Full wwPDB X-ray Structure Validation Report ⓘ

Nov 14, 2023 – 01:15 AM JST

PDB ID	:	5YOY
Title	:	Crystal structure of the human tumor necrosis factor in complex with golimumab Fv
Authors	:	Ono, M.; Horita, S.; Sato, Y.; Nomura, Y.; Iwata, S.; Nomura, N.
Deposited on	:	2017-10-31
Resolution	:	2.73 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
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.

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

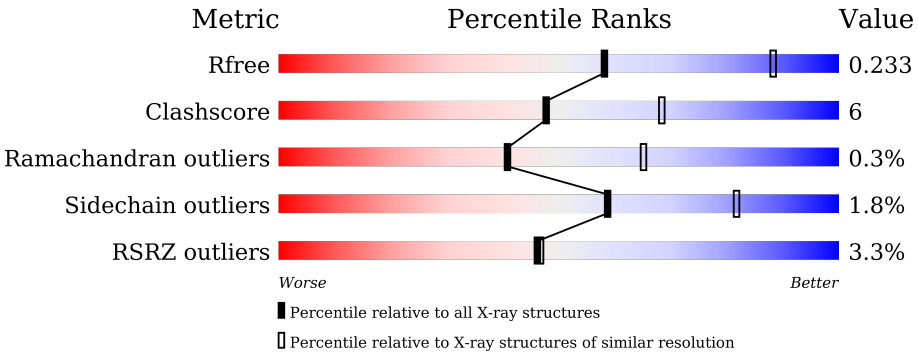
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.73 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	3359 (2.74-2.70)
Clashscore	141614	3686 (2.74-2.70)
Ramachandran outliers	138981	3622 (2.74-2.70)
Sidechain outliers	138945	3623 (2.74-2.70)
RSRZ outliers	127900	3276 (2.74-2.70)

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 >=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 <=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	173	5% 70% 17% • 11%
1	B	173	2% 74% 13% • 11%
1	C	173	5% 72% 17% 11%
1	J	173	5% 71% 18% 12%
1	K	173	7% 66% 21% • 12%
1	L	173	3% 65% 22% • 12%

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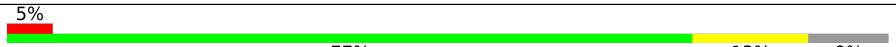
Mol	Chain	Length	Quality of chain
2	D	119	
2	E	119	
2	F	119	
2	M	119	
2	N	119	
2	O	119	
3	G	129	
3	H	129	
3	I	129	
3	P	129	
3	Q	129	
3	R	129	

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 18116 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 Tumor necrosis factor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	154	Total	C	N	O	S	0	0	0
			1202	765	209	226	2			
1	B	154	Total	C	N	O	S	0	0	0
			1202	765	209	226	2			
1	C	154	Total	C	N	O	S	0	0	0
			1202	765	209	226	2			
1	J	153	Total	C	N	O	S	0	0	0
			1196	762	208	224	2			
1	K	153	Total	C	N	O	S	0	0	0
			1196	762	208	224	2			
1	L	153	Total	C	N	O	S	0	0	0
			1196	762	208	224	2			

There are 96 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-7	ASP	-	expression tag	UNP P01375
A	-6	TYR	-	expression tag	UNP P01375
A	-5	LYS	-	expression tag	UNP P01375
A	-4	ASP	-	expression tag	UNP P01375
A	-3	ASP	-	expression tag	UNP P01375
A	-2	ASP	-	expression tag	UNP P01375
A	-1	ASP	-	expression tag	UNP P01375
A	0	LYS	-	cloning artifact	UNP P01375
A	158	THR	-	cloning artifact	UNP P01375
A	159	SER	-	cloning artifact	UNP P01375
A	160	GLU	-	cloning artifact	UNP P01375
A	161	ASN	-	cloning artifact	UNP P01375
A	162	LEU	-	cloning artifact	UNP P01375
A	163	TYR	-	cloning artifact	UNP P01375
A	164	PHE	-	cloning artifact	UNP P01375
A	165	GLN	-	cloning artifact	UNP P01375
B	-7	ASP	-	expression tag	UNP P01375

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-6	TYR	-	expression tag	UNP P01375
B	-5	LYS	-	expression tag	UNP P01375
B	-4	ASP	-	expression tag	UNP P01375
B	-3	ASP	-	expression tag	UNP P01375
B	-2	ASP	-	expression tag	UNP P01375
B	-1	ASP	-	expression tag	UNP P01375
B	0	LYS	-	cloning artifact	UNP P01375
B	158	THR	-	cloning artifact	UNP P01375
B	159	SER	-	cloning artifact	UNP P01375
B	160	GLU	-	cloning artifact	UNP P01375
B	161	ASN	-	cloning artifact	UNP P01375
B	162	LEU	-	cloning artifact	UNP P01375
B	163	TYR	-	cloning artifact	UNP P01375
B	164	PHE	-	cloning artifact	UNP P01375
B	165	GLN	-	cloning artifact	UNP P01375
C	-7	ASP	-	expression tag	UNP P01375
C	-6	TYR	-	expression tag	UNP P01375
C	-5	LYS	-	expression tag	UNP P01375
C	-4	ASP	-	expression tag	UNP P01375
C	-3	ASP	-	expression tag	UNP P01375
C	-2	ASP	-	expression tag	UNP P01375
C	-1	ASP	-	expression tag	UNP P01375
C	0	LYS	-	cloning artifact	UNP P01375
C	158	THR	-	cloning artifact	UNP P01375
C	159	SER	-	cloning artifact	UNP P01375
C	160	GLU	-	cloning artifact	UNP P01375
C	161	ASN	-	cloning artifact	UNP P01375
C	162	LEU	-	cloning artifact	UNP P01375
C	163	TYR	-	cloning artifact	UNP P01375
C	164	PHE	-	cloning artifact	UNP P01375
C	165	GLN	-	cloning artifact	UNP P01375
J	-7	ASP	-	expression tag	UNP P01375
J	-6	TYR	-	expression tag	UNP P01375
J	-5	LYS	-	expression tag	UNP P01375
J	-4	ASP	-	expression tag	UNP P01375
J	-3	ASP	-	expression tag	UNP P01375
J	-2	ASP	-	expression tag	UNP P01375
J	-1	ASP	-	expression tag	UNP P01375
J	0	LYS	-	cloning artifact	UNP P01375
J	158	THR	-	cloning artifact	UNP P01375
J	159	SER	-	cloning artifact	UNP P01375
J	160	GLU	-	cloning artifact	UNP P01375

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Chain	Residue	Modelled	Actual	Comment	Reference
J	161	ASN	-	cloning artifact	UNP P01375
J	162	LEU	-	cloning artifact	UNP P01375
J	163	TYR	-	cloning artifact	UNP P01375
J	164	PHE	-	cloning artifact	UNP P01375
J	165	GLN	-	cloning artifact	UNP P01375
K	-7	ASP	-	expression tag	UNP P01375
K	-6	TYR	-	expression tag	UNP P01375
K	-5	LYS	-	expression tag	UNP P01375
K	-4	ASP	-	expression tag	UNP P01375
K	-3	ASP	-	expression tag	UNP P01375
K	-2	ASP	-	expression tag	UNP P01375
K	-1	ASP	-	expression tag	UNP P01375
K	0	LYS	-	cloning artifact	UNP P01375
K	158	THR	-	cloning artifact	UNP P01375
K	159	SER	-	cloning artifact	UNP P01375
K	160	GLU	-	cloning artifact	UNP P01375
K	161	ASN	-	cloning artifact	UNP P01375
K	162	LEU	-	cloning artifact	UNP P01375
K	163	TYR	-	cloning artifact	UNP P01375
K	164	PHE	-	cloning artifact	UNP P01375
K	165	GLN	-	cloning artifact	UNP P01375
L	-7	ASP	-	expression tag	UNP P01375
L	-6	TYR	-	expression tag	UNP P01375
L	-5	LYS	-	expression tag	UNP P01375
L	-4	ASP	-	expression tag	UNP P01375
L	-3	ASP	-	expression tag	UNP P01375
L	-2	ASP	-	expression tag	UNP P01375
L	-1	ASP	-	expression tag	UNP P01375
L	0	LYS	-	cloning artifact	UNP P01375
L	158	THR	-	cloning artifact	UNP P01375
L	159	SER	-	cloning artifact	UNP P01375
L	160	GLU	-	cloning artifact	UNP P01375
L	161	ASN	-	cloning artifact	UNP P01375
L	162	LEU	-	cloning artifact	UNP P01375
L	163	TYR	-	cloning artifact	UNP P01375
L	164	PHE	-	cloning artifact	UNP P01375
L	165	GLN	-	cloning artifact	UNP P01375

- Molecule 2 is a protein called Golimumab light chain variable region.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	108	Total	C	N	O	S	0	0	0
			834	530	140	162	2			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	108	Total	C	N	O	S	0	0	0
			834	530	140	162	2			
2	F	108	Total	C	N	O	S	0	0	0
			834	530	140	162	2			
2	M	108	Total	C	N	O	S	0	0	0
			834	530	140	162	2			
2	N	108	Total	C	N	O	S	0	0	0
			834	530	140	162	2			
2	O	108	Total	C	N	O	S	0	0	0
			834	530	140	162	2			

- Molecule 3 is a protein called Golimumab heavy chain variable region.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	G	126	Total	C	N	O	S	0	0	0
			973	610	171	186	6			
3	H	126	Total	C	N	O	S	0	0	0
			973	610	171	186	6			
3	I	125	Total	C	N	O	S	0	0	0
			967	607	170	184	6			
3	P	126	Total	C	N	O	S	0	0	0
			973	610	171	186	6			
3	Q	126	Total	C	N	O	S	0	0	0
			973	610	171	186	6			
3	R	126	Total	C	N	O	S	0	0	0
			973	610	171	186	6			

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	2	Total	O	0	0
			2	2		
4	B	6	Total	O	0	0
			6	6		
4	C	7	Total	O	0	0
			7	7		
4	D	8	Total	O	0	0
			8	8		
4	E	2	Total	O	0	0
			2	2		
4	F	1	Total	O	0	0
			1	1		

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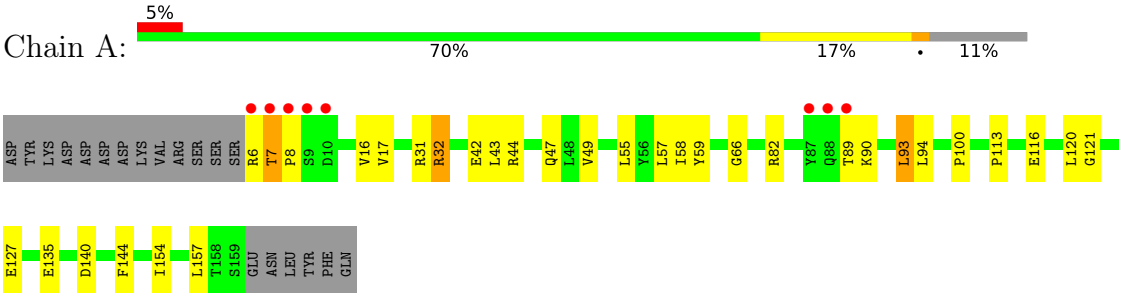
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	G	9	Total O 9 9	0	0
4	H	4	Total O 4 4	0	0
4	I	6	Total O 6 6	0	0
4	J	2	Total O 2 2	0	0
4	K	5	Total O 5 5	0	0
4	L	6	Total O 6 6	0	0
4	M	11	Total O 11 11	0	0
4	N	3	Total O 3 3	0	0
4	P	7	Total O 7 7	0	0
4	Q	6	Total O 6 6	0	0
4	R	1	Total O 1 1	0	0

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.

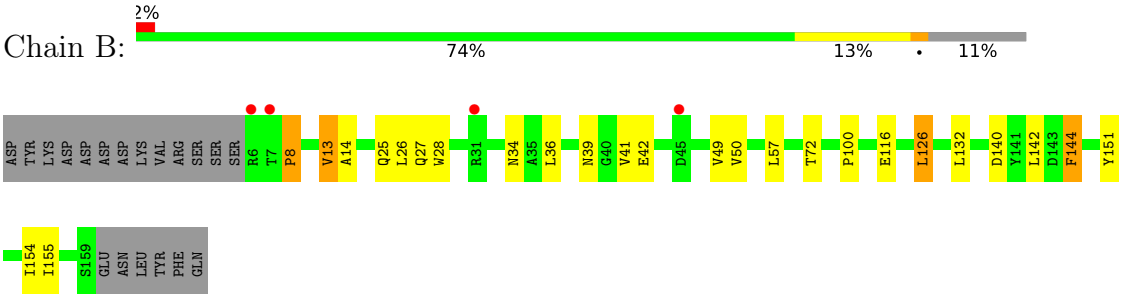
• Molecule 1: Tumor necrosis factor

Chain A:



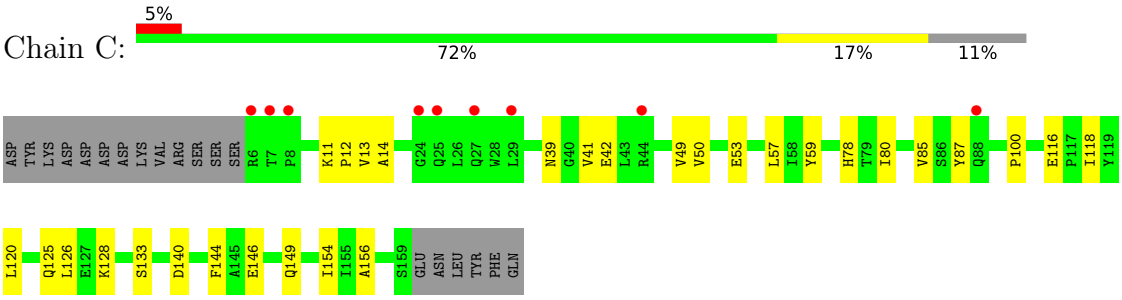
• Molecule 1: Tumor necrosis factor

Chain B:



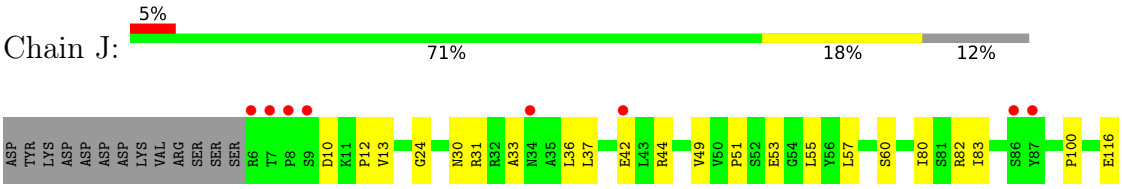
• Molecule 1: Tumor necrosis factor

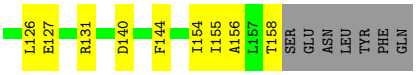
Chain C:



• Molecule 1: Tumor necrosis factor

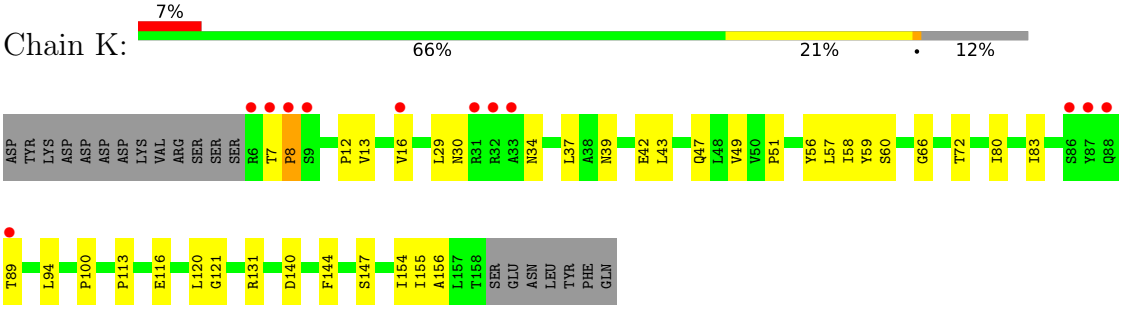
Chain J:





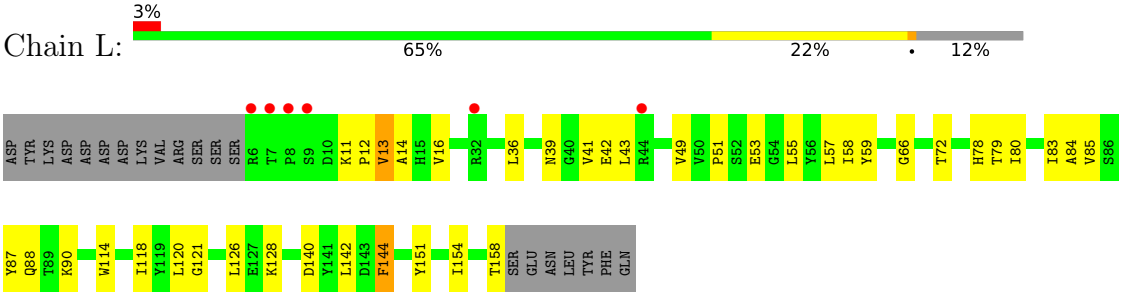
• Molecule 1: Tumor necrosis factor

Chain K:



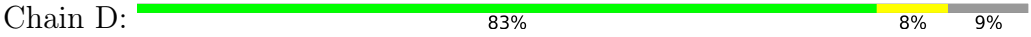
• Molecule 1: Tumor necrosis factor

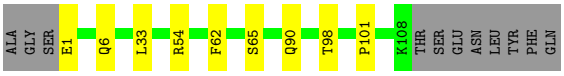
Chain L:



• Molecule 2: Golimumab light chain variable region

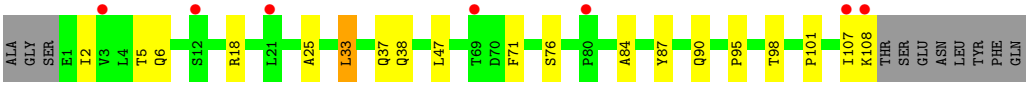
Chain D:





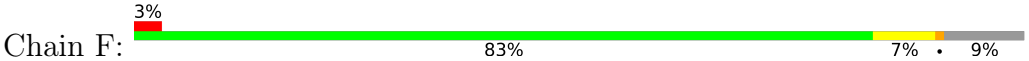
• Molecule 2: Golimumab light chain variable region

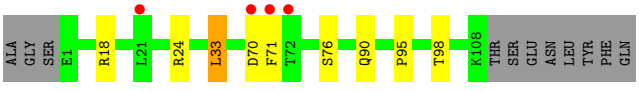
Chain E:



• Molecule 2: Golimumab light chain variable region

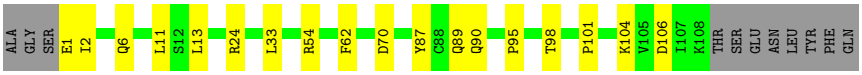
Chain F:



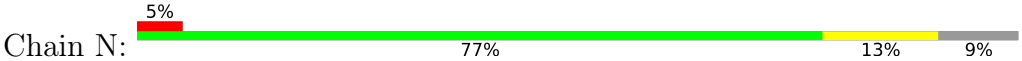


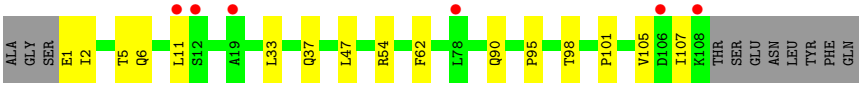
• Molecule 2: Golimumab light chain variable region

Chain M:

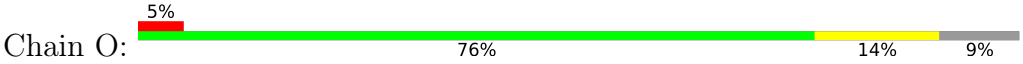


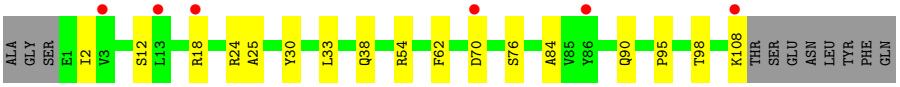
• Molecule 2: Golimumab light chain variable region



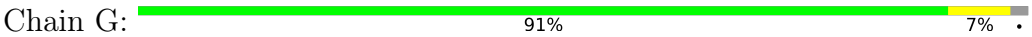


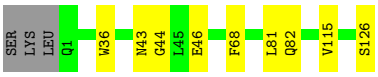
• Molecule 2: Golimumab light chain variable region



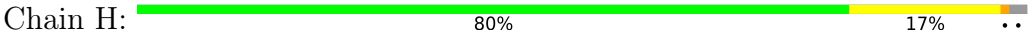


• Molecule 3: Golimumab heavy chain variable region

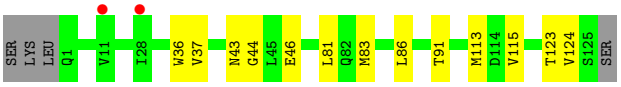




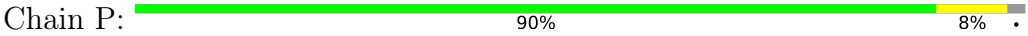
• Molecule 3: Golimumab heavy chain variable region



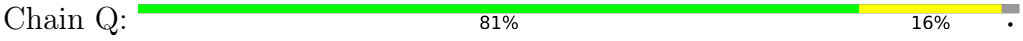
• Molecule 3: Golimumab heavy chain variable region

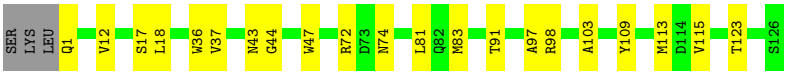


• Molecule 3: Golimumab heavy chain variable region

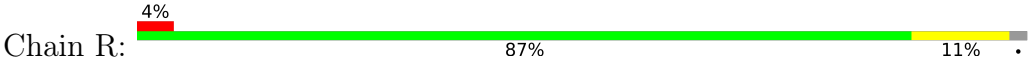


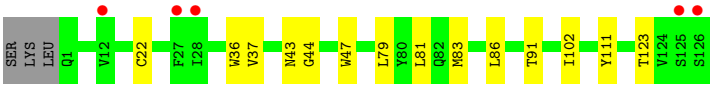
• Molecule 3: Golimumab heavy chain variable region





• Molecule 3: Golimumab heavy chain variable region





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	133.64Å 85.30Å 135.96Å 90.00° 101.61° 90.00°	Depositor
Resolution (Å)	46.25 – 2.73 46.25 – 2.73	Depositor EDS
% Data completeness (in resolution range)	97.1 (46.25-2.73) 97.1 (46.25-2.73)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.61 (at 2.73Å)	Xtriage
Refinement program	PHENIX dev_2210	Depositor
R, R_{free}	0.190 , 0.234 0.191 , 0.233	Depositor DCC
R_{free} test set	3936 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å^2)	65.9	Xtriage
Anisotropy	0.354	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 41.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.29$	Xtriage
Estimated twinning fraction	0.026 for l,-k,h	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	18116	wwPDB-VP
Average B, all atoms (Å^2)	77.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.72% 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, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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	0.27	0/1229	0.51	0/1674
1	B	0.29	0/1229	0.51	0/1674
1	C	0.28	0/1229	0.50	0/1674
1	J	0.26	0/1223	0.49	0/1666
1	K	0.27	0/1223	0.50	0/1666
1	L	0.28	0/1223	0.50	0/1666
2	D	0.28	0/857	0.52	0/1169
2	E	0.27	0/857	0.48	0/1169
2	F	0.27	0/857	0.48	0/1169
2	M	0.29	0/857	0.54	0/1169
2	N	0.26	0/857	0.49	0/1169
2	O	0.27	0/857	0.48	0/1169
3	G	0.30	0/995	0.52	0/1345
3	H	0.28	0/995	0.50	0/1345
3	I	0.26	0/989	0.50	0/1337
3	P	0.29	0/995	0.50	0/1345
3	Q	0.28	0/995	0.51	0/1345
3	R	0.26	0/995	0.48	0/1345
All	All	0.28	0/18462	0.50	0/25096

There are no bond length outliers.

There are no bond angle outliers.

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	1202	0	1197	25	0
1	B	1202	0	1197	17	0
1	C	1202	0	1197	21	0
1	J	1196	0	1192	23	0
1	K	1196	0	1192	23	0
1	L	1196	0	1192	22	0
2	D	834	0	809	5	0
2	E	834	0	809	10	0
2	F	834	0	809	6	0
2	M	834	0	809	12	0
2	N	834	0	809	7	0
2	O	834	0	809	10	0
3	G	973	0	926	6	0
3	H	973	0	926	15	0
3	I	967	0	921	7	0
3	P	973	0	926	7	0
3	Q	973	0	926	11	0
3	R	973	0	926	8	0
4	A	2	0	0	0	0
4	B	6	0	0	1	0
4	C	7	0	0	1	0
4	D	8	0	0	2	0
4	E	2	0	0	0	0
4	F	1	0	0	0	0
4	G	9	0	0	2	0
4	H	4	0	0	0	0
4	I	6	0	0	1	0
4	J	2	0	0	0	0
4	K	5	0	0	2	0
4	L	6	0	0	0	0
4	M	11	0	0	1	0
4	N	3	0	0	1	0
4	P	7	0	0	1	0
4	Q	6	0	0	1	0
4	R	1	0	0	0	0
All	All	18116	0	17572	216	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 (216) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:30:ASN:OD1	4:K:201:HOH:O	1.90	0.88
1:B:28:TRP:O	4:B:201:HOH:O	1.91	0.88
2:N:1:GLU:N	4:N:201:HOH:O	2.09	0.84
1:L:13:VAL:HG13	1:L:36:LEU:HD13	1.65	0.79
3:G:46:GLU:OE1	4:G:201:HOH:O	2.00	0.78
2:F:90:GLN:HE21	2:F:98:THR:HB	1.48	0.77
2:M:89:GLN:HE22	3:P:113:MET:HE3	1.49	0.76
2:D:65:SER:OG	4:D:201:HOH:O	2.03	0.75
3:G:126:SER:HA	4:G:205:HOH:O	1.87	0.74
2:E:90:GLN:HE21	2:E:98:THR:HB	1.54	0.72
2:E:6:GLN:HB2	2:E:101:PRO:HD2	1.71	0.72
2:N:90:GLN:HE21	2:N:98:THR:HB	1.55	0.71
2:O:90:GLN:HE21	2:O:98:THR:HB	1.55	0.70
1:L:84:ALA:HB3	1:L:87:TYR:HB2	1.72	0.70
1:K:147:SER:O	4:K:202:HOH:O	2.11	0.69
2:O:2:ILE:HG22	2:O:95:PRO:HD2	1.74	0.69
1:A:44:ARG:HH12	1:L:85:VAL:HG11	1.58	0.69
2:M:54:ARG:NH1	2:M:62:PHE:O	2.26	0.69
2:D:90:GLN:HE21	2:D:98:THR:HB	1.59	0.68
1:J:82:ARG:NH2	1:K:34:ASN:OD1	2.27	0.67
1:B:13:VAL:HG13	1:B:36:LEU:HD13	1.75	0.67
1:K:47:GLN:OE1	1:K:131:ARG:NH1	2.29	0.66
1:C:42:GLU:HB2	1:C:49:VAL:HB	1.79	0.65
2:M:104:LYS:NZ	2:M:106:ASP:OD2	2.29	0.65
2:D:54:ARG:NH1	2:D:62:PHE:O	2.30	0.65
2:M:90:GLN:HE21	2:M:98:THR:HB	1.62	0.64
2:O:12:SER:HB3	2:O:108:LYS:HB2	1.79	0.64
1:A:17:VAL:HG21	1:A:32:ARG:HD2	1.79	0.64
2:F:24:ARG:NH1	2:F:70:ASP:OD2	2.31	0.63
1:A:100:PRO:HB3	1:A:116:GLU:HG3	1.79	0.63
3:R:43:ASN:OD1	3:R:44:GLY:N	2.29	0.63
2:M:24:ARG:NH2	2:M:70:ASP:OD1	2.32	0.63
3:I:91:THR:HG23	3:I:123:THR:HA	1.82	0.62
1:B:50:VAL:HG21	1:B:126:LEU:HD23	1.82	0.61
1:J:42:GLU:HB2	1:J:49:VAL:HB	1.82	0.61
1:A:82:ARG:NH1	1:A:127:GLU:OE1	2.34	0.61
1:A:82:ARG:HB2	1:A:93:LEU:HD21	1.84	0.60
2:N:54:ARG:NH1	2:N:62:PHE:O	2.34	0.60
1:B:100:PRO:HB3	1:B:116:GLU:HG3	1.84	0.58
2:M:6:GLN:HB2	2:M:101:PRO:HD2	1.85	0.58
1:L:140:ASP:OD1	1:L:140:ASP:N	2.37	0.57
1:K:16:VAL:HG12	1:K:30:ASN:HB3	1.85	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:2:ILE:HG22	2:E:95:PRO:HD2	1.86	0.57
2:E:6:GLN:HE22	2:E:87:TYR:HA	1.68	0.57
2:O:18:ARG:HD2	2:O:76:SER:HA	1.87	0.57
3:R:91:THR:HG23	3:R:123:THR:HA	1.87	0.57
1:C:12:PRO:HA	1:C:39:ASN:HB2	1.88	0.56
3:Q:1:GLN:NE2	4:Q:203:HOH:O	2.37	0.56
3:H:14:PRO:HD3	3:H:125:SER:O	2.06	0.56
1:J:100:PRO:HB3	1:J:116:GLU:HG3	1.88	0.55
3:P:43:ASN:OD1	3:P:44:GLY:N	2.31	0.55
1:B:140:ASP:OD1	1:B:140:ASP:N	2.38	0.55
1:C:50:VAL:HG21	1:C:126:LEU:HD13	1.89	0.55
1:K:12:PRO:HA	1:K:39:ASN:HB2	1.89	0.55
1:J:82:ARG:NH1	1:J:127:GLU:OE1	2.39	0.55
2:D:6:GLN:HB2	2:D:101:PRO:HD2	1.88	0.55
2:M:1:GLU:N	4:M:204:HOH:O	2.38	0.55
1:A:82:ARG:NH2	1:B:34:ASN:OD1	2.40	0.54
1:C:85:VAL:O	4:C:201:HOH:O	2.18	0.54
3:I:43:ASN:OD1	3:I:44:GLY:N	2.32	0.54
1:K:12:PRO:HG2	1:K:156:ALA:HB3	1.88	0.54
3:G:43:ASN:OD1	3:G:44:GLY:N	2.32	0.54
1:L:42:GLU:HB2	1:L:49:VAL:HB	1.90	0.53
2:D:1:GLU:O	4:D:202:HOH:O	2.19	0.53
1:C:128:LYS:HZ1	1:J:44:ARG:HH12	1.54	0.53
2:N:11:LEU:HB3	2:N:105:VAL:HG22	1.90	0.53
3:H:53:TYR:O	3:H:72:ARG:NH1	2.42	0.53
1:A:140:ASP:OD1	1:A:140:ASP:N	2.42	0.53
2:E:2:ILE:HD11	2:E:25:ALA:HB1	1.91	0.53
1:A:31:ARG:HG3	1:J:33:ALA:HB1	1.89	0.52
1:A:44:ARG:HH21	1:L:128:LYS:HE3	1.74	0.52
1:J:13:VAL:HG23	1:J:155:ILE:HB	1.90	0.52
1:J:57:LEU:O	1:J:154:ILE:HA	2.09	0.52
3:Q:91:THR:HG23	3:Q:123:THR:HA	1.92	0.52
1:L:57:LEU:O	1:L:154:ILE:HA	2.10	0.52
2:N:6:GLN:HB2	2:N:101:PRO:HD2	1.92	0.52
1:L:12:PRO:HA	1:L:39:ASN:HB2	1.92	0.52
3:H:72:ARG:NH1	3:H:74:ASN:OD1	2.42	0.52
1:J:140:ASP:OD1	1:J:140:ASP:N	2.37	0.52
3:H:98:ARG:HG2	3:H:115:VAL:HG12	1.92	0.51
3:H:43:ASN:OD1	3:H:44:GLY:N	2.35	0.51
3:R:83:MET:HE2	3:R:86:LEU:HD21	1.93	0.51
1:J:30:ASN:HD22	1:J:37:LEU:HD23	1.76	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:140:ASP:OD1	1:K:140:ASP:N	2.42	0.51
3:Q:12:VAL:HG21	3:Q:18:LEU:HD22	1.93	0.51
2:M:11:LEU:HG	2:M:13:LEU:CD2	2.42	0.50
1:L:11:LYS:H	1:L:39:ASN:ND2	2.09	0.50
1:A:6:ARG:NE	1:C:125:GLN:HE22	2.10	0.50
1:B:42:GLU:HB2	1:B:49:VAL:HB	1.93	0.50
1:J:53:GLU:HA	1:J:126:LEU:O	2.11	0.50
3:R:36:TRP:CE2	3:R:81:LEU:HB2	2.46	0.50
1:A:42:GLU:HB2	1:A:49:VAL:HB	1.94	0.49
3:H:34:MET:HB3	3:H:79:LEU:HD22	1.94	0.49
1:L:14:ALA:HB2	1:L:41:VAL:HG11	1.94	0.49
1:J:13:VAL:HG13	1:J:36:LEU:HD13	1.93	0.49
1:J:83:ILE:HB	1:J:131:ARG:HB2	1.94	0.49
3:H:91:THR:HG23	3:H:123:THR:HA	1.94	0.49
1:K:66:GLY:O	1:K:113:PRO:HA	2.13	0.49
3:Q:43:ASN:OD1	3:Q:44:GLY:N	2.35	0.49
1:A:16:VAL:HG11	1:A:43:LEU:HD12	1.94	0.49
1:B:57:LEU:O	1:B:154:ILE:HA	2.13	0.49
1:K:13:VAL:HG23	1:K:155:ILE:HB	1.95	0.49
1:K:56:TYR:CZ	1:K:156:ALA:HB2	2.48	0.49
1:K:83:ILE:HB	1:K:131:ARG:HB2	1.94	0.49
1:C:140:ASP:N	1:C:140:ASP:OD1	2.44	0.48
3:Q:36:TRP:NE1	3:Q:81:LEU:HB2	2.28	0.48
2:O:2:ILE:HD11	2:O:25:ALA:HB1	1.94	0.48
1:C:11:LYS:O	1:C:13:VAL:HG23	2.13	0.48
1:C:100:PRO:HB3	1:C:116:GLU:HG3	1.95	0.48
3:Q:37:VAL:HG22	3:Q:47:TRP:HA	1.95	0.48
3:I:83:MET:HE2	3:I:86:LEU:HD21	1.95	0.47
1:L:83:ILE:HD11	1:L:90:LYS:HE2	1.95	0.47
3:I:37:VAL:HG21	3:I:113:MET:HE1	1.96	0.47
2:E:37:GLN:HB2	2:E:47:LEU:HD11	1.94	0.47
1:K:43:LEU:HA	1:K:47:GLN:O	2.13	0.47
1:A:57:LEU:O	1:A:154:ILE:HA	2.14	0.47
3:P:97:ALA:HB1	3:P:113:MET:HB3	1.97	0.47
1:A:6:ARG:NH2	1:J:37:LEU:HB3	2.29	0.47
1:C:146:GLU:HB2	1:C:149:GLN:NE2	2.30	0.47
3:H:12:VAL:HG21	3:H:18:LEU:HD22	1.96	0.47
3:P:126:SER:HA	4:P:204:HOH:O	2.15	0.47
1:B:14:ALA:HB2	1:B:41:VAL:HG11	1.97	0.47
3:R:37:VAL:HG22	3:R:47:TRP:HA	1.97	0.47
2:E:38:GLN:O	2:E:84:ALA:HB1	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:12:PRO:HD2	1:J:156:ALA:HB3	1.97	0.46
1:L:58:ILE:O	1:L:121:GLY:HA2	2.15	0.46
1:A:90:LYS:NZ	1:A:135:GLU:OE2	2.38	0.46
1:C:78:HIS:HB3	1:C:118:ILE:HG21	1.95	0.46
1:L:66:GLY:HA3	1:L:114:TRP:CE2	2.50	0.46
1:C:57:LEU:O	1:C:154:ILE:HA	2.15	0.46
1:J:30:ASN:OD1	1:J:31:ARG:N	2.48	0.46
2:O:38:GLN:O	2:O:84:ALA:HB1	2.16	0.46
1:B:142:LEU:HD23	1:B:144:PHE:HE2	1.81	0.46
1:J:24:GLY:O	2:O:30:TYR:OH	2.28	0.46
1:L:66:GLY:HA3	1:L:114:TRP:CZ2	2.51	0.46
1:C:14:ALA:HB2	1:C:41:VAL:HG11	1.98	0.46
1:L:59:TYR:HA	1:L:120:LEU:O	2.16	0.46
1:A:82:ARG:CB	1:A:93:LEU:HD21	2.45	0.45
1:K:60:SER:HB3	1:K:80:ILE:HD11	1.97	0.45
1:C:146:GLU:HB2	1:C:149:GLN:CD	2.37	0.45
1:K:100:PRO:HB3	1:K:116:GLU:HG3	1.98	0.45
3:Q:72:ARG:HD3	3:Q:74:ASN:OD1	2.17	0.45
1:L:142:LEU:HD23	1:L:144:PHE:HE2	1.81	0.45
3:H:51:MET:SD	3:H:72:ARG:HB3	2.57	0.45
1:C:80:ILE:HA	1:C:133:SER:O	2.16	0.44
2:F:33:LEU:HD22	2:F:71:PHE:CD2	2.52	0.44
3:H:17:SER:HA	3:H:83:MET:O	2.17	0.44
2:O:24:ARG:NH1	2:O:70:ASP:OD2	2.51	0.44
1:C:128:LYS:NZ	1:J:44:ARG:HH12	2.14	0.44
2:E:18:ARG:HG3	2:E:76:SER:HA	1.99	0.44
3:P:91:THR:HG23	3:P:123:THR:HA	1.99	0.44
2:M:89:GLN:HE22	3:P:113:MET:CE	2.24	0.44
1:B:25:GLN:HE21	1:B:27:GLN:HE21	1.65	0.44
1:C:128:LYS:HZ1	1:J:44:ARG:NH1	2.16	0.44
1:B:26:LEU:HD13	1:B:142:LEU:HD21	2.00	0.44
1:A:7:THR:OG1	1:A:8:PRO:HD2	2.18	0.43
2:F:18:ARG:HG2	2:F:76:SER:O	2.18	0.43
1:L:55:LEU:HB2	1:L:158:THR:HG23	2.00	0.43
1:B:8:PRO:HD2	1:B:39:ASN:HD21	1.83	0.43
1:J:60:SER:HB3	1:J:80:ILE:HD11	1.99	0.43
2:M:11:LEU:HG	2:M:13:LEU:HD21	1.99	0.43
1:A:58:ILE:O	1:A:121:GLY:HA2	2.18	0.43
3:G:68:PHE:HA	3:G:82:GLN:O	2.18	0.43
2:N:95:PRO:HG2	2:N:98:THR:OG1	2.18	0.43
1:A:55:LEU:HD13	1:B:13:VAL:HG21	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:36:TRP:CE2	3:H:81:LEU:HB2	2.53	0.43
3:H:83:MET:HE2	3:H:86:LEU:HD21	1.99	0.43
1:C:12:PRO:HD2	1:C:156:ALA:HB3	2.00	0.43
1:K:57:LEU:O	1:K:154:ILE:HA	2.18	0.43
3:Q:97:ALA:HB1	3:Q:113:MET:HB3	2.00	0.43
1:K:7:THR:OG1	1:K:8:PRO:HD3	2.19	0.43
3:G:36:TRP:CE2	3:G:81:LEU:HB2	2.54	0.43
1:B:126:LEU:HD21	1:B:132:LEU:HD21	2.00	0.42
3:I:86:LEU:HB3	3:I:124:VAL:HG21	2.01	0.42
3:P:34:MET:HB3	3:P:79:LEU:HD22	2.01	0.42
1:C:53:GLU:HA	1:C:126:LEU:O	2.19	0.42
1:K:42:GLU:HB2	1:K:49:VAL:HB	2.02	0.42
1:L:53:GLU:HA	1:L:126:LEU:O	2.19	0.42
1:A:157:LEU:HD12	1:B:155:ILE:HD13	2.00	0.42
1:K:58:ILE:O	1:K:121:GLY:HA2	2.19	0.42
3:H:103:ALA:HB2	3:H:109:TYR:CD2	2.55	0.42
3:I:46:GLU:HA	4:I:201:HOH:O	2.19	0.42
3:Q:103:ALA:HB2	3:Q:109:TYR:CD2	2.55	0.42
3:R:83:MET:HB3	3:R:86:LEU:HD21	2.02	0.42
3:R:102:ILE:HD12	3:R:111:TYR:HE2	1.84	0.42
1:A:94:LEU:HD22	1:B:151:TYR:CZ	2.55	0.42
1:C:128:LYS:HZ3	1:J:44:ARG:HH22	1.67	0.42
1:A:6:ARG:HH21	1:J:37:LEU:HB3	1.84	0.42
2:F:33:LEU:HD22	2:F:71:PHE:CG	2.54	0.42
2:O:54:ARG:NH1	2:O:62:PHE:O	2.53	0.42
1:K:94:LEU:HD22	1:L:151:TYR:CZ	2.54	0.42
3:I:36:TRP:CE2	3:I:81:LEU:HB2	2.55	0.41
3:Q:17:SER:HA	3:Q:83:MET:O	2.19	0.41
2:F:95:PRO:HG2	2:F:98:THR:OG1	2.20	0.41
3:H:83:MET:HB3	3:H:86:LEU:HD21	2.01	0.41
1:A:43:LEU:HA	1:A:47:GLN:O	2.20	0.41
3:G:36:TRP:NE1	3:G:81:LEU:HB2	2.34	0.41
2:M:2:ILE:H	2:M:95:PRO:HD3	1.85	0.41
1:L:58:ILE:HG22	1:L:80:ILE:HD13	2.03	0.41
1:K:30:ASN:HD22	1:K:37:LEU:HB3	1.86	0.41
3:R:22:CYS:HB3	3:R:79:LEU:HB3	2.01	0.41
2:E:33:LEU:HD13	2:E:71:PHE:CD1	2.56	0.41
2:N:37:GLN:HB2	2:N:47:LEU:HD11	2.02	0.41
1:A:66:GLY:O	1:A:113:PRO:HA	2.21	0.41
3:H:86:LEU:HD23	3:H:86:LEU:HA	1.89	0.41
1:J:55:LEU:HB2	1:J:158:THR:HG23	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:59:TYR:HA	1:K:120:LEU:O	2.21	0.41
2:M:6:GLN:HE22	2:M:87:TYR:HA	1.86	0.41
2:E:107:ILE:HG22	2:E:108:LYS:H	1.86	0.41
1:C:59:TYR:HA	1:C:120:LEU:O	2.21	0.40
1:L:16:VAL:HG11	1:L:43:LEU:HD12	2.03	0.40
3:Q:98:ARG:HG2	3:Q:115:VAL:HG12	2.02	0.40
1:A:59:TYR:HA	1:A:120:LEU:O	2.20	0.40
1:L:78:HIS:HB3	1:L:118:ILE:HG21	2.03	0.40
1:K:29:LEU:HD23	1:K:29:LEU:HA	1.90	0.40
2:O:95:PRO:HG2	2:O:98:THR:OG1	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	152/173 (88%)	143 (94%)	9 (6%)	0	100	100
1	B	152/173 (88%)	142 (93%)	9 (6%)	1 (1%)	22	45
1	C	152/173 (88%)	144 (95%)	8 (5%)	0	100	100
1	J	151/173 (87%)	144 (95%)	5 (3%)	2 (1%)	12	28
1	K	151/173 (87%)	141 (93%)	8 (5%)	2 (1%)	12	28
1	L	151/173 (87%)	144 (95%)	6 (4%)	1 (1%)	22	45
2	D	106/119 (89%)	102 (96%)	4 (4%)	0	100	100
2	E	106/119 (89%)	101 (95%)	5 (5%)	0	100	100
2	F	106/119 (89%)	100 (94%)	6 (6%)	0	100	100
2	M	106/119 (89%)	100 (94%)	6 (6%)	0	100	100
2	N	106/119 (89%)	101 (95%)	5 (5%)	0	100	100
2	O	106/119 (89%)	101 (95%)	5 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	G	124/129 (96%)	122 (98%)	2 (2%)	0	100	100
3	H	124/129 (96%)	120 (97%)	4 (3%)	0	100	100
3	I	123/129 (95%)	120 (98%)	3 (2%)	0	100	100
3	P	124/129 (96%)	122 (98%)	2 (2%)	0	100	100
3	Q	124/129 (96%)	121 (98%)	3 (2%)	0	100	100
3	R	124/129 (96%)	120 (97%)	4 (3%)	0	100	100
All	All	2288/2526 (91%)	2188 (96%)	94 (4%)	6 (0%)	41	65

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	8	PRO
1	J	10	ASP
1	K	8	PRO
1	J	51	PRO
1	K	51	PRO
1	L	51	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	130/149 (87%)	125 (96%)	5 (4%)	33	60
1	B	130/149 (87%)	126 (97%)	4 (3%)	40	68
1	C	130/149 (87%)	128 (98%)	2 (2%)	65	85
1	J	129/149 (87%)	128 (99%)	1 (1%)	81	92
1	K	129/149 (87%)	126 (98%)	3 (2%)	50	77
1	L	129/149 (87%)	124 (96%)	5 (4%)	32	59
2	D	91/100 (91%)	90 (99%)	1 (1%)	73	89
2	E	91/100 (91%)	89 (98%)	2 (2%)	52	78
2	F	91/100 (91%)	90 (99%)	1 (1%)	73	89

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
2	M	91/100 (91%)	90 (99%)	1 (1%)	73 89
2	N	91/100 (91%)	87 (96%)	4 (4%)	28 54
2	O	91/100 (91%)	90 (99%)	1 (1%)	73 89
3	G	100/103 (97%)	99 (99%)	1 (1%)	76 90
3	H	100/103 (97%)	99 (99%)	1 (1%)	76 90
3	I	99/103 (96%)	98 (99%)	1 (1%)	76 90
3	P	100/103 (97%)	99 (99%)	1 (1%)	76 90
3	Q	100/103 (97%)	100 (100%)	0	100 100
3	R	100/103 (97%)	100 (100%)	0	100 100
All	All	1922/2112 (91%)	1888 (98%)	34 (2%)	59 82

All (34) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	THR
1	A	32	ARG
1	A	89	THR
1	A	93	LEU
1	A	144	PHE
1	B	13	VAL
1	B	72	THR
1	B	126	LEU
1	B	144	PHE
1	C	87	TYR
1	C	144	PHE
2	D	33	LEU
2	E	5	THR
2	E	33	LEU
2	F	33	LEU
3	G	115	VAL
3	H	72	ARG
3	I	115	VAL
1	J	144	PHE
1	K	72	THR
1	K	89	THR
1	K	144	PHE
1	L	13	VAL
1	L	72	THR
1	L	79	THR

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Mol	Chain	Res	Type
1	L	88	GLN
1	L	144	PHE
2	M	33	LEU
2	N	2	ILE
2	N	5	THR
2	N	33	LEU
2	N	107	ILE
2	O	33	LEU
3	P	115	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	27	GLN
1	C	88	GLN
1	C	125	GLN
2	D	53	ASN
2	D	93	ASN
1	J	27	GLN
1	K	88	GLN
1	L	88	GLN
2	M	53	ASN
2	M	89	GLN
2	O	53	ASN

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 monosaccharides in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

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

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} 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	154/173 (89%)	0.43	8 (5%) 27 26	45, 80, 136, 197	0
1	B	154/173 (89%)	0.14	4 (2%) 56 57	44, 65, 113, 141	0
1	C	154/173 (89%)	0.32	9 (5%) 23 22	47, 79, 139, 165	0
1	J	153/173 (88%)	0.35	8 (5%) 27 26	46, 82, 142, 195	0
1	K	153/173 (88%)	0.40	12 (7%) 13 11	48, 75, 136, 201	0
1	L	153/173 (88%)	0.17	6 (3%) 39 39	46, 71, 122, 173	0
2	D	108/119 (90%)	-0.23	0 100 100	39, 53, 83, 115	0
2	E	108/119 (90%)	0.33	7 (6%) 18 18	50, 84, 132, 141	0
2	F	108/119 (90%)	0.32	4 (3%) 41 41	68, 101, 124, 134	0
2	M	108/119 (90%)	-0.28	0 100 100	41, 54, 85, 93	0
2	N	108/119 (90%)	0.43	6 (5%) 24 23	45, 84, 137, 152	0
2	O	108/119 (90%)	0.45	6 (5%) 24 23	59, 93, 126, 141	0
3	G	126/129 (97%)	-0.22	0 100 100	40, 58, 83, 104	0
3	H	126/129 (97%)	-0.15	0 100 100	43, 64, 89, 104	0
3	I	125/129 (96%)	0.01	2 (1%) 72 74	52, 89, 112, 126	0
3	P	126/129 (97%)	-0.14	0 100 100	42, 58, 85, 100	0
3	Q	126/129 (97%)	-0.20	0 100 100	43, 61, 82, 99	0
3	R	126/129 (97%)	0.25	5 (3%) 38 37	54, 95, 127, 149	0
All	All	2324/2526 (92%)	0.14	77 (3%) 46 47	39, 73, 124, 201	0

All (77) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	6	ARG	11.0
1	L	6	ARG	9.5
1	A	8	PRO	9.0

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Mol	Chain	Res	Type	RSRZ
1	K	7	THR	7.5
1	J	8	PRO	6.7
1	J	6	ARG	6.1
1	A	7	THR	5.9
1	A	88	GLN	5.9
1	K	8	PRO	5.8
1	J	9	SER	5.4
1	L	9	SER	5.3
2	E	107	ILE	5.2
1	A	87	TYR	5.0
2	O	108	LYS	5.0
1	L	8	PRO	4.9
1	C	88	GLN	4.6
1	C	7	THR	4.6
1	B	6	ARG	4.5
1	K	32	ARG	4.5
1	J	87	TYR	4.5
1	K	9	SER	4.4
3	I	28	ILE	4.3
1	K	33	ALA	4.2
2	O	13	LEU	4.0
2	N	11	LEU	3.9
3	R	126	SER	3.9
1	J	7	THR	3.9
1	K	31	ARG	3.7
1	K	87	TYR	3.6
1	K	88	GLN	3.6
2	F	70	ASP	3.5
1	C	29	LEU	3.4
1	J	86	SER	3.4
1	C	25	GLN	3.2
2	E	80	PRO	3.2
2	O	70	ASP	3.1
1	B	7	THR	3.0
1	J	34	ASN	3.0
2	O	86	TYR	2.9
1	A	9	SER	2.9
2	O	3	VAL	2.8
1	C	6	ARG	2.8
1	C	24	GLY	2.8
2	N	12	SER	2.8
1	C	44	ARG	2.8

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Mol	Chain	Res	Type	RSRZ
2	E	12	SER	2.7
1	C	8	PRO	2.6
2	E	108	LYS	2.6
1	L	7	THR	2.6
2	F	71	PHE	2.6
2	N	19	ALA	2.5
1	K	89	THR	2.5
1	A	10	ASP	2.5
1	K	6	ARG	2.5
2	E	69	THR	2.5
3	R	125	SER	2.5
1	B	45	ASP	2.4
1	A	89	THR	2.3
2	N	78	LEU	2.3
2	F	21	LEU	2.3
2	F	72	THR	2.3
2	E	3	VAL	2.3
1	K	86	SER	2.3
2	N	108	LYS	2.3
1	L	44	ARG	2.3
1	K	16	VAL	2.3
2	N	106	ASP	2.2
3	R	27	PHE	2.2
1	L	32	ARG	2.2
2	E	21	LEU	2.2
1	B	31	ARG	2.1
1	J	42	GLU	2.1
3	R	12	VAL	2.1
2	O	18	ARG	2.1
3	R	28	ILE	2.0
3	I	11	VAL	2.0
1	C	27	GLN	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 monosaccharides in this entry.

6.4 Ligands

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.