



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 10:07 AM GMT

PDB ID : 3KYK  
Title : Crystal structure of li33 Igg1 Fab  
Authors : Silvian, L.F.; Pepinsky, R.B.; Walus, L.  
Deposited on : 2009-12-06  
Resolution : 3.20 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

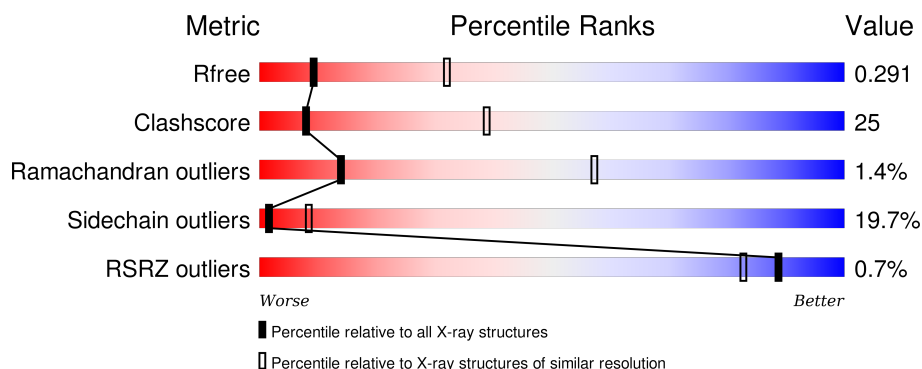
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 3.20 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	1124 (3.24-3.16)
Clashscore	102246	1024 (3.22-3.18)
Ramachandran outliers	100387	1004 (3.22-3.18)
Sidechain outliers	100360	1003 (3.22-3.18)
RSRZ outliers	91569	1129 (3.24-3.16)

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	H	227	
2	L	214	

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 3309 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 Heavy Chain Li33 IgG1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	H	220	Total	C	N	O	S	3	0	0
			1633	1040	273	314	6			

- Molecule 2 is a protein called Light Chain Li33 IgG1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	L	211	Total	C	N	O	S	0	0	0
			1618	1012	273	328	5			

- 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		

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

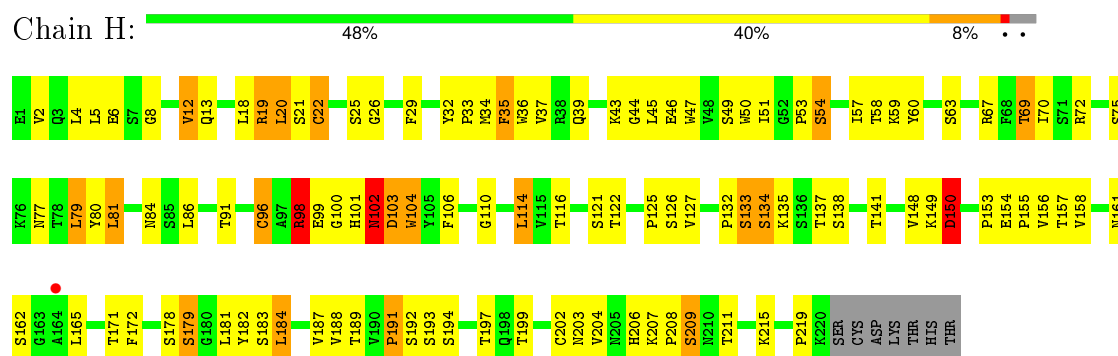
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	H	14	Total	O	0	0
			14	14		
4	L	24	Total	O	0	0
			24	24		

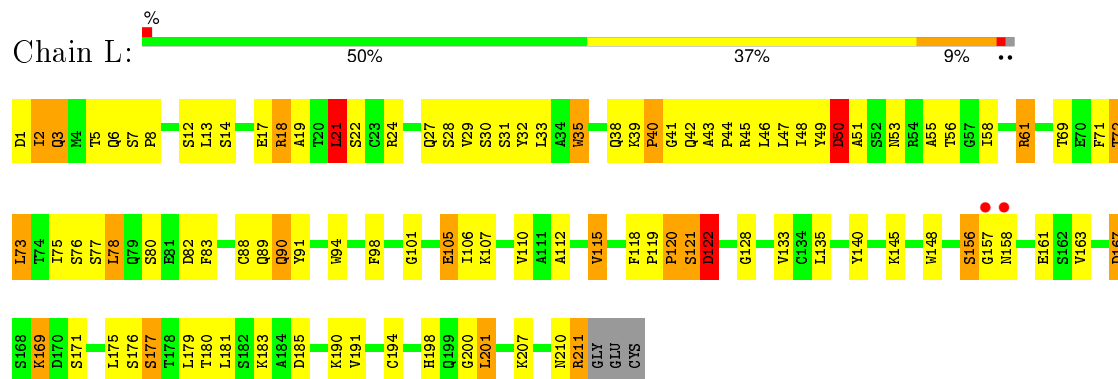
### 3 Residue-property plots

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 ( $\text{RSRZ} > 2$ ). 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: Heavy Chain Li33 IgG1



#### • Molecule 2: Light Chain Li33 IgG1



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 65 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	90.63 Å 90.63 Å 215.04 Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	44.34 – 3.20 44.34 – 3.20	Depositor EDS
% Data completeness (in resolution range)	99.9 (44.34-3.20) 99.9 (44.34-3.20)	Depositor EDS
$R_{merge}$	0.22	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	5.21 (at 3.19 Å)	Xtriage
Refinement program	REFMAC 5.5.0088	Depositor
R, $R_{free}$	0.194 , 0.290 0.193 , 0.291	Depositor DCC
$R_{free}$ test set	441 reflections (5.02%)	DCC
Wilson B-factor (Å <sup>2</sup> )	34.1	Xtriage
Anisotropy	0.263	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.38 , 48.4	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 9258 reflections	Xtriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	3309	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	18.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.01% 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: 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	H	1.05	3/1677 (0.2%)	1.13	10/2286 (0.4%)
2	L	1.14	5/1654 (0.3%)	1.08	4/2248 (0.2%)
All	All	1.10	8/3331 (0.2%)	1.11	14/4534 (0.3%)

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	L	0	1

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	L	17	GLU	CG-CD	11.34	1.69	1.51
1	H	96	CYS	CB-SG	-11.18	1.63	1.82
2	L	17	GLU	CB-CG	9.03	1.69	1.52
2	L	3	GLN	CG-CD	6.10	1.65	1.51
2	L	3	GLN	CB-CG	5.72	1.68	1.52
1	H	102	ASN	CB-CG	5.28	1.63	1.51
1	H	54	SER	CA-CB	5.18	1.60	1.52
2	L	190	LYS	CB-CG	5.07	1.66	1.52

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	103	ASP	N-CA-C	-8.64	87.67	111.00
1	H	96	CYS	CA-CB-SG	-7.10	101.21	114.00
2	L	50	ASP	CB-CG-OD1	-6.81	112.17	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	215	LYS	CB-CA-C	6.74	123.88	110.40
2	L	91	TYR	N-CA-C	6.39	128.25	111.00
1	H	114	LEU	CA-CB-CG	5.85	128.76	115.30
2	L	21	LEU	CA-CB-CG	5.60	128.18	115.30
1	H	150	ASP	N-CA-C	-5.53	96.06	111.00
1	H	102	ASN	N-CA-C	5.49	125.83	111.00
1	H	103	ASP	CB-CG-OD1	5.45	123.20	118.30
1	H	98	ARG	NE-CZ-NH1	-5.30	117.65	120.30
2	L	211	ARG	NE-CZ-NH1	5.16	122.88	120.30
1	H	72	ARG	NE-CZ-NH2	5.08	122.84	120.30
1	H	209	SER	N-CA-C	-5.08	97.30	111.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	L	40	PRO	Peptide

## 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	H	1633	0	1580	82	4
2	L	1618	0	1554	86	0
3	H	15	0	0	1	0
3	L	5	0	0	0	0
4	H	14	0	0	3	0
4	L	24	0	0	6	0
All	All	3309	0	3134	159	4

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 25.

All (159) 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:L:7:SER:HB2	2:L:22:SER:HB2	1.29	1.14
2:L:7:SER:CB	2:L:22:SER:HB2	1.87	1.05
1:H:36:TRP:HD1	1:H:70:ILE:HD12	1.16	1.04
2:L:7:SER:HB3	2:L:8:PRO:HD3	1.42	1.00
2:L:121:SER:O	2:L:122:ASP:HB2	1.60	0.98
1:H:36:TRP:CD1	1:H:70:ILE:HD12	2.06	0.91
2:L:161:GLU:HG3	4:L:229:HOH:O	1.70	0.91
2:L:18:ARG:HG2	2:L:76:SER:O	1.72	0.90
2:L:18:ARG:CB	2:L:18:ARG:HH21	1.86	0.89
2:L:18:ARG:NH2	2:L:18:ARG:CB	2.41	0.84
2:L:18:ARG:HB3	2:L:18:ARG:NH2	1.92	0.83
1:H:187:VAL:HG11	2:L:135:LEU:HD11	1.60	0.82
1:H:102:ASN:N	1:H:103:ASP:CG	2.33	0.82
1:H:100:GLY:O	1:H:103:ASP:HA	1.81	0.81
1:H:51:ILE:HG13	1:H:58:THR:HG22	1.64	0.79
1:H:101:HIS:HA	1:H:103:ASP:OD1	1.83	0.77
1:H:50:TRP:HZ3	1:H:57:ILE:HG22	1.49	0.77
1:H:154:GLU:N	1:H:155:PRO:CD	2.48	0.76
1:H:102:ASN:N	1:H:103:ASP:OD2	2.22	0.72
1:H:158:VAL:HG22	1:H:204:VAL:HG22	1.70	0.72
2:L:120:PRO:O	2:L:121:SER:CB	2.36	0.72
2:L:18:ARG:HB2	2:L:18:ARG:HH21	1.53	0.72
1:H:110:GLY:O	2:L:43:ALA:HB2	1.92	0.69
1:H:133:SER:HB2	4:L:222:HOH:O	1.93	0.68
1:H:33:PRO:HG3	1:H:53:PRO:HD3	1.75	0.67
2:L:157:GLY:HA2	2:L:158:ASN:CG	2.14	0.67
2:L:112:ALA:HB1	2:L:201:LEU:HD13	1.77	0.66
2:L:28:SER:HA	2:L:69:THR:HG22	1.79	0.65
1:H:36:TRP:HD1	1:H:70:ILE:CD1	2.03	0.65
1:H:6:GLU:HA	1:H:21:SER:O	1.96	0.65
2:L:121:SER:O	2:L:122:ASP:CB	2.37	0.64
1:H:102:ASN:H	1:H:103:ASP:CG	1.98	0.63
2:L:1:ASP:O	2:L:2:ILE:C	2.36	0.63
2:L:157:GLY:HA2	2:L:158:ASN:OD1	1.98	0.63
2:L:105:GLU:HB2	4:L:216:HOH:O	1.99	0.63
1:H:110:GLY:O	2:L:43:ALA:CB	2.48	0.62
1:H:99:GLU:OE2	1:H:103:ASP:HB3	1.98	0.62
1:H:43:LYS:HG3	1:H:44:GLY:H	1.64	0.62
2:L:80:SER:HA	2:L:106:ILE:HD13	1.80	0.62
1:H:101:HIS:CA	1:H:103:ASP:OD1	2.46	0.62
2:L:41:GLY:HA2	4:L:234:HOH:O	1.99	0.61
2:L:39:LYS:HB2	2:L:42:GLN:HE21	1.65	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:7:SER:HB3	2:L:8:PRO:CD	2.25	0.61
2:L:157:GLY:HA2	2:L:158:ASN:CB	2.32	0.60
2:L:30:SER:OG	2:L:31:SER:N	2.30	0.60
2:L:115:VAL:O	2:L:115:VAL:CG2	2.50	0.60
2:L:50:ASP:O	2:L:51:ALA:HB3	2.01	0.60
2:L:55:ALA:HB3	2:L:58:ILE:HG13	1.84	0.59
1:H:21:SER:HA	1:H:79:LEU:O	2.03	0.59
1:H:165:LEU:HD21	1:H:188:VAL:HG21	1.83	0.59
2:L:128:GLY:O	2:L:183:LYS:HB3	2.03	0.58
1:H:8:GLY:O	1:H:18:LEU:HD11	2.03	0.58
1:H:50:TRP:CZ3	1:H:57:ILE:HG22	2.36	0.58
1:H:154:GLU:N	1:H:155:PRO:HD3	2.17	0.58
1:H:43:LYS:HG3	1:H:44:GLY:N	2.19	0.58
1:H:29:PHE:HE1	1:H:34:MET:HE3	1.68	0.58
1:H:103:ASP:O	1:H:104:TRP:CB	2.51	0.58
1:H:59:LYS:HE2	3:H:229:SO4:O2	2.03	0.58
2:L:175:LEU:HD23	2:L:176:SER:N	2.18	0.58
1:H:126:SER:N	1:H:149:LYS:O	2.26	0.58
1:H:103:ASP:O	1:H:104:TRP:HB2	2.04	0.57
1:H:35:PHE:CZ	1:H:106:PHE:CZ	2.92	0.57
1:H:67:ARG:HG2	1:H:84:ASN:O	2.05	0.57
2:L:18:ARG:NH1	4:L:217:HOH:O	2.11	0.57
1:H:2:VAL:HA	1:H:26:GLY:HA3	1.87	0.57
2:L:77:SER:O	2:L:78:LEU:C	2.41	0.56
1:H:150:ASP:HA	1:H:182:TYR:O	2.05	0.56
2:L:115:VAL:HG23	2:L:115:VAL:O	2.06	0.56
2:L:107:LYS:HA	2:L:140:TYR:OH	2.06	0.56
2:L:6:GLN:NE2	2:L:88:CYS:H	2.04	0.55
2:L:7:SER:HB2	2:L:22:SER:CB	2.19	0.55
1:H:148:VAL:O	1:H:183:SER:HA	2.07	0.55
1:H:47:TRP:CZ3	1:H:49:SER:HA	2.42	0.55
1:H:36:TRP:CD1	1:H:70:ILE:CD1	2.85	0.54
1:H:32:TYR:CD2	1:H:98:ARG:HD2	2.43	0.54
2:L:19:ALA:HB3	2:L:75:ILE:HB	1.90	0.53
1:H:13:GLN:HG3	4:H:233:HOH:O	2.07	0.53
1:H:19:ARG:HA	1:H:81:LEU:O	2.08	0.53
2:L:33:LEU:HD22	2:L:71:PHE:CG	2.44	0.52
1:H:104:TRP:CZ3	2:L:94:TRP:CZ3	2.97	0.52
1:H:104:TRP:CZ3	2:L:94:TRP:HZ3	2.28	0.51
1:H:153:PRO:C	1:H:155:PRO:HD2	2.31	0.51
2:L:61:ARG:NH1	2:L:82:ASP:OD1	2.43	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:132:PRO:HG2	1:H:219:PRO:HA	1.92	0.51
1:H:133:SER:CB	4:L:222:HOH:O	2.57	0.51
1:H:12:VAL:HG21	1:H:86:LEU:HD13	1.91	0.51
2:L:148:TRP:HE1	2:L:177:SER:HB3	1.74	0.51
1:H:179:SER:HB2	1:H:181:LEU:H	1.75	0.51
2:L:6:GLN:NE2	2:L:88:CYS:N	2.58	0.51
2:L:210:ASN:O	2:L:211:ARG:CB	2.59	0.51
2:L:210:ASN:O	2:L:211:ARG:HG3	2.10	0.51
1:H:135:LYS:HD3	2:L:207:LYS:HE3	1.91	0.51
1:H:29:PHE:CE1	1:H:34:MET:HE3	2.47	0.50
1:H:29:PHE:HB3	1:H:77:ASN:OD1	2.10	0.50
2:L:14:SER:HA	2:L:107:LYS:O	2.12	0.50
2:L:7:SER:HB3	2:L:22:SER:HB2	1.83	0.50
1:H:154:GLU:N	1:H:155:PRO:HD2	2.27	0.49
2:L:33:LEU:HD22	2:L:71:PHE:CD2	2.48	0.49
1:H:133:SER:O	1:H:137:THR:OG1	2.27	0.49
2:L:120:PRO:O	2:L:121:SER:OG	2.28	0.49
2:L:32:TYR:O	2:L:90:GLN:O	2.30	0.49
1:H:172:PHE:H	1:H:172:PHE:HD1	1.58	0.49
2:L:35:TRP:CD1	2:L:73:LEU:HD22	2.48	0.48
2:L:1:ASP:O	2:L:3:GLN:N	2.46	0.48
1:H:51:ILE:HB	1:H:70:ILE:HG12	1.95	0.48
1:H:209:SER:O	1:H:211:THR:N	2.47	0.48
2:L:49:TYR:O	2:L:53:ASN:HB3	2.14	0.48
2:L:43:ALA:O	2:L:44:PRO:C	2.52	0.48
1:H:187:VAL:HG11	2:L:135:LEU:CD1	2.40	0.47
1:H:106:PHE:HE1	2:L:98:PHE:HZ	1.62	0.47
1:H:172:PHE:CD1	1:H:172:PHE:N	2.82	0.47
1:H:101:HIS:CE1	4:H:240:HOH:O	2.67	0.47
2:L:21:LEU:O	2:L:72:THR:HA	2.14	0.47
2:L:49:TYR:O	2:L:50:ASP:CB	2.63	0.47
2:L:210:ASN:O	2:L:211:ARG:HB2	2.15	0.46
1:H:60:TYR:OH	1:H:69:THR:HA	2.14	0.46
1:H:29:PHE:CE1	1:H:34:MET:CE	2.99	0.46
2:L:110:VAL:HG11	2:L:200:GLY:HA2	1.97	0.46
2:L:47:LEU:HA	2:L:58:ILE:HD12	1.97	0.45
2:L:120:PRO:O	2:L:121:SER:HB3	2.15	0.45
1:H:37:VAL:HG23	1:H:46:GLU:O	2.17	0.45
2:L:118:PHE:HB2	2:L:133:VAL:HB	1.98	0.45
2:L:49:TYR:O	2:L:50:ASP:HB2	2.15	0.45
1:H:106:PHE:HE1	2:L:98:PHE:CZ	2.35	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:46:LEU:O	2:L:58:ILE:HD11	2.18	0.44
2:L:29:VAL:O	2:L:29:VAL:CG1	2.65	0.44
1:H:125:PRO:HD2	1:H:211:THR:HG21	2.00	0.44
1:H:103:ASP:O	1:H:104:TRP:CD1	2.70	0.44
1:H:35:PHE:CZ	1:H:106:PHE:CE1	3.06	0.44
1:H:206:HIS:HD2	1:H:209:SER:OG	2.00	0.44
2:L:89:GLN:HG3	2:L:98:PHE:CE2	2.52	0.44
2:L:119:PRO:HA	2:L:120:PRO:HD3	1.69	0.43
2:L:6:GLN:HE22	2:L:88:CYS:N	2.16	0.43
2:L:39:LYS:CB	2:L:42:GLN:HE21	2.30	0.43
2:L:112:ALA:HB1	2:L:201:LEU:CD1	2.46	0.43
1:H:18:LEU:HD12	1:H:19:ARG:H	1.83	0.43
2:L:156:SER:O	2:L:158:ASN:OD1	2.37	0.43
1:H:191:PRO:O	1:H:194:SER:OG	2.29	0.43
2:L:6:GLN:OE1	2:L:101:GLY:N	2.42	0.43
1:H:39:GLN:HB2	1:H:45:LEU:HD23	2.01	0.42
2:L:148:TRP:CD2	2:L:179:LEU:HB2	2.54	0.42
2:L:38:GLN:OE1	2:L:44:PRO:HD3	2.19	0.42
2:L:169:LYS:HB2	2:L:169:LYS:HE2	1.73	0.42
1:H:35:PHE:CE1	1:H:106:PHE:CZ	3.08	0.42
1:H:103:ASP:O	1:H:104:TRP:CG	2.73	0.41
2:L:167:ASP:O	2:L:171:SER:HA	2.20	0.41
1:H:184:LEU:HD12	1:H:184:LEU:C	2.40	0.41
1:H:134:SER:OG	4:H:232:HOH:O	2.19	0.41
1:H:102:ASN:N	1:H:103:ASP:OD1	2.54	0.41
1:H:91:THR:HG23	1:H:116:THR:HA	2.03	0.41
1:H:161:ASN:O	1:H:162:SER:HB2	2.20	0.41
1:H:6:GLU:HG2	1:H:22:CYS:SG	2.61	0.41
2:L:2:ILE:HG12	2:L:27:GLN:CG	2.51	0.41
1:H:20:LEU:O	1:H:80:TYR:HA	2.20	0.41
1:H:127:VAL:HG12	1:H:127:VAL:O	2.20	0.41
2:L:40:PRO:HA	2:L:41:GLY:HA2	1.82	0.41
2:L:13:LEU:HB2	2:L:78:LEU:HD12	2.04	0.40
2:L:38:GLN:OE1	2:L:42:GLN:O	2.39	0.40
2:L:198:HIS:O	2:L:201:LEU:HB2	2.22	0.40

All (4) 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)
1:H:101:HIS:NE2	1:H:101:HIS:NE2[10_555]	0.89	1.31

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:101:HIS:CD2	1:H:101:HIS:CD2[10_555]	1.13	1.07
1:H:101:HIS:CD2	1:H:101:HIS:NE2[10_555]	1.47	0.73
1:H:101:HIS:CE1	1:H:101:HIS:NE2[10_555]	2.03	0.17

## 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	H	218/227 (96%)	197 (90%)	18 (8%)	3 (1%)	14	57
2	L	209/214 (98%)	182 (87%)	24 (12%)	3 (1%)	14	57
All	All	427/441 (97%)	379 (89%)	42 (10%)	6 (1%)	14	57

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	H	104	TRP
2	L	121	SER
2	L	122	ASP
1	H	179	SER
1	H	191	PRO
2	L	2	ILE

### 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	H	180/191 (94%)	141 (78%)	39 (22%)	1	6
2	L	181/185 (98%)	149 (82%)	32 (18%)	2	11
All	All	361/376 (96%)	290 (80%)	71 (20%)	1	8

All (71) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	H	4	LEU
1	H	5	LEU
1	H	12	VAL
1	H	19	ARG
1	H	20	LEU
1	H	22	CYS
1	H	25	SER
1	H	35	PHE
1	H	54	SER
1	H	63	SER
1	H	69	THR
1	H	75	SER
1	H	79	LEU
1	H	81	LEU
1	H	96	CYS
1	H	98	ARG
1	H	102	ASN
1	H	114	LEU
1	H	121	SER
1	H	122	THR
1	H	133	SER
1	H	134	SER
1	H	138	SER
1	H	141	THR
1	H	150	ASP
1	H	156	VAL
1	H	157	THR
1	H	171	THR
1	H	178	SER
1	H	184	LEU
1	H	189	THR
1	H	192	SER
1	H	193	SER
1	H	197	THR
1	H	199	THR

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Mol	Chain	Res	Type
1	H	202	CYS
1	H	203	ASN
1	H	207	LYS
1	H	208	PRO
2	L	5	THR
2	L	12	SER
2	L	18	ARG
2	L	21	LEU
2	L	24	ARG
2	L	35	TRP
2	L	45	ARG
2	L	48	ILE
2	L	50	ASP
2	L	56	THR
2	L	61	ARG
2	L	72	THR
2	L	73	LEU
2	L	78	LEU
2	L	83	PHE
2	L	90	GLN
2	L	105	GLU
2	L	115	VAL
2	L	120	PRO
2	L	122	ASP
2	L	145	LYS
2	L	156	SER
2	L	163	VAL
2	L	167	ASP
2	L	169	LYS
2	L	177	SER
2	L	180	THR
2	L	181	LEU
2	L	185	ASP
2	L	191	VAL
2	L	194	CYS
2	L	201	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	H	39	GLN
1	H	82	GLN

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Mol	Chain	Res	Type
1	H	206	HIS
2	L	38	GLN
2	L	42	GLN
2	L	166	GLN
2	L	199	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

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	$\# Z  > 2$
3	SO4	H	228	-	4,4,4	0.34	0	6,6,6	0.51	0
3	SO4	H	229	-	4,4,4	0.31	0	6,6,6	0.40	0
3	SO4	H	230	-	4,4,4	0.32	0	6,6,6	0.67	0
3	SO4	L	215	-	4,4,4	0.26	0	6,6,6	0.57	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
3	SO4	H	228	-	-	0/0/0/0	0/0/0/0
3	SO4	H	229	-	-	0/0/0/0	0/0/0/0
3	SO4	H	230	-	-	0/0/0/0	0/0/0/0
3	SO4	L	215	-	-	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.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	H	229	SO4	1	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 [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

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	H	220/227 (96%)	-0.35	1 (0%) 91 87	7, 18, 34, 38	3 (1%)
2	L	211/214 (98%)	-0.24	2 (0%) 85 78	5, 16, 32, 39	0
All	All	431/441 (97%)	-0.29	3 (0%) 89 83	5, 17, 33, 39	3 (0%)

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	L	157	GLY	2.5
1	H	164	ALA	2.1
2	L	158	ASN	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
3	SO4	H	230	5/5	0.95	0.17	-0.41	48,49,49,50	0
3	SO4	L	215	5/5	0.93	0.19	-0.77	51,51,52,52	0
3	SO4	H	228	5/5	0.99	0.09	-2.21	25,25,26,27	0
3	SO4	H	229	5/5	0.97	0.11	-	38,39,39,40	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.