,27,27,28	0
2	SO4	B	1002	5/5	0.98	0.06	-1.52	31,34,34,35	0
2	SO4	A	1001	5/5	0.99	0.05	-1.75	33,35,36,37	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.