Full wwPDB X-ray Structure Validation Report ⓘ

Jun 26, 2024 – 06:45 AM EDT

PDB ID	:	6VMK
Title	:	Crystal structure of human Complement Factor D with anti-Factor D Fab 20D12
Authors	:	Wu, P.; Harris, S.F.; Eigenbrot, C.
Deposited on	:	2020-01-28
Resolution	:	3.01 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:

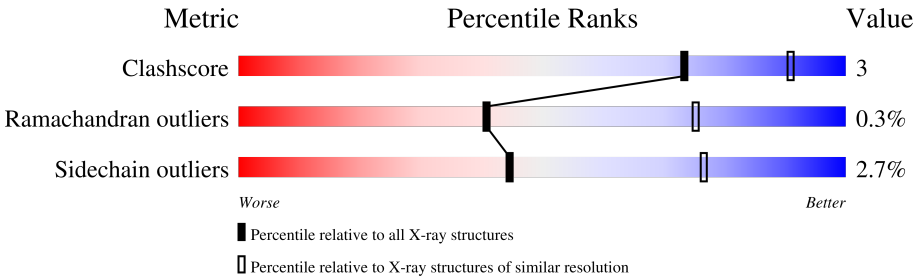
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	FAILED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

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 3.01 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	141614	2734 (3.04-3.00)
Ramachandran outliers	138981	2640 (3.04-3.00)
Sidechain outliers	138945	2643 (3.04-3.00)

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%

Note EDS failed to run properly.

Mol	Chain	Length	Quality of chain
1	C	228	84% 15% .
1	F	228	88% 11%
1	I	228	91% 9%
1	N	228	91% 9%
1	Q	228	88% 12%
1	T	228	89% 10%
1	W	228	88% 12%
1	X	228	88% 12%

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Mol	Chain	Length	Quality of chain
1	a	228	98%
1	d	228	99%
1	g	228	99%
1	j	228	97%
1	m	228	99%
1	p	228	99%
1	s	228	100%
1	v	228	98%
2	A	214	84% 15%
2	D	214	87% 12%
2	G	214	91% 8%
2	J	214	88% 11%
2	L	214	87% 12%
2	O	214	91% 8%
2	R	214	91% 8%
2	U	214	87% 11%
2	Y	214	87% 12%
2	b	214	95%
2	e	214	95% 5%
2	h	214	96%
2	k	214	96%
2	n	214	97%
2	q	214	97%
2	t	214	97%
3	B	223	87% 8%

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Mol	Chain	Length	Quality of chain
3	E	223	87% 7%
3	H	223	87% 8%
3	K	223	87% 8%
3	M	223	86% 9%
3	P	223	85% 9%
3	S	223	89% 6%
3	V	223	89% 6%
3	Z	223	87% 8%
3	c	223	93%
3	f	223	93%
3	i	223	94%
3	l	223	93%
3	o	223	92%
3	r	223	94%
3	u	223	94%

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 80635 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 Complement factor D.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	W	228	Total	C	N	O	S	0	1	0
			1713	1058	325	320	10			
1	C	228	Total	C	N	O	S	0	1	0
			1713	1058	325	320	10			
1	F	228	Total	C	N	O	S	0	1	0
			1713	1058	325	320	10			
1	I	228	Total	C	N	O	S	0	1	0
			1713	1058	325	320	10			
1	N	228	Total	C	N	O	S	0	1	0
			1713	1058	325	320	10			
1	Q	228	Total	C	N	O	S	0	1	0
			1713	1058	325	320	10			
1	T	228	Total	C	N	O	S	0	1	0
			1713	1058	325	320	10			
1	X	228	Total	C	N	O	S	0	1	0
			1713	1058	325	320	10			
1	a	228	Total	C	N	O	S	0	1	0
			1713	1058	325	320	10			
1	d	228	Total	C	N	O	S	0	1	0
			1713	1058	325	320	10			
1	g	228	Total	C	N	O	S	0	1	0
			1713	1058	325	320	10			
1	j	228	Total	C	N	O	S	0	1	0
			1713	1058	325	320	10			
1	m	228	Total	C	N	O	S	0	1	0
			1713	1058	325	320	10			
1	p	228	Total	C	N	O	S	0	1	0
			1713	1058	325	320	10			
1	s	228	Total	C	N	O	S	0	1	0
			1713	1058	325	320	10			
1	v	228	Total	C	N	O	S	0	1	0
			1713	1058	325	320	10			

- Molecule 2 is a protein called Fab Y49R light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	L	213	Total	C	N	O	S	0	0	0
			1634	1017	277	335	5			
2	A	213	Total	C	N	O	S	0	0	0
			1634	1017	277	335	5			
2	D	213	Total	C	N	O	S	0	0	0
			1634	1017	277	335	5			
2	G	213	Total	C	N	O	S	0	0	0
			1634	1017	277	335	5			
2	J	213	Total	C	N	O	S	0	0	0
			1634	1017	277	335	5			
2	O	213	Total	C	N	O	S	0	0	0
			1634	1017	277	335	5			
2	R	213	Total	C	N	O	S	0	0	0
			1634	1017	277	335	5			
2	U	213	Total	C	N	O	S	0	0	0
			1634	1017	277	335	5			
2	Y	213	Total	C	N	O	S	0	0	0
			1634	1017	277	335	5			
2	b	213	Total	C	N	O	S	0	0	0
			1634	1017	277	335	5			
2	e	213	Total	C	N	O	S	0	0	0
			1634	1017	277	335	5			
2	h	213	Total	C	N	O	S	0	0	0
			1634	1017	277	335	5			
2	k	213	Total	C	N	O	S	0	0	0
			1634	1017	277	335	5			
2	n	213	Total	C	N	O	S	0	0	0
			1634	1017	277	335	5			
2	q	213	Total	C	N	O	S	0	0	0
			1634	1017	277	335	5			
2	t	213	Total	C	N	O	S	0	0	0
			1634	1017	277	335	5			

- Molecule 3 is a protein called Fab Y49R heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	M	213	Total	C	N	O	S	0	0	0
			1589	1006	260	318	5			
3	B	213	Total	C	N	O	S	0	0	0
			1589	1006	260	318	5			
3	E	213	Total	C	N	O	S	0	0	0
			1589	1006	260	318	5			

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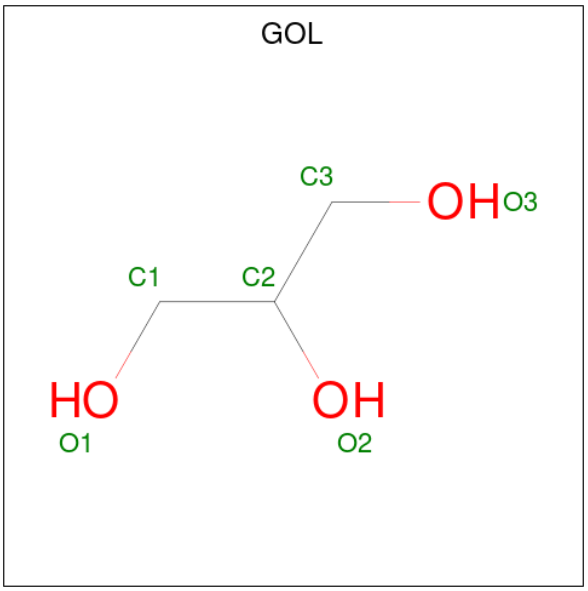
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	H	213	Total	C	N	O	S	0	0	0
			1589	1006	260	318	5			
3	K	213	Total	C	N	O	S	0	0	0
			1589	1006	260	318	5			
3	P	213	Total	C	N	O	S	0	0	0
			1589	1006	260	318	5			
3	S	213	Total	C	N	O	S	0	0	0
			1589	1006	260	318	5			
3	V	213	Total	C	N	O	S	0	0	0
			1589	1006	260	318	5			
3	Z	213	Total	C	N	O	S	0	0	0
			1589	1006	260	318	5			
3	c	213	Total	C	N	O	S	0	0	0
			1589	1006	260	318	5			
3	f	213	Total	C	N	O	S	0	0	0
			1589	1006	260	318	5			
3	i	213	Total	C	N	O	S	0	0	0
			1589	1006	260	318	5			
3	l	213	Total	C	N	O	S	0	0	0
			1589	1006	260	318	5			
3	o	213	Total	C	N	O	S	0	0	0
			1589	1006	260	318	5			
3	r	213	Total	C	N	O	S	0	0	0
			1589	1006	260	318	5			
3	u	213	Total	C	N	O	S	0	0	0
			1589	1006	260	318	5			

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	W	1	Total	C	O	0	0
			6	3	3		
4	C	1	Total	C	O	0	0
			6	3	3		
4	F	1	Total	C	O	0	0
			6	3	3		
4	I	1	Total	C	O	0	0
			6	3	3		
4	N	1	Total	C	O	0	0
			6	3	3		
4	Q	1	Total	C	O	0	0
			6	3	3		
4	T	1	Total	C	O	0	0
			6	3	3		
4	X	1	Total	C	O	0	0
			6	3	3		
4	a	1	Total	C	O	0	0
			6	3	3		
4	d	1	Total	C	O	0	0
			6	3	3		
4	g	1	Total	C	O	0	0
			6	3	3		
4	j	1	Total	C	O	0	0
			6	3	3		
4	m	1	Total	C	O	0	0
			6	3	3		
4	p	1	Total	C	O	0	0
			6	3	3		

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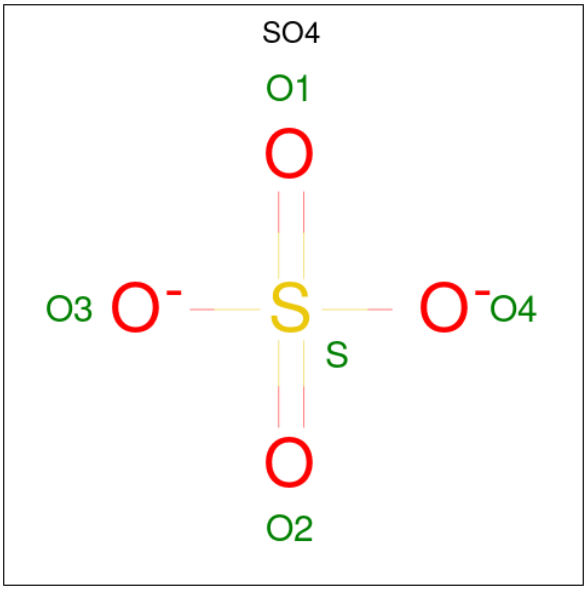
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	s	1	Total C O 6 3 3	0	0
4	v	1	Total C O 6 3 3	0	0

- Molecule 5 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	W	1	Total O S 5 4 1	0	0
5	C	1	Total O S 5 4 1	0	0
5	N	1	Total O S 5 4 1	0	0
5	Q	1	Total O S 5 4 1	0	0
5	T	1	Total O S 5 4 1	0	0
5	X	1	Total O S 5 4 1	0	0
5	g	1	Total O S 5 4 1	0	0
5	j	1	Total O S 5 4 1	0	0
5	m	1	Total O S 5 4 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	p	1	Total O S 5 4 1	0	0
5	s	1	Total O S 5 4 1	0	0
5	v	1	Total O S 5 4 1	0	0

- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	W	50	Total O 50 50	0	0
6	L	28	Total O 28 28	0	0
6	M	36	Total O 36 36	0	0
6	C	42	Total O 42 42	0	0
6	A	39	Total O 39 39	0	0
6	B	32	Total O 32 32	0	0
6	F	37	Total O 37 37	0	0
6	D	34	Total O 34 34	0	0
6	E	27	Total O 27 27	0	0
6	I	33	Total O 33 33	0	0
6	G	31	Total O 31 31	0	0
6	H	24	Total O 24 24	0	0
6	N	55	Total O 55 55	0	0
6	J	16	Total O 16 16	0	0
6	K	17	Total O 17 17	0	0
6	Q	49	Total O 49 49	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	O	24	Total O 24 24	0	0
6	P	12	Total O 12 12	0	0
6	T	41	Total O 41 41	0	0
6	R	26	Total O 26 26	0	0
6	S	11	Total O 11 11	0	0
6	X	44	Total O 44 44	0	0
6	U	36	Total O 36 36	0	0
6	V	20	Total O 20 20	0	0
6	a	48	Total O 48 48	0	0
6	Y	37	Total O 37 37	0	0
6	Z	31	Total O 31 31	0	0
6	d	40	Total O 40 40	0	0
6	b	34	Total O 34 34	0	0
6	c	36	Total O 36 36	0	0
6	g	41	Total O 41 41	0	0
6	e	20	Total O 20 20	0	0
6	f	17	Total O 17 17	0	0
6	j	42	Total O 42 42	0	0
6	h	31	Total O 31 31	0	0
6	i	20	Total O 20 20	0	0
6	m	30	Total O 30 30	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	k	27	Total O 27 27	0	0
6	l	21	Total O 21 21	0	0
6	p	47	Total O 47 47	0	0
6	n	30	Total O 30 30	0	0
6	o	24	Total O 24 24	0	0
6	s	44	Total O 44 44	0	0
6	q	21	Total O 21 21	0	0
6	r	13	Total O 13 13	0	0
6	v	35	Total O 35 35	0	0
6	t	23	Total O 23 23	0	0
6	u	27	Total O 27 27	0	0

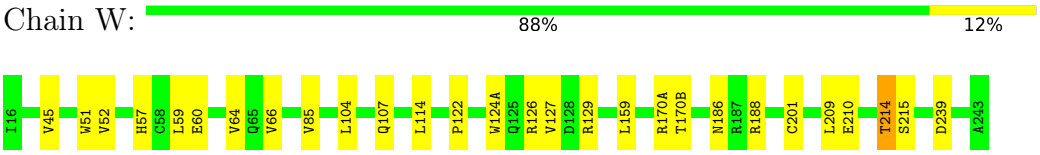
3 Residue-property plots (i)

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. 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. 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.

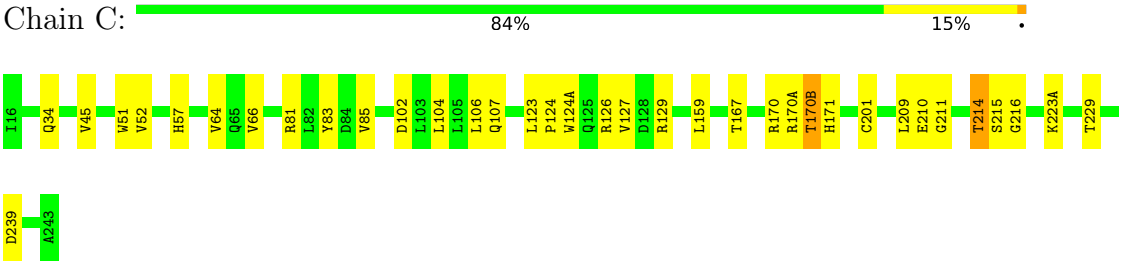
• Molecule 1: Complement factor D

Chain W:



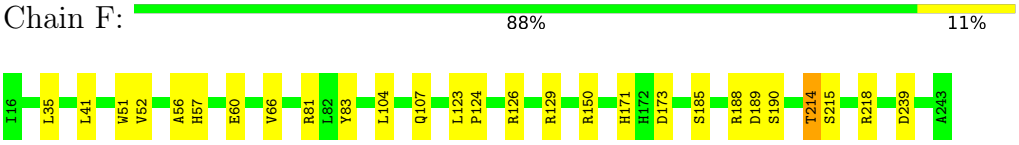
• Molecule 1: Complement factor D

Chain C:



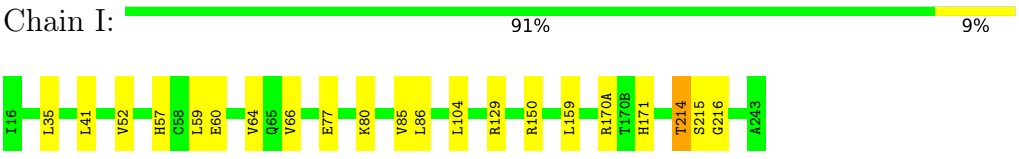
• Molecule 1: Complement factor D

Chain F:



• Molecule 1: Complement factor D

Chain I:

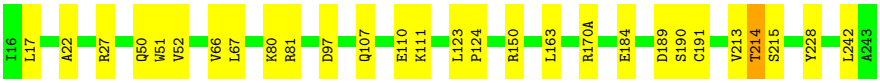


• Molecule 1: Complement factor D

Chain N:

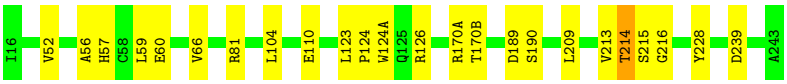
• Molecule 1: Complement factor D

Chain Q:



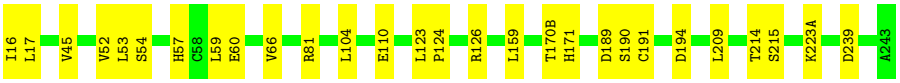
• Molecule 1: Complement factor D

Chain T:



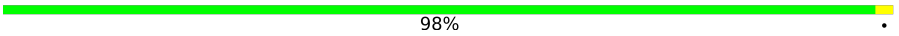
• Molecule 1: Complement factor D

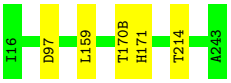
Chain X:



• Molecule 1: Complement factor D

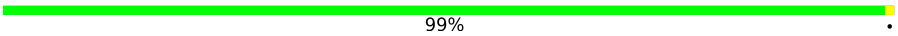
Chain a:





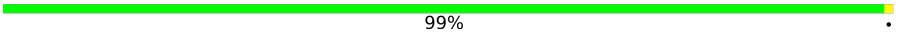
• Molecule 1: Complement factor D

Chain d:



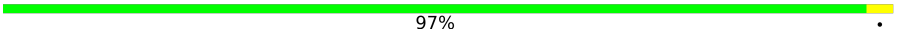
• Molecule 1: Complement factor D

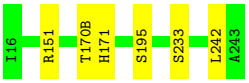
Chain g:



• Molecule 1: Complement factor D

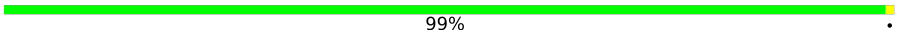
Chain j:

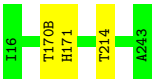




• Molecule 1: Complement factor D

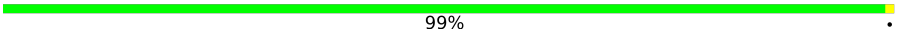
Chain m:

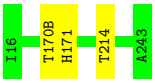




• Molecule 1: Complement factor D

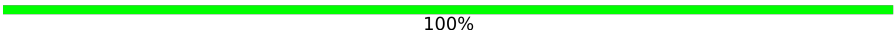
Chain p:





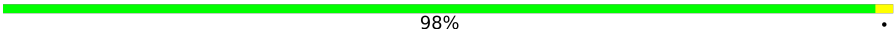
• Molecule 1: Complement factor D

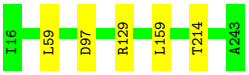
Chain s:



• Molecule 1: Complement factor D

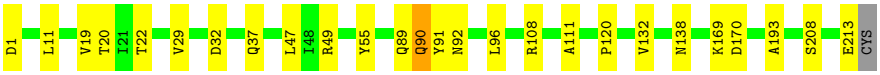
Chain v:





• Molecule 2: Fab Y49R light chain

Chain L:

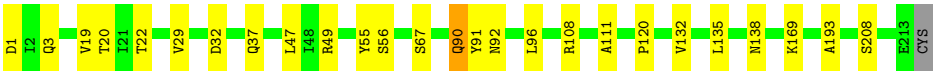


• Molecule 2: Fab Y49R light chain

Chain A:

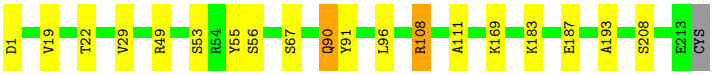
• Molecule 2: Fab Y49R light chain

Chain D:



• Molecule 2: Fab Y49R light chain

Chain G:

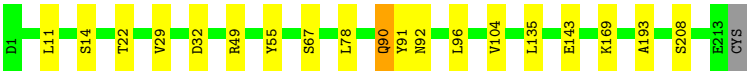


• Molecule 2: Fab Y49R light chain

Chain J:

• Molecule 2: Fab Y49R light chain

Chain O:



• Molecule 2: Fab Y49R light chain

Chain R:

• Molecule 2: Fab Y49R light chain

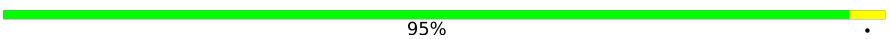
Chain U:

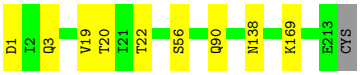
• Molecule 2: Fab Y49R light chain

Chain Y:

• Molecule 2: Fab Y49R light chain

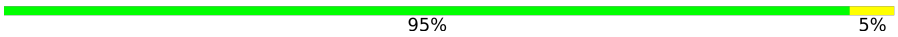
Chain b:

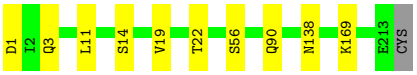




• Molecule 2: Fab Y49R light chain

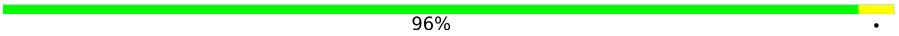
Chain e:

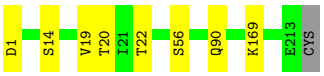




• Molecule 2: Fab Y49R light chain

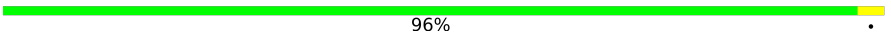
Chain h:

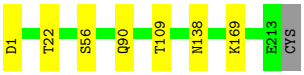




• Molecule 2: Fab Y49R light chain

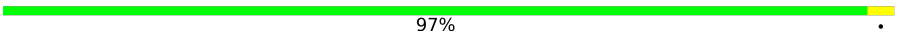
Chain k:

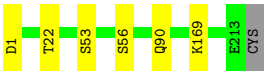




• Molecule 2: Fab Y49R light chain

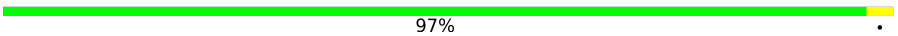
Chain n:

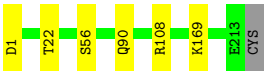




• Molecule 2: Fab Y49R light chain

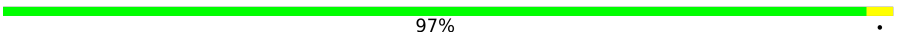
Chain q:

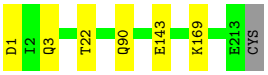




• Molecule 2: Fab Y49R light chain

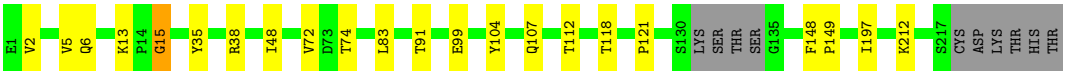
Chain t:





• Molecule 3: Fab Y49R heavy chain

Chain M:

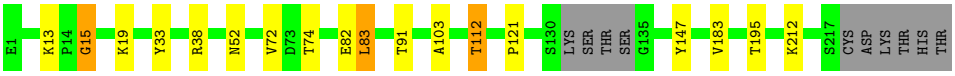


• Molecule 3: Fab Y49R heavy chain

Chain B:

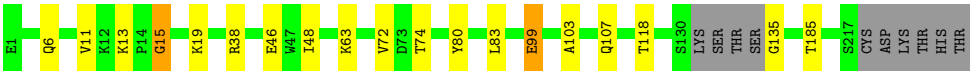
• Molecule 3: Fab Y49R heavy chain

Chain E:



• Molecule 3: Fab Y49R heavy chain

Chain H:

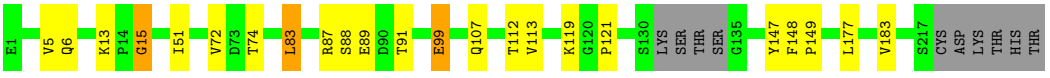


• Molecule 3: Fab Y49R heavy chain

Chain K:

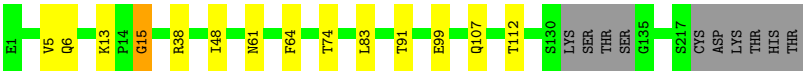
• Molecule 3: Fab Y49R heavy chain

Chain P:



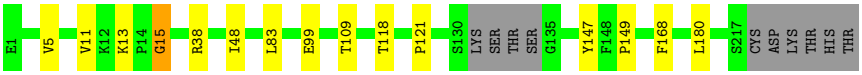
• Molecule 3: Fab Y49R heavy chain

Chain S:



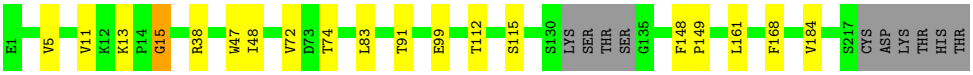
• Molecule 3: Fab Y49R heavy chain

Chain V:



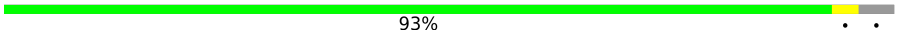
• Molecule 3: Fab Y49R heavy chain

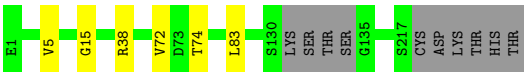
Chain Z:



• Molecule 3: Fab Y49R heavy chain

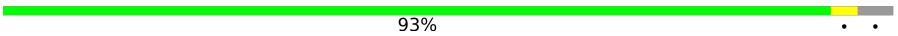
Chain c:





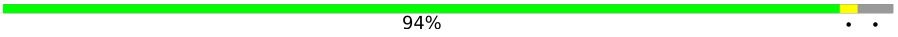
• Molecule 3: Fab Y49R heavy chain

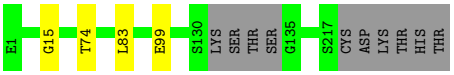
Chain f:



• Molecule 3: Fab Y49R heavy chain

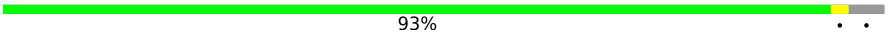
Chain i:

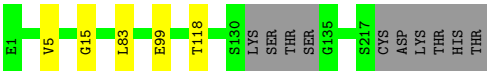




• Molecule 3: Fab Y49R heavy chain

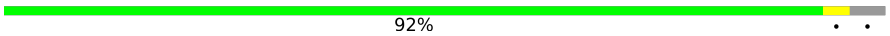
Chain l:

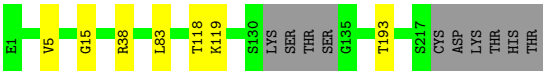




• Molecule 3: Fab Y49R heavy chain

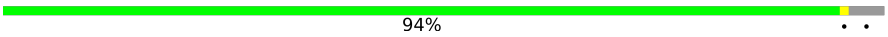
Chain o:





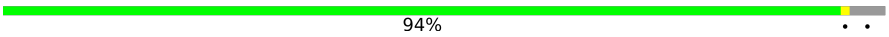
• Molecule 3: Fab Y49R heavy chain

Chain r:



• Molecule 3: Fab Y49R heavy chain

Chain u:



4 Data and refinement statistics (i)

EDS failed to run properly - this section is therefore incomplete.

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α, β, γ	263.70Å 301.45Å 458.84Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.93 – 3.01	Depositor
% Data completeness (in resolution range)	99.9 (49.93-3.01)	Depositor
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.63 (at 3.01Å)	Xtriage
Refinement program	PHENIX 1.12-2829_final	Depositor
R, R_{free}	0.174 , 0.215	Depositor
Wilson B-factor (Å^2)	55.3	Xtriage
Anisotropy	0.038	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	80635	wwPDB-VP
Average B, all atoms (Å^2)	66.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 31.27 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.1383e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[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

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, 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	C	0.25	0/1753	0.45	0/2385
1	F	0.25	0/1753	0.44	0/2385
1	I	0.25	0/1753	0.44	0/2385
1	N	0.25	0/1753	0.44	0/2385
1	Q	0.25	0/1753	0.44	0/2385
1	T	0.25	0/1753	0.44	0/2385
1	W	0.25	0/1753	0.45	0/2385
1	X	0.24	0/1753	0.43	0/2385
1	a	0.25	0/1753	0.43	0/2385
1	d	0.25	0/1753	0.44	0/2385
1	g	0.25	0/1753	0.44	0/2385
1	j	0.25	0/1753	0.45	0/2385
1	m	0.24	0/1753	0.43	0/2385
1	p	0.25	0/1753	0.44	0/2385
1	s	0.25	0/1753	0.44	0/2385
1	v	0.25	0/1753	0.45	0/2385
2	A	0.25	0/1668	0.45	0/2263
2	D	0.26	0/1668	0.46	0/2263
2	G	0.25	0/1668	0.46	0/2263
2	J	0.25	0/1668	0.45	0/2263
2	L	0.25	0/1668	0.45	0/2263
2	O	0.25	0/1668	0.46	0/2263
2	R	0.25	0/1668	0.45	0/2263
2	U	0.26	0/1668	0.45	0/2263
2	Y	0.26	0/1668	0.46	0/2263
2	b	0.25	0/1668	0.46	0/2263
2	e	0.25	0/1668	0.45	0/2263
2	h	0.25	0/1668	0.47	0/2263
2	k	0.25	0/1668	0.46	0/2263
2	n	0.26	0/1668	0.46	0/2263
2	q	0.25	0/1668	0.45	0/2263
2	t	0.25	0/1668	0.45	0/2263

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
3	B	0.25	0/1627	0.47	0/2217
3	E	0.26	0/1627	0.48	0/2217
3	H	0.26	0/1627	0.47	0/2217
3	K	0.25	0/1627	0.46	0/2217
3	M	0.26	0/1627	0.47	0/2217
3	P	0.26	0/1627	0.46	0/2217
3	S	0.26	0/1627	0.46	0/2217
3	V	0.25	0/1627	0.47	0/2217
3	Z	0.25	0/1627	0.47	0/2217
3	c	0.26	0/1627	0.48	0/2217
3	f	0.25	0/1627	0.46	0/2217
3	i	0.26	0/1627	0.46	0/2217
3	l	0.25	0/1627	0.47	0/2217
3	o	0.26	0/1627	0.48	0/2217
3	r	0.25	0/1627	0.45	0/2217
3	u	0.25	0/1627	0.46	0/2217
All	All	0.25	0/80768	0.45	0/109840

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 (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	C	1713	0	1696	19	0
1	F	1713	0	1696	15	0
1	I	1713	0	1696	12	0
1	N	1713	0	1696	13	0
1	Q	1713	0	1696	15	0
1	T	1713	0	1696	16	0
1	W	1713	0	1696	15	0
1	X	1713	0	1696	16	0
1	a	1713	0	1696	0	0

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Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	d	1713	0	1696	0	0
1	g	1713	0	1696	0	0
1	j	1713	0	1696	0	0
1	m	1713	0	1696	0	0
1	p	1713	0	1696	0	0
1	s	1713	0	1696	0	0
1	v	1713	0	1696	0	0
2	A	1634	0	1582	14	0
2	D	1634	0	1582	13	0
2	G	1634	0	1582	9	0
2	J	1634	0	1582	12	0
2	L	1634	0	1582	12	0
2	O	1634	0	1582	10	0
2	R	1634	0	1582	8	0
2	U	1634	0	1582	11	0
2	Y	1634	0	1582	14	0
2	b	1634	0	1582	0	0
2	e	1634	0	1582	0	0
2	h	1634	0	1582	0	0
2	k	1634	0	1582	0	0
2	n	1634	0	1582	0	0
2	q	1634	0	1582	0	0
2	t	1634	0	1582	0	0
3	B	1589	0	1554	9	0
3	E	1589	0	1554	9	0
3	H	1589	0	1554	9	0
3	K	1589	0	1554	10	0
3	M	1589	0	1554	11	0
3	P	1589	0	1554	13	0
3	S	1589	0	1554	7	0
3	V	1589	0	1554	7	0
3	Z	1589	0	1554	7	0
3	c	1589	0	1554	0	0
3	f	1589	0	1554	0	0
3	i	1589	0	1554	0	0
3	l	1589	0	1554	0	0
3	o	1589	0	1554	0	0
3	r	1589	0	1554	0	0
3	u	1589	0	1554	0	0
4	C	6	0	8	0	0
4	F	6	0	8	0	0
4	I	6	0	8	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	N	6	0	8	0	0
4	Q	6	0	8	0	0
4	T	6	0	8	0	0
4	W	6	0	8	0	0
4	X	6	0	8	0	0
4	a	6	0	8	0	0
4	d	6	0	8	0	0
4	g	6	0	8	0	0
4	j	6	0	8	0	0
4	m	6	0	8	0	0
4	p	6	0	8	0	0
4	s	6	0	8	0	0
4	v	6	0	8	0	0
5	C	5	0	0	0	0
5	N	5	0	0	1	0
5	Q	5	0	0	0	0
5	T	5	0	0	0	0
5	W	5	0	0	0	0
5	X	5	0	0	0	0
5	g	5	0	0	0	0
5	j	5	0	0	0	0
5	m	5	0	0	0	0
5	p	5	0	0	0	0
5	s	5	0	0	0	0
5	v	5	0	0	0	0
6	A	39	0	0	3	0
6	B	32	0	0	0	0
6	C	42	0	0	0	0
6	D	34	0	0	0	0
6	E	27	0	0	0	0
6	F	37	0	0	1	0
6	G	31	0	0	0	0
6	H	24	0	0	2	0
6	I	33	0	0	0	0
6	J	16	0	0	0	0
6	K	17	0	0	1	0
6	L	28	0	0	0	0
6	M	36	0	0	2	0
6	N	55	0	0	3	0
6	O	24	0	0	0	0
6	P	12	0	0	0	0
6	Q	49	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	R	26	0	0	0	0
6	S	11	0	0	0	0
6	T	41	0	0	1	0
6	U	36	0	0	0	0
6	V	20	0	0	1	0
6	W	50	0	0	0	0
6	X	44	0	0	1	0
6	Y	37	0	0	1	0
6	Z	31	0	0	0	0
6	a	48	0	0	0	0
6	b	34	0	0	0	0
6	c	36	0	0	0	0
6	d	40	0	0	0	0
6	e	20	0	0	0	0
6	f	17	0	0	0	0
6	g	41	0	0	0	0
6	h	31	0	0	0	0
6	i	20	0	0	0	0
6	j	42	0	0	0	0
6	k	27	0	0	0	0
6	l	21	0	0	0	0
6	m	30	0	0	0	0
6	n	30	0	0	0	0
6	o	24	0	0	0	0
6	p	47	0	0	0	0
6	q	21	0	0	0	0
6	r	13	0	0	0	0
6	s	44	0	0	0	0
6	t	23	0	0	0	0
6	u	27	0	0	0	0
6	v	35	0	0	0	0
All	All	80635	0	77440	284	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 3.

All (284) 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:I:150:ARG:HG3	2:O:67:SER:HB3	1.64	0.79
2:G:67:SER:HB3	1:Q:150:ARG:HG3	1.70	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:194:CYS:SG	6:A:301:HOH:O	2.50	0.69
2:D:67:SER:HB3	1:N:150:ARG:HG3	1.75	0.67
1:N:81:ARG:NH2	1:N:110:GLU:OE2	2.28	0.67
1:F:150:ARG:HG3	2:J:67:SER:HB3	1.75	0.67
1:X:52:VAL:HG21	1:X:66:VAL:HG11	1.78	0.66
3:H:38:ARG:HB2	3:H:48:ILE:HD11	1.77	0.65
1:T:52:VAL:HG21	1:T:66:VAL:HG11	1.80	0.64
1:C:201:CYS:HB2	1:C:210:GLU:HG3	1.80	0.62
1:C:215:SER:OG	1:C:216:GLY:N	2.32	0.61
3:K:87:ARG:O	3:K:89:GLU:N	2.30	0.61
2:R:32:ASP:HB2	2:R:92:ASN:HB2	1.83	0.60
2:G:183:LYS:NZ	2:G:187:GLU:OE2	2.34	0.60
2:O:49:ARG:HD3	2:O:55:TYR:CZ	2.37	0.60
2:U:6:GLN:O	2:U:100:GLN:NE2	2.34	0.60
1:N:52:VAL:HG21	1:N:66:VAL:HG11	1.83	0.60
1:Q:123:LEU:HD12	1:Q:124:PRO:HD2	1.84	0.59
2:G:49:ARG:HD3	2:G:55:TYR:CZ	2.37	0.59
1:T:215:SER:OG	1:T:216:GLY:N	2.35	0.59
2:G:91:TYR:HA	2:G:96:LEU:HG	1.85	0.59
2:J:49:ARG:HD3	2:J:55:TYR:CZ	2.37	0.59
2:A:49:ARG:HD3	2:A:55:TYR:CZ	2.37	0.59
1:W:126:ARG:NH1	1:W:239:ASP:OD2	2.36	0.59
1:I:215:SER:OG	1:I:216:GLY:N	2.36	0.58
1:C:170(A):ARG:NH1	3:B:99:GLU:OE2	2.35	0.58
2:A:108:ARG:NH1	2:A:109:THR:O	2.36	0.58
1:Q:52:VAL:HG21	1:Q:66:VAL:HG11	1.85	0.58
2:L:49:ARG:HD3	2:L:55:TYR:CZ	2.39	0.58
3:M:38:ARG:HB2	3:M:48:ILE:HD11	1.85	0.57
1:F:52:VAL:HG21	1:F:66:VAL:HG11	1.86	0.57
1:W:201:CYS:HB2	1:W:210:GLU:HG3	1.86	0.57
1:W:214:THR:HG23	1:W:215:SER:H	1.68	0.57
2:Y:120:PRO:HD3	2:Y:132:VAL:HG22	1.86	0.57
3:Z:91:THR:HG23	3:Z:112:THR:HA	1.87	0.57
2:Y:49:ARG:HD3	2:Y:55:TYR:CZ	2.40	0.56
2:R:49:ARG:HD3	2:R:55:TYR:CZ	2.41	0.56
1:W:170(A):ARG:NH2	2:L:89:GLN:OE1	2.36	0.56
3:Z:38:ARG:HB2	3:Z:48:ILE:HD11	1.88	0.56
3:M:91:THR:HG23	3:M:112:THR:HA	1.88	0.55
1:C:57:HIS:HD2	1:C:102:ASP:OD2	1.90	0.55
2:J:108:ARG:HH21	2:J:111:ALA:HB2	1.71	0.55
1:T:170(A):ARG:NH1	3:S:99:GLU:OE2	2.39	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:U:49:ARG:HD3	2:U:55:TYR:CZ	2.41	0.54
1:Q:81:ARG:NH2	1:Q:110:GLU:OE2	2.36	0.54
1:I:52:VAL:HG21	1:I:66:VAL:HG11	1.90	0.54
2:J:29:VAL:HG11	2:J:90:GLN:HG3	1.89	0.54
1:C:170(A):ARG:NH2	2:A:89:GLN:OE1	2.39	0.54
3:K:38:ARG:HB2	3:K:48:ILE:HD11	1.90	0.53
3:S:6:GLN:H	3:S:107:GLN:HE22	1.53	0.53
1:X:123:LEU:HD12	1:X:124:PRO:HD2	1.90	0.53
2:D:29:VAL:HG11	2:D:90:GLN:HG3	1.90	0.53
2:G:108:ARG:HH21	2:G:111:ALA:HB2	1.73	0.53
1:N:214:THR:HG23	1:N:215:SER:H	1.73	0.53
2:U:32:ASP:HB2	2:U:92:ASN:HB2	1.89	0.53
3:B:6:GLN:H	3:B:107:GLN:HE22	1.56	0.53
3:E:91:THR:HG23	3:E:112:THR:HA	1.90	0.53
1:T:126:ARG:NH2	6:T:401:HOH:O	2.41	0.53
2:L:49:ARG:HD3	2:L:55:TYR:CE1	2.43	0.53
3:V:11:VAL:HG21	3:V:149:PRO:HG3	1.90	0.53
2:L:32:ASP:HB2	2:L:92:ASN:HB2	1.91	0.53
2:J:32:ASP:HB2	2:J:92:ASN:HB2	1.90	0.53
2:R:193:ALA:HB2	2:R:208:SER:HB3	1.91	0.52
2:U:91:TYR:HA	2:U:96:LEU:HG	1.90	0.52
2:Y:37:GLN:HB2	2:Y:47:LEU:HD11	1.92	0.52
3:H:6:GLN:H	3:H:107:GLN:HE22	1.58	0.52
3:S:38:ARG:HB2	3:S:48:ILE:HD11	1.91	0.52
3:P:87:ARG:O	3:P:89:GLU:N	2.38	0.52
3:P:88:SER:HA	3:P:113:VAL:HB	1.91	0.52
3:B:38:ARG:HB2	3:B:48:ILE:HD11	1.92	0.52
2:D:49:ARG:HD3	2:D:55:TYR:CZ	2.44	0.52
3:S:91:THR:HG23	3:S:112:THR:HA	1.92	0.52
2:L:91:TYR:HA	2:L:96:LEU:HG	1.92	0.52
2:D:91:TYR:HA	2:D:96:LEU:HG	1.92	0.52
2:Y:32:ASP:HB2	2:Y:92:ASN:HB2	1.91	0.52
2:R:91:TYR:HA	2:R:96:LEU:HG	1.92	0.51
1:X:81:ARG:NH2	1:X:110:GLU:OE2	2.43	0.51
1:W:170(A):ARG:NH1	3:M:99:GLU:OE2	2.43	0.51
2:J:37:GLN:HB2	2:J:47:LEU:HD11	1.91	0.51
3:P:91:THR:HG23	3:P:112:THR:HA	1.93	0.51
1:I:64:VAL:HG12	1:I:85:VAL:HG21	1.92	0.51
3:V:38:ARG:HB3	3:V:48:ILE:HD11	1.92	0.51
1:X:123:LEU:HD23	1:X:209:LEU:HB2	1.94	0.51
2:U:145:LYS:HB3	2:U:197:THR:HB	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Y:91:TYR:HA	2:Y:96:LEU:HG	1.91	0.50
1:X:126:ARG:NH1	1:X:239:ASP:OD2	2.43	0.50
1:C:127:VAL:HG12	1:C:129:ARG:HG2	1.93	0.50
2:A:32:ASP:HB2	2:A:92:ASN:HB2	1.93	0.50
2:O:11:LEU:HD22	2:O:104:VAL:HG22	1.94	0.50
1:F:218:ARG:NH2	6:F:401:HOH:O	2.43	0.50
2:A:49:ARG:HD3	2:A:55:TYR:CE1	2.47	0.50
2:D:120:PRO:HD3	2:D:132:VAL:HG22	1.94	0.50
3:K:91:THR:HG23	3:K:112:THR:HA	1.94	0.50
1:W:64:VAL:HG12	1:W:85:VAL:HG21	1.94	0.50
1:I:170(A):ARG:NH1	3:H:99:GLU:OE2	2.37	0.50
2:J:94:TYR:OH	3:K:50:GLU:OE2	2.20	0.49
1:C:170(B):THR:HG22	1:C:223(A):LYS:HE2	1.94	0.49
1:X:214:THR:HG23	1:X:215:SER:H	1.76	0.49
3:V:118:THR:HG22	3:V:149:PRO:HD3	1.93	0.49
1:F:126:ARG:NH1	1:F:239:ASP:OD2	2.45	0.49
3:E:33:TYR:CZ	3:E:52:ASN:HB2	2.48	0.49
2:D:49:ARG:HD3	2:D:55:TYR:CE1	2.47	0.49
1:Q:189:ASP:OD1	1:Q:190:SER:N	2.41	0.49
2:O:32:ASP:HB2	2:O:92:ASN:HB2	1.95	0.49
2:O:91:TYR:HA	2:O:96:LEU:HG	1.95	0.49
1:T:123:LEU:HD12	1:T:124:PRO:HD2	1.94	0.49
2:R:29:VAL:HG11	2:R:90:GLN:HG3	1.95	0.49
3:E:13:LYS:O	3:E:15:GLY:N	2.41	0.48
3:P:6:GLN:H	3:P:107:GLN:HE22	1.60	0.48
1:T:189:ASP:OD1	1:T:190:SER:N	2.45	0.48
3:M:13:LYS:O	3:M:15:GLY:N	2.42	0.48
1:C:52:VAL:HG21	1:C:66:VAL:HG11	1.96	0.48
1:T:59:LEU:HD22	1:T:104:LEU:HD21	1.94	0.48
2:J:91:TYR:HA	2:J:96:LEU:HG	1.95	0.48
1:C:124(A):TRP:HA	1:C:209:LEU:HB3	1.94	0.48
1:W:127:VAL:HG12	1:W:129:ARG:HG2	1.96	0.48
1:Q:214:THR:HG23	1:Q:215:SER:H	1.79	0.48
2:Y:158:ASN:HD22	2:Y:181:LEU:HD21	1.79	0.48
1:X:45:VAL:HG13	1:X:53:LEU:HB3	1.95	0.47
1:C:51:TRP:CH2	1:C:107:GLN:HB2	2.48	0.47
2:U:193:ALA:HB2	2:U:208:SER:HB3	1.96	0.47
1:T:213:VAL:HG22	1:T:228:TYR:CE2	2.49	0.47
1:C:123:LEU:HD12	1:C:124:PRO:HD2	1.96	0.47
3:M:6:GLN:H	3:M:107:GLN:HE22	1.63	0.47
1:C:214:THR:HG23	1:C:215:SER:H	1.80	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:57:HIS:HA	1:F:60:GLU:HG3	1.95	0.47
1:I:57:HIS:HA	1:I:60:GLU:HG3	1.97	0.47
1:N:123:LEU:HD12	1:N:124:PRO:HD2	1.95	0.47
1:Q:51:TRP:CH2	1:Q:107:GLN:HB2	2.50	0.47
3:S:13:LYS:O	3:S:15:GLY:N	2.46	0.47
1:N:57:HIS:HA	1:N:60:GLU:HG3	1.97	0.47
2:O:29:VAL:HG11	2:O:90:GLN:HG3	1.96	0.47
1:C:81:ARG:HD3	1:C:83:TYR:CZ	2.50	0.46
1:W:57:HIS:HA	1:W:60:GLU:HG3	1.96	0.46
2:L:29:VAL:HG11	2:L:90:GLN:HG3	1.97	0.46
2:D:193:ALA:HB2	2:D:208:SER:HB3	1.97	0.46
2:G:29:VAL:HG11	2:G:90:GLN:HG3	1.96	0.46
3:K:121:PRO:HB3	3:K:147:TYR:HB3	1.97	0.46
1:F:51:TRP:CH2	1:F:107:GLN:HB2	2.51	0.46
1:Q:67:LEU:HD11	1:Q:80:LYS:HG2	1.97	0.46
2:L:120:PRO:HD3	2:L:132:VAL:HG22	1.97	0.46
2:U:29:VAL:HG11	2:U:90:GLN:HG3	1.97	0.46
1:F:81:ARG:HD3	1:F:83:TYR:CZ	2.51	0.46
1:X:126:ARG:NH2	6:X:402:HOH:O	2.49	0.46
2:A:37:GLN:HB2	2:A:47:LEU:HD11	1.98	0.46
3:H:118:THR:HB	6:H:322:HOH:O	2.15	0.46
2:J:108:ARG:NH2	2:J:111:ALA:HB2	2.31	0.46
3:M:118:THR:HB	6:M:327:HOH:O	2.14	0.46
2:U:108:ARG:HH21	2:U:111:ALA:HB2	1.80	0.45
2:R:11:LEU:HD22	2:R:104:VAL:HG22	1.98	0.45
3:M:121:PRO:O	6:M:301:HOH:O	2.20	0.45
2:A:91:TYR:HA	2:A:96:LEU:HG	1.98	0.45
2:Y:49:ARG:HD3	2:Y:55:TYR:CE1	2.51	0.45
3:H:13:LYS:O	3:H:15:GLY:N	2.48	0.45
1:T:81:ARG:NH2	1:T:110:GLU:OE2	2.48	0.45
1:W:51:TRP:CH2	1:W:107:GLN:HB2	2.51	0.45
2:D:108:ARG:NH2	2:D:111:ALA:HB2	2.32	0.45
3:S:6:GLN:H	3:S:107:GLN:NE2	2.14	0.45
2:U:49:ARG:HD3	2:U:55:TYR:CE1	2.51	0.45
2:Y:61:ARG:NE	2:Y:82:ASP:OD2	2.44	0.45
1:W:124(A):TRP:HA	1:W:209:LEU:HB3	1.98	0.45
1:C:64:VAL:HG12	1:C:85:VAL:HG21	1.99	0.45
1:N:213:VAL:HG22	1:N:228:TYR:CE2	2.51	0.45
2:D:55:TYR:CZ	3:E:103:ALA:HB2	2.52	0.45
2:G:49:ARG:HD3	2:G:55:TYR:CE1	2.51	0.45
1:F:123:LEU:HD12	1:F:124:PRO:HD2	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:91:THR:HG23	3:B:112:THR:HA	1.98	0.44
3:Z:13:LYS:O	3:Z:15:GLY:N	2.46	0.44
3:B:83:LEU:HD23	3:B:83:LEU:HA	1.82	0.44
1:Q:17:LEU:HB2	1:Q:191:CYS:SG	2.58	0.44
1:X:59:LEU:HD22	1:X:104:LEU:HD21	1.99	0.44
2:Y:162:SER:HB3	6:Y:301:HOH:O	2.16	0.44
1:I:77:GLU:HB2	1:I:80:LYS:HG3	1.98	0.44
1:N:51:TRP:CH2	1:N:107:GLN:HB2	2.52	0.44
1:X:16:ILE:N	1:X:194:ASP:OD2	2.51	0.44
1:N:16:ILE:N	6:N:407:HOH:O	2.50	0.44
1:N:81:ARG:HD3	1:N:83:TYR:CZ	2.53	0.44
2:Y:54:ARG:HD3	2:Y:62:PHE:O	2.17	0.44
2:D:37:GLN:HB2	2:D:47:LEU:HD11	1.98	0.44
2:G:193:ALA:HB2	2:G:208:SER:HB3	1.98	0.44
2:O:135:LEU:HD22	3:P:183:VAL:HG11	2.00	0.44
1:T:56:ALA:HA	1:T:104:LEU:HB2	1.99	0.44
1:T:57:HIS:HA	1:T:60:GLU:HG3	1.99	0.44
3:Z:161:LEU:HD21	3:Z:184:VAL:HG21	2.00	0.44
2:L:108:ARG:HH21	2:L:111:ALA:HB2	1.83	0.44
1:T:124(A):TRP:HA	1:T:209:LEU:HB3	1.99	0.44
2:A:193:ALA:HB2	2:A:208:SER:HB3	2.00	0.44
1:Q:213:VAL:HG22	1:Q:228:TYR:CE2	2.53	0.44
3:P:119:LYS:HD2	3:P:177:LEU:HD21	2.00	0.44
1:W:52:VAL:HG21	1:W:66:VAL:HG11	2.00	0.44
2:O:193:ALA:HB2	2:O:208:SER:HB3	2.00	0.43
2:R:54:ARG:HD3	2:R:62:PHE:O	2.18	0.43
1:W:126:ARG:HH12	1:W:239:ASP:CG	2.21	0.43
2:D:135:LEU:HD22	3:E:183:VAL:HG11	2.00	0.43
1:Q:22:ALA:HB1	1:Q:27:ARG:NH1	2.33	0.43
2:J:90:GLN:HE21	2:J:90:GLN:HB3	1.71	0.43
1:X:54:SER:O	1:X:104:LEU:N	2.49	0.43
3:V:109:THR:HA	6:V:315:HOH:O	2.19	0.43
3:M:35:TYR:CD1	3:M:99:GLU:HG2	2.54	0.43
1:C:126:ARG:NH1	1:C:239:ASP:OD2	2.48	0.43
1:T:214:THR:HG23	1:T:215:SER:H	1.83	0.43
2:O:49:ARG:HD3	2:O:55:TYR:CE1	2.53	0.43
3:M:197:ILE:HG12	3:M:212:LYS:HA	2.00	0.43
2:J:193:ALA:HB2	2:J:208:SER:HB3	2.00	0.43
2:Y:176:SER:HB3	3:Z:168:PHE:CE2	2.53	0.43
1:F:189:ASP:OD1	1:F:190:SER:N	2.50	0.43
1:C:167:THR:O	1:C:171:HIS:HD2	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:K:148:PHE:HA	3:K:149:PRO:HA	1.82	0.43
1:Q:170(A):ARG:HD3	3:P:99:GLU:OE2	2.19	0.43
1:W:186:ASN:C	1:W:188:ARG:H	2.23	0.43
2:Y:29:VAL:HG11	2:Y:90:GLN:HG3	2.00	0.43
2:L:37:GLN:HB2	2:L:47:LEU:HD11	1.99	0.42
3:K:208:LYS:HE2	3:K:208:LYS:HB3	1.89	0.42
3:M:2:VAL:HB	3:M:104:TYR:CZ	2.54	0.42
3:P:83:LEU:HD23	3:P:83:LEU:HA	1.89	0.42
1:X:57:HIS:HA	1:X:60:GLU:HG3	2.01	0.42
3:B:148:PHE:HA	3:B:149:PRO:HA	1.82	0.42
3:H:19:LYS:HE2	3:H:80:TYR:CD1	2.53	0.42
5:N:302:SO4:O3	6:N:401:HOH:O	2.20	0.42
2:A:2:ILE:HD12	2:A:93:ASN:HB3	2.01	0.42
2:D:32:ASP:HB2	2:D:92:ASN:HB2	2.01	0.42
2:G:55:TYR:CZ	3:H:103:ALA:HB2	2.54	0.42
2:A:204:PRO:HD3	6:A:325:HOH:O	2.19	0.42
1:F:129:ARG:HG3	1:I:129:ARG:NH1	2.34	0.42
1:Q:163:LEU:HD13	1:Q:184:GLU:HG2	2.02	0.42
2:L:193:ALA:HB2	2:L:208:SER:HB3	2.02	0.42
1:T:213:VAL:HG22	1:T:228:TYR:HE2	1.84	0.42
1:F:56:ALA:HA	1:F:104:LEU:HB2	2.01	0.42
1:Q:50:GLN:HG3	1:Q:111:LYS:HA	2.02	0.42
1:F:173:ASP:OD2	2:D:49:ARG:NE	2.49	0.42
1:N:56:ALA:HA	1:N:104:LEU:HB2	2.02	0.42
3:V:13:LYS:O	3:V:15:GLY:N	2.48	0.42
3:B:141:GLY:HA2	3:B:156:TRP:CH2	2.55	0.42
3:K:39:GLN:HB2	3:K:45:LEU:HD23	2.02	0.42
1:X:171:HIS:HA	1:X:223(A):LYS:O	2.20	0.42
3:E:121:PRO:HB3	3:E:147:TYR:HB3	2.02	0.41
1:Q:170(A):ARG:NH1	3:P:99:GLU:OE2	2.47	0.41
2:L:108:ARG:HD2	2:L:170:ASP:O	2.20	0.41
1:X:17:LEU:HB2	1:X:191:CYS:SG	2.60	0.41
2:L:213:GLU:OE1	2:L:213:GLU:N	2.53	0.41
3:M:148:PHE:HA	3:M:149:PRO:HA	1.83	0.41
1:F:214:THR:HG23	1:F:215:SER:H	1.84	0.41
1:X:57:HIS:HE1	1:X:214:THR:O	2.04	0.41
3:K:13:LYS:O	3:K:15:GLY:N	2.54	0.41
2:U:163:VAL:HG22	2:U:175:LEU:HD12	2.03	0.41
3:H:46:GLU:OE2	3:H:63:LYS:NZ	2.41	0.41
2:A:207:LYS:O	6:A:301:HOH:O	2.22	0.41
3:E:195:THR:HG23	3:E:212:LYS:NZ	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:T:124(A):TRP:HB3	1:T:209:LEU:HD23	2.03	0.41
1:X:189:ASP:OD1	1:X:190:SER:N	2.53	0.41
1:F:35:LEU:HB2	1:F:41:LEU:HD22	2.03	0.41
2:R:49:ARG:HD3	2:R:55:TYR:CE1	2.55	0.41
2:U:176:SER:HB3	3:V:168:PHE:CZ	2.56	0.41
1:C:211:GLY:HA2	1:C:229:THR:O	2.20	0.41
2:A:118:PHE:HA	2:A:119:PRO:HD3	1.95	0.41
1:I:86:LEU:HD12	1:I:86:LEU:HA	1.95	0.41
3:P:121:PRO:HB3	3:P:147:TYR:HB3	2.01	0.41
1:C:170:ARG:NH2	3:B:50:GLU:OE1	2.50	0.41
1:I:35:LEU:HB2	1:I:41:LEU:HD22	2.04	0.41
3:H:135:GLY:N	6:H:302:HOH:O	2.53	0.41
3:P:13:LYS:O	3:P:15:GLY:N	2.49	0.41
1:F:185:SER:HA	1:F:188:ARG:O	2.20	0.40
3:E:83:LEU:HD23	3:E:83:LEU:HA	1.94	0.40
3:P:51:ILE:HD13	3:P:72:VAL:HG23	2.02	0.40
3:V:121:PRO:HB3	3:V:147:TYR:HB3	2.04	0.40
1:C:104:LEU:HD21	1:C:106:LEU:HD21	2.02	0.40
1:N:215:SER:HB2	6:N:409:HOH:O	2.22	0.40
1:W:59:LEU:HD22	1:W:104:LEU:HD21	2.02	0.40
1:I:59:LEU:HD22	1:I:104:LEU:HD21	2.04	0.40
1:I:214:THR:HG23	1:I:215:SER:H	1.86	0.40
3:P:148:PHE:HA	3:P:149:PRO:HA	1.87	0.40
2:Y:96:LEU:HB2	3:Z:47:TRP:CD2	2.57	0.40
1:W:114:LEU:HD22	1:W:122:PRO:HD3	2.04	0.40
2:A:29:VAL:HG11	2:A:90:GLN:HG3	2.02	0.40
3:E:19:LYS:HG3	3:E:82:GLU:HG3	2.02	0.40
1:N:242:LEU:HD12	1:N:242:LEU:HA	1.89	0.40
2:J:49:ARG:HD3	2:J:55:TYR:CE1	2.57	0.40
3:K:109:THR:HA	6:K:313:HOH:O	2.21	0.40
3:Z:148:PHE:HA	3:Z:149:PRO:HA	1.84	0.40
3:B:35:TYR:CD1	3:B:99:GLU:HG2	2.56	0.40
2:O:78:LEU:HD12	2:O:78:LEU:HA	1.94	0.40
1:T:126:ARG:NH1	1:T:239:ASP:OD2	2.54	0.40
3:S:61:ASN:HB3	3:S:64:PHE:HD2	1.87	0.40
2:Y:90:GLN:HE21	2:Y:90:GLN:HB3	1.77	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	C	227/228 (100%)	220 (97%)	7 (3%)	0	100	100
1	F	227/228 (100%)	218 (96%)	9 (4%)	0	100	100
1	I	227/228 (100%)	217 (96%)	10 (4%)	0	100	100
1	N	227/228 (100%)	220 (97%)	7 (3%)	0	100	100
1	Q	227/228 (100%)	218 (96%)	9 (4%)	0	100	100
1	T	227/228 (100%)	220 (97%)	7 (3%)	0	100	100
1	W	227/228 (100%)	215 (95%)	12 (5%)	0	100	100
1	X	227/228 (100%)	217 (96%)	10 (4%)	0	100	100
1	a	227/228 (100%)	215 (95%)	12 (5%)	0	100	100
1	d	227/228 (100%)	215 (95%)	12 (5%)	0	100	100
1	g	227/228 (100%)	220 (97%)	6 (3%)	1 (0%)	34	71
1	j	227/228 (100%)	220 (97%)	7 (3%)	0	100	100
1	m	227/228 (100%)	218 (96%)	9 (4%)	0	100	100
1	p	227/228 (100%)	219 (96%)	8 (4%)	0	100	100
1	s	227/228 (100%)	219 (96%)	8 (4%)	0	100	100
1	v	227/228 (100%)	219 (96%)	8 (4%)	0	100	100
2	A	211/214 (99%)	198 (94%)	12 (6%)	1 (0%)	29	66
2	D	211/214 (99%)	200 (95%)	10 (5%)	1 (0%)	29	66
2	G	211/214 (99%)	199 (94%)	12 (6%)	0	100	100
2	J	211/214 (99%)	202 (96%)	7 (3%)	2 (1%)	17	53
2	L	211/214 (99%)	203 (96%)	7 (3%)	1 (0%)	29	66
2	O	211/214 (99%)	198 (94%)	12 (6%)	1 (0%)	29	66
2	R	211/214 (99%)	198 (94%)	13 (6%)	0	100	100
2	U	211/214 (99%)	202 (96%)	8 (4%)	1 (0%)	29	66
2	Y	211/214 (99%)	201 (95%)	9 (4%)	1 (0%)	29	66

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	b	211/214 (99%)	203 (96%)	7 (3%)	1 (0%)	29	66
2	e	211/214 (99%)	201 (95%)	9 (4%)	1 (0%)	29	66
2	h	211/214 (99%)	199 (94%)	12 (6%)	0	100	100
2	k	211/214 (99%)	200 (95%)	10 (5%)	1 (0%)	29	66
2	n	211/214 (99%)	203 (96%)	8 (4%)	0	100	100
2	q	211/214 (99%)	200 (95%)	11 (5%)	0	100	100
2	t	211/214 (99%)	202 (96%)	8 (4%)	1 (0%)	29	66
3	B	209/223 (94%)	202 (97%)	7 (3%)	0	100	100
3	E	209/223 (94%)	199 (95%)	9 (4%)	1 (0%)	29	66
3	H	209/223 (94%)	201 (96%)	7 (3%)	1 (0%)	29	66
3	K	209/223 (94%)	199 (95%)	8 (4%)	2 (1%)	15	50
3	M	209/223 (94%)	200 (96%)	8 (4%)	1 (0%)	29	66
3	P	209/223 (94%)	195 (93%)	13 (6%)	1 (0%)	29	66
3	S	209/223 (94%)	198 (95%)	10 (5%)	1 (0%)	29	66
3	V	209/223 (94%)	199 (95%)	9 (4%)	1 (0%)	29	66
3	Z	209/223 (94%)	199 (95%)	9 (4%)	1 (0%)	29	66
3	c	209/223 (94%)	202 (97%)	6 (3%)	1 (0%)	29	66
3	f	209/223 (94%)	201 (96%)	7 (3%)	1 (0%)	29	66
3	i	209/223 (94%)	198 (95%)	10 (5%)	1 (0%)	29	66
3	l	209/223 (94%)	198 (95%)	10 (5%)	1 (0%)	29	66
3	o	209/223 (94%)	200 (96%)	7 (3%)	2 (1%)	15	50
3	r	209/223 (94%)	198 (95%)	11 (5%)	0	100	100
3	u	209/223 (94%)	200 (96%)	9 (4%)	0	100	100
All	All	10352/10640 (97%)	9888 (96%)	436 (4%)	28 (0%)	41	75

All (28) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	o	118	THR
2	A	138	ASN
3	E	15	GLY
3	P	15	GLY
3	Z	15	GLY
3	f	15	GLY

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Mol	Chain	Res	Type
3	i	15	GLY
3	o	15	GLY
2	L	138	ASN
2	D	138	ASN
2	J	143	GLU
2	O	143	GLU
3	S	15	GLY
3	V	15	GLY
2	b	138	ASN
2	k	138	ASN
3	M	15	GLY
2	J	138	ASN
3	K	88	SER
2	U	138	ASN
2	Y	143	GLU
2	e	138	ASN
3	l	15	GLY
2	t	143	GLU
3	H	15	GLY
3	K	15	GLY
3	c	15	GLY
1	g	143	ILE

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	183/182 (100%)	178 (97%)	5 (3%)	44	76
1	F	183/182 (100%)	181 (99%)	2 (1%)	73	90
1	I	183/182 (100%)	180 (98%)	3 (2%)	62	86
1	N	183/182 (100%)	181 (99%)	2 (1%)	73	90
1	Q	183/182 (100%)	180 (98%)	3 (2%)	62	86
1	T	183/182 (100%)	181 (99%)	2 (1%)	73	90
1	W	183/182 (100%)	179 (98%)	4 (2%)	52	80

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	X	183/182 (100%)	181 (99%)	2 (1%)	73	90
1	a	183/182 (100%)	178 (97%)	5 (3%)	44	76
1	d	183/182 (100%)	181 (99%)	2 (1%)	73	90
1	g	183/182 (100%)	181 (99%)	2 (1%)	73	90
1	j	183/182 (100%)	177 (97%)	6 (3%)	38	72
1	m	183/182 (100%)	180 (98%)	3 (2%)	62	86
1	p	183/182 (100%)	180 (98%)	3 (2%)	62	86
1	s	183/182 (100%)	182 (100%)	1 (0%)	88	96
1	v	183/182 (100%)	178 (97%)	5 (3%)	44	76
2	A	187/188 (100%)	176 (94%)	11 (6%)	19	52
2	D	187/188 (100%)	179 (96%)	8 (4%)	29	64
2	G	187/188 (100%)	179 (96%)	8 (4%)	29	64
2	J	187/188 (100%)	178 (95%)	9 (5%)	25	60
2	L	187/188 (100%)	180 (96%)	7 (4%)	34	69
2	O	187/188 (100%)	183 (98%)	4 (2%)	53	81
2	R	187/188 (100%)	181 (97%)	6 (3%)	39	73
2	U	187/188 (100%)	179 (96%)	8 (4%)	29	64
2	Y	187/188 (100%)	179 (96%)	8 (4%)	29	64
2	b	187/188 (100%)	179 (96%)	8 (4%)	29	64
2	e	187/188 (100%)	178 (95%)	9 (5%)	25	60
2	h	187/188 (100%)	179 (96%)	8 (4%)	29	64
2	k	187/188 (100%)	181 (97%)	6 (3%)	39	73
2	n	187/188 (100%)	181 (97%)	6 (3%)	39	73
2	q	187/188 (100%)	181 (97%)	6 (3%)	39	73
2	t	187/188 (100%)	182 (97%)	5 (3%)	44	76
3	B	178/188 (95%)	173 (97%)	5 (3%)	43	76
3	E	178/188 (95%)	173 (97%)	5 (3%)	43	76
3	H	178/188 (95%)	172 (97%)	6 (3%)	37	72
3	K	178/188 (95%)	175 (98%)	3 (2%)	60	85
3	M	178/188 (95%)	174 (98%)	4 (2%)	52	80
3	P	178/188 (95%)	174 (98%)	4 (2%)	52	80

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	S	178/188 (95%)	175 (98%)	3 (2%)	60	85
3	V	178/188 (95%)	174 (98%)	4 (2%)	52	80
3	Z	178/188 (95%)	171 (96%)	7 (4%)	32	67
3	c	178/188 (95%)	173 (97%)	5 (3%)	43	76
3	f	178/188 (95%)	173 (97%)	5 (3%)	43	76
3	i	178/188 (95%)	175 (98%)	3 (2%)	60	85
3	l	178/188 (95%)	174 (98%)	4 (2%)	52	80
3	o	178/188 (95%)	173 (97%)	5 (3%)	43	76
3	r	178/188 (95%)	175 (98%)	3 (2%)	60	85
3	u	178/188 (95%)	175 (98%)	3 (2%)	60	85
All	All	8768/8928 (98%)	8532 (97%)	236 (3%)	44	76

All (236) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	W	45	VAL
1	W	159	LEU
1	W	170(B)	THR
1	W	214	THR
2	L	1	ASP
2	L	11	LEU
2	L	19	VAL
2	L	20	THR
2	L	22	THR
2	L	90	GLN
2	L	169	LYS
3	M	5	VAL
3	M	72	VAL
3	M	74	THR
3	M	83	LEU
1	C	34	GLN
1	C	45	VAL
1	C	159	LEU
1	C	170(B)	THR
1	C	214	THR
2	A	3	GLN
2	A	11	LEU
2	A	14	SER

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Mol	Chain	Res	Type
2	A	19	VAL
2	A	20	THR
2	A	22	THR
2	A	56	SER
2	A	90	GLN
2	A	105	GLU
2	A	132	VAL
2	A	169	LYS
3	B	5	VAL
3	B	17	SER
3	B	72	VAL
3	B	74	THR
3	B	83	LEU
1	F	171	HIS
1	F	214	THR
2	D	1	ASP
2	D	3	GLN
2	D	19	VAL
2	D	20	THR
2	D	22	THR
2	D	56	SER
2	D	90	GLN
2	D	169	LYS
3	E	38	ARG
3	E	72	VAL
3	E	74	THR
3	E	83	LEU
3	E	112	THR
1	I	159	LEU
1	I	171	HIS
1	I	214	THR
2	G	1	ASP
2	G	19	VAL
2	G	22	THR
2	G	53	SER
2	G	56	SER
2	G	90	GLN
2	G	108	ARG
2	G	169	LYS
3	H	11	VAL
3	H	72	VAL
3	H	74	THR

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Mol	Chain	Res	Type
3	H	83	LEU
3	H	99	GLU
3	H	185	THR
1	N	233	SER
1	N	242	LEU
2	J	1	ASP
2	J	11	LEU
2	J	19	VAL
2	J	22	THR
2	J	90	GLN
2	J	106	ILE
2	J	108	ARG
2	J	169	LYS
2	J	185	ASP
3	K	83	LEU
3	K	99	GLU
3	K	112	THR
1	Q	97	ASP
1	Q	214	THR
1	Q	242	LEU
2	O	14	SER
2	O	22	THR
2	O	90	GLN
2	O	169	LYS
3	P	5	VAL
3	P	74	THR
3	P	83	LEU
3	P	99	GLU
1	T	170(B)	THR
1	T	214	THR
2	R	1	ASP
2	R	3	GLN
2	R	14	SER
2	R	56	SER
2	R	90	GLN
2	R	169	LYS
3	S	5	VAL
3	S	74	THR
3	S	83	LEU
1	X	159	LEU
1	X	170(B)	THR
2	U	1	ASP

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Mol	Chain	Res	Type
2	U	3	GLN
2	U	14	SER
2	U	22	THR
2	U	56	SER
2	U	90	GLN
2	U	108	ARG
2	U	169	LYS
3	V	5	VAL
3	V	83	LEU
3	V	99	GLU
3	V	180	LEU
1	a	97	ASP
1	a	159	LEU
1	a	170(B)	THR
1	a	171	HIS
1	a	214	THR
2	Y	1	ASP
2	Y	19	VAL
2	Y	20	THR
2	Y	22	THR
2	Y	56	SER
2	Y	90	GLN
2	Y	169	LYS
2	Y	176	SER
3	Z	5	VAL
3	Z	11	VAL
3	Z	72	VAL
3	Z	74	THR
3	Z	83	LEU
3	Z	99	GLU
3	Z	115	SER
1	d	45	VAL
1	d	214	THR
2	b	1	ASP
2	b	3	GLN
2	b	19	VAL
2	b	20	THR
2	b	22	THR
2	b	56	SER
2	b	90	GLN
2	b	169	LYS
3	c	5	VAL

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Mol	Chain	Res	Type
3	c	38	ARG
3	c	72	VAL
3	c	74	THR
3	c	83	LEU
1	g	214	THR
1	g	233	SER
2	e	1	ASP
2	e	3	GLN
2	e	11	LEU
2	e	14	SER
2	e	19	VAL
2	e	22	THR
2	e	56	SER
2	e	90	GLN
2	e	169	LYS
3	f	5	VAL
3	f	43	GLN
3	f	83	LEU
3	f	99	GLU
3	f	112	THR
1	j	151	ARG
1	j	170(B)	THR
1	j	171	HIS
1	j	195	SER
1	j	233	SER
1	j	242	LEU
2	h	1	ASP
2	h	14	SER
2	h	19	VAL
2	h	20	THR
2	h	22	THR
2	h	56	SER
2	h	90	GLN
2	h	169	LYS
3	i	74	THR
3	i	83	LEU
3	i	99	GLU
1	m	170(B)	THR
1	m	171	HIS
1	m	214	THR
2	k	1	ASP
2	k	22	THR

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Mol	Chain	Res	Type
2	k	56	SER
2	k	90	GLN
2	k	109	THR
2	k	169	LYS
3	l	5	VAL
3	l	83	LEU
3	l	99	GLU
3	l	118	THR
1	p	170(B)	THR
1	p	171	HIS
1	p	214	THR
2	n	1	ASP
2	n	22	THR
2	n	53	SER
2	n	56	SER
2	n	90	GLN
2	n	169	LYS
3	o	5	VAL
3	o	38	ARG
3	o	83	LEU
3	o	119	LYS
3	o	193	THR
1	s	214	THR
2	q	1	ASP
2	q	22	THR
2	q	56	SER
2	q	90	GLN
2	q	108	ARG
2	q	169	LYS
3	r	74	THR
3	r	83	LEU
3	r	99	GLU
1	v	59	LEU
1	v	97	ASP
1	v	129	ARG
1	v	159	LEU
1	v	214	THR
2	t	1	ASP
2	t	3	GLN
2	t	22	THR
2	t	90	GLN
2	t	169	LYS

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Mol	Chain	Res	Type
3	u	5	VAL
3	u	83	LEU
3	u	99	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
2	G	199	GLN
2	q	3	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

28 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	$\#\|Z\| > 2$
5	SO4	X	302	-	4,4,4	0.15	0	6,6,6	0.08	0
4	GOL	I	301	-	5,5,5	0.87	0	5,5,5	1.07	0
4	GOL	Q	301	-	5,5,5	0.89	0	5,5,5	1.00	0
4	GOL	d	301	-	5,5,5	0.90	0	5,5,5	1.02	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
4	GOL	W	301	-	5,5,5	0.91	0	5,5,5	0.97	0
4	GOL	j	301	-	5,5,5	0.93	0	5,5,5	1.03	0
4	GOL	a	301	-	5,5,5	0.89	0	5,5,5	0.99	0
4	GOL	X	301	-	5,5,5	0.90	0	5,5,5	1.03	0
5	SO4	g	302	-	4,4,4	0.16	0	6,6,6	0.08	0
5	SO4	T	302	-	4,4,4	0.12	0	6,6,6	0.10	0
5	SO4	N	302	-	4,4,4	0.14	0	6,6,6	0.06	0
4	GOL	N	301	-	5,5,5	0.96	0	5,5,5	0.96	0
5	SO4	p	302	-	4,4,4	0.15	0	6,6,6	0.08	0
4	GOL	v	301	-	5,5,5	0.88	0	5,5,5	1.01	0
4	GOL	C	301	-	5,5,5	0.94	0	5,5,5	0.98	0
5	SO4	v	302	-	4,4,4	0.12	0	6,6,6	0.11	0
4	GOL	m	301	-	5,5,5	0.87	0	5,5,5	1.01	0
5	SO4	s	302	-	4,4,4	0.16	0	6,6,6	0.08	0
4	GOL	F	301	-	5,5,5	0.93	0	5,5,5	0.98	0
4	GOL	g	301	-	5,5,5	0.86	0	5,5,5	1.03	0
5	SO4	C	302	-	4,4,4	0.17	0	6,6,6	0.10	0
5	SO4	Q	302	-	4,4,4	0.12	0	6,6,6	0.10	0
4	GOL	T	301	-	5,5,5	0.87	0	5,5,5	1.05	0
5	SO4	m	302	-	4,4,4	0.15	0	6,6,6	0.06	0
5	SO4	W	302	-	4,4,4	0.17	0	6,6,6	0.07	0
4	GOL	s	301	-	5,5,5	0.88	0	5,5,5	1.04	0
4	GOL	p	301	-	5,5,5	0.89	0	5,5,5	0.97	0
5	SO4	j	302	-	4,4,4	0.16	0	6,6,6	0.09	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	GOL	j	301	-	-	4/4/4/4	-
4	GOL	N	301	-	-	2/4/4/4	-
4	GOL	T	301	-	-	2/4/4/4	-
4	GOL	a	301	-	-	4/4/4/4	-
4	GOL	I	301	-	-	2/4/4/4	-
4	GOL	Q	301	-	-	2/4/4/4	-
4	GOL	C	301	-	-	2/4/4/4	-
4	GOL	X	301	-	-	4/4/4/4	-
4	GOL	d	301	-	-	2/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	GOL	m	301	-	-	4/4/4/4	-
4	GOL	p	301	-	-	0/4/4/4	-
4	GOL	s	301	-	-	0/4/4/4	-
4	GOL	v	301	-	-	0/4/4/4	-
4	GOL	W	301	-	-	2/4/4/4	-
4	GOL	F	301	-	-	3/4/4/4	-
4	GOL	g	301	-	-	3/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (36) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	I	301	GOL	O1-C1-C2-C3
4	N	301	GOL	O1-C1-C2-C3
4	Q	301	GOL	C1-C2-C3-O3
4	Q	301	GOL	O2-C2-C3-O3
4	T	301	GOL	C1-C2-C3-O3
4	X	301	GOL	O1-C1-C2-C3
4	a	301	GOL	C1-C2-C3-O3
4	d	301	GOL	O1-C1-C2-C3
4	g	301	GOL	O1-C1-C2-C3
4	j	301	GOL	C1-C2-C3-O3
4	X	301	GOL	O2-C2-C3-O3
4	j	301	GOL	O2-C2-C3-O3
4	W	301	GOL	C1-C2-C3-O3
4	C	301	GOL	C1-C2-C3-O3
4	F	301	GOL	C1-C2-C3-O3
4	X	301	GOL	C1-C2-C3-O3
4	a	301	GOL	O1-C1-C2-C3
4	j	301	GOL	O1-C1-C2-C3
4	m	301	GOL	C1-C2-C3-O3
4	W	301	GOL	O2-C2-C3-O3
4	I	301	GOL	O1-C1-C2-O2
4	d	301	GOL	O1-C1-C2-O2
4	F	301	GOL	O2-C2-C3-O3
4	N	301	GOL	O1-C1-C2-O2
4	T	301	GOL	O2-C2-C3-O3
4	j	301	GOL	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
4	C	301	GOL	O2-C2-C3-O3
4	a	301	GOL	O2-C2-C3-O3
4	m	301	GOL	O1-C1-C2-O2
4	m	301	GOL	O2-C2-C3-O3
4	F	301	GOL	O1-C1-C2-C3
4	X	301	GOL	O1-C1-C2-O2
4	a	301	GOL	O1-C1-C2-O2
4	g	301	GOL	O1-C1-C2-O2
4	g	301	GOL	C1-C2-C3-O3
4	m	301	GOL	O1-C1-C2-C3

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	N	302	SO4	1	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS failed to run properly - this section is therefore empty.

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

EDS failed to run properly - this section is therefore empty.

6.3 Carbohydrates

EDS failed to run properly - this section is therefore empty.

6.4 Ligands

EDS failed to run properly - this section is therefore empty.

6.5 Other polymers

EDS failed to run properly - this section is therefore empty.