



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 28, 2023 – 11:36 AM EDT

PDB ID : 3L7F  
Title : Structure of IL-13 antibody H2L6, A humanized variant OF C836  
Authors : Teplyakov, A.; Obmolova, G.; Malia, T.; Gilliland, G.L.  
Deposited on : 2009-12-28  
Resolution : 2.60 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

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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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 : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.35  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.35

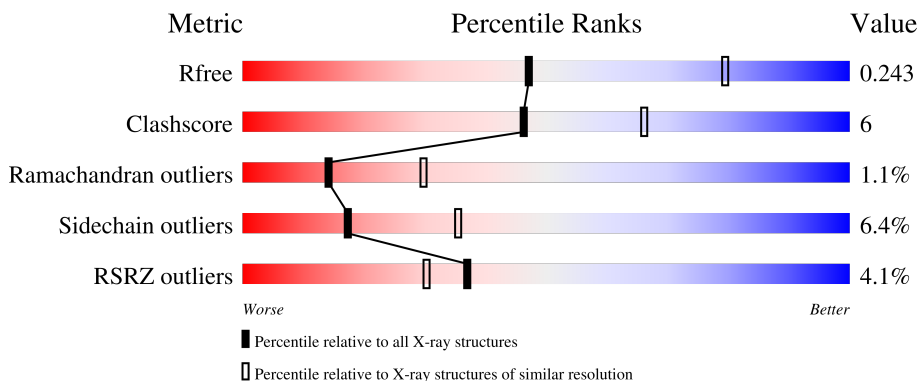
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*


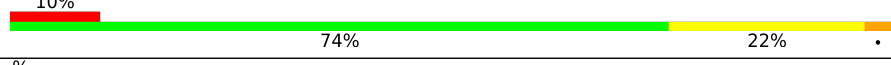



The reported resolution of this entry is 2.60 Å.

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.



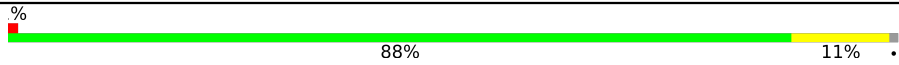
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (2.60-2.60)

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 of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. 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	214	 4% 75% 21%
1	D	214	 10% 74% 22%
1	L	214	 0% 82% 15%
2	B	224	 3% 81% 16%
2	E	224	 5% 79% 18%

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Mol	Chain	Length	Quality of chain
2	H	224	 <p>A horizontal bar chart representing the quality of chain. The bar is 88% green and 11% yellow. A small red square is at the start, and a small grey square is at the end. The percentage values '88%' and '11%' are printed below the bar. A '%' symbol is at the top left of the bar area.</p>

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 10198 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 H2L6 LIGHT CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	L	213	1646	1035	275	332	4	0	0	0
1	A	213	1646	1035	275	332	4	0	0	0
1	D	213	1646	1035	275	332	4	0	0	0

- Molecule 2 is a protein called H2L6 HEAVY CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	H	222	1677	1070	272	327	8	0	0	0
2	B	221	1672	1067	271	326	8	0	0	0
2	E	221	1672	1067	271	326	8	0	0	0

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



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

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

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

- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	L	56	Total O 56 56	0	0
5	H	31	Total O 31 31	0	0
5	A	37	Total O 37 37	0	0
5	B	44	Total O 44 44	0	0
5	D	37	Total O 37 37	0	0

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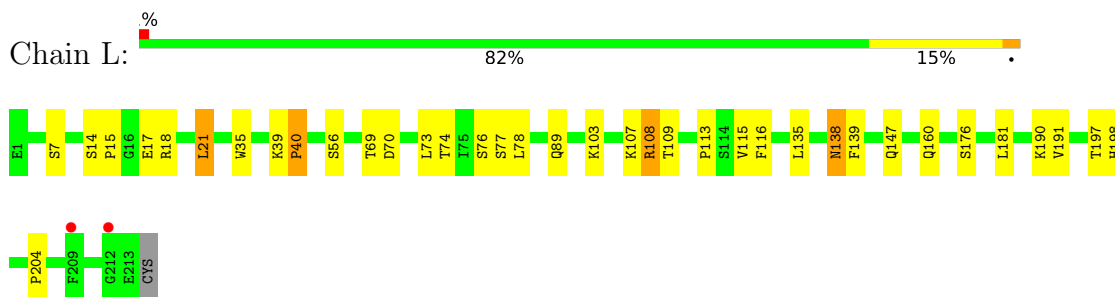
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<b>Mol</b>	<b>Chain</b>	<b>Residues</b>	<b>Atoms</b>		<b>ZeroOcc</b>	<b>AltConf</b>
5	E	18	Total	O	0	0
			18	18		

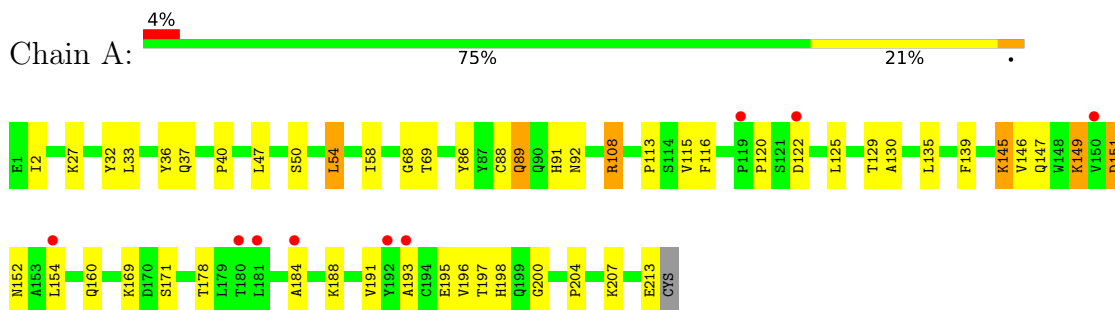
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes 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.

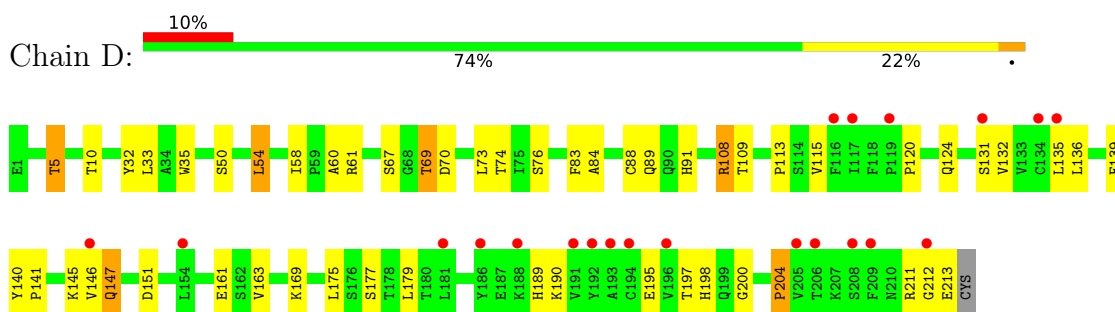
- Molecule 1: H2L6 LIGHT CHAIN



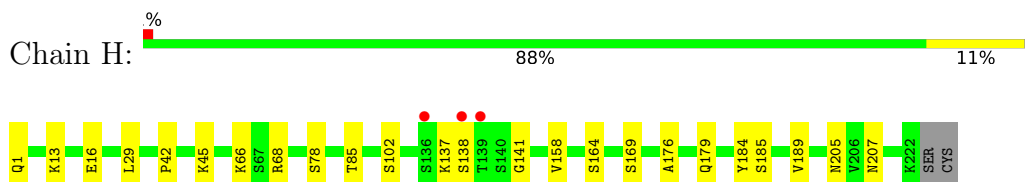
- Molecule 1: H2L6 LIGHT CHAIN




- Molecule 1: H2L6 LIGHT CHAIN

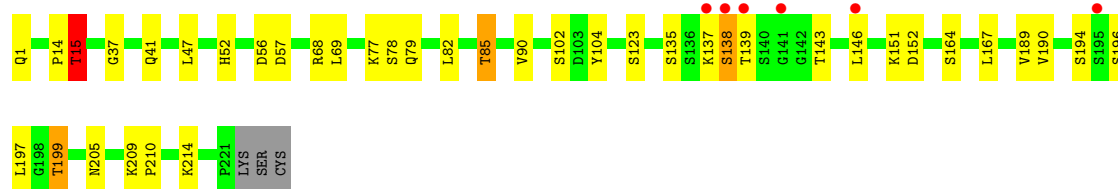


- Molecule 2: H2L6 HEAVY CHAIN




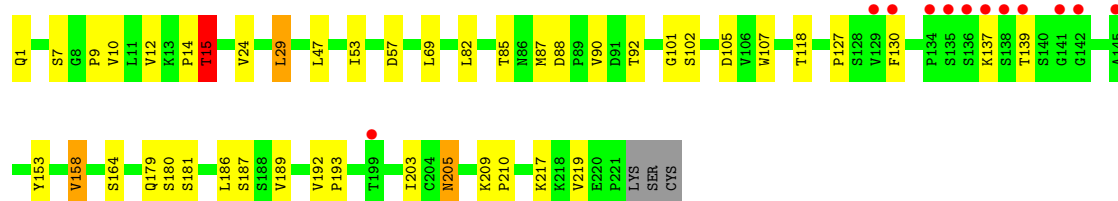
- Molecule 2: H2L6 HEAVY CHAIN

Chain B:  3% 81% 16% ..



- Molecule 2: H2L6 HEAVY CHAIN

Chain E:  5% 79% 18% ..





## 4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	69.64Å 228.16Å 234.00Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	15.00 – 2.60 66.61 – 2.60	Depositor EDS
% Data completeness (in resolution range)	93.0 (15.00-2.60) 97.1 (66.61-2.60)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.87 (at 2.62Å)	Xtrriage
Refinement program	REFMAC 5.2.0005	Depositor
R, $R_{free}$	0.205 , 0.243 0.207 , 0.243	Depositor DCC
$R_{free}$ test set	2281 reflections (4.06%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	46.1	Xtrriage
Anisotropy	0.122	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 60.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.52$ , $\langle L^2 \rangle = 0.35$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	10198	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	52.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.15% 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, 0.333 respectively for untwinned datasets, and 0.375, 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: CA, SO4, PCA

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	0.48	0/1683	0.63	0/2285
1	D	0.54	0/1683	0.65	0/2285
1	L	0.54	0/1683	0.70	1/2285 (0.0%)
2	B	0.53	0/1710	0.63	0/2343
2	E	0.48	0/1710	0.62	0/2343
2	H	0.52	0/1715	0.65	0/2350
All	All	0.52	0/10184	0.65	1/13891 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	21	LEU	CA-CB-CG	5.66	128.32	115.30

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	1646	0	1605	30	0
1	D	1646	0	1605	36	0
1	L	1646	0	1605	19	0
2	B	1672	0	1655	22	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	E	1672	0	1655	23	0
2	H	1677	0	1657	10	0
3	D	5	0	0	0	0
3	H	5	0	0	0	0
3	L	5	0	0	1	0
4	D	1	0	0	0	0
5	A	37	0	0	0	0
5	B	44	0	0	0	0
5	D	37	0	0	1	0
5	E	18	0	0	0	0
5	H	31	0	0	0	0
5	L	56	0	0	1	0
All	All	10198	0	9782	125	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 6.

All (125) 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:B:14:PRO:O	2:B:15:THR:HB	1.65	0.95
2:E:164:SER:HA	2:E:205:ASN:HD21	1.33	0.93
2:H:164:SER:H	2:H:205:ASN:HD21	1.21	0.87
2:E:14:PRO:O	2:E:15:THR:HB	1.77	0.84
1:A:149:LYS:HB2	1:A:193:ALA:HB3	1.61	0.80
2:B:164:SER:H	2:B:205:ASN:HD21	1.29	0.79
2:E:164:SER:HA	2:E:205:ASN:ND2	1.98	0.77
1:A:147:GLN:HB3	1:A:195:GLU:HB3	1.67	0.76
1:D:69:THR:HG22	1:D:70:ASP:OD1	1.90	0.72
1:A:108:ARG:HG2	1:A:171:SER:HB2	1.72	0.71
2:E:164:SER:CA	2:E:205:ASN:HD21	2.03	0.71
1:D:197:THR:HG22	1:D:204:PRO:HB3	1.75	0.69
1:L:135:LEU:HD22	2:H:189:VAL:HG11	1.75	0.68
1:D:50:SER:H	1:D:91:HIS:HE1	1.42	0.66
2:H:164:SER:H	2:H:205:ASN:ND2	1.92	0.66
1:A:54:LEU:HD22	1:A:58:ILE:HB	1.78	0.65
1:L:138:ASN:HD22	1:L:138:ASN:N	1.93	0.65
1:D:147:GLN:HB3	1:D:195:GLU:HB3	1.80	0.64
1:A:197:THR:HG22	1:A:204:PRO:HB3	1.81	0.63
1:L:190:LYS:HG3	1:L:191:VAL:HG23	1.80	0.62
1:A:151:ASP:HA	1:A:191:VAL:HB	1.83	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:120:PRO:HD3	1:D:132:VAL:HG22	1.83	0.61
1:D:50:SER:H	1:D:91:HIS:CE1	2.18	0.60
1:A:145:LYS:HE3	1:A:146:VAL:H	1.68	0.58
1:D:69:THR:CG2	1:D:70:ASP:OD1	2.51	0.58
1:D:124:GLN:HG3	2:E:130:PHE:CE1	2.38	0.58
2:E:92:THR:HG23	2:E:118:THR:HA	1.86	0.58
2:H:68:ARG:HD2	2:H:85:THR:O	2.05	0.57
1:L:103:LYS:HE2	5:L:260:HOH:O	2.04	0.57
2:B:14:PRO:O	2:B:15:THR:CB	2.48	0.57
2:E:24:VAL:HG11	2:E:29:LEU:HD13	1.86	0.56
2:E:14:PRO:O	2:E:15:THR:CB	2.52	0.56
2:B:167:LEU:HD21	2:B:190:VAL:HG21	1.86	0.56
2:E:69:LEU:HD22	2:E:82:LEU:HD11	1.88	0.55
1:A:54:LEU:CD2	1:A:58:ILE:HB	2.37	0.54
1:L:18:ARG:HG2	1:L:76:SER:HA	1.89	0.54
2:B:164:SER:H	2:B:205:ASN:ND2	2.01	0.54
1:D:131:SER:HA	1:D:179:LEU:O	2.09	0.53
3:L:1002:SO4:O3	1:D:67:SER:HB3	2.10	0.52
1:L:69:THR:HG22	1:L:70:ASP:OD1	2.10	0.52
1:A:37:GLN:HB2	1:A:47:LEU:HD11	1.90	0.52
1:L:135:LEU:CD2	2:H:189:VAL:HG11	2.39	0.52
2:B:135:SER:O	2:B:139:THR:OG1	2.26	0.52
2:E:101:GLY:HA3	2:E:107:TRP:CZ3	2.46	0.51
2:E:192:VAL:HB	2:E:193:PRO:HD2	1.92	0.51
2:B:41:GLN:HB2	2:B:47:LEU:HD23	1.91	0.51
1:D:140:TYR:CG	1:D:141:PRO:HA	2.46	0.51
1:A:160:GLN:N	1:A:178:THR:O	2.43	0.51
2:B:196:SER:HA	2:B:199:THR:OG1	2.10	0.51
1:D:35:TRP:CE2	1:D:73:LEU:HB2	2.46	0.50
1:D:151:ASP:HB2	1:D:189:HIS:HB3	1.94	0.50
1:L:39:LYS:HB3	1:L:40:PRO:HD2	1.94	0.49
1:D:135:LEU:HD21	2:E:189:VAL:HG11	1.93	0.49
1:D:108:ARG:HD2	1:D:140:TYR:CB	2.42	0.49
1:A:146:VAL:HG22	1:A:196:VAL:HG22	1.94	0.49
1:L:108:ARG:HD3	1:L:109:THR:O	2.12	0.49
1:L:138:ASN:N	1:L:138:ASN:ND2	2.61	0.49
1:A:198:HIS:CD2	1:A:200:GLY:H	2.32	0.48
1:A:151:ASP:N	1:A:191:VAL:O	2.40	0.48
1:D:198:HIS:CD2	1:D:200:GLY:H	2.31	0.48
1:D:5:THR:HG23	5:D:248:HOH:O	2.13	0.48
1:D:147:GLN:HE21	1:D:147:GLN:HA	1.78	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:50:SER:H	1:A:91:HIS:HE1	1.62	0.47
1:A:116:PHE:CD2	2:B:138:SER:HB2	2.49	0.47
2:B:151:LYS:HG2	2:B:152:ASP:OD1	2.15	0.47
1:D:91:HIS:HD2	2:E:105:ASP:OD1	1.97	0.47
1:L:113:PRO:HB3	1:L:139:PHE:HB3	1.97	0.47
2:B:104:TYR:OH	1:D:76:SER:O	2.15	0.47
2:H:179:GLN:OE1	2:H:185:SER:HB2	2.14	0.47
1:A:2:ILE:HG13	1:A:27:LYS:HE2	1.96	0.47
1:A:135:LEU:HD22	2:B:189:VAL:HG11	1.96	0.47
1:A:116:PHE:HD2	2:B:138:SER:HB2	1.79	0.46
1:D:163:VAL:HG22	1:D:175:LEU:HD12	1.98	0.46
2:B:69:LEU:HD22	2:B:82:LEU:HD11	1.96	0.46
1:D:147:GLN:HA	1:D:147:GLN:NE2	2.31	0.46
2:E:12:VAL:HG11	2:E:87:MET:HG3	1.95	0.46
1:A:147:GLN:N	1:A:195:GLU:O	2.48	0.46
2:B:164:SER:N	2:B:205:ASN:HD21	2.07	0.46
1:D:113:PRO:HB3	1:D:139:PHE:HB3	1.98	0.46
1:A:50:SER:H	1:A:91:HIS:CE1	2.33	0.46
2:B:56:ASP:O	2:B:57:ASP:HB2	2.15	0.46
1:A:213:GLU:OE2	2:B:137:LYS:NZ	2.47	0.45
1:D:135:LEU:HD21	2:E:189:VAL:CG1	2.46	0.45
1:A:113:PRO:HB3	1:A:139:PHE:HB3	1.98	0.45
2:E:53:ILE:HD11	2:E:57:ASP:OD1	2.17	0.45
1:D:54:LEU:HD22	1:D:58:ILE:HB	1.99	0.45
1:L:35:TRP:CE2	1:L:73:LEU:HB2	2.53	0.44
2:B:68:ARG:HD2	2:B:85:THR:O	2.17	0.44
1:A:115:VAL:HG13	1:A:207:LYS:HE3	1.99	0.44
2:E:203:ILE:HA	2:E:217:LYS:O	2.17	0.44
1:A:113:PRO:HD3	1:A:198:HIS:CD2	2.53	0.44
2:B:37:GLY:HA2	2:B:52:HIS:HA	1.99	0.44
1:L:116:PHE:HD2	2:H:138:SER:HA	1.83	0.43
1:D:33:LEU:HD11	1:D:88:CYS:HB2	2.00	0.43
1:A:36:TYR:HE2	1:A:89:GLN:HE21	1.65	0.43
2:H:13:LYS:HB2	2:H:16:GLU:CD	2.38	0.43
1:D:54:LEU:HD11	1:D:60:ALA:HA	2.00	0.43
2:H:42:PRO:HB2	2:H:45:LYS:HB2	2.00	0.43
1:A:125:LEU:HD21	1:A:130:ALA:HB2	2.01	0.43
1:L:77:SER:O	1:L:78:LEU:C	2.55	0.42
1:A:120:PRO:HG3	1:A:130:ALA:HB1	2.01	0.42
2:B:77:LYS:O	2:B:79:GLN:HG3	2.18	0.42
1:D:135:LEU:C	1:D:136:LEU:HD12	2.40	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:83:PHE:O	1:D:84:ALA:HB2	2.20	0.42
1:D:108:ARG:HD3	1:D:109:THR:O	2.19	0.42
1:D:135:LEU:CD2	2:E:189:VAL:HG11	2.50	0.42
1:L:14:SER:O	1:L:17:GLU:HG2	2.20	0.42
1:L:113:PRO:HD3	1:L:198:HIS:CD2	2.55	0.41
1:D:161:GLU:HG2	1:D:175:LEU:HD21	2.03	0.41
2:H:176:ALA:HB1	2:H:184:TYR:HB3	2.01	0.41
2:B:209:LYS:N	2:B:210:PRO:CD	2.84	0.41
2:E:179:GLN:C	2:E:181:SER:H	2.23	0.41
2:E:209:LYS:N	2:E:210:PRO:CD	2.83	0.41
1:L:15:PRO:HD3	1:L:107:LYS:O	2.21	0.41
1:L:197:THR:HG22	1:L:204:PRO:HG3	2.01	0.41
1:A:32:TYR:HB2	1:A:92:ASN:HB2	2.02	0.41
1:A:37:GLN:HG3	1:A:86:TYR:CE2	2.55	0.41
1:A:33:LEU:HD21	1:A:88:CYS:HB2	2.02	0.41
2:E:158:VAL:HG12	2:E:186:LEU:HD21	2.02	0.41
2:B:104:TYR:CZ	1:D:76:SER:O	2.73	0.41
1:D:136:LEU:HD21	1:D:146:VAL:HG22	2.03	0.41
1:D:32:TYR:HB3	1:D:91:HIS:CD2	2.55	0.41
1:D:189:HIS:O	1:D:211:ARG:NH1	2.53	0.40
1:L:18:ARG:HH22	2:E:105:ASP:CG	2.25	0.40
2:E:127:PRO:HB3	2:E:153:TYR:HB3	2.03	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	211/214 (99%)	199 (94%)	9 (4%)	3 (1%)	<b>11</b> <b>22</b>
1	D	211/214 (99%)	198 (94%)	12 (6%)	1 (0%)	29 52
1	L	211/214 (99%)	199 (94%)	10 (5%)	2 (1%)	<b>17</b> <b>35</b>

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	219/224 (98%)	202 (92%)	14 (6%)	3 (1%)	11	22
2	E	219/224 (98%)	200 (91%)	16 (7%)	3 (1%)	11	22
2	H	220/224 (98%)	209 (95%)	9 (4%)	2 (1%)	17	35
All	All	1291/1314 (98%)	1207 (94%)	70 (5%)	14 (1%)	14	30

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	L	40	PRO
2	H	141	GLY
2	E	15	THR
2	B	138	SER
2	B	197	LEU
2	E	9	PRO
1	A	40	PRO
1	A	184	ALA
1	L	56	SER
2	B	15	THR
1	D	212	GLY
2	E	180	SER
2	H	29	LEU
1	A	68	GLY

### 5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	186/187 (100%)	173 (93%)	13 (7%)	15	30
1	D	186/187 (100%)	170 (91%)	16 (9%)	10	20
1	L	186/187 (100%)	175 (94%)	11 (6%)	19	39
2	B	192/195 (98%)	181 (94%)	11 (6%)	20	41
2	E	192/195 (98%)	177 (92%)	15 (8%)	12	25
2	H	192/195 (98%)	185 (96%)	7 (4%)	35	61

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	1134/1146 (99%)	1061 (94%)	73 (6%)	17 35

All (73) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	7	SER
1	L	21	LEU
1	L	74	THR
1	L	89	GLN
1	L	108	ARG
1	L	115	VAL
1	L	138	ASN
1	L	147	GLN
1	L	160	GLN
1	L	176	SER
1	L	181	LEU
2	H	66	LYS
2	H	78	SER
2	H	102	SER
2	H	137	LYS
2	H	158	VAL
2	H	169	SER
2	H	207	ASN
1	A	54	LEU
1	A	69	THR
1	A	89	GLN
1	A	108	ARG
1	A	122	ASP
1	A	129	THR
1	A	145	LYS
1	A	149	LYS
1	A	151	ASP
1	A	152	ASN
1	A	154	LEU
1	A	169	LYS
1	A	188	LYS
2	B	15	THR
2	B	78	SER
2	B	85	THR
2	B	90	VAL
2	B	102	SER
2	B	123	SER

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
2	B	143	THR
2	B	146	LEU
2	B	194	SER
2	B	199	THR
2	B	214	LYS
1	D	5	THR
1	D	10	THR
1	D	54	LEU
1	D	61	ARG
1	D	69	THR
1	D	74	THR
1	D	89	GLN
1	D	108	ARG
1	D	115	VAL
1	D	145	LYS
1	D	147	GLN
1	D	169	LYS
1	D	177	SER
1	D	190	LYS
1	D	204	PRO
1	D	213	GLU
2	E	7	SER
2	E	10	VAL
2	E	15	THR
2	E	29	LEU
2	E	47	LEU
2	E	85	THR
2	E	88	ASP
2	E	90	VAL
2	E	102	SER
2	E	137	LYS
2	E	139	THR
2	E	158	VAL
2	E	187	SER
2	E	205	ASN
2	E	219	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	L	89	GLN
1	L	124	GLN

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Mol	Chain	Res	Type
1	L	138	ASN
1	L	189	HIS
1	L	198	HIS
2	H	205	ASN
2	H	212	ASN
1	A	89	GLN
1	A	91	HIS
1	A	124	GLN
1	A	138	ASN
1	A	147	GLN
1	A	155	GLN
1	A	160	GLN
1	A	198	HIS
2	B	205	ASN
1	D	89	GLN
1	D	91	HIS
1	D	124	GLN
1	D	147	GLN
1	D	198	HIS
2	E	205	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

3 non-standard protein/DNA/RNA residues 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	PCA	H	1	2	7,8,9	1.82	1 (14%)	9,10,12	2.05	3 (33%)
2	PCA	B	1	2	7,8,9	1.70	1 (14%)	9,10,12	2.43	6 (66%)
2	PCA	E	1	2	7,8,9	1.88	1 (14%)	9,10,12	2.22	5 (55%)

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	PCA	H	1	2	-	0/0/11/13	0/1/1/1
2	PCA	B	1	2	-	0/0/11/13	0/1/1/1
2	PCA	E	1	2	-	0/0/11/13	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	1	PCA	CD-N	4.82	1.47	1.34
2	H	1	PCA	CD-N	4.62	1.46	1.34
2	B	1	PCA	CD-N	4.37	1.46	1.34

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	1	PCA	CA-N-CD	-3.60	101.24	113.58
2	E	1	PCA	CA-N-CD	-3.54	101.47	113.58
2	B	1	PCA	CB-CA-C	-3.30	108.17	112.70
2	B	1	PCA	OE-CD-CG	-3.21	121.16	126.76
2	E	1	PCA	OE-CD-CG	-3.16	121.24	126.76
2	B	1	PCA	CA-N-CD	-3.04	103.17	113.58
2	B	1	PCA	CG-CD-N	2.80	115.65	108.39
2	H	1	PCA	OE-CD-CG	-2.78	121.91	126.76
2	B	1	PCA	CB-CA-N	2.70	111.05	103.30
2	E	1	PCA	CG-CD-N	2.51	114.88	108.39
2	E	1	PCA	CB-CA-N	2.50	110.47	103.30
2	H	1	PCA	CB-CG-CD	-2.35	100.62	104.40
2	E	1	PCA	CB-CA-C	-2.20	109.67	112.70
2	B	1	PCA	O-C-CA	-2.10	119.27	124.78

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 1 is monoatomic - leaving 3 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	SO4	D	1003	-	4,4,4	0.15	0	6,6,6	0.31	0
3	SO4	L	1002	-	4,4,4	0.14	0	6,6,6	0.36	0
3	SO4	H	1001	-	4,4,4	0.21	0	6,6,6	0.22	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	L	1002	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	A	213/214 (99%)	0.07	9 (4%) 36 29	24, 48, 97, 99	0
1	D	213/214 (99%)	0.36	21 (9%) 7 5	25, 51, 99, 99	0
1	L	213/214 (99%)	-0.24	2 (0%) 84 82	25, 44, 74, 94	0
2	B	220/224 (98%)	-0.21	6 (2%) 54 48	27, 41, 93, 99	0
2	E	220/224 (98%)	-0.04	12 (5%) 25 19	32, 56, 98, 99	0
2	H	221/224 (98%)	-0.43	3 (1%) 75 71	26, 41, 67, 99	0
All	All	1300/1314 (98%)	-0.09	53 (4%) 37 30	24, 46, 97, 99	0

All (53) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	L	212	GLY	5.8
1	D	193	ALA	5.8
1	D	192	TYR	5.2
2	E	135	SER	4.9
1	D	181	LEU	4.9
1	A	192	TYR	4.6
1	D	206	THR	4.5
1	A	122	ASP	4.3
1	D	194	CYS	4.3
1	D	196	VAL	4.2
2	E	141	GLY	4.2
2	B	138	SER	4.0
2	E	138	SER	3.6
1	D	135	LEU	3.6
2	E	136	SER	3.5
1	A	181	LEU	3.4
1	D	116	PHE	3.4
1	D	208	SER	3.3
1	L	209	PHE	3.3

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Mol	Chain	Res	Type	RSRZ
1	D	209	PHE	3.2
2	E	134	PRO	3.1
2	B	137	LYS	3.1
2	H	138	SER	2.9
1	A	180	THR	2.9
1	A	193	ALA	2.9
1	D	188	LYS	2.9
2	E	199	THR	2.8
1	A	184	ALA	2.8
1	D	212	GLY	2.7
1	D	119	PRO	2.7
1	D	131	SER	2.7
2	E	139	THR	2.5
1	D	134	CYS	2.5
1	A	150	VAL	2.4
1	D	146	VAL	2.4
2	E	142	GLY	2.4
2	B	141	GLY	2.4
2	E	130	PHE	2.3
2	E	145	ALA	2.3
1	D	205	VAL	2.3
2	H	139	THR	2.2
2	E	137	LYS	2.2
1	A	119	PRO	2.2
1	A	154	LEU	2.2
1	D	186	TYR	2.2
2	H	136	SER	2.2
1	D	117	ILE	2.2
2	B	195	SER	2.1
1	D	191	VAL	2.1
2	E	129	VAL	2.1
2	B	139	THR	2.1
1	D	154	LEU	2.0
2	B	146	LEU	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains [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. 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	B-factors( $\text{\AA}^2$ )	Q<0.9
2	PCA	H	1	8/9	0.90	0.22	51,60,68,84	0
2	PCA	E	1	8/9	0.96	0.09	50,57,60,64	0
2	PCA	B	1	8/9	0.98	0.15	40,45,49,58	0

### 6.3 Carbohydrates [i](#)

There are no monosaccharides 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. 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	B-factors( $\text{\AA}^2$ )	Q<0.9
4	CA	D	1004	1/1	0.93	0.16	58,58,58,58	0
3	SO4	H	1001	5/5	0.95	0.13	41,51,63,74	0
3	SO4	D	1003	5/5	0.97	0.17	61,76,83,99	0
3	SO4	L	1002	5/5	0.99	0.22	47,75,99,99	0

### 6.5 Other polymers [i](#)

There are no such residues in this entry.