Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 06:36 AM GMT

PDB ID	:	2XQB
Title	:	CRYSTAL STRUCTURE OF ANTI-IL-15 ANTIBODY IN COMPLEX WITH HUMAN IL-15
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Deposited on	:	2010-09-01
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 (i) symbol.

The following versions of software and data (see references (i)) were used in the production of this report:

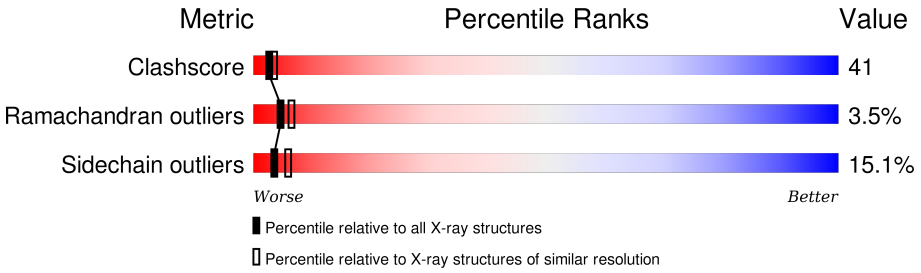
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	FAILED
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation 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))
Clashscore	102246	2679 (2.60-2.60)
Ramachandran outliers	100387	2635 (2.60-2.60)
Sidechain outliers	100360	2635 (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 <=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.

Note EDS failed to run properly.

Mol	Chain	Length	Quality of chain
1	A	114	33% 45% 12% • 8%
2	H	236	51% 36% 9% •
3	L	211	48% 37% 10% •

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 4063 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 INTERLEUKIN 15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	105	785	495	123	161	6	0	0	0

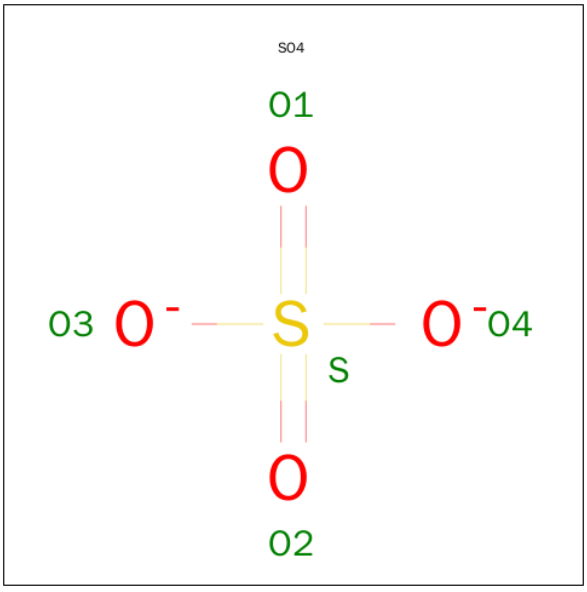
- Molecule 2 is a protein called ANTI-IL-15 ANTIBODY.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	H	227	1696	1075	281	333	7	0	0	0

- Molecule 3 is a protein called ANTI-IL-15 ANTIBODY.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	L	202	1501	944	247	306	4	0	0	0

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



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

- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	5	Total O 5 5	0	0
5	H	46	Total O 46 46	0	0
5	L	15	Total O 15 15	0	0

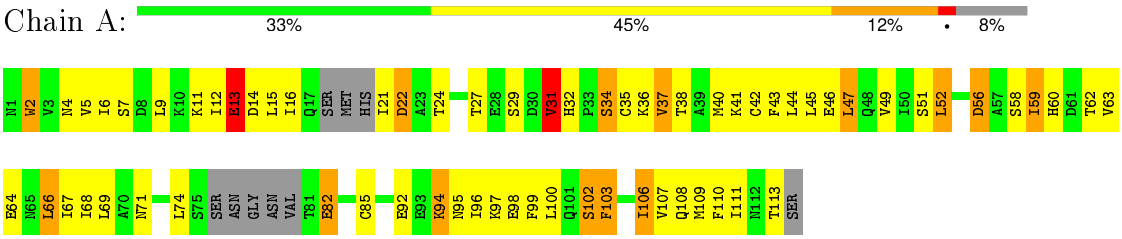
3 Residue-property plots (i)

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.

Note EDS failed to run properly.

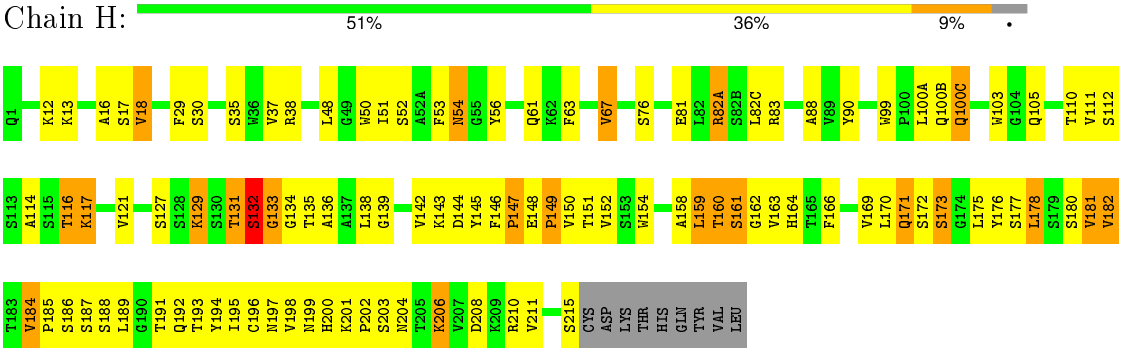
- Molecule 1: INTERLEUKIN 15

Chain A:



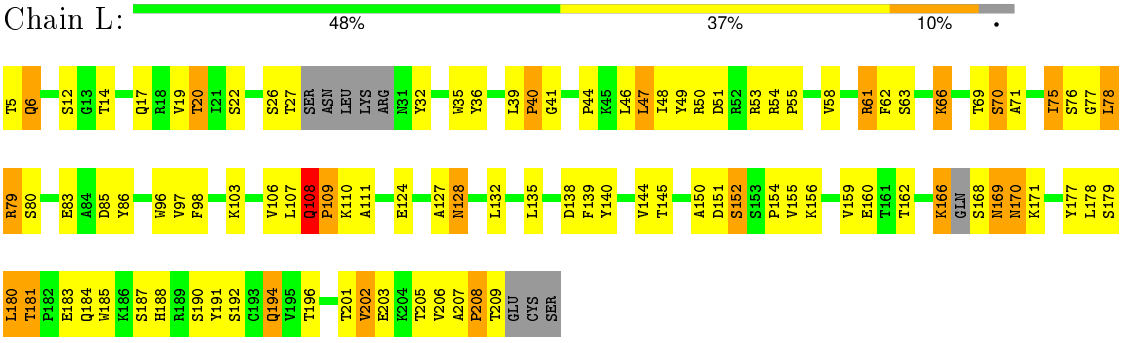
- Molecule 2: ANTI-IL-15 ANTIBODY

Chain H:



- Molecule 3: ANTI-IL-15 ANTIBODY

Chain L:



4 Data and refinement statistics (i)

EDS failed to run properly - this section will therefore be incomplete.

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	185.19Å 43.75Å 70.09Å 90.00° 95.95° 90.00°	Depositor
Resolution (Å)	69.71 – 2.60	Depositor
% Data completeness (in resolution range)	99.0 (69.71-2.60)	Depositor
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.42 (at 2.62Å)	Xtriage
Refinement program	REFMAC 5.4.0069	Depositor
R, R_{free}	0.244 , 0.318	Depositor
Wilson B-factor (Å^2)	48.0	Xtriage
Anisotropy	0.420	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.34$	Xtriage
Outliers	1 of 17425 reflections (0.006%)	Xtriage
Total number of atoms	4063	wwPDB-VP
Average B, all atoms (Å^2)	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.67% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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	A	0.48	0/792	0.89	0/1072
2	H	0.54	0/1742	0.88	1/2380 (0.0%)
3	L	0.46	0/1540	0.85	1/2108 (0.0%)
All	All	0.50	0/4074	0.87	2/5560 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	H	132	SER	CB-CA-C	-6.59	97.57	110.10
3	L	108	GLN	C-N-CD	-5.92	107.57	120.60

There are no chirality outliers.

There are no planarity outliers.

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	A	785	0	735	84	0
2	H	1696	0	1642	135	0
3	L	1501	0	1416	115	0
4	H	10	0	0	0	0
4	L	5	0	0	0	0
5	A	5	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	H	46	0	0	2	0
5	L	15	0	0	0	0
All	All	4063	0	3793	317	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 41.

All (317) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:131:THR:HG23	2:H:136:ALA:CB	1.84	1.08
2:H:171:GLN:HG3	2:H:175:LEU:O	1.59	1.03
2:H:132:SER:OG	2:H:133:GLY:N	1.78	0.96
2:H:131:THR:HG23	2:H:136:ALA:HB2	1.48	0.92
1:A:12:ILE:C	1:A:14:ASP:H	1.72	0.92
2:H:18:VAL:CG2	2:H:82(C):LEU:HD11	1.99	0.92
2:H:131:THR:CG2	2:H:136:ALA:HB2	2.00	0.91
2:H:138:LEU:HD13	2:H:211:VAL:HG11	1.52	0.91
3:L:49:TYR:CD1	3:L:50:ARG:HG3	2.06	0.90
1:A:5:VAL:HG13	1:A:66:LEU:CD1	2.03	0.89
2:H:131:THR:HG23	2:H:136:ALA:CA	2.03	0.89
2:H:127:SER:O	2:H:131:THR:OG1	1.90	0.88
2:H:181:VAL:CG2	3:L:135:LEU:HD13	2.04	0.87
3:L:49:TYR:HD1	3:L:50:ARG:HG3	1.39	0.86
2:H:18:VAL:HG23	2:H:82(C):LEU:HD11	1.56	0.86
1:A:6:ILE:HD11	1:A:108:GLN:HE22	1.44	0.81
2:H:131:THR:HG23	2:H:136:ALA:HA	1.62	0.80
1:A:66:LEU:HD12	1:A:66:LEU:O	1.82	0.79
3:L:110:LYS:CG	3:L:111:ALA:H	1.96	0.78
2:H:181:VAL:HG21	3:L:135:LEU:HD13	1.65	0.78
1:A:103:PHE:O	1:A:107:VAL:HG23	1.82	0.78
2:H:170:LEU:HD13	2:H:176:TYR:CE2	2.18	0.78
2:H:116:THR:HG22	5:H:2034:HOH:O	1.83	0.77
2:H:138:LEU:HD13	2:H:211:VAL:CG1	2.14	0.76
1:A:14:ASP:C	1:A:16:ILE:H	1.89	0.76
3:L:54:ARG:HD3	3:L:62:PHE:O	1.85	0.76
3:L:110:LYS:CG	3:L:111:ALA:N	2.47	0.76
1:A:96:ILE:O	1:A:100:LEU:HG	1.85	0.76
3:L:110:LYS:HG3	3:L:111:ALA:H	1.50	0.75
1:A:6:ILE:CD1	1:A:108:GLN:HE22	2.00	0.75
1:A:5:VAL:HG13	1:A:66:LEU:HD13	1.67	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:151:ASP:CG	3:L:188:HIS:HD1	1.92	0.73
2:H:170:LEU:HD13	2:H:176:TYR:CZ	2.24	0.73
2:H:169:VAL:HG23	3:L:162:THR:HG22	1.70	0.73
2:H:159:LEU:HD11	2:H:182:VAL:HG21	1.71	0.73
1:A:4:ASN:HB2	1:A:69:LEU:HD13	1.72	0.72
3:L:139:PHE:CE2	3:L:144:VAL:HG23	2.24	0.71
2:H:195:ILE:HD11	2:H:210:ARG:CB	2.20	0.71
1:A:12:ILE:C	1:A:14:ASP:N	2.41	0.71
2:H:181:VAL:HG22	3:L:135:LEU:HD13	1.71	0.71
1:A:59:ILE:O	1:A:63:VAL:HG13	1.90	0.71
2:H:178:LEU:C	2:H:178:LEU:HD23	2.11	0.71
3:L:159:VAL:HG22	3:L:178:LEU:HD13	1.73	0.70
2:H:144:ASP:HB3	2:H:175:LEU:HD13	1.74	0.70
3:L:169:ASN:O	3:L:170:ASN:CB	2.38	0.70
1:A:13:GLU:HB2	1:A:100:LEU:CD1	2.22	0.69
2:H:191:THR:HG22	2:H:192:GLN:N	2.07	0.69
3:L:169:ASN:HB3	3:L:171:LYS:HD2	1.72	0.69
1:A:6:ILE:HD11	1:A:108:GLN:NE2	2.07	0.69
1:A:5:VAL:HG13	1:A:66:LEU:HD11	1.72	0.69
1:A:2:TRP:HA	1:A:2:TRP:CE3	2.28	0.68
1:A:14:ASP:O	1:A:16:ILE:N	2.25	0.68
1:A:102:SER:O	1:A:106:ILE:HG22	1.94	0.68
1:A:13:GLU:HA	1:A:100:LEU:CD1	2.24	0.68
2:H:139:GLY:HA2	2:H:154:TRP:CZ2	2.29	0.68
2:H:52:SER:HB3	2:H:54:ASN:ND2	2.09	0.67
1:A:29:SER:C	1:A:31:VAL:H	1.96	0.67
2:H:18:VAL:HG22	2:H:82(C):LEU:HD11	1.75	0.67
3:L:75:ILE:HD11	3:L:78:LEU:HD21	1.76	0.67
3:L:110:LYS:HG2	3:L:111:ALA:N	2.09	0.67
3:L:169:ASN:O	3:L:170:ASN:HB2	1.94	0.66
1:A:106:ILE:HG12	1:A:106:ILE:O	1.95	0.66
2:H:12:LYS:HE2	2:H:17:SER:O	1.96	0.66
3:L:205:THR:CG2	3:L:206:VAL:N	2.58	0.66
2:H:150:VAL:CG2	2:H:178:LEU:HD13	2.26	0.65
3:L:79:ARG:HG2	3:L:79:ARG:NH1	2.12	0.64
2:H:142:VAL:HB	2:H:178:LEU:HD22	1.80	0.64
3:L:169:ASN:CB	3:L:171:LYS:HD2	2.28	0.64
3:L:183:GLU:O	3:L:187:SER:HB3	1.98	0.64
1:A:43:PHE:HB3	1:A:103:PHE:CE1	2.33	0.63
2:H:132:SER:HA	2:H:135:THR:O	1.98	0.63
1:A:27:THR:HB	1:A:94:LYS:HG3	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:75:ILE:HD11	3:L:78:LEU:CD2	2.28	0.63
2:H:169:VAL:CG2	3:L:162:THR:HG22	2.28	0.63
3:L:185:TRP:CH2	3:L:208:PRO:HA	2.34	0.63
2:H:152:VAL:HG11	2:H:180:SER:CB	2.29	0.63
2:H:121:VAL:HG21	2:H:198:VAL:HG21	1.80	0.63
2:H:138:LEU:CD1	2:H:211:VAL:HG11	2.27	0.63
2:H:127:SER:C	2:H:129:LYS:H	2.01	0.62
1:A:56:ASP:OD1	1:A:58:SER:OG	2.17	0.62
1:A:51:SER:HA	1:A:59:ILE:HD11	1.80	0.62
1:A:14:ASP:C	1:A:16:ILE:N	2.52	0.62
3:L:169:ASN:HB3	3:L:171:LYS:CD	2.29	0.62
3:L:207:ALA:O	3:L:209:THR:N	2.23	0.62
1:A:111:ILE:C	1:A:113:THR:H	2.00	0.62
1:A:13:GLU:HB2	1:A:100:LEU:HD12	1.81	0.62
2:H:131:THR:CG2	2:H:136:ALA:CB	2.64	0.61
3:L:169:ASN:CG	3:L:171:LYS:HD2	2.21	0.61
1:A:12:ILE:O	1:A:14:ASP:N	2.34	0.61
2:H:121:VAL:CG2	2:H:198:VAL:HG21	2.30	0.61
2:H:160:THR:O	2:H:161:SER:O	2.19	0.60
1:A:52:LEU:HD22	3:L:55:PRO:HB3	1.83	0.60
1:A:4:ASN:HB2	1:A:69:LEU:CD1	2.31	0.60
1:A:66:LEU:HD12	1:A:66:LEU:C	2.19	0.60
2:H:159:LEU:C	2:H:159:LEU:HD12	2.22	0.60
3:L:83:GLU:HG3	3:L:106:VAL:H	1.67	0.60
1:A:47:LEU:HD23	1:A:47:LEU:O	2.02	0.60
3:L:169:ASN:C	3:L:171:LYS:H	2.06	0.59
1:A:82:GLU:HG3	1:A:85:CYS:SG	2.42	0.59
3:L:169:ASN:HB3	3:L:171:LYS:CG	2.32	0.59
3:L:107:LEU:HA	3:L:140:TYR:OH	2.03	0.59
2:H:169:VAL:HG23	3:L:162:THR:CG2	2.31	0.58
2:H:131:THR:CG2	2:H:136:ALA:CA	2.78	0.58
1:A:13:GLU:HB2	1:A:100:LEU:HD13	1.86	0.58
2:H:166:PHE:HE1	2:H:181:VAL:CG2	2.16	0.58
2:H:145:TYR:CZ	2:H:150:VAL:HG22	2.37	0.58
3:L:79:ARG:HG2	3:L:79:ARG:HH11	1.68	0.58
3:L:69:THR:O	3:L:70:SER:HB3	2.05	0.57
2:H:131:THR:CG2	2:H:136:ALA:HA	2.31	0.57
2:H:171:GLN:CG	2:H:175:LEU:O	2.45	0.57
2:H:161:SER:C	2:H:163:VAL:H	2.07	0.57
3:L:76:SER:OG	3:L:77:GLY:N	2.34	0.57
3:L:181:THR:H	3:L:184:GLN:HB2	1.70	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:19:VAL:HG12	3:L:20:THR:H	1.69	0.56
2:H:81:GLU:OE2	2:H:82(A):ARG:NH2	2.38	0.56
3:L:179:SER:C	3:L:180:LEU:HD23	2.25	0.56
3:L:79:ARG:CG	3:L:79:ARG:HH11	2.19	0.56
2:H:150:VAL:HG23	2:H:178:LEU:CD1	2.35	0.56
1:A:52:LEU:HD13	3:L:49:TYR:CE2	2.41	0.56
2:H:139:GLY:HA2	2:H:154:TRP:CH2	2.41	0.55
3:L:194:GLN:HG2	3:L:194:GLN:O	2.05	0.55
1:A:106:ILE:O	1:A:110:PHE:HD1	1.89	0.55
1:A:5:VAL:CG1	1:A:66:LEU:HD11	2.35	0.55
2:H:138:LEU:HD12	2:H:138:LEU:C	2.27	0.55
3:L:51:ASP:OD1	3:L:66:LYS:HD2	2.06	0.54
2:H:133:GLY:C	2:H:135:THR:H	2.11	0.54
2:H:54:ASN:HD22	2:H:56:TYR:H	1.53	0.54
2:H:171:GLN:C	2:H:173:SER:H	2.11	0.54
2:H:195:ILE:HG22	2:H:197:ASN:ND2	2.22	0.54
1:A:36:LYS:HG3	1:A:110:PHE:CZ	2.43	0.54
1:A:43:PHE:CE1	1:A:106:ILE:HG21	2.44	0.53
2:H:116:THR:HG23	5:H:2033:HOH:O	2.08	0.53
2:H:134:GLY:C	2:H:186:SER:HB2	2.29	0.53
3:L:79:ARG:O	3:L:106:VAL:HG21	2.08	0.53
2:H:159:LEU:HD11	2:H:182:VAL:CG2	2.38	0.53
1:A:37:VAL:HG22	1:A:74:LEU:HD22	1.91	0.53
2:H:195:ILE:HG22	2:H:197:ASN:HD21	1.73	0.53
1:A:47:LEU:O	1:A:47:LEU:CD2	2.58	0.52
2:H:166:PHE:HE1	2:H:181:VAL:HG23	1.74	0.52
3:L:35:TRP:HB2	3:L:48:ILE:HB	1.91	0.52
2:H:131:THR:HB	2:H:132:SER:HB3	1.90	0.52
1:A:51:SER:HB3	1:A:60:HIS:CD2	2.44	0.52
3:L:132:LEU:HD13	3:L:180:LEU:HD21	1.92	0.52
1:A:27:THR:HG23	1:A:43:PHE:CE2	2.45	0.52
3:L:14:THR:O	3:L:17:GLN:HB2	2.10	0.52
3:L:145:THR:HB	3:L:196:THR:HB	1.92	0.52
3:L:152:SER:O	3:L:154:PRO:HD3	2.10	0.52
1:A:12:ILE:HD11	1:A:62:THR:HG22	1.91	0.51
2:H:18:VAL:HG23	2:H:82(C):LEU:HD21	1.92	0.51
1:A:13:GLU:CA	1:A:100:LEU:CD1	2.88	0.51
1:A:2:TRP:HA	1:A:2:TRP:HE3	1.72	0.51
3:L:150:ALA:O	3:L:151:ASP:HB2	2.10	0.51
3:L:132:LEU:HB2	3:L:178:LEU:HB3	1.91	0.51
3:L:155:VAL:HG22	3:L:156:LYS:N	2.25	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:139:PHE:CE2	3:L:144:VAL:CG2	2.94	0.51
3:L:190:SER:OG	3:L:191:TYR:N	2.44	0.51
3:L:36:TYR:CE2	3:L:46:LEU:HD13	2.45	0.51
1:A:5:VAL:CG1	1:A:66:LEU:CD1	2.85	0.51
2:H:131:THR:HG21	2:H:136:ALA:HB2	1.87	0.50
2:H:50:TRP:CG	2:H:51:ILE:N	2.78	0.50
3:L:50:ARG:O	3:L:51:ASP:HB2	2.09	0.50
1:A:98:GLU:O	1:A:102:SER:HB2	2.11	0.50
1:A:11:LYS:O	1:A:14:ASP:HB2	2.12	0.50
1:A:92:GLU:HB3	1:A:94:LYS:HE3	1.94	0.50
2:H:189:LEU:C	2:H:191:THR:H	2.14	0.50
3:L:17:GLN:O	3:L:78:LEU:HB2	2.11	0.50
3:L:155:VAL:CG2	3:L:156:LYS:N	2.75	0.50
1:A:2:TRP:CD1	1:A:110:PHE:HB3	2.47	0.50
2:H:150:VAL:HG23	2:H:178:LEU:HD13	1.92	0.50
3:L:138:ASP:OD1	3:L:171:LYS:HD3	2.12	0.50
1:A:29:SER:C	1:A:31:VAL:N	2.65	0.50
3:L:188:HIS:HB2	3:L:191:TYR:CE2	2.46	0.50
2:H:185:PRO:C	2:H:187:SER:H	2.15	0.50
1:A:13:GLU:HA	1:A:100:LEU:HD12	1.91	0.49
2:H:63:PHE:HB3	2:H:67:VAL:HG22	1.93	0.49
3:L:180:LEU:HD23	3:L:180:LEU:N	2.26	0.49
3:L:207:ALA:C	3:L:209:THR:H	2.13	0.49
1:A:4:ASN:O	1:A:7:SER:OG	2.30	0.49
3:L:144:VAL:HG12	3:L:145:THR:N	2.27	0.49
2:H:12:LYS:O	2:H:111:VAL:HA	2.13	0.49
3:L:80:SER:HA	3:L:106:VAL:HG11	1.95	0.49
3:L:49:TYR:CE1	3:L:50:ARG:HG3	2.47	0.49
3:L:159:VAL:HG22	3:L:178:LEU:CD1	2.40	0.49
2:H:52:SER:CB	2:H:54:ASN:ND2	2.75	0.49
3:L:32:TYR:CE2	3:L:50:ARG:HD3	2.47	0.49
2:H:134:GLY:O	2:H:186:SER:N	2.35	0.49
1:A:13:GLU:O	1:A:13:GLU:CG	2.61	0.48
2:H:144:ASP:HB3	2:H:175:LEU:CD1	2.44	0.48
1:A:41:LYS:HD2	2:H:100(A):LEU:HD21	1.95	0.48
1:A:29:SER:HA	1:A:31:VAL:HG22	1.96	0.48
3:L:151:ASP:OD2	3:L:188:HIS:ND1	2.29	0.48
1:A:42:CYS:O	1:A:46:GLU:HG2	2.14	0.48
2:H:195:ILE:CD1	2:H:210:ARG:HA	2.45	0.47
2:H:184:VAL:HG21	2:H:189:LEU:HD21	1.96	0.47
3:L:205:THR:HG23	3:L:206:VAL:N	2.27	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:47:LEU:C	1:A:47:LEU:CD2	2.82	0.47
3:L:66:LYS:CG	3:L:71:ALA:HB2	2.43	0.47
2:H:185:PRO:C	2:H:187:SER:N	2.68	0.47
1:A:13:GLU:CB	1:A:100:LEU:CD1	2.92	0.47
2:H:164:HIS:HE1	2:H:166:PHE:HA	1.80	0.47
2:H:103:TRP:CZ3	3:L:44:PRO:HG2	2.50	0.47
1:A:45:LEU:CD1	2:H:100(B):GLN:HB3	2.45	0.47
3:L:127:ALA:O	3:L:128:ASN:CB	2.63	0.47
1:A:32:HIS:C	1:A:34:SER:N	2.68	0.46
1:A:9:LEU:O	1:A:13:GLU:HB3	2.15	0.46
2:H:188:SER:O	2:H:192:GLN:N	2.48	0.46
2:H:184:VAL:HG21	2:H:189:LEU:CD2	2.45	0.46
2:H:171:GLN:C	2:H:173:SER:N	2.66	0.46
2:H:133:GLY:O	2:H:135:THR:HG23	2.16	0.46
1:A:56:ASP:OD1	1:A:59:ILE:HG23	2.15	0.46
1:A:43:PHE:HB3	1:A:103:PHE:CZ	2.50	0.46
3:L:169:ASN:HB3	3:L:171:LYS:HG3	1.98	0.46
3:L:132:LEU:O	3:L:177:TYR:HA	2.16	0.46
2:H:147:PRO:HB2	2:H:148:GLU:H	1.59	0.46
1:A:111:ILE:C	1:A:113:THR:N	2.69	0.46
2:H:159:LEU:HD11	2:H:163:VAL:HG23	1.98	0.46
2:H:159:LEU:HD12	2:H:160:THR:N	2.31	0.45
1:A:21:ILE:O	1:A:22:ASP:CB	2.64	0.45
3:L:205:THR:HG22	3:L:206:VAL:N	2.31	0.45
2:H:112:SER:C	2:H:114:ALA:H	2.20	0.45
2:H:117:LYS:HE2	2:H:144:ASP:O	2.17	0.45
2:H:197:ASN:ND2	2:H:208:ASP:OD1	2.44	0.45
2:H:52:SER:C	2:H:53:PHE:H	2.20	0.45
3:L:166:LYS:HE3	3:L:166:LYS:HB2	1.38	0.45
3:L:166:LYS:O	3:L:168:SER:N	2.50	0.45
2:H:88:ALA:HB3	2:H:90:TYR:CE1	2.51	0.45
3:L:66:LYS:HG2	3:L:71:ALA:HB2	1.99	0.45
2:H:162:GLY:O	2:H:182:VAL:HA	2.17	0.45
2:H:145:TYR:CZ	2:H:150:VAL:CG2	3.00	0.45
2:H:154:TRP:CH2	2:H:196:CYS:HB3	2.52	0.45
3:L:76:SER:C	3:L:78:LEU:H	2.19	0.45
2:H:99:TRP:HB2	2:H:100(B):GLN:HG3	1.98	0.45
3:L:85:ASP:OD1	3:L:103:LYS:HD2	2.16	0.45
2:H:150:VAL:HG21	2:H:178:LEU:HD13	1.98	0.45
2:H:201:LYS:N	2:H:202:PRO:CD	2.79	0.44
2:H:181:VAL:HG12	2:H:182:VAL:H	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:180:LEU:HA	3:L:184:GLN:OE1	2.17	0.44
2:H:139:GLY:HA3	2:H:180:SER:O	2.18	0.44
2:H:143:LYS:HA	2:H:177:SER:OG	2.17	0.44
2:H:161:SER:OG	2:H:162:GLY:N	2.47	0.44
3:L:26:SER:O	3:L:27:THR:O	2.36	0.44
2:H:13:LYS:O	2:H:16:ALA:HB3	2.18	0.44
2:H:37:VAL:HG12	2:H:38:ARG:N	2.32	0.44
2:H:142:VAL:HB	2:H:178:LEU:CD2	2.47	0.44
2:H:195:ILE:HG13	2:H:210:ARG:HA	2.00	0.44
3:L:61:ARG:HB3	3:L:76:SER:O	2.17	0.44
3:L:19:VAL:HG12	3:L:20:THR:N	2.32	0.44
2:H:185:PRO:O	2:H:187:SER:N	2.51	0.43
1:A:64:GLU:O	1:A:68:ILE:HG13	2.17	0.43
3:L:151:ASP:OD1	3:L:188:HIS:HB3	2.18	0.43
3:L:109:PRO:HB2	3:L:110:LYS:H	1.55	0.43
1:A:13:GLU:CB	1:A:100:LEU:HD13	2.48	0.43
3:L:207:ALA:HA	3:L:208:PRO:HD3	1.92	0.43
1:A:46:GLU:O	1:A:49:VAL:HB	2.19	0.43
3:L:19:VAL:HG21	3:L:78:LEU:HD11	2.00	0.43
2:H:63:PHE:O	2:H:67:VAL:HG22	2.18	0.43
1:A:51:SER:OG	1:A:63:VAL:HG21	2.19	0.43
2:H:184:VAL:HG23	2:H:185:PRO:N	2.33	0.43
3:L:97:VAL:HG12	3:L:98:PHE:N	2.34	0.43
3:L:39:LEU:HB3	3:L:40:PRO:HD2	2.01	0.42
1:A:5:VAL:O	1:A:9:LEU:HG	2.20	0.42
2:H:139:GLY:HA2	2:H:154:TRP:HZ2	1.80	0.42
3:L:75:ILE:CD1	3:L:78:LEU:HD21	2.46	0.42
2:H:116:THR:HA	2:H:146:PHE:O	2.20	0.42
2:H:152:VAL:HG11	2:H:180:SER:HB3	2.00	0.42
2:H:166:PHE:HE1	2:H:181:VAL:HG21	1.85	0.42
2:H:12:LYS:O	2:H:112:SER:N	2.52	0.42
3:L:194:GLN:HB2	3:L:203:GLU:HG3	2.01	0.42
3:L:6:GLN:HB3	3:L:22:SER:O	2.19	0.42
1:A:40:MET:O	1:A:44:LEU:HG	2.19	0.42
2:H:48:LEU:HD23	2:H:48:LEU:N	2.35	0.42
3:L:47:LEU:O	3:L:55:PRO:HD2	2.19	0.42
2:H:103:TRP:CE3	3:L:44:PRO:HD2	2.54	0.42
2:H:148:GLU:HA	2:H:149:PRO:HA	1.66	0.42
3:L:51:ASP:CG	3:L:66:LYS:HD2	2.39	0.42
1:A:95:ASN:C	1:A:97:LYS:H	2.22	0.42
2:H:171:GLN:O	2:H:173:SER:N	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:166:PHE:CE1	2:H:181:VAL:HG23	2.53	0.42
3:L:78:LEU:HA	3:L:78:LEU:HD23	1.65	0.42
3:L:19:VAL:HG21	3:L:78:LEU:CD1	2.48	0.42
2:H:150:VAL:HG13	2:H:200:HIS:CD2	2.55	0.42
3:L:40:PRO:HB2	3:L:41:GLY:H	1.62	0.42
1:A:59:ILE:HG13	1:A:60:HIS:N	2.35	0.42
2:H:100(C):GLN:OE1	3:L:96:TRP:NE1	2.53	0.42
1:A:52:LEU:HD13	3:L:49:TYR:CD2	2.55	0.41
3:L:178:LEU:HG	3:L:180:LEU:CD2	2.50	0.41
2:H:203:SER:O	2:H:204:ASN:HB2	2.20	0.41
2:H:163:VAL:O	2:H:163:VAL:HG12	2.19	0.41
2:H:189:LEU:C	2:H:191:THR:N	2.74	0.41
3:L:124:GLU:O	3:L:127:ALA:HB3	2.20	0.41
2:H:188:SER:HB2	2:H:192:GLN:HB3	2.02	0.41
2:H:127:SER:C	2:H:129:LYS:N	2.69	0.41
2:H:194:TYR:O	2:H:195:ILE:HD12	2.21	0.41
2:H:100(C):GLN:OE1	3:L:96:TRP:CD1	2.74	0.41
1:A:67:ILE:O	1:A:71:ASN:HB2	2.21	0.41
1:A:27:THR:HG21	1:A:102:SER:HB2	2.02	0.41
2:H:129:LYS:HE3	3:L:206:VAL:HG12	2.02	0.41
1:A:52:LEU:HD23	1:A:52:LEU:HA	1.85	0.41
3:L:53:ARG:HD2	3:L:53:ARG:HA	1.80	0.41
3:L:202:VAL:O	3:L:202:VAL:HG22	2.20	0.41
2:H:169:VAL:HG11	3:L:160:GLU:HB3	2.03	0.41
3:L:55:PRO:HG2	3:L:58:VAL:HG21	2.03	0.41
1:A:99:PHE:HD2	1:A:100:LEU:HD23	1.85	0.40
3:L:181:THR:N	3:L:184:GLN:HB2	2.34	0.40
2:H:121:VAL:HG22	2:H:198:VAL:HG21	2.02	0.40
3:L:201:THR:O	3:L:201:THR:HG23	2.21	0.40
2:H:178:LEU:CD2	2:H:178:LEU:C	2.82	0.40
3:L:170:ASN:HA	3:L:170:ASN:HD22	1.56	0.40
2:H:199:ASN:OD1	2:H:206:LYS:HD3	2.21	0.40
3:L:86:TYR:N	3:L:86:TYR:CD1	2.89	0.40
1:A:37:VAL:HA	1:A:110:PHE:HZ	1.85	0.40
1:A:32:HIS:C	1:A:34:SER:H	2.22	0.40
2:H:29:PHE:CD2	2:H:76:SER:HA	2.57	0.40
2:H:145:TYR:CE1	2:H:150:VAL:HG22	2.56	0.40
1:A:38:THR:N	1:A:82:GLU:OE1	2.54	0.40
2:H:195:ILE:O	2:H:195:ILE:HG22	2.21	0.40
3:L:127:ALA:O	3:L:128:ASN:HB3	2.21	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	99/114 (87%)	89 (90%)	6 (6%)	4 (4%)	4	4
2	H	225/236 (95%)	201 (89%)	16 (7%)	8 (4%)	4	6
3	L	196/211 (93%)	179 (91%)	11 (6%)	6 (3%)	5	8
All	All	520/561 (93%)	469 (90%)	33 (6%)	18 (4%)	4	6

All (18) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	15	LEU
2	H	161	SER
3	L	40	PRO
3	L	78	LEU
3	L	108	GLN
3	L	109	PRO
1	A	13	GLU
1	A	22	ASP
2	H	133	GLY
2	H	158	ALA
3	L	70	SER
1	A	31	VAL
2	H	61	GLN
2	H	132	SER
3	L	208	PRO
2	H	149	PRO
2	H	182	VAL
2	H	147	PRO

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	86/107 (80%)	68 (79%)	18 (21%)	1 2
2	H	188/200 (94%)	161 (86%)	27 (14%)	4 7
3	L	164/180 (91%)	143 (87%)	21 (13%)	5 10
All	All	438/487 (90%)	372 (85%)	66 (15%)	3 6

All (66) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	TRP
1	A	13	GLU
1	A	24	THR
1	A	31	VAL
1	A	34	SER
1	A	35	CYS
1	A	37	VAL
1	A	47	LEU
1	A	52	LEU
1	A	56	ASP
1	A	59	ILE
1	A	66	LEU
1	A	82	GLU
1	A	94	LYS
1	A	102	SER
1	A	103	PHE
1	A	106	ILE
1	A	109	MET
2	H	18	VAL
2	H	30	SER
2	H	35	SER
2	H	54	ASN
2	H	67	VAL
2	H	82(A)	ARG
2	H	83	ARG
2	H	100(C)	GLN
2	H	105	GLN
2	H	110	THR
2	H	116	THR
2	H	117	LYS
2	H	129	LYS

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Mol	Chain	Res	Type
2	H	131	THR
2	H	132	SER
2	H	151	THR
2	H	159	LEU
2	H	160	THR
2	H	171	GLN
2	H	172	SER
2	H	173	SER
2	H	178	LEU
2	H	181	VAL
2	H	184	VAL
2	H	193	THR
2	H	206	LYS
2	H	215	SER
3	L	5	THR
3	L	6	GLN
3	L	12	SER
3	L	20	THR
3	L	47	LEU
3	L	61	ARG
3	L	63	SER
3	L	66	LYS
3	L	75	ILE
3	L	79	ARG
3	L	108	GLN
3	L	128	ASN
3	L	152	SER
3	L	166	LYS
3	L	169	ASN
3	L	170	ASN
3	L	180	LEU
3	L	181	THR
3	L	192	SER
3	L	194	GLN
3	L	202	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	4	ASN
1	A	108	GLN
2	H	54	ASN

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Mol	Chain	Res	Type
2	H	61	GLN
2	H	64	GLN
2	H	192	GLN
3	L	128	ASN
3	L	170	ASN
3	L	194	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

3 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	$\#\|Z\| > 2$
4	SO4	H	1216	-	4,4,4	0.18	0	6,6,6	0.16	0
4	SO4	H	1217	-	4,4,4	0.32	0	6,6,6	0.12	0
4	SO4	L	1210	-	4,4,4	0.20	0	6,6,6	0.13	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
4	SO4	H	1216	-	-	0/0/0/0	0/0/0/0
4	SO4	H	1217	-	-	0/0/0/0	0/0/0/0
4	SO4	L	1210	-	-	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

EDS failed to run properly - this section will therefore be empty.

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

EDS failed to run properly - this section will therefore be empty.

6.3 Carbohydrates

EDS failed to run properly - this section will therefore be empty.

6.4 Ligands

EDS failed to run properly - this section will therefore be empty.

6.5 Other polymers

EDS failed to run properly - this section will therefore be empty.