



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 10:12 AM GMT

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
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

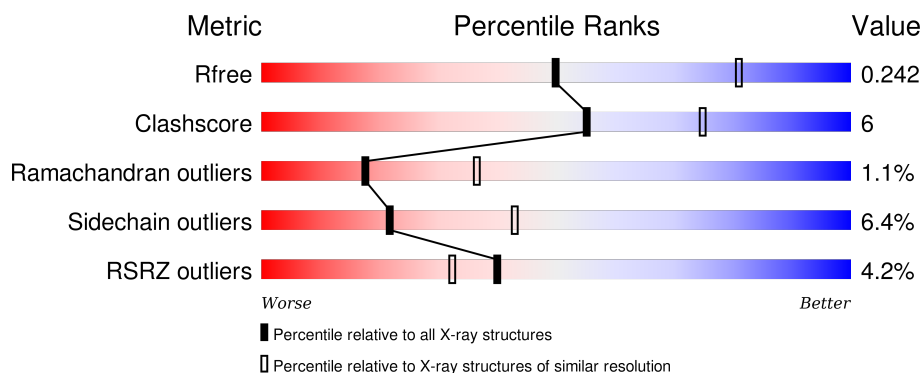
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	91344	2328 (2.60-2.60)
Clashscore	102246	2679 (2.60-2.60)
Ramachandran outliers	100387	2635 (2.60-2.60)
Sidechain outliers	100360	2635 (2.60-2.60)
RSRZ outliers	91569	2334 (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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 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	214	<div> <div>4%</div> <div>75%</div> <div>21%</div> <div>.</div> </div>
1	D	214	<div> <div>10%</div> <div>74%</div> <div>22%</div> <div>.</div> </div>
1	L	214	<div> <div>%</div> <div>82%</div> <div>15%</div> <div>.</div> </div>
2	B	224	<div> <div>3%</div> <div>81%</div> <div>16%</div> <div>..</div> </div>
2	E	224	<div> <div>5%</div> <div>79%</div> <div>18%</div> <div>..</div> </div>

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	H	224	 % 89% 10%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	SO4	L	1002	-	-	-	X

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
1	L	213	Total	C	N	O	S	0	0	0
			1646	1035	275	332	4			
1	A	213	Total	C	N	O	S	0	0	0
			1646	1035	275	332	4			
1	D	213	Total	C	N	O	S	0	0	0
			1646	1035	275	332	4			

- Molecule 2 is a protein called H2L6 HEAVY CHAIN.

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

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



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

- Molecule 5 is water.

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

Continued on next page...

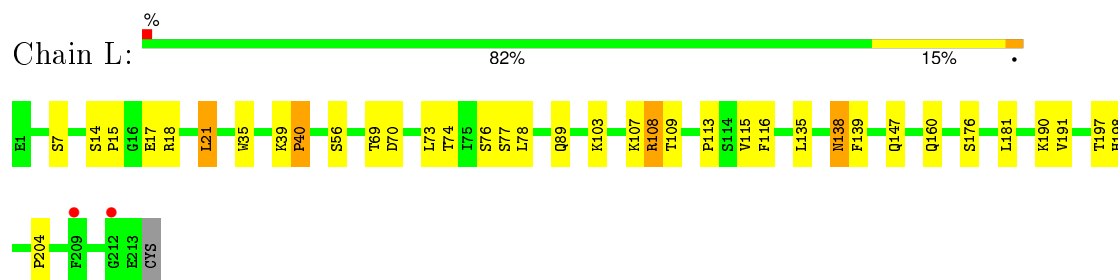
Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	E	18	Total	O	0	0
			18	18		

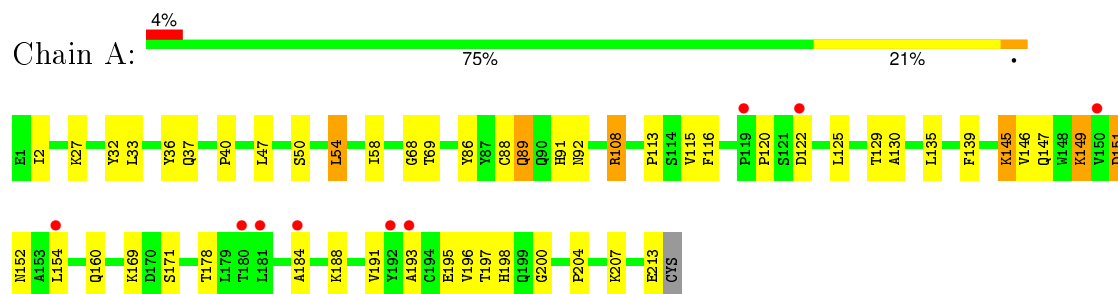
3 Residue-property plots

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.

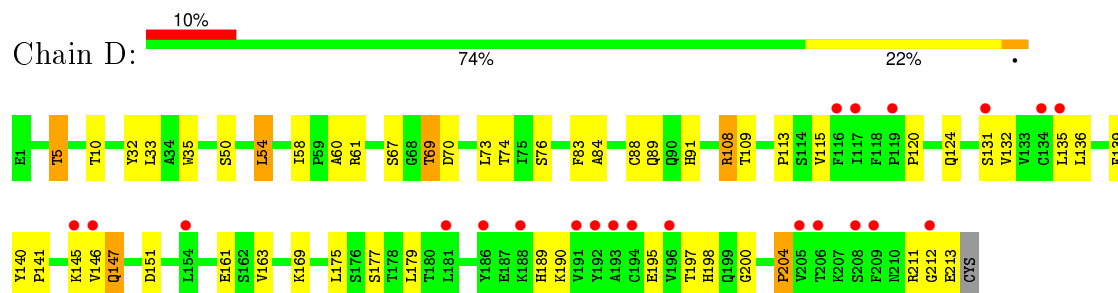
• Molecule 1: H2L6 LIGHT CHAIN



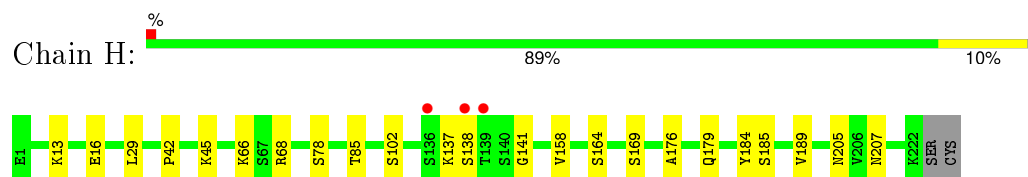
• Molecule 1: H2L6 LIGHT CHAIN



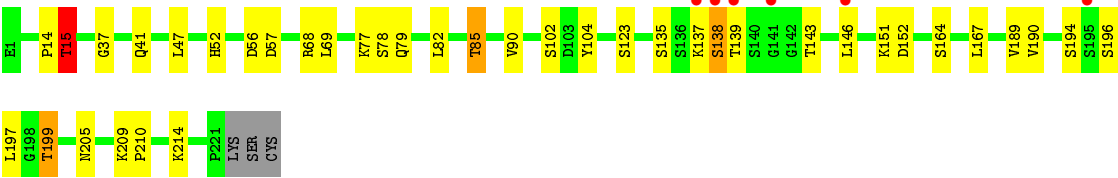
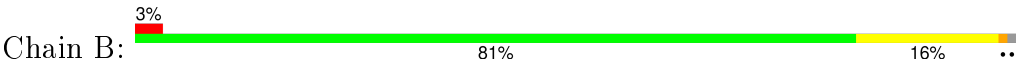
• Molecule 1: H2L6 LIGHT CHAIN



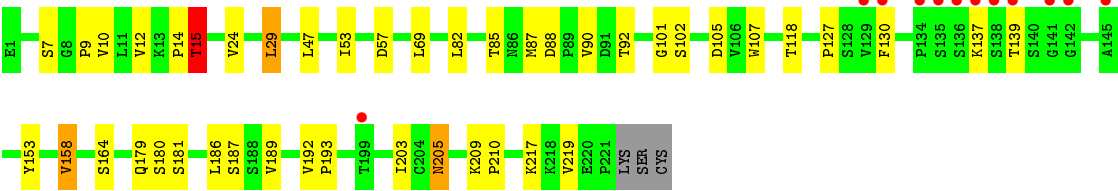
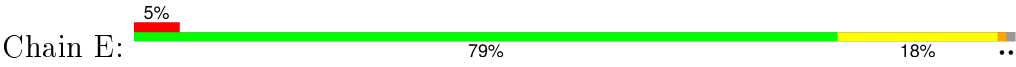
• Molecule 2: H2L6 HEAVY CHAIN



• Molecule 2: H2L6 HEAVY CHAIN



• Molecule 2: H2L6 HEAVY CHAIN



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	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
$\langle I/\sigma(I) \rangle$ ¹	1.87 (at 2.62Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.205 , 0.243 0.205 , 0.242	Depositor DCC
R_{free} test set	2269 reflections (4.24%)	DCC
Wilson B-factor (Å ²)	46.1	Xtriage
Anisotropy	0.122	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 60.4	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.52$, $\langle L^2 \rangle = 0.35$	Xtriage
Outliers	0 of 56166 reflections	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	10198	wwPDB-VP
Average B, all atoms (Å ²)	52.0	wwPDB-VP

Xtriage'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.*

¹Intensities estimated from amplitudes.

²Theoretical 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: CA, PCA, 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	0.48	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

Continued on next page...

Continued from previous page...

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:N	1:L:138:ASN:HD22	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

Continued on next page...

Continued from previous page...

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:A:37:GLN:HB2	1:A:47:LEU:HD11	1.90	0.52
1:L:69:THR:HG22	1:L:70:ASP:OD1	2.10	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:192:VAL:HB	2:E:193:PRO:HD2	1.92	0.51
2:E:101:GLY:HA3	2:E:107:TRP:CZ3	2.46	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:HA	1:D:147:GLN:HE21	1.78	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:50:SER:H	1:A:91:HIS:HE1	1.62	0.47
2:B:151:LYS:HG2	2:B:152:ASP:OD1	2.15	0.47
1:A:116:PHE:CD2	2:B:138:SER:HB2	2.49	0.47
1:D:91:HIS:HD2	2:E:105:ASP:OD1	1.97	0.47
2:B:104:TYR:OH	1:D:76:SER:O	2.15	0.47
1:L:113:PRO:HB3	1:L:139:PHE:HB3	1.97	0.47
1:A:2:ILE:HG13	1:A:27:LYS:HE2	1.96	0.47
2:H:179:GLN:OE1	2:H:185:SER:HB2	2.14	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
2:B:164:SER:N	2:B:205:ASN:HD21	2.07	0.46
1:A:147:GLN:N	1:A:195:GLU:O	2.48	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
2:B:68:ARG:HD2	2:B:85:THR:O	2.17	0.44
1:L:35:TRP:CE2	1:L:73:LEU:HB2	2.53	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: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:L:77:SER:O	1:L:78:LEU:C	2.55	0.42
1:D:135:LEU:C	1:D:136:LEU:HD12	2.40	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:D:83:PHE:O	1:D:84:ALA:HB2	2.20	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: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
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
1:A:37:GLN:HG3	1:A:86:TYR:CE2	2.55	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:L:15:PRO:HD3	1:L:107:LYS:O	2.21	0.41
2:E:158:VAL:HG12	2:E:186:LEU:HD21	2.02	0.41
1:A:33:LEU:HD21	1:A:88:CYS:HB2	2.02	0.41
1:D:136:LEU:HD21	1:D:146:VAL:HG22	2.03	0.41
2:B:104:TYR:CZ	1:D:76:SER:O	2.73	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%)	14	28
1	D	211/214 (99%)	198 (94%)	12 (6%)	1 (0%)	34	60
1	L	211/214 (99%)	199 (94%)	10 (5%)	2 (1%)	21	42

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	219/224 (98%)	202 (92%)	14 (6%)	3 (1%)	14	28
2	E	219/224 (98%)	200 (91%)	16 (7%)	3 (1%)	14	28
2	H	220/224 (98%)	209 (95%)	9 (4%)	2 (1%)	21	42
All	All	1291/1314 (98%)	1207 (94%)	70 (5%)	14 (1%)	17	36

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 ⓘ

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%)	19	37
1	D	186/187 (100%)	170 (91%)	16 (9%)	13	25
1	L	186/187 (100%)	175 (94%)	11 (6%)	24	47
2	B	192/195 (98%)	181 (94%)	11 (6%)	25	49
2	E	192/195 (98%)	177 (92%)	15 (8%)	16	30
2	H	192/195 (98%)	185 (96%)	7 (4%)	42	71

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
All	All	1134/1146 (99%)	1061 (94%)	73 (6%)	22	43

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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
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

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

Mol	Chain	Res	Type
1	L	89	GLN
1	L	124	GLN

Continued on next page...

Continued from previous page...

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 ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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	B	1	2	7,8,9	1.45	1 (14%)	9,10,12	2.28	6 (66%)
2	PCA	E	1	2	7,8,9	1.60	1 (14%)	9,10,12	2.08	4 (44%)
2	PCA	H	1	2	7,8,9	1.55	1 (14%)	9,10,12	1.92	3 (33%)

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	B	1	2	-	0/0/11/13	0/1/1/1
2	PCA	E	1	2	-	0/0/11/13	0/1/1/1
2	PCA	H	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	B	1	PCA	CD-N	3.71	1.46	1.33
2	H	1	PCA	CD-N	3.92	1.46	1.33
2	E	1	PCA	CD-N	4.09	1.47	1.33

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	1	PCA	CA-N-CD	-3.75	101.24	113.81
2	E	1	PCA	CA-N-CD	-3.68	101.47	113.81
2	B	1	PCA	CB-CA-C	-3.36	108.17	112.76
2	B	1	PCA	CA-N-CD	-3.18	103.17	113.81
2	B	1	PCA	OE-CD-CG	-2.53	121.16	126.81
2	E	1	PCA	OE-CD-CG	-2.49	121.24	126.81
2	B	1	PCA	O-C-CA	-2.33	119.27	125.44
2	E	1	PCA	CB-CA-C	-2.26	109.67	112.76
2	H	1	PCA	OE-CD-CG	-2.20	121.91	126.81
2	H	1	PCA	O-C-CA	-2.10	119.90	125.44
2	B	1	PCA	CG-CD-N	2.11	115.65	108.04
2	E	1	PCA	CB-CA-N	2.49	110.47	103.20
2	B	1	PCA	CB-CA-N	2.69	111.05	103.20

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 ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry

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	0.32	0
3	SO4	H	1001	-	4,4,4	0.23	0	6,6,6	0.26	0
3	SO4	L	1002	-	4,4,4	0.17	0	6,6,6	0.28	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	D	1003	-	-	0/0/0/0	0/0/0/0
3	SO4	H	1001	-	-	0/0/0/0	0/0/0/0
3	SO4	L	1002	-	-	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	L	1002	SO4	1	0

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, 95th 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 ²)	Q<0.9
1	A	213/214 (99%)	0.10	9 (4%) 40 32	24, 48, 97, 99	0
1	D	213/214 (99%)	0.40	22 (10%) 9 5	25, 51, 99, 99	0
1	L	213/214 (99%)	-0.21	2 (0%) 85 83	25, 44, 74, 94	0
2	B	220/224 (98%)	-0.18	6 (2%) 58 51	27, 41, 93, 99	0
2	E	220/224 (98%)	-0.01	12 (5%) 29 21	32, 56, 98, 99	0
2	H	221/224 (98%)	-0.40	3 (1%) 78 74	26, 41, 67, 99	0
All	All	1300/1314 (98%)	-0.05	54 (4%) 40 32	24, 46, 97, 99	0

All (54) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	L	212	GLY	5.9
1	D	193	ALA	5.9
1	D	192	TYR	5.3
2	E	135	SER	5.0
1	D	181	LEU	4.9
1	A	192	TYR	4.6
1	D	206	THR	4.6
1	A	122	ASP	4.5
1	D	194	CYS	4.4
1	D	196	VAL	4.3
2	E	141	GLY	4.2
2	B	138	SER	4.1
1	D	135	LEU	3.6
2	E	138	SER	3.6
2	E	136	SER	3.5
1	D	116	PHE	3.5
1	A	181	LEU	3.4
1	D	208	SER	3.4
1	L	209	PHE	3.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	209	PHE	3.2
2	B	137	LYS	3.1
2	E	134	PRO	3.1
1	A	180	THR	3.0
2	H	138	SER	3.0
1	D	188	LYS	2.9
1	A	193	ALA	2.9
1	A	184	ALA	2.9
2	E	199	THR	2.9
1	D	212	GLY	2.8
1	D	119	PRO	2.8
1	D	131	SER	2.7
2	E	139	THR	2.6
1	D	134	CYS	2.6
2	B	141	GLY	2.5
2	E	142	GLY	2.5
1	A	150	VAL	2.5
1	D	146	VAL	2.5
2	E	145	ALA	2.4
2	E	130	PHE	2.3
2	E	137	LYS	2.3
1	D	205	VAL	2.3
2	H	139	THR	2.3
1	D	186	TYR	2.3
1	A	119	PRO	2.3
2	H	136	SER	2.2
1	A	154	LEU	2.2
1	D	117	ILE	2.2
1	D	191	VAL	2.2
2	B	195	SER	2.2
2	E	129	VAL	2.1
2	B	139	THR	2.1
1	D	154	LEU	2.1
1	D	145	LYS	2.1
2	B	146	LEU	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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, 95th 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(\AA^2)	Q<0.9
2	PCA	B	1	8/9	0.98	0.15	-	40,45,49,58	0
2	PCA	E	1	8/9	0.96	0.09	-	50,57,60,64	0
2	PCA	H	1	8/9	0.90	0.22	-	51,60,68,84	0

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, 95th 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(\AA^2)	Q<0.9
3	SO4	L	1002	5/5	0.99	0.22	6.77	47,75,99,99	0
3	SO4	D	1003	5/5	0.97	0.17	1.64	61,76,83,99	0
3	SO4	H	1001	5/5	0.95	0.13	-	41,51,63,74	0
4	CA	D	1004	1/1	0.93	0.16	-	58,58,58,58	0

6.5 Other polymers [i](#)

There are no such residues in this entry.