



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 06:01 PM UTC

PDB ID : 6VMK / pdb_00006vmk
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 : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

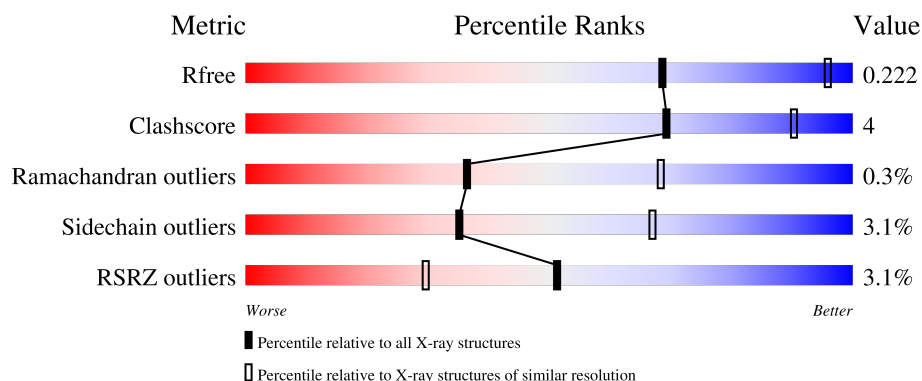
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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.



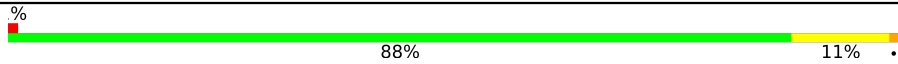
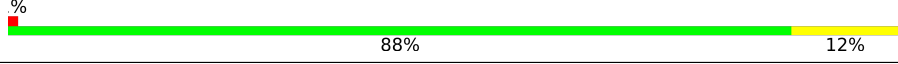
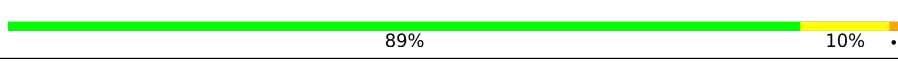
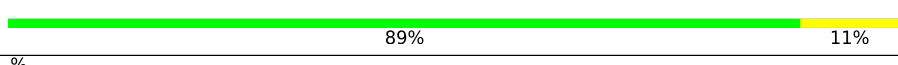
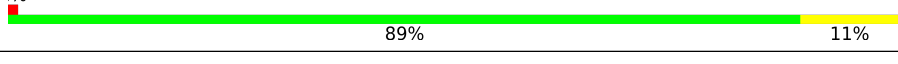
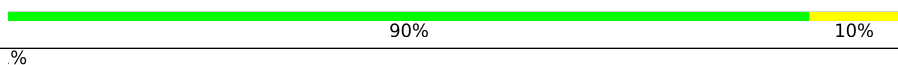
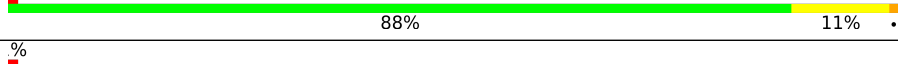
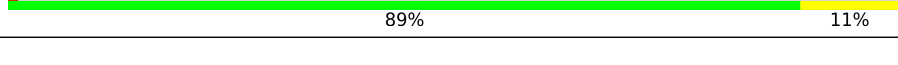
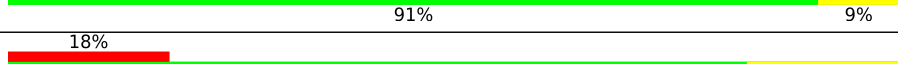
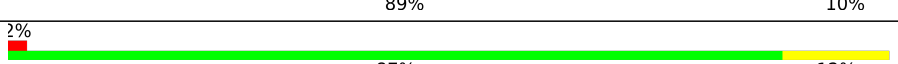
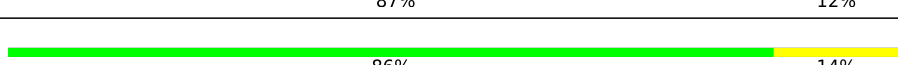
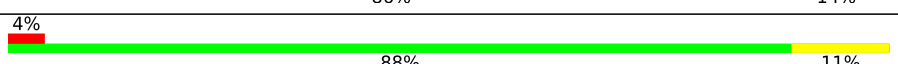
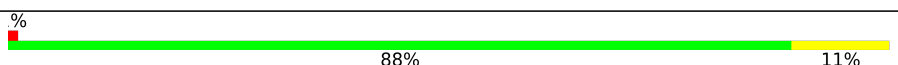
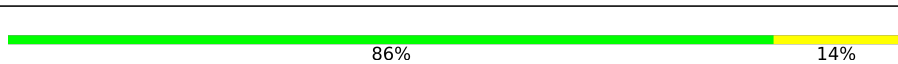
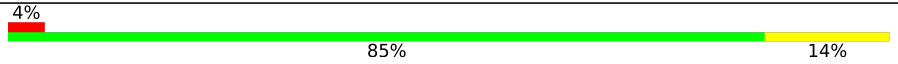
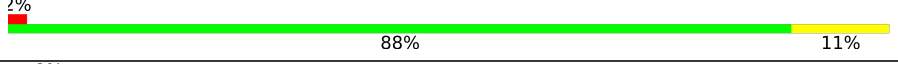
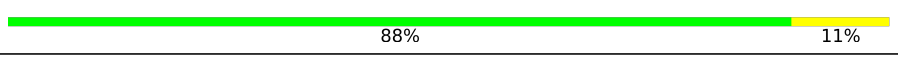
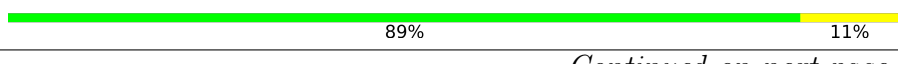
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	3131 (3.04-3.00)
Clashscore	190562	3444 (3.04-3.00)
Ramachandran outliers	187476	3319 (3.04-3.00)
Sidechain outliers	187428	3322 (3.04-3.00)
RSRZ outliers	180081	3130 (3.04-3.00)

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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	C	228	
1	F	228	
1	I	228	
1	N	228	
1	Q	228	

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Mol	Chain	Length	Quality of chain
1	T	228	
1	W	228	
1	X	228	
1	a	228	
1	d	228	
1	g	228	
1	j	228	
1	m	228	
1	p	228	
1	s	228	
1	v	228	
2	A	214	
2	D	214	
2	G	214	
2	J	214	
2	L	214	
2	O	214	
2	R	214	
2	U	214	
2	Y	214	
2	b	214	
2	e	214	
2	h	214	
2	k	214	
2	n	214	

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Mol	Chain	Length	Quality of chain
2	q	214	
2	t	214	
3	B	223	
3	E	223	
3	H	223	
3	K	223	
3	M	223	
3	P	223	
3	S	223	
3	V	223	
3	Z	223	
3	c	223	
3	f	223	
3	i	223	
3	l	223	
3	o	223	
3	r	223	
3	u	223	

2 Entry composition

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.

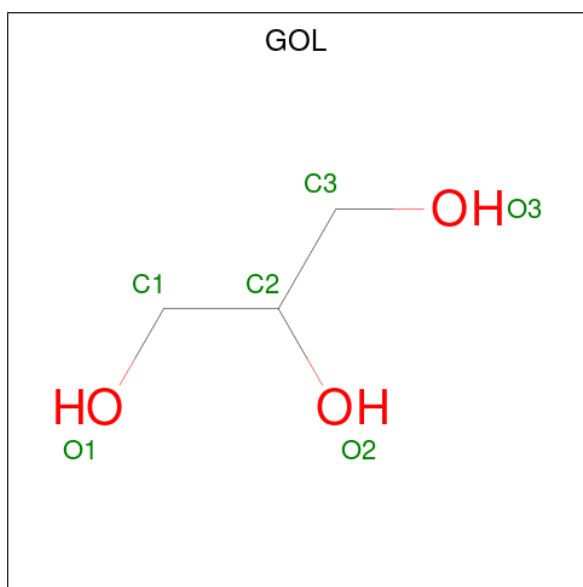
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	M	213	Total	C	N	O	S	0	0	0
			1589	1006	260	318	5			
3	B	213	Total	C	N	O	S	0	0	0
			1589	1006	260	318	5			
3	E	213	Total	C	N	O	S	0	0	0
			1589	1006	260	318	5			

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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 (CCD ID: GOL) (formula: $C_3H_8O_3$).



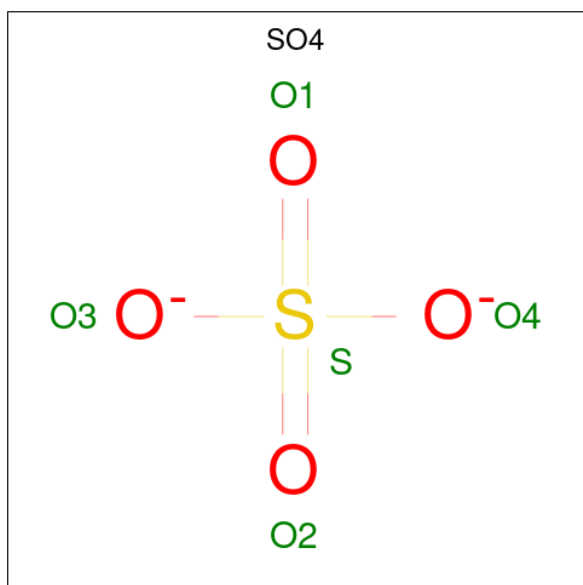
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	W	1	Total	C	O	0	0
			6	3	3		
4	C	1	Total	C	O	0	0
			6	3	3		
4	F	1	Total	C	O	0	0
			6	3	3		
4	I	1	Total	C	O	0	0
			6	3	3		
4	N	1	Total	C	O	0	0
			6	3	3		
4	Q	1	Total	C	O	0	0
			6	3	3		
4	T	1	Total	C	O	0	0
			6	3	3		
4	X	1	Total	C	O	0	0
			6	3	3		
4	a	1	Total	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	0	0
			6	3	3		
4	v	1	Total	C	O	0	0
			6	3	3		

- Molecule 5 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



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

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

- Molecule 6 is water.

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

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

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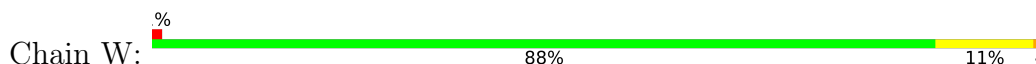
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	k	27	Total 27	O 27	0	0
6	l	21	Total 21	O 21	0	0
6	p	47	Total 47	O 47	0	0
6	n	30	Total 30	O 30	0	0
6	o	24	Total 24	O 24	0	0
6	s	44	Total 44	O 44	0	0
6	q	21	Total 21	O 21	0	0
6	r	13	Total 13	O 13	0	0
6	v	35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

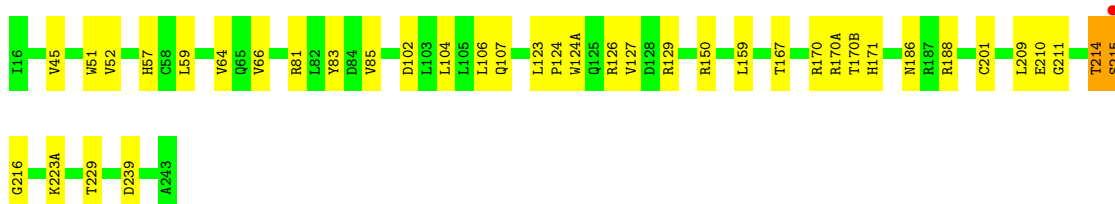
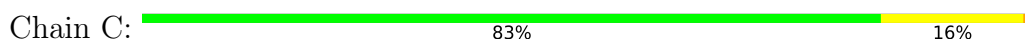
3 Residue-property plots [i](#)

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 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.

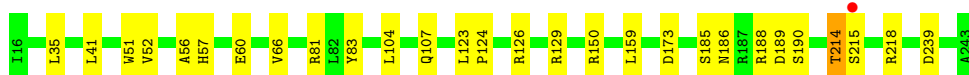
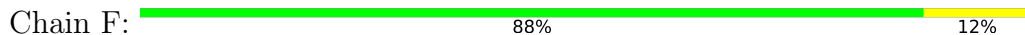
- Molecule 1: Complement factor D



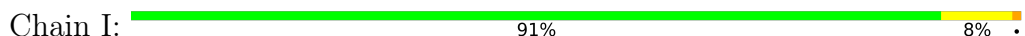
- Molecule 1: Complement factor D



- Molecule 1: Complement factor D



- Molecule 1: Complement factor D

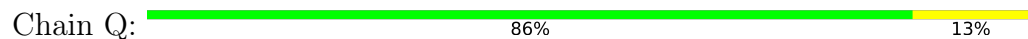


- Molecule 1: Complement factor D

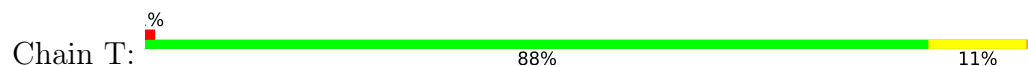




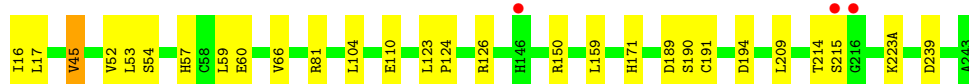
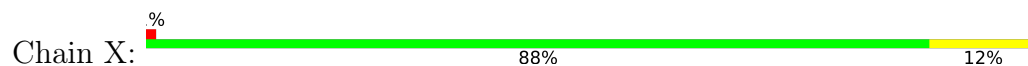
- Molecule 1: Complement factor D



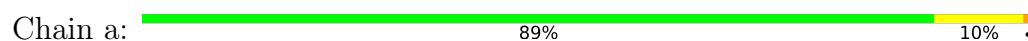
- Molecule 1: Complement factor D



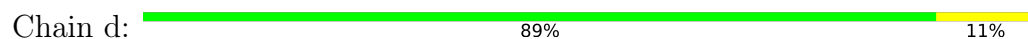
- Molecule 1: Complement factor D



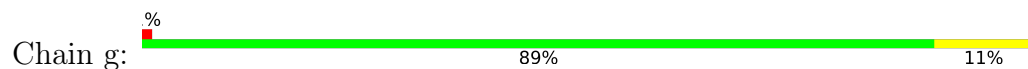
- Molecule 1: Complement factor D



- Molecule 1: Complement factor D



- Molecule 1: Complement factor D



- Molecule 1: Complement factor D

Chain j:  90% 10%



- Molecule 1: Complement factor D

Chain m:  87% 13%



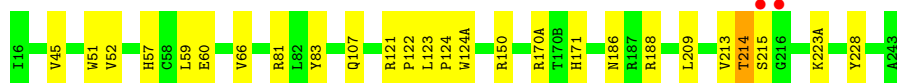
- Molecule 1: Complement factor D

Chain p:  88% 11%



- Molecule 1: Complement factor D

Chain s:  89% 11%



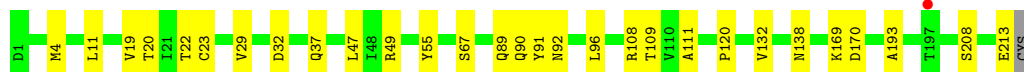
- Molecule 1: Complement factor D

Chain v:  91% 9%



- Molecule 2: Fab Y49R light chain

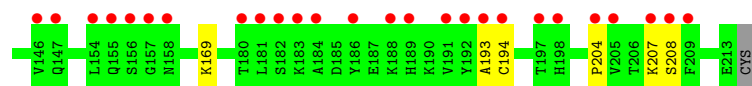
Chain L:  86% 14%



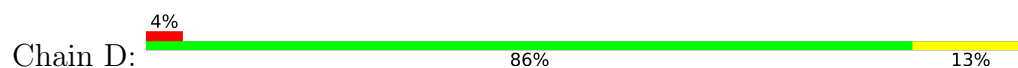
- Molecule 2: Fab Y49R light chain

Chain A:  18% 83% 17%

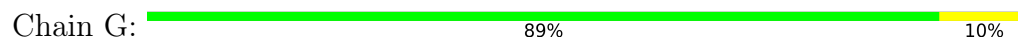




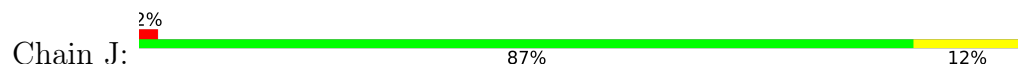
- Molecule 2: Fab Y49R light chain



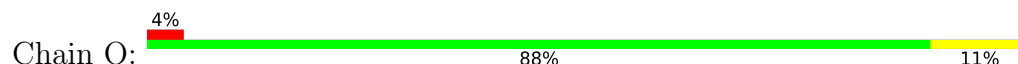
- Molecule 2: Fab Y49R light chain



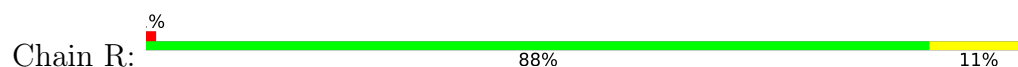
- Molecule 2: Fab Y49R light chain



- Molecule 2: Fab Y49R light chain

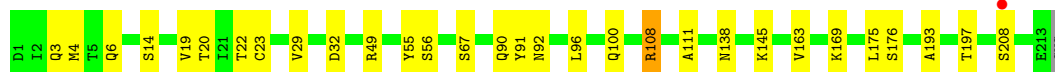


- Molecule 2: Fab Y49R light chain



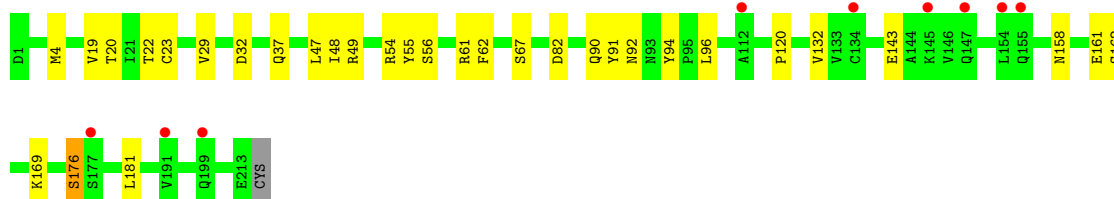
- Molecule 2: Fab Y49R light chain

Chain U:  86% 14%



• Molecule 2: Fab Y49R light chain

Chain Y:  4% 85% 14%



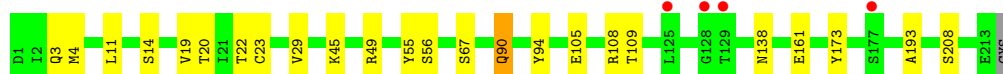
• Molecule 2: Fab Y49R light chain

Chain b:  87% 12%



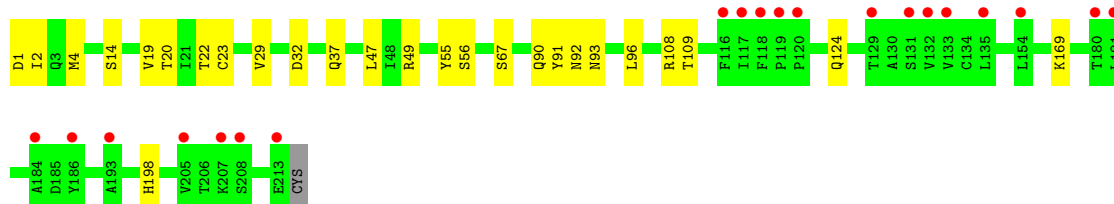
• Molecule 2: Fab Y49R light chain

Chain e:  2% 88% 11%



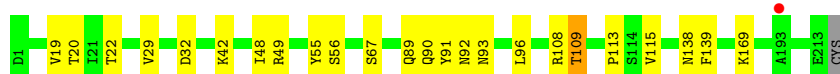
• Molecule 2: Fab Y49R light chain

Chain h:  9% 87% 12%



• Molecule 2: Fab Y49R light chain

Chain k:  88% 11%

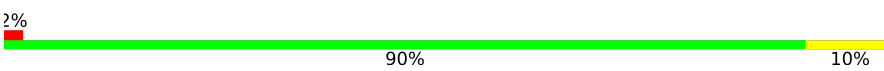


- Molecule 2: Fab Y49R light chain

Chain n:  89% 11%



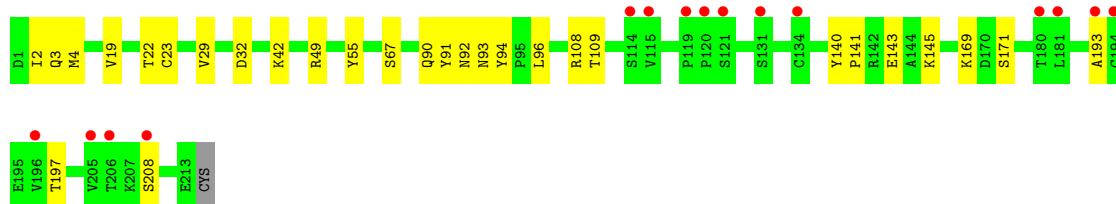
- Molecule 2: Fab Y49R light chain

Chain q:  2% 90% 10%



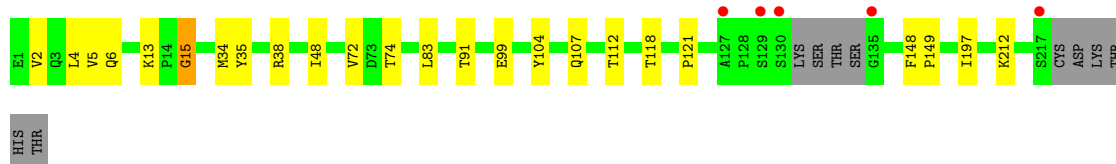
- Molecule 2: Fab Y49R light chain

Chain t:  7% 86% 14%



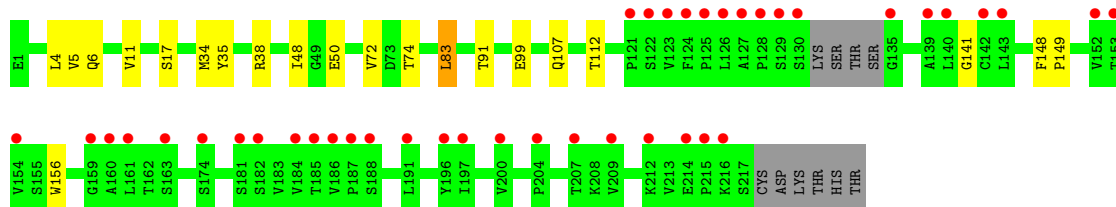
- Molecule 3: Fab Y49R heavy chain

Chain M:  2% 85% 10% .



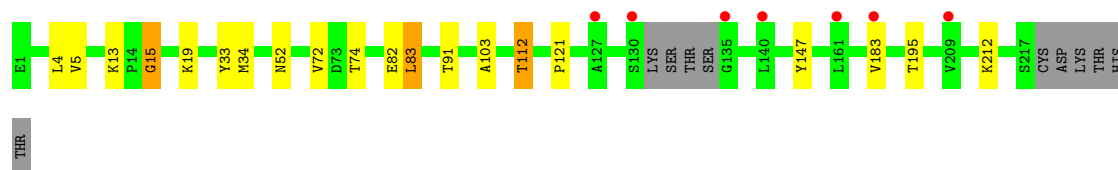
- Molecule 3: Fab Y49R heavy chain

Chain B:  18% 86% 9% .

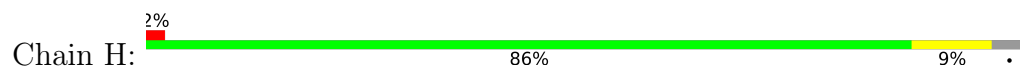


- Molecule 3: Fab Y49R heavy chain

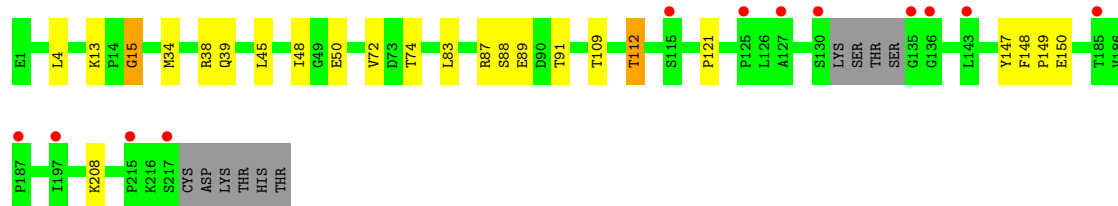
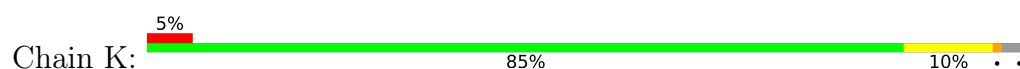
Chain E:  3% 87% 8% . .



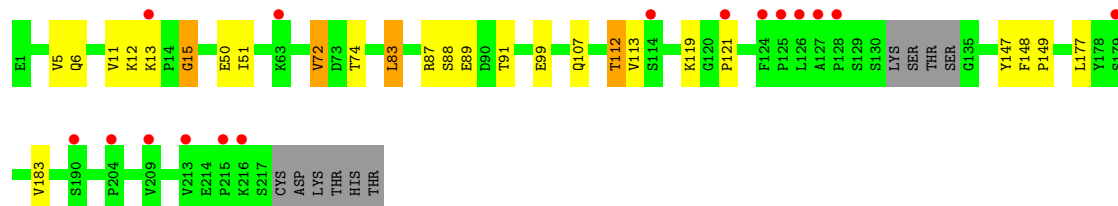
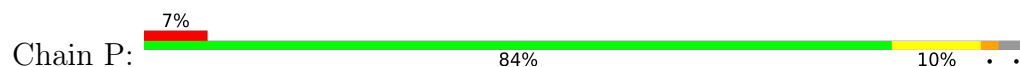
- Molecule 3: Fab Y49R heavy chain



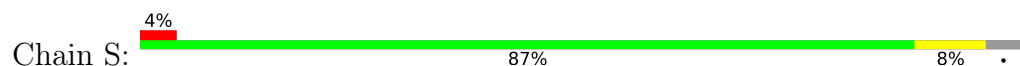
- Molecule 3: Fab Y49R heavy chain



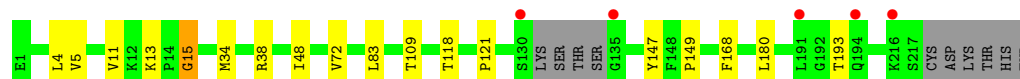
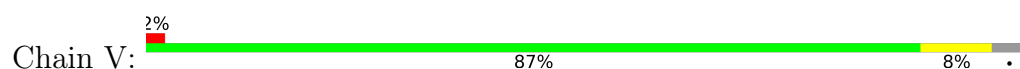
- Molecule 3: Fab Y49R heavy chain



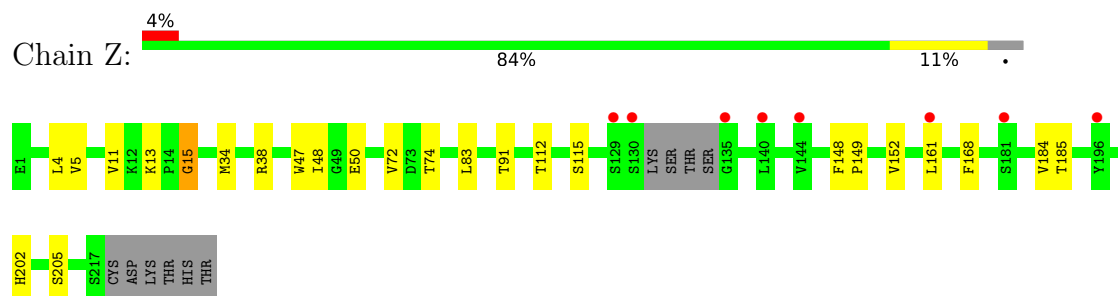
- Molecule 3: Fab Y49R heavy chain



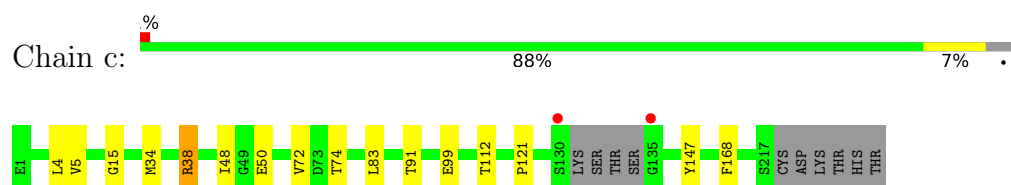
- Molecule 3: Fab Y49R heavy chain



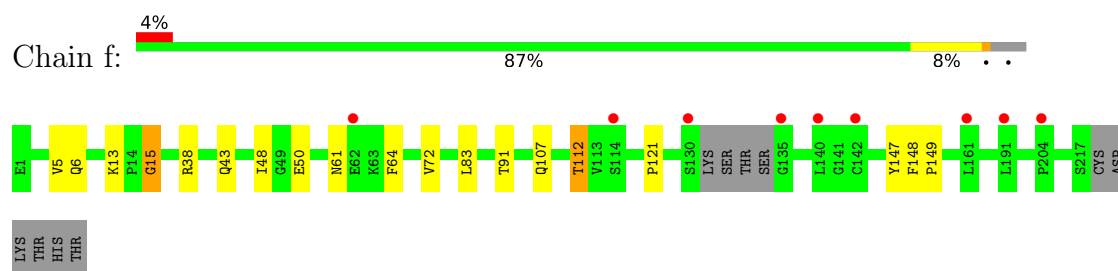
- Molecule 3: Fab Y49R heavy chain



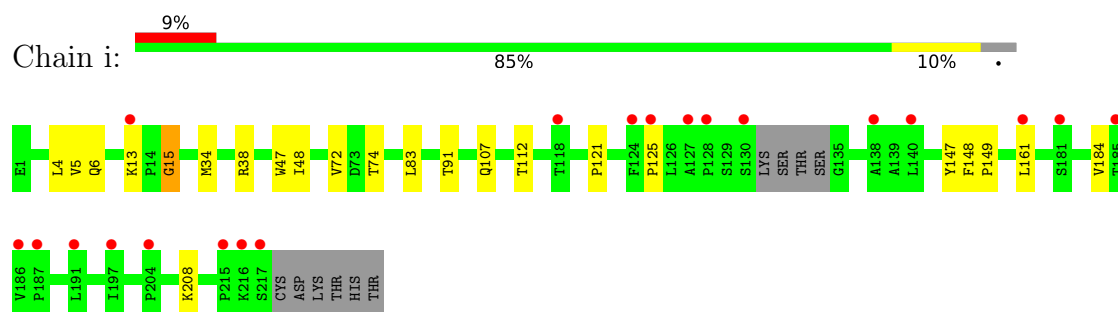
- Molecule 3: Fab Y49R heavy chain



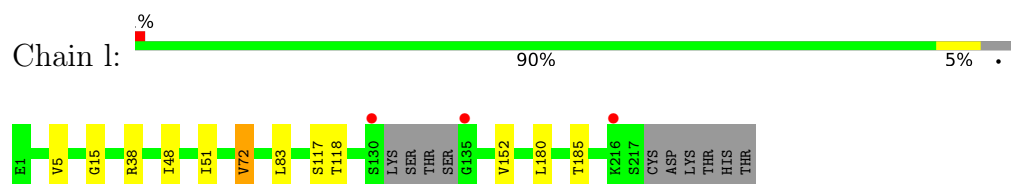
- Molecule 3: Fab Y49R heavy chain



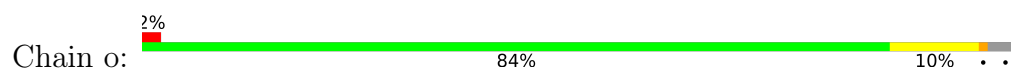
- Molecule 3: Fab Y49R heavy chain

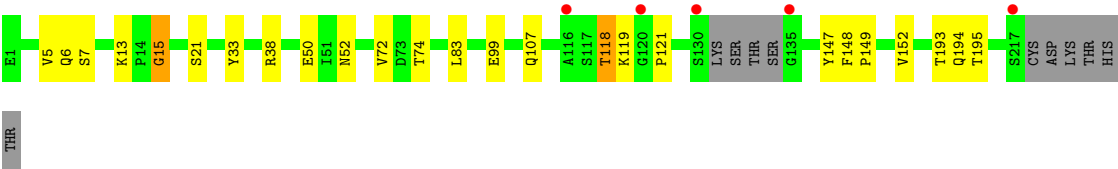


- Molecule 3: Fab Y49R heavy chain

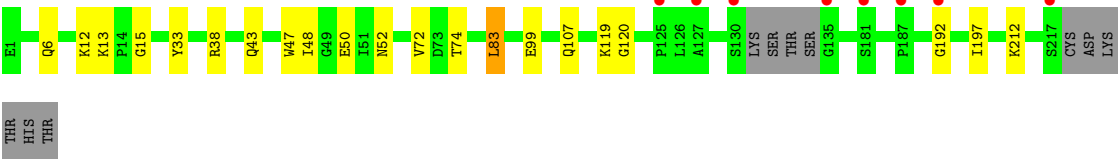
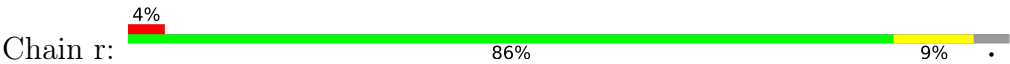


- Molecule 3: Fab Y49R heavy chain

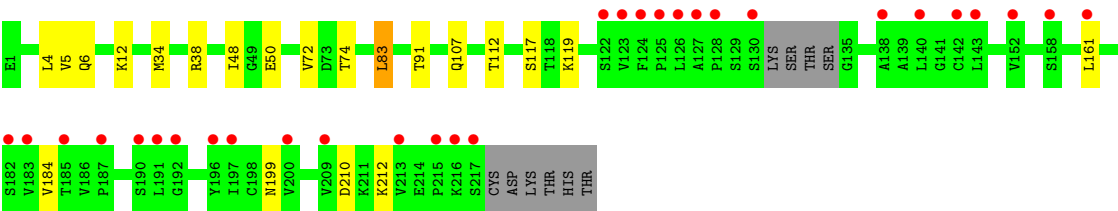
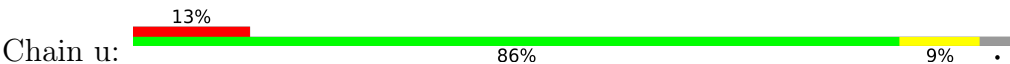




• Molecule 3: Fab Y49R heavy chain



• Molecule 3: Fab Y49R heavy chain



4 Data and refinement statistics

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 49.93 – 3.01	Depositor EDS
% Data completeness (in resolution range)	99.9 (49.93-3.01) 99.9 (49.93-3.01)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.63 (at 3.01Å)	Xtriage
Refinement program	PHENIX 1.12-2829_final	Depositor
R, R_{free}	0.174 , 0.215 0.180 , 0.222	Depositor DCC
R_{free} test set	2180 reflections (0.61%)	wwPDB-VP
Wilson B-factor (Å ²)	55.3	Xtriage
Anisotropy	0.038	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 64.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
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.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: SO4, GOL

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	0.14	0/1753	0.41	1/2385 (0.0%)
1	F	0.12	0/1753	0.32	0/2385
1	I	0.13	0/1753	0.33	0/2385
1	N	0.13	0/1753	0.33	0/2385
1	Q	0.13	0/1753	0.33	0/2385
1	T	0.13	0/1753	0.37	1/2385 (0.0%)
1	W	0.13	0/1753	0.34	0/2385
1	X	0.13	0/1753	0.34	0/2385
1	a	0.13	0/1753	0.34	1/2385 (0.0%)
1	d	0.13	0/1753	0.33	0/2385
1	g	0.13	0/1753	0.34	0/2385
1	j	0.13	0/1753	0.34	0/2385
1	m	0.12	0/1753	0.35	1/2385 (0.0%)
1	p	0.12	0/1753	0.32	0/2385
1	s	0.12	0/1753	0.32	0/2385
1	v	0.14	0/1753	0.34	0/2385
2	A	0.12	0/1668	0.33	0/2263
2	D	0.12	0/1668	0.33	0/2263
2	G	0.11	0/1668	0.32	0/2263
2	J	0.10	0/1668	0.31	0/2263
2	L	0.12	0/1668	0.32	0/2263
2	O	0.11	0/1668	0.32	0/2263
2	R	0.11	0/1668	0.31	0/2263
2	U	0.11	0/1668	0.32	0/2263
2	Y	0.12	0/1668	0.32	0/2263
2	b	0.12	0/1668	0.32	0/2263
2	e	0.10	0/1668	0.31	0/2263
2	h	0.11	0/1668	0.32	0/2263
2	k	0.11	0/1668	0.32	0/2263
2	n	0.11	0/1668	0.32	0/2263
2	q	0.11	0/1668	0.31	0/2263
2	t	0.11	0/1668	0.32	0/2263

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
3	B	0.11	0/1627	0.31	0/2217
3	E	0.11	0/1627	0.31	0/2217
3	H	0.11	0/1627	0.31	0/2217
3	K	0.11	0/1627	0.30	0/2217
3	M	0.11	0/1627	0.30	0/2217
3	P	0.10	0/1627	0.30	0/2217
3	S	0.10	0/1627	0.29	0/2217
3	V	0.10	0/1627	0.29	0/2217
3	Z	0.11	0/1627	0.31	0/2217
3	c	0.11	0/1627	0.33	0/2217
3	f	0.10	0/1627	0.29	0/2217
3	i	0.11	0/1627	0.31	0/2217
3	l	0.10	0/1627	0.31	0/2217
3	o	0.11	0/1627	0.35	0/2217
3	r	0.09	0/1627	0.28	0/2217
3	u	0.10	0/1627	0.29	0/2217
All	All	0.12	0/80768	0.32	4/109840 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	215	SER	CB-CA-C	-9.85	105.22	116.54
1	T	215	SER	CB-CA-C	-7.63	106.86	117.23
1	m	215	SER	CB-CA-C	-5.70	109.98	116.54
1	a	215	SER	CB-CA-C	-5.02	110.41	117.23

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	21	0
1	F	1713	0	1696	16	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	I	1713	0	1696	12	0
1	N	1713	0	1696	13	0
1	Q	1713	0	1696	16	0
1	T	1713	0	1696	18	0
1	W	1713	0	1696	16	0
1	X	1713	0	1696	17	0
1	a	1713	0	1696	14	0
1	d	1713	0	1696	16	0
1	g	1713	0	1696	13	0
1	j	1713	0	1696	11	0
1	m	1713	0	1696	16	0
1	p	1713	0	1696	16	0
1	s	1713	0	1696	14	0
1	v	1713	0	1696	8	0
2	A	1634	0	1582	16	0
2	D	1634	0	1582	16	0
2	G	1634	0	1582	10	0
2	J	1634	0	1582	13	0
2	L	1634	0	1582	14	0
2	O	1634	0	1582	12	0
2	R	1634	0	1582	10	0
2	U	1634	0	1582	13	0
2	Y	1634	0	1582	17	0
2	b	1634	0	1582	14	0
2	e	1634	0	1582	10	0
2	h	1634	0	1582	13	0
2	k	1634	0	1582	12	0
2	n	1634	0	1582	10	0
2	q	1634	0	1582	11	0
2	t	1634	0	1582	17	0
3	B	1589	0	1554	10	0
3	E	1589	0	1554	10	0
3	H	1589	0	1554	9	0
3	K	1589	0	1554	11	0
3	M	1589	0	1554	12	0
3	P	1589	0	1554	14	0
3	S	1589	0	1554	9	0
3	V	1589	0	1554	8	0
3	Z	1589	0	1554	10	0
3	c	1589	0	1554	7	0
3	f	1589	0	1554	9	0
3	i	1589	0	1554	12	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	l	1589	0	1554	3	0
3	o	1589	0	1554	13	0
3	r	1589	0	1554	12	0
3	u	1589	0	1554	9	0
4	C	6	0	8	0	0
4	F	6	0	8	0	0
4	I	6	0	8	0	0
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	1	0
4	d	6	0	8	2	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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
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	1	0
6	b	34	0	0	0	0
6	c	36	0	0	0	0
6	d	40	0	0	1	0
6	e	20	0	0	1	0
6	f	17	0	0	0	0
6	g	41	0	0	0	0
6	h	31	0	0	3	0
6	i	20	0	0	1	0
6	j	42	0	0	0	0
6	k	27	0	0	1	0
6	l	21	0	0	1	0
6	m	30	0	0	1	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	1	0
6	s	44	0	0	0	0
6	t	23	0	0	1	0
6	u	27	0	0	1	0
6	v	35	0	0	0	0
All	All	80635	0	77440	551	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 4.

All (551) 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:W:150:ARG:HG3	2:k:67:SER:HB3	1.63	0.81
1:d:150:ARG:HG3	2:e:67:SER:HB3	1.64	0.80
1:l:150:ARG:HG3	2:O:67:SER:HB3	1.64	0.79
1:a:150:ARG:HG3	2:h:67:SER:HB3	1.66	0.78
2:b:67:SER:HB3	1:g:150:ARG:HG3	1.66	0.77
2:A:67:SER:HB3	1:p:150:ARG:HG3	1.66	0.77
2:L:67:SER:HB3	1:m:150:ARG:HG3	1.67	0.77
1:X:150:ARG:HG3	2:q:67:SER:HB3	1.67	0.76
2:G:67:SER:HB3	1:Q:150:ARG:HG3	1.70	0.74
2:Y:67:SER:HB3	1:j:150:ARG:HG3	1.69	0.72
2:R:67:SER:HB3	1:v:150:ARG:HG3	1.71	0.72
1:C:150:ARG:HG3	2:n:67:SER:HB3	1.72	0.71
1:T:150:ARG:HG3	2:t:67:SER:HB3	1.72	0.70
2:U:67:SER:HB3	1:s:150:ARG:HG3	1.72	0.70
2:A:194:CYS:SG	6:A:301:HOH:O	2.50	0.69
1:p:123:LEU:HD12	1:p:124:PRO:HD2	1.75	0.68
3:i:91:THR:HG23	3:i:112:THR:HA	1.75	0.67
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
2:h:198:HIS:ND1	6:h:301:HOH:O	2.28	0.67
1:g:52:VAL:HG21	1:g:66:VAL:HG11	1.77	0.67
1:X:52:VAL:HG21	1:X:66:VAL:HG11	1.78	0.66
3:f:91:THR:HG23	3:f:112:THR:HA	1.78	0.66
3:H:38:ARG:HB2	3:H:48:ILE:HD11	1.77	0.65
1:j:52:VAL:HG21	1:j:66:VAL:HG11	1.78	0.65
2:b:49:ARG:HD3	2:b:55:TYR:CZ	2.32	0.65
2:q:49:ARG:HD3	2:q:55:TYR:CZ	2.32	0.65
3:l:117:SER:O	6:l:301:HOH:O	2.13	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
2:e:49:ARG:HD3	2:e:55:TYR:CZ	2.34	0.62
3:K:87:ARG:O	3:K:89:GLU:N	2.30	0.61
3:S:194:GLN:NE2	2:b:200:GLY:O	2.34	0.61
3:f:38:ARG:HB2	3:f:48:ILE:HD11	1.83	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:d:52:VAL:HG21	1:d:66:VAL:HG11	1.83	0.60
1:v:52:VAL:HG21	1:v:66:VAL:HG11	1.82	0.60
2:t:91:TYR:HA	2:t:96:LEU:HG	1.84	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
1:a:52:VAL:HG21	1:a:66:VAL:HG11	1.83	0.59
1:j:81:ARG:NH2	1:j:110:GLU:OE2	2.31	0.59
2:n:49:ARG:HD3	2:n:55:TYR:CZ	2.37	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
1:m:52:VAL:HG21	1:m:66:VAL:HG11	1.83	0.59
1:p:170(A):ARG:NH1	3:o:99:GLU:OE2	2.36	0.59
2:t:49:ARG:HD3	2:t:55:TYR:CZ	2.38	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
2:h:124:GLN:NE2	6:h:302:HOH:O	2.32	0.59
3:r:6:GLN:H	3:r:107:GLN:HE22	1.52	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
3:f:6:GLN:H	3:f:107:GLN:HE22	1.51	0.58
2:L:49:ARG:HD3	2:L:55:TYR:CZ	2.39	0.58
1:s:123:LEU:HD12	1:s:124:PRO:HD2	1.85	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
3:i:6:GLN:H	3:i:107:GLN:HE22	1.50	0.57
3:u:38:ARG:HB2	3:u:48:ILE:HD11	1.86	0.57
1:W:201:CYS:HB2	1:W:210:GLU:HG3	1.86	0.57
2:h:1:ASP:N	6:h:303:HOH:O	2.36	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
1:C:215:SER:OG	1:C:216:GLY:N	2.32	0.56
1:g:67:LEU:HD11	1:g:80:LYS:HG2	1.87	0.56
2:Y:49:ARG:HD3	2:Y:55:TYR:CZ	2.40	0.56
2:e:105:GLU:OE1	2:e:173:TYR:OH	2.21	0.56
2:k:49:ARG:HD3	2:k:55:TYR:CZ	2.40	0.56
1:I:215:SER:OG	1:I:216:GLY:N	2.36	0.56
2:R:49:ARG:HD3	2:R:55:TYR:CZ	2.41	0.56
2:t:32:ASP:HB2	2:t:92:ASN:HB2	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:b:91:TYR:HA	2:b:96:LEU:HG	1.87	0.55
3:o:118:THR:H	3:o:148:PHE:HD1	1.54	0.55
3:M:91:THR:HG23	3:M:112:THR:HA	1.88	0.55
2:h:29:VAL:HG11	2:h:90:GLN:HG3	1.89	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
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
3:Z:202:HIS:ND1	3:Z:205:SER:OG	2.32	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:p:52:VAL:HG21	1:p:66:VAL:HG11	1.90	0.54
1:C:170(A):ARG:NH2	2:A:89:GLN:OE1	2.39	0.54
1:s:52:VAL:HG21	1:s:66:VAL:HG11	1.89	0.53
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
2:n:91:TYR:HA	2:n:96:LEU:HG	1.91	0.53
1:X:123:LEU:HD12	1:X:124:PRO:HD2	1.90	0.53
2:h:49:ARG:HD3	2:h:55:TYR:CZ	2.42	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
1:p:57:HIS:HD2	1:p:102:ASP:OD2	1.92	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
1:j:214:THR:HG23	1:j:215:SER:H	1.74	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
2:q:32:ASP:HB2	2:q:92:ASN:HB2	1.90	0.52
3:H:6:GLN:H	3:H:107:GLN:HE22	1.58	0.52
2:k:91:TYR:HA	2:k:96:LEU:HG	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:S:38:ARG:HB2	3:S:48:ILE:HD11	1.91	0.52
1:m:123:LEU:HD12	1:m:124:PRO:HD2	1.91	0.52
3:i:13:LYS:O	3:i:15:GLY:N	2.41	0.52
3:P:87:ARG:O	3:P:89:GLU:N	2.38	0.52
2:t:108:ARG:NH1	2:t:109:THR:O	2.43	0.52
3:P:88:SER:HA	3:P:113:VAL:HB	1.91	0.52
2:b:193:ALA:HB2	2:b:208:SER:HB3	1.90	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:D:4:MET:HE3	2:D:23:CYS:SG	2.50	0.51
2:J:37:GLN:HB2	2:J:47:LEU:HD11	1.91	0.51
2:e:94:TYR:OH	3:f:50:GLU:OE2	2.22	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
1:d:189:ASP:OD1	1:d:190:SER:N	2.43	0.51
3:V:38:ARG:HB3	3:V:48:ILE:HD11	1.92	0.51
2:h:108:ARG:NH1	2:h:109:THR:O	2.42	0.51
1:a:123:LEU:HD12	1:a:124:PRO:HD2	1.93	0.51
3:i:38:ARG:HB2	3:i: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
2:Y:91:TYR:HA	2:Y:96:LEU:HG	1.91	0.50
1:j:81:ARG:HD3	1:j:83:TYR:CZ	2.46	0.50
1:X:126:ARG:NH1	1:X:239:ASP:OD2	2.43	0.50
2:U:4:MET:HE3	2:U:23:CYS:SG	2.51	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
2:b:94:TYR:OH	3:c:50:GLU:OE2	2.29	0.50
1:j:57:HIS:HA	1:j:60:GLU:HG3	1.93	0.50
2:R:4:MET:HE3	2:R:23:CYS:SG	2.52	0.50
2:t:4:MET:HE3	2:t:23:CYS:SG	2.52	0.50
1:F:218:ARG:NH2	6:F:401:HOH:O	2.43	0.50
1:a:201:CYS:HB2	1:a:210:GLU:HG3	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:b:37:GLN:HB2	2:b:47:LEU:HD11	1.92	0.50
2:k:49:ARG:HD3	2:k:55:TYR:CE1	2.46	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:b:32:ASP:HB2	2:b:92:ASN:HB2	1.94	0.50
2:G:4:MET:HE3	2:G:23:CYS:SG	2.51	0.49
3:l:38:ARG:HB2	3:l:48:ILE:HD11	1.93	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
1:d:214:THR:HG23	1:d:215:SER:H	1.78	0.49
2:k:32:ASP:HB2	2:k:92:ASN:HB2	1.93	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:b:4:MET:HE3	2:b:23:CYS:SG	2.53	0.49
2:h:4:MET:HE3	2:h:23:CYS:SG	2.53	0.49
1:d:59:LEU:HD22	1:d:104:LEU:HD21	1.95	0.49
2:R:29:VAL:HG11	2:R:90:GLN:HG3	1.95	0.49
3:V:4:LEU:HD13	3:V:34:MET:HE1	1.95	0.49
1:p:186:ASN:C	1:p:188:ARG:H	2.21	0.49
2:n:32:ASP:HB2	2:n:92:ASN:HB2	1.94	0.49
3:E:13:LYS:O	3:E:15:GLY:N	2.41	0.48
1:g:214:THR:HG23	1:g:215:SER:H	1.78	0.48
1:v:123:LEU:HD12	1:v:124:PRO:HD2	1.95	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
1:W:126:ARG:HH12	1:W:239:ASP:CG	2.21	0.48
2:J:91:TYR:HA	2:J:96:LEU:HG	1.95	0.48
1:m:218:ARG:NH2	6:m:401:HOH:O	2.43	0.48
1:C:124(A):TRP:HA	1:C:209:LEU:HB3	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:t:171:SER:O	6:t:301:HOH:O	2.19	0.48
3:u:91:THR:HG23	3:u:112:THR:HA	1.96	0.48
3:u:212:LYS:O	6:u:301:HOH:O	2.20	0.48
2:Y:158:ASN:HD22	2:Y:181:LEU:HD21	1.79	0.48
2:t:94:TYR:OH	3:u:50:GLU:OE2	2.31	0.48
1:X:45:VAL:HG13	1:X:53:LEU:HB3	1.95	0.47
3:f:61:ASN:HB3	3:f:64:PHE:HD2	1.79	0.47
1:j:49:GLU:OE1	1:j:111:LYS:HE2	2.14	0.47
2:k:42:LYS:NZ	6:k:302:HOH:O	2.47	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
3:i:121:PRO:HB3	3:i:147:TYR:HB3	1.96	0.47
1:s:214:THR:HG23	1:s:215:SER:H	1.78	0.47
1:W:186:ASN:C	1:W:188:ARG:H	2.23	0.47
1:T:213:VAL:HG22	1:T:228:TYR:CE2	2.49	0.47
1:m:189:ASP:OD1	1:m:190:SER:N	2.48	0.47
2:k:29:VAL:HG11	2:k:90:GLN:HG3	1.96	0.47
3:r:192:GLY:N	6:r:301:HOH:O	2.46	0.47
2:q:91:TYR:HA	2:q:96:LEU:HG	1.97	0.47
1:C:123:LEU:HD12	1:C:124:PRO:HD2	1.96	0.47
1:j:51:TRP:CH2	1:j:107:GLN:HB2	2.48	0.47
1:s:124(A):TRP:HA	1:s:209:LEU:HB3	1.97	0.47
2:L:4:MET:HE3	2:L:23:CYS:SG	2.53	0.47
1:s:213:VAL:HG22	1:s:228:TYR:CE2	2.50	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
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
1:a:180:LEU:HD23	1:a:229:THR:HA	1.96	0.47
3:S:13:LYS:O	3:S:15:GLY:N	2.46	0.47
3:Z:4:LEU:HD22	3:Z:34:MET:HE1	1.97	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
2:e:193:ALA:HB2	2:e:208:SER:HB3	1.96	0.47
3:f:121:PRO:HB3	3:f:147:TYR:HB3	1.97	0.47
1:m:81:ARG:NH2	1:m:110:GLU:OE2	2.47	0.47
3:u:161:LEU:HD21	3:u:184:VAL:HG21	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:81:ARG:HD3	1:C:83:TYR:CZ	2.50	0.46
2:J:94:TYR:OH	3:K:50:GLU:OE2	2.20	0.46
2:q:94:TYR:OH	3:r:50:GLU:OE2	2.32	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
3:S:4:LEU:HD13	3:S:34:MET:HE1	1.97	0.46
3:r:119:LYS:NZ	3:r:120:GLY:O	2.47	0.46
1:v:51:TRP:CH2	1:v:107:GLN:HB2	2.51	0.46
1:Q:67:LEU:HD11	1:Q:80:LYS:HG2	1.97	0.46
1:m:57:HIS:HD2	1:m:102:ASP:OD2	1.99	0.46
1:s:171:HIS:HA	1:s:223(A):LYS:O	2.16	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:v:57:HIS:HA	1:v:60:GLU:HG3	1.98	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:b:90:GLN:NE2	2:b:97:THR:OG1	2.47	0.46
2:e:29:VAL:HG11	2:e:90:GLN:HG3	1.97	0.46
2:t:29:VAL:HG11	2:t:90:GLN:HG3	1.97	0.46
3:M:4:LEU:HD13	3:M:34:MET:HE1	1.98	0.46
2:A:37:GLN:HB2	2:A:47:LEU:HD11	1.98	0.46
1:s:57:HIS:HA	1:s:60:GLU:HG3	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:o:33:TYR:CZ	3:o:52:ASN:HB2	2.51	0.46
1:a:59:LEU:HD22	1:a:104:LEU:HD21	1.97	0.46
1:a:195:SER:HG	4:a:301:GOL:HO2	1.62	0.46
2:Y:94:TYR:OH	3:Z:50:GLU:OE2	2.33	0.46
1:m:180:LEU:HD23	1:m:229:THR:HA	1.98	0.46
3:u:6:GLN:H	3:u:107:GLN:HE22	1.64	0.46
3:M:118:THR:HB	6:M:327:HOH:O	2.14	0.46
1:a:81:ARG:HD3	1:a:83:TYR:CZ	2.50	0.46
2:e:108:ARG:NH1	2:e:109:THR:O	2.46	0.46
2:n:29:VAL:HG11	2:n:90:GLN:HG3	1.98	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
2:h:32:ASP:HB2	2:h:92:ASN:HB2	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:d:57:HIS:HA	1:d:60:GLU:HG3	1.97	0.45
3:i:125:PRO:HB3	6:i:303:HOH:O	2.16	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
3:f:13:LYS:O	3:f:15:GLY:N	2.44	0.45
1:p:81:ARG:HD3	1:p:83:TYR:CZ	2.52	0.45
1:W:124(A):TRP:HA	1:W:209:LEU:HB3	1.98	0.45
1:s:51:TRP:CH2	1:s:107:GLN:HB2	2.52	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
1:g:57:HIS:HA	1:g:60:GLU:HG3	1.99	0.45
2:h:91:TYR:HA	2:h:96:LEU:HG	1.99	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
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:i:208:LYS:HE2	3:i:208:LYS:HB3	1.87	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
2:n:90:GLN:OE1	2:n:92:ASN:N	2.50	0.44
2:n:94:TYR:OH	3:o:50:GLU:OE2	2.32	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
1:a:214:THR:HG23	1:a:215:SER:H	1.82	0.44
2:Y:54:ARG:HD3	2:Y:62:PHE:O	2.17	0.44
1:d:16:ILE:N	1:d:194:ASP:OD2	2.50	0.44
2:q:120:PRO:HD3	2:q:132:VAL:HG22	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:t:49:ARG:HD3	2:t:55:TYR:CE1	2.53	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
1:Q:186:ASN:C	1:Q:188:ARG:H	2.25	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
3:i:6:GLN:H	3:i:107:GLN:NE2	2.15	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
1:a:186:ASN:C	1:a:188:ARG:H	2.26	0.44
2:e:4:MET:HE3	2:e:23:CYS:SG	2.57	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:a:189:ASP:OD1	1:a:190:SER:N	2.50	0.44
3:c:121:PRO:HB3	3:c:147:TYR:HB3	1.99	0.44
1:W:52:VAL:HG21	1:W:66:VAL:HG11	2.00	0.44
2:Y:4:MET:HE3	2:Y:23:CYS:SG	2.57	0.44
1:g:180:LEU:HD23	1:g:229:THR:HA	2.00	0.44
2:k:90:GLN:OE1	2:k:93:ASN:N	2.49	0.44
2:t:108:ARG:HG2	2:t:109:THR:N	2.32	0.44
2:A:4:MET:HE3	2:A:23:CYS:SG	2.58	0.43
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:d:56:ALA:HA	1:d:104:LEU:HB2	1.99	0.43
4:d:301:GOL:H2	6:d:406:HOH:O	2.18	0.43
1:p:59:LEU:HD22	1:p:104:LEU:HD21	2.00	0.43
2:q:29:VAL:HG11	2:q:90:GLN:HG3	1.99	0.43
1:v:81:ARG:HD3	1:v:83:TYR:CZ	2.53	0.43
1:d:57:HIS:NE2	4:d:301:GOL:H32	2.34	0.43
1:d:213:VAL:HG22	1:d:228:TYR:CE2	2.52	0.43
1:g:189:ASP:OD1	1:g:190:SER:N	2.49	0.43
2:k:113:PRO:HB3	2:k:139:PHE:HB3	2.00	0.43
3:o:118:THR:HA	3:o:148:PHE:O	2.18	0.43
1:s:81:ARG:HD3	1:s:83:TYR:CZ	2.53	0.43
1:v:126:ARG:NH1	1:v:239:ASP:OD2	2.50	0.43
1:C:186:ASN:C	1:C:188:ARG:H	2.26	0.43
3:B:4:LEU:HD13	3:B:34:MET:HE1	2.00	0.43
2:D:135:LEU:HD22	3:E:183:VAL:HG11	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:22:ALA:HB1	1:Q:27:ARG:NH1	2.33	0.43
2:O:4:MET:HE3	2:O:23:CYS:SG	2.58	0.43
1:m:186:ASN:C	1:m:188:ARG:H	2.26	0.43
3:E:4:LEU:HD22	3:E:34:MET:HE1	2.01	0.43
2:J:90:GLN:HE21	2:J:90:GLN:HB3	1.71	0.43
3:K:4:LEU:HD13	3:K:34:MET:HE1	1.99	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:h:96:LEU:HB2	3:i:47:TRP:CD2	2.53	0.43
2:O:49:ARG:HD3	2:O:55:TYR:CE1	2.53	0.43
3:c:38:ARG:HB3	3:c:48:ILE:HD11	2.01	0.43
2:e:45:LYS:NZ	6:e:302:HOH:O	2.51	0.43
3:o:121:PRO:HB3	3:o:147:TYR:HB3	2.00	0.43
3:M:197:ILE:HG12	3:M:212:LYS:HA	2.00	0.43
2:D:201:LEU:O	3:o:194:GLN:NE2	2.51	0.43
2:J:193:ALA:HB2	2:J:208:SER:HB3	2.00	0.43
1:a:51:TRP:CH2	1:a:107:GLN:HB2	2.54	0.43
2:Y:176:SER:HB3	3:Z:168:PHE:CE2	2.53	0.43
3:c:4:LEU:HD13	3:c:34:MET:HE1	2.01	0.43
1:g:135:LEU:HD13	1:g:159:LEU:HD23	2.01	0.43
1:j:180:LEU:HD23	1:j:229:THR:HA	2.00	0.43
1:p:56:ALA:HA	1:p:104:LEU:HB2	2.01	0.43
2:n:37:GLN:HB2	2:n:47:LEU:HD11	2.00	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
2:J:4:MET:HE3	2:J:23:CYS:SG	2.59	0.43
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:s:213:VAL:HG22	1:s:228:TYR:HE2	1.84	0.43
2:O:94:TYR:OH	3:P:50:GLU:OE2	2.27	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
1:d:171:HIS:O	1:d:224:LYS:NZ	2.46	0.42
1:m:64:VAL:HG12	1:m:85:VAL:HG21	2.01	0.42
2:k:108:ARG:HG3	2:k:109:THR:O	2.19	0.42
3:u:83:LEU:HD23	3:u:83:LEU:HA	1.91	0.42
3:u:199:ASN:ND2	3:u:210:ASP:OD1	2.39	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:g:56:ALA:HA	1:g:104:LEU:HB2	2.01	0.42
1:m:51:TRP:CH2	1:m:107:GLN:HB2	2.53	0.42
3:o:13:LYS:O	3:o:15:GLY:N	2.46	0.42
2:q:193:ALA:HB2	2:q:208:SER:HB3	2.01	0.42
3:r:33:TYR:CZ	3:r:52:ASN:HB2	2.54	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
1:T:186:ASN:C	1:T:188:ARG:H	2.28	0.42
1:a:56:ALA:HA	1:a:104:LEU:HB2	2.01	0.42
2:t:42:LYS:HE2	2:t:42:LYS:HB3	1.83	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
3:f:148:PHE:HA	3:f:149:PRO:HA	1.83	0.42
1:j:56:ALA:HA	1:j:104:LEU:HB2	2.02	0.42
1:m:32:SER:HB3	1:m:67:LEU:HB3	2.01	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
1:m:213:VAL:HG22	1:m:228:TYR:CE2	2.54	0.42
1:s:186:ASN:C	1:s:188:ARG:H	2.28	0.42
3:r:6:GLN:H	3:r:107:GLN:NE2	2.15	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:d:213:VAL:HG22	1:d:228:TYR:HE2	1.84	0.42
1:s:170(A):ARG:HD3	3:r:99:GLU:OE2	2.20	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
3:i:161:LEU:HD21	3:i:184:VAL:HG21	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
1:p:51:TRP:CH2	1:p:107:GLN:HB2	2.55	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
2:b:49:ARG:HD3	2:b:55:TYR:CE1	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:b:176:SER:HB3	3:c:168:PHE:CZ	2.55	0.42
2:h:37:GLN:HB2	2:h:47:LEU:HD11	2.01	0.42
1:v:214:THR:HG23	1:v:215:SER:H	1.85	0.42
2:t:90:GLN:OE1	2:t:93:ASN:N	2.49	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
1:d:129:ARG:HD3	1:d:129:ARG:HA	1.90	0.41
1:p:189:ASP:OD1	1:p:190:SER:N	2.53	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:d:186:ASN:C	1:d:188:ARG:H	2.27	0.41
1:g:49:GLU:HG2	1:g:114:LEU:HD21	2.03	0.41
1:g:129:ARG:HD3	1:g:129:ARG:HA	1.90	0.41
3:i:148:PHE:HA	3:i:149:PRO:HA	1.80	0.41
1:m:57:HIS:HA	1:m:60:GLU:HG3	2.01	0.41
2:n:193:ALA:HB2	2:n:208:SER:HB3	2.02	0.41
2:q:4:MET:SD	2:q:90:GLN:HB2	2.60	0.41
3:r:83:LEU:HD23	3:r:83:LEU:HA	1.89	0.41
2:t:2:ILE:HD12	2:t:93:ASN:HB3	2.03	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
1:d:170(A):ARG:NH1	3:c:99:GLU:OE2	2.49	0.41
3:r:38:ARG:HB2	3:r:48:ILE:HD11	2.03	0.41
2:D:202:SER:HB3	3:o:195:THR:H	1.85	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:o:6:GLN:H	3:o:107:GLN:HE22	1.69	0.41
3:c:91:THR:HG23	3:c:112:THR:HA	2.03	0.41
1:g:51:TRP:CH2	1:g:107:GLN:HB2	2.56	0.41
2:t:140:TYR:CD1	2:t:141:PRO:HA	2.55	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
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
2:k:90:GLN:HE21	2:k:90:GLN:HB3	1.75	0.41
3:l:51:ILE:HD13	3:l:72:VAL:HG23	2.03	0.41
3:o:148:PHE:HA	3:o:149:PRO:HA	1.85	0.41
3:r:13:LYS:O	3:r:15:GLY:N	2.54	0.41
2:t:145:LYS:HB3	2:t:197:THR:HB	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:u:4:LEU:HD13	3:u:34:MET:HE1	2.03	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:d:170(B):THR:HG23	2:b:91:TYR:HD1	1.86	0.41
2:b:90:GLN:HE21	2:b:90:GLN:HB3	1.69	0.41
2:q:78:LEU:HD12	2:q:78:LEU:HA	1.90	0.41
3:r:197:ILE:HG12	3:r:212:LYS:HA	2.03	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:H:4:LEU:HD13	3:H:34:MET:HE1	2.03	0.41
3:P:121:PRO:HB3	3:P:147:TYR:HB3	2.01	0.41
1:g:186:ASN:C	1:g:188:ARG:H	2.29	0.41
3:i:4:LEU:HD13	3:i:34:MET:HE1	2.02	0.41
1:m:170(A):ARG:NH2	2:k:89:GLN:OE1	2.48	0.41
1:p:104:LEU:HD21	1:p:106:LEU:HD21	2.02	0.41
2:t:193:ALA:HB2	2:t:208:SER:HB3	2.03	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
3:f:6:GLN:H	3:f:107:GLN:NE2	2.19	0.40
1:p:81:ARG:NH2	1:p:110:GLU:OE2	2.52	0.40
1:p:214:THR:HG23	1:p:215:SER:H	1.86	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:a:188:ARG:HD2	6:a:437:HOH:O	2.21	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
2:e:49:ARG:HD3	2:e:55:TYR:CE1	2.56	0.40
2:h:2:ILE:HD12	2:h:93:ASN:HB3	2.03	0.40
2:n:120:PRO:HD3	2:n:132:VAL:HG22	2.03	0.40
1:s:121:ARG:HA	1:s:122:PRO:HD3	1.98	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:q:96:LEU:HB2	3:r:47:TRP:CD2	2.56	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
1:j:59:LEU:HD22	1:j:104:LEU:HD21	2.03	0.40
1:m:213:VAL:HG22	1:m:228:TYR:HE2	1.86	0.40
1:p:170(A):ARG:HD3	3:o:99:GLU:CD	2.46	0.40
3:B:35:TYR:CD1	3:B:99:GLU:HG2	2.56	0.40
1:F:186:ASN:C	1:F:188:ARG:H	2.30	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
1:p:126:ARG:NH1	1:p:239:ASP:OD2	2.55	0.40
3:o:7:SER:HB3	3:o:21:SER:OG	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	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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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%)	30	63
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%)	24	59
2	D	211/214 (99%)	200 (95%)	10 (5%)	1 (0%)	24	59
2	G	211/214 (99%)	199 (94%)	12 (6%)	0	100	100
2	J	211/214 (99%)	202 (96%)	7 (3%)	2 (1%)	14	46
2	L	211/214 (99%)	203 (96%)	7 (3%)	1 (0%)	24	59
2	O	211/214 (99%)	198 (94%)	12 (6%)	1 (0%)	24	59
2	R	211/214 (99%)	198 (94%)	13 (6%)	0	100	100
2	U	211/214 (99%)	202 (96%)	8 (4%)	1 (0%)	24	59
2	Y	211/214 (99%)	201 (95%)	9 (4%)	1 (0%)	24	59
2	b	211/214 (99%)	203 (96%)	7 (3%)	1 (0%)	24	59
2	e	211/214 (99%)	201 (95%)	9 (4%)	1 (0%)	24	59
2	h	211/214 (99%)	199 (94%)	12 (6%)	0	100	100
2	k	211/214 (99%)	200 (95%)	10 (5%)	1 (0%)	24	59
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%)	24	59
3	B	209/223 (94%)	202 (97%)	7 (3%)	0	100	100
3	E	209/223 (94%)	199 (95%)	9 (4%)	1 (0%)	24	59
3	H	209/223 (94%)	201 (96%)	7 (3%)	1 (0%)	24	59
3	K	209/223 (94%)	199 (95%)	8 (4%)	2 (1%)	12	43

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	M	209/223 (94%)	200 (96%)	8 (4%)	1 (0%)	24	59
3	P	209/223 (94%)	195 (93%)	13 (6%)	1 (0%)	24	59
3	S	209/223 (94%)	198 (95%)	10 (5%)	1 (0%)	24	59
3	V	209/223 (94%)	199 (95%)	9 (4%)	1 (0%)	24	59
3	Z	209/223 (94%)	199 (95%)	9 (4%)	1 (0%)	24	59
3	c	209/223 (94%)	202 (97%)	6 (3%)	1 (0%)	24	59
3	f	209/223 (94%)	201 (96%)	7 (3%)	1 (0%)	24	59
3	i	209/223 (94%)	198 (95%)	10 (5%)	1 (0%)	24	59
3	l	209/223 (94%)	198 (95%)	10 (5%)	1 (0%)	24	59
3	o	209/223 (94%)	200 (96%)	7 (3%)	2 (1%)	12	43
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%)	36	68

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
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

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Mol	Chain	Res	Type
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 ⓘ

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%)	179 (98%)	4 (2%)	45	73
1	F	183/182 (100%)	181 (99%)	2 (1%)	65	82
1	I	183/182 (100%)	179 (98%)	4 (2%)	45	73
1	N	183/182 (100%)	179 (98%)	4 (2%)	45	73
1	Q	183/182 (100%)	178 (97%)	5 (3%)	39	70
1	T	183/182 (100%)	180 (98%)	3 (2%)	55	78
1	W	183/182 (100%)	179 (98%)	4 (2%)	45	73
1	X	183/182 (100%)	181 (99%)	2 (1%)	65	82
1	a	183/182 (100%)	178 (97%)	5 (3%)	39	70
1	d	183/182 (100%)	179 (98%)	4 (2%)	45	73
1	g	183/182 (100%)	181 (99%)	2 (1%)	65	82
1	j	183/182 (100%)	179 (98%)	4 (2%)	45	73
1	m	183/182 (100%)	181 (99%)	2 (1%)	65	82
1	p	183/182 (100%)	179 (98%)	4 (2%)	45	73
1	s	183/182 (100%)	180 (98%)	3 (2%)	55	78
1	v	183/182 (100%)	176 (96%)	7 (4%)	29	62
2	A	187/188 (100%)	177 (95%)	10 (5%)	20	52
2	D	187/188 (100%)	181 (97%)	6 (3%)	34	66

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	G	187/188 (100%)	179 (96%)	8 (4%)	26	59
2	J	187/188 (100%)	179 (96%)	8 (4%)	26	59
2	L	187/188 (100%)	181 (97%)	6 (3%)	34	66
2	O	187/188 (100%)	181 (97%)	6 (3%)	34	66
2	R	187/188 (100%)	178 (95%)	9 (5%)	23	56
2	U	187/188 (100%)	179 (96%)	8 (4%)	26	59
2	Y	187/188 (100%)	179 (96%)	8 (4%)	26	59
2	b	187/188 (100%)	178 (95%)	9 (5%)	23	56
2	e	187/188 (100%)	178 (95%)	9 (5%)	23	56
2	h	187/188 (100%)	181 (97%)	6 (3%)	34	66
2	k	187/188 (100%)	179 (96%)	8 (4%)	26	59
2	n	187/188 (100%)	180 (96%)	7 (4%)	30	63
2	q	187/188 (100%)	182 (97%)	5 (3%)	39	70
2	t	187/188 (100%)	183 (98%)	4 (2%)	47	74
3	B	178/188 (95%)	172 (97%)	6 (3%)	32	64
3	E	178/188 (95%)	173 (97%)	5 (3%)	38	69
3	H	178/188 (95%)	171 (96%)	7 (4%)	28	61
3	K	178/188 (95%)	173 (97%)	5 (3%)	38	69
3	M	178/188 (95%)	174 (98%)	4 (2%)	45	73
3	P	178/188 (95%)	171 (96%)	7 (4%)	28	61
3	S	178/188 (95%)	174 (98%)	4 (2%)	45	73
3	V	178/188 (95%)	173 (97%)	5 (3%)	38	69
3	Z	178/188 (95%)	170 (96%)	8 (4%)	24	57
3	c	178/188 (95%)	173 (97%)	5 (3%)	38	69
3	f	178/188 (95%)	173 (97%)	5 (3%)	38	69
3	i	178/188 (95%)	174 (98%)	4 (2%)	45	73
3	l	178/188 (95%)	171 (96%)	7 (4%)	28	61
3	o	178/188 (95%)	170 (96%)	8 (4%)	24	57
3	r	178/188 (95%)	173 (97%)	5 (3%)	38	69
3	u	178/188 (95%)	171 (96%)	7 (4%)	28	61
All	All	8768/8928 (98%)	8500 (97%)	268 (3%)	35	67

All (268) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	W	45	VAL
1	W	59	LEU
1	W	159	LEU
1	W	214	THR
2	L	11	LEU
2	L	19	VAL
2	L	20	THR
2	L	22	THR
2	L	109	THR
2	L	169	LYS
3	M	5	VAL
3	M	72	VAL
3	M	74	THR
3	M	83	LEU
1	C	45	VAL
1	C	59	LEU
1	C	159	LEU
1	C	214	THR
2	A	3	GLN
2	A	11	LEU
2	A	14	SER
2	A	19	VAL
2	A	20	THR
2	A	22	THR
2	A	56	SER
2	A	105	GLU
2	A	132	VAL
2	A	169	LYS
3	B	5	VAL
3	B	11	VAL
3	B	17	SER
3	B	72	VAL
3	B	74	THR
3	B	83	LEU
1	F	159	LEU
1	F	214	THR
2	D	3	GLN
2	D	19	VAL
2	D	20	THR
2	D	22	THR
2	D	56	SER
2	D	90	GLN

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Mol	Chain	Res	Type
3	E	5	VAL
3	E	72	VAL
3	E	74	THR
3	E	83	LEU
3	E	112	THR
1	I	45	VAL
1	I	59	LEU
1	I	159	LEU
1	I	214	THR
2	G	19	VAL
2	G	20	THR
2	G	22	THR
2	G	48	ILE
2	G	53	SER
2	G	56	SER
2	G	108	ARG
2	G	169	LYS
3	H	5	VAL
3	H	11	VAL
3	H	43	GLN
3	H	72	VAL
3	H	74	THR
3	H	83	LEU
3	H	185	THR
1	N	45	VAL
1	N	59	LEU
1	N	233	SER
1	N	242	LEU
2	J	11	LEU
2	J	14	SER
2	J	19	VAL
2	J	20	THR
2	J	22	THR
2	J	90	GLN
2	J	106	ILE
2	J	169	LYS
3	K	72	VAL
3	K	74	THR
3	K	83	LEU
3	K	112	THR
3	K	150	GLU
1	Q	17	LEU

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Mol	Chain	Res	Type
1	Q	45	VAL
1	Q	159	LEU
1	Q	214	THR
1	Q	242	LEU
2	O	14	SER
2	O	19	VAL
2	O	20	THR
2	O	22	THR
2	O	90	GLN
2	O	169	LYS
3	P	5	VAL
3	P	11	VAL
3	P	12	LYS
3	P	72	VAL
3	P	74	THR
3	P	83	LEU
3	P	112	THR
1	T	45	VAL
1	T	59	LEU
1	T	214	THR
2	R	3	GLN
2	R	11	LEU
2	R	14	SER
2	R	19	VAL
2	R	20	THR
2	R	22	THR
2	R	48	ILE
2	R	56	SER
2	R	169	LYS
3	S	5	VAL
3	S	72	VAL
3	S	74	THR
3	S	83	LEU
1	X	45	VAL
1	X	159	LEU
2	U	3	GLN
2	U	14	SER
2	U	19	VAL
2	U	20	THR
2	U	22	THR
2	U	56	SER
2	U	108	ARG

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Mol	Chain	Res	Type
2	U	169	LYS
3	V	5	VAL
3	V	72	VAL
3	V	83	LEU
3	V	180	LEU
3	V	193	THR
1	a	45	VAL
1	a	59	LEU
1	a	138	VAL
1	a	159	LEU
1	a	214	THR
2	Y	19	VAL
2	Y	20	THR
2	Y	22	THR
2	Y	48	ILE
2	Y	56	SER
2	Y	161	GLU
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	115	SER
3	Z	152	VAL
3	Z	185	THR
1	d	17	LEU
1	d	45	VAL
1	d	159	LEU
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	48	ILE
2	b	56	SER
2	b	90	GLN
2	b	169	LYS
3	c	5	VAL
3	c	38	ARG

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Mol	Chain	Res	Type
3	c	72	VAL
3	c	74	THR
3	c	83	LEU
1	g	214	THR
1	g	233	SER
2	e	3	GLN
2	e	11	LEU
2	e	14	SER
2	e	19	VAL
2	e	20	THR
2	e	22	THR
2	e	56	SER
2	e	90	GLN
2	e	161	GLU
3	f	5	VAL
3	f	43	GLN
3	f	72	VAL
3	f	83	LEU
3	f	112	THR
1	j	159	LEU
1	j	195	SER
1	j	233	SER
1	j	242	LEU
2	h	14	SER
2	h	19	VAL
2	h	20	THR
2	h	22	THR
2	h	56	SER
2	h	169	LYS
3	i	5	VAL
3	i	72	VAL
3	i	74	THR
3	i	83	LEU
1	m	45	VAL
1	m	214	THR
2	k	19	VAL
2	k	20	THR
2	k	22	THR
2	k	48	ILE
2	k	56	SER
2	k	109	THR
2	k	115	VAL

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Mol	Chain	Res	Type
2	k	169	LYS
3	l	5	VAL
3	l	72	VAL
3	l	83	LEU
3	l	118	THR
3	l	152	VAL
3	l	180	LEU
3	l	185	THR
1	p	45	VAL
1	p	59	LEU
1	p	159	LEU
1	p	214	THR
2	n	19	VAL
2	n	20	THR
2	n	22	THR
2	n	48	ILE
2	n	53	SER
2	n	56	SER
2	n	169	LYS
3	o	5	VAL
3	o	38	ARG
3	o	72	VAL
3	o	74	THR
3	o	83	LEU
3	o	119	LYS
3	o	152	VAL
3	o	193	THR
1	s	45	VAL
1	s	59	LEU
1	s	214	THR
2	q	19	VAL
2	q	22	THR
2	q	56	SER
2	q	108	ARG
2	q	169	LYS
3	r	12	LYS
3	r	43	GLN
3	r	72	VAL
3	r	74	THR
3	r	83	LEU
1	v	17	LEU
1	v	45	VAL

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Mol	Chain	Res	Type
1	v	59	LEU
1	v	129	ARG
1	v	129(A)	ASP
1	v	159	LEU
1	v	214	THR
2	t	3	GLN
2	t	19	VAL
2	t	22	THR
2	t	169	LYS
3	u	5	VAL
3	u	12	LYS
3	u	72	VAL
3	u	74	THR
3	u	83	LEU
3	u	117	SER
3	u	119	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (57) such sidechains are listed below:

Mol	Chain	Res	Type
1	W	34	GLN
2	L	93	ASN
2	L	124	GLN
1	C	146	HIS
2	A	37	GLN
2	A	92	ASN
3	B	59	ASN
2	D	79	GLN
2	D	93	ASN
3	E	166	HIS
1	I	107	GLN
2	G	27	GLN
2	G	92	ASN
2	G	93	ASN
2	G	199	GLN
3	H	59	ASN
2	J	3	GLN
2	J	93	ASN
3	K	59	ASN
1	Q	107	GLN
2	O	3	GLN
2	O	93	ASN

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Mol	Chain	Res	Type
3	P	59	ASN
2	R	27	GLN
2	R	37	GLN
2	R	92	ASN
2	R	93	ASN
3	S	59	ASN
3	S	194	GLN
2	U	93	ASN
2	U	138	ASN
3	V	166	HIS
2	Y	38	GLN
2	Y	92	ASN
2	Y	93	ASN
3	Z	39	GLN
3	Z	59	ASN
2	b	3	GLN
2	b	92	ASN
3	c	59	ASN
2	e	93	ASN
3	f	59	ASN
1	j	34	GLN
2	h	93	ASN
2	h	199	GLN
3	i	59	ASN
2	k	3	GLN
2	k	93	ASN
3	l	3	GLN
2	n	3	GLN
2	n	93	ASN
3	o	59	ASN
2	q	3	GLN
2	q	79	GLN
2	q	93	ASN
1	v	107	GLN
2	t	93	ASN

5.3.3 RNA ⓘ

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 oligosaccharides 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	$\# Z > 2$
4	GOL	C	301	-	5,5,5	0.98	0	5,5,5	1.05	0
4	GOL	v	301	-	5,5,5	0.90	0	5,5,5	1.09	0
4	GOL	X	301	-	5,5,5	0.93	0	5,5,5	1.11	0
5	SO4	X	302	-	4,4,4	0.25	0	6,6,6	0.10	0
5	SO4	j	302	-	4,4,4	0.26	0	6,6,6	0.06	0
5	SO4	g	302	-	4,4,4	0.26	0	6,6,6	0.07	0
5	SO4	N	302	-	4,4,4	0.23	0	6,6,6	0.07	0
5	SO4	C	302	-	4,4,4	0.27	0	6,6,6	0.10	0
4	GOL	I	301	-	5,5,5	0.89	0	5,5,5	1.16	0
4	GOL	j	301	-	5,5,5	0.96	0	5,5,5	1.11	0
4	GOL	m	301	-	5,5,5	0.90	0	5,5,5	1.09	0
5	SO4	s	302	-	4,4,4	0.26	0	6,6,6	0.11	0
4	GOL	T	301	-	5,5,5	0.90	0	5,5,5	1.13	1 (20%)
5	SO4	v	302	-	4,4,4	0.23	0	6,6,6	0.11	0
4	GOL	g	301	-	5,5,5	0.89	0	5,5,5	1.11	0
5	SO4	Q	302	-	4,4,4	0.22	0	6,6,6	0.11	0
4	GOL	F	301	-	5,5,5	0.97	0	5,5,5	1.05	0
4	GOL	d	301	-	5,5,5	0.93	0	5,5,5	1.09	0
4	GOL	p	301	-	5,5,5	0.92	0	5,5,5	1.05	0
4	GOL	W	301	-	5,5,5	0.95	0	5,5,5	1.05	0
5	SO4	T	302	-	4,4,4	0.22	0	6,6,6	0.11	0
4	GOL	N	301	-	5,5,5	1.01	0	5,5,5	1.03	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	SO4	m	302	-	4,4,4	0.26	0	6,6,6	0.09	0
4	GOL	s	301	-	5,5,5	0.91	0	5,5,5	1.12	0
4	GOL	Q	301	-	5,5,5	0.93	0	5,5,5	1.08	0
4	GOL	a	301	-	5,5,5	0.93	0	5,5,5	1.06	0
5	SO4	W	302	-	4,4,4	0.27	0	6,6,6	0.09	0
5	SO4	p	302	-	4,4,4	0.25	0	6,6,6	0.10	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	C	301	-	-	2/4/4/4	-
4	GOL	v	301	-	-	0/4/4/4	-
4	GOL	j	301	-	-	4/4/4/4	-
4	GOL	m	301	-	-	3/4/4/4	-
4	GOL	N	301	-	-	2/4/4/4	-
4	GOL	T	301	-	-	2/4/4/4	-
4	GOL	s	301	-	-	0/4/4/4	-
4	GOL	g	301	-	-	2/4/4/4	-
4	GOL	Q	301	-	-	2/4/4/4	-
4	GOL	X	301	-	-	4/4/4/4	-
4	GOL	a	301	-	-	4/4/4/4	-
4	GOL	F	301	-	-	3/4/4/4	-
4	GOL	d	301	-	-	2/4/4/4	-
4	GOL	I	301	-	-	2/4/4/4	-
4	GOL	p	301	-	-	0/4/4/4	-
4	GOL	W	301	-	-	2/4/4/4	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	T	301	GOL	C3-C2-C1	-2.00	104.45	111.80

There are no chirality outliers.

All (34) 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	a	301	GOL	C1-C2-C3-O3
4	d	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	O1-C1-C2-C3
4	X	301	GOL	C1-C2-C3-O3
4	a	301	GOL	O1-C1-C2-C3
4	g	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
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

There are no ring outliers.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	N	302	SO4	1	0
4	d	301	GOL	2	0
4	a	301	GOL	1	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ > 2	OWAB(Å ²)	Q < 0.9
1	C	228/228 (100%)	-0.81	1 (0%) 88 76	23, 37, 67, 85	1 (0%)
1	F	228/228 (100%)	-0.53	1 (0%) 88 76	32, 49, 74, 106	1 (0%)
1	I	228/228 (100%)	-0.74	1 (0%) 88 76	24, 44, 70, 113	1 (0%)
1	N	228/228 (100%)	-0.81	1 (0%) 88 76	21, 35, 64, 99	1 (0%)
1	Q	228/228 (100%)	-0.82	1 (0%) 88 76	26, 37, 66, 103	1 (0%)
1	T	228/228 (100%)	-0.58	2 (0%) 81 61	30, 44, 76, 123	1 (0%)
1	W	228/228 (100%)	-0.83	2 (0%) 81 61	19, 37, 67, 105	1 (0%)
1	X	228/228 (100%)	-0.50	3 (1%) 75 53	28, 49, 83, 107	1 (0%)
1	a	228/228 (100%)	-0.85	1 (0%) 88 76	24, 37, 64, 90	1 (0%)
1	d	228/228 (100%)	-0.73	1 (0%) 88 76	26, 41, 73, 86	1 (0%)
1	g	228/228 (100%)	-0.83	2 (0%) 81 61	23, 36, 67, 99	1 (0%)
1	j	228/228 (100%)	-0.89	0 100 100	22, 35, 61, 100	1 (0%)
1	m	228/228 (100%)	-0.51	2 (0%) 81 61	35, 51, 82, 104	1 (0%)
1	p	228/228 (100%)	-0.69	2 (0%) 81 61	29, 41, 71, 94	1 (0%)
1	s	228/228 (100%)	-0.65	2 (0%) 81 61	20, 46, 74, 105	1 (0%)
1	v	228/228 (100%)	-0.76	1 (0%) 88 76	27, 42, 70, 98	1 (0%)
2	A	213/214 (99%)	0.40	38 (17%) 4 2	25, 66, 179, 238	0
2	D	213/214 (99%)	-0.01	9 (4%) 40 22	18, 67, 139, 165	0
2	G	213/214 (99%)	-0.35	0 100 100	19, 63, 117, 151	0
2	J	213/214 (99%)	-0.03	4 (1%) 66 43	27, 74, 138, 157	0
2	L	213/214 (99%)	-0.15	1 (0%) 87 72	29, 65, 131, 152	0
2	O	213/214 (99%)	0.03	8 (3%) 44 24	28, 69, 149, 176	0
2	R	213/214 (99%)	-0.05	3 (1%) 73 51	30, 68, 138, 179	0
2	U	213/214 (99%)	-0.38	1 (0%) 87 72	27, 53, 115, 133	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
2	Y	213/214 (99%)	0.02	9 (4%) 40 22	23, 65, 147, 186	0
2	b	213/214 (99%)	-0.34	1 (0%) 87 72	25, 56, 122, 157	0
2	e	213/214 (99%)	-0.04	4 (1%) 66 43	26, 74, 151, 193	0
2	h	213/214 (99%)	0.16	20 (9%) 14 7	25, 68, 160, 189	0
2	k	213/214 (99%)	-0.08	1 (0%) 87 72	27, 62, 143, 162	0
2	n	213/214 (99%)	-0.39	0 100 100	24, 52, 111, 128	0
2	q	213/214 (99%)	0.18	5 (2%) 61 38	36, 82, 159, 171	0
2	t	213/214 (99%)	0.23	15 (7%) 22 11	26, 71, 173, 198	0
3	B	213/223 (95%)	0.43	41 (19%) 3 2	29, 57, 188, 227	0
3	E	213/223 (95%)	-0.02	7 (3%) 49 28	32, 67, 136, 160	0
3	H	213/223 (95%)	-0.18	5 (2%) 61 38	29, 63, 128, 155	0
3	K	213/223 (95%)	0.36	12 (5%) 30 15	33, 87, 157, 177	0
3	M	213/223 (95%)	-0.29	5 (2%) 61 38	29, 64, 123, 146	0
3	P	213/223 (95%)	0.50	16 (7%) 20 10	38, 95, 168, 195	0
3	S	213/223 (95%)	0.27	9 (4%) 40 22	40, 81, 140, 178	0
3	V	213/223 (95%)	-0.27	5 (2%) 61 38	33, 59, 116, 173	0
3	Z	213/223 (95%)	0.06	8 (3%) 44 24	28, 62, 147, 164	0
3	c	213/223 (95%)	-0.39	2 (0%) 81 61	24, 53, 114, 140	0
3	f	213/223 (95%)	0.39	9 (4%) 40 22	37, 92, 168, 192	0
3	i	213/223 (95%)	0.40	20 (9%) 14 7	34, 83, 183, 224	0
3	l	213/223 (95%)	-0.06	3 (1%) 73 51	38, 74, 117, 149	0
3	o	213/223 (95%)	-0.17	5 (2%) 61 38	29, 62, 114, 141	0
3	r	213/223 (95%)	0.22	8 (3%) 44 24	45, 94, 140, 165	0
3	u	213/223 (95%)	0.35	30 (14%) 6 3	36, 69, 183, 227	0
All	All	10464/10640 (98%)	-0.23	327 (3%) 51 30	18, 52, 144, 238	16 (0%)

All (327) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	B	127	ALA	5.3
3	B	140	LEU	4.9
3	B	161	LEU	4.8
2	t	114	SER	4.7
1	X	215	SER	4.7

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Mol	Chain	Res	Type	RSRZ
3	B	128	PRO	4.6
3	u	124	PHE	4.5
2	A	132	VAL	4.4
2	A	194	CYS	4.4
3	u	185	THR	4.4
1	W	215	SER	4.4
2	A	120	PRO	4.4
3	B	122	SER	4.3
2	Y	134	CYS	4.3
3	u	122	SER	4.2
1	T	215	SER	4.2
3	V	130	SER	4.1
1	N	215	SER	4.1
2	A	131	SER	4.0
2	A	193	ALA	4.0
3	u	128	PRO	3.9
3	B	129	SER	3.9
3	B	125	PRO	3.9
3	P	125	PRO	3.9
2	A	116	PHE	3.9
2	A	134	CYS	3.9
3	i	125	PRO	3.9
3	Z	130	SER	3.9
2	Y	155	GLN	3.8
2	A	180	THR	3.8
3	B	215	PRO	3.8
3	E	135	GLY	3.8
2	t	121	SER	3.7
3	l	130	SER	3.7
3	r	130	SER	3.7
2	A	205	VAL	3.7
3	B	123	VAL	3.7
1	T	216	GLY	3.7
2	Y	191	VAL	3.6
2	A	186	TYR	3.6
3	B	187	PRO	3.6
3	P	127	ALA	3.6
3	u	182	SER	3.6
3	K	135	GLY	3.6
3	u	196	TYR	3.5
2	Y	199	GLN	3.5
2	R	208	SER	3.5

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Mol	Chain	Res	Type	RSRZ
2	t	134	CYS	3.5
2	e	177	SER	3.5
2	A	133	VAL	3.4
3	B	139	ALA	3.4
2	A	121	SER	3.4
2	D	122	ASP	3.4
2	Y	154	LEU	3.4
2	D	199	GLN	3.4
3	B	124	PHE	3.3
2	A	154	LEU	3.3
3	Z	140	LEU	3.3
3	u	130	SER	3.3
3	V	135	GLY	3.3
3	B	207	THR	3.3
3	i	127	ALA	3.3
1	X	216	GLY	3.3
3	B	186	VAL	3.2
3	c	130	SER	3.2
2	h	133	VAL	3.2
2	A	129	THR	3.2
3	B	143	LEU	3.2
2	h	119	PRO	3.2
2	L	197	THR	3.2
3	r	135	GLY	3.2
2	t	115	VAL	3.2
3	i	128	PRO	3.2
3	H	212	LYS	3.1
1	W	216	GLY	3.1
3	S	191	LEU	3.1
3	B	196	TYR	3.1
3	P	209	VAL	3.1
3	S	130	SER	3.1
3	l	135	GLY	3.1
1	I	215	SER	3.1
2	t	120	PRO	3.1
1	d	215	SER	3.1
3	S	189	SER	3.1
2	A	182	SER	3.0
3	K	187	PRO	3.0
3	u	140	LEU	3.0
3	K	127	ALA	3.0
3	u	216	LYS	3.0

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Mol	Chain	Res	Type	RSRZ
2	A	209	PHE	3.0
3	B	142	CYS	3.0
3	B	153	THR	3.0
3	E	127	ALA	2.9
3	E	130	SER	2.9
3	B	185	THR	2.9
2	J	125	LEU	2.9
2	A	197	THR	2.9
3	u	123	VAL	2.9
2	h	116	PHE	2.9
3	u	143	LEU	2.9
2	h	120	PRO	2.8
2	A	146	VAL	2.8
3	B	154	VAL	2.8
3	S	127	ALA	2.8
3	B	135	GLY	2.8
3	B	204	PRO	2.8
2	A	118	PHE	2.8
2	A	188	LYS	2.8
3	f	114	SER	2.8
1	m	60	GLU	2.8
3	H	214	GLU	2.8
3	f	140	LEU	2.8
3	i	185	THR	2.8
1	C	215	SER	2.8
3	B	174	SER	2.8
3	S	217	SER	2.8
3	f	130	SER	2.8
3	B	214	GLU	2.8
2	h	117	ILE	2.8
3	P	124	PHE	2.7
2	b	119	PRO	2.7
3	B	121	PRO	2.7
2	A	157	GLY	2.7
3	B	212	LYS	2.7
3	i	138	ALA	2.7
3	i	215	PRO	2.7
1	p	215	SER	2.7
3	B	182	SER	2.7
3	u	192	GLY	2.7
3	c	135	GLY	2.7
2	h	131	SER	2.7

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Mol	Chain	Res	Type	RSRZ
3	B	191	LEU	2.7
3	Z	135	GLY	2.7
3	B	126	LEU	2.7
3	f	161	LEU	2.7
2	t	119	PRO	2.6
3	B	216	LYS	2.6
1	g	215	SER	2.6
2	Y	177	SER	2.6
2	q	154	LEU	2.6
2	t	193	ALA	2.6
3	B	209	VAL	2.6
3	K	125	PRO	2.6
1	s	216	GLY	2.6
2	A	181	LEU	2.6
3	i	186	VAL	2.6
1	v	215	SER	2.6
3	u	209	VAL	2.6
3	B	188	SER	2.6
3	o	130	SER	2.6
3	B	200	VAL	2.6
2	A	207	LYS	2.6
3	P	13	LYS	2.6
2	A	158	ASN	2.6
3	E	161	LEU	2.6
2	h	193	ALA	2.6
1	F	215	SER	2.5
3	S	135	GLY	2.5
2	h	180	THR	2.5
3	K	197	ILE	2.5
2	D	154	LEU	2.5
2	J	154	LEU	2.5
3	K	130	SER	2.5
3	o	217	SER	2.5
3	u	190	SER	2.5
2	A	198	HIS	2.5
3	P	121	PRO	2.5
2	A	208	SER	2.5
3	B	130	SER	2.5
3	Z	181	SER	2.5
2	A	191	VAL	2.5
3	i	124	PHE	2.5
3	i	187	PRO	2.5

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Mol	Chain	Res	Type	RSRZ
2	A	147	GLN	2.5
3	r	217	SER	2.5
2	h	118	PHE	2.5
2	t	180	THR	2.5
3	S	216	LYS	2.5
3	l	216	LYS	2.5
3	u	187	PRO	2.5
3	P	213	VAL	2.5
3	u	217	SER	2.4
2	A	119	PRO	2.4
2	q	120	PRO	2.4
3	P	128	PRO	2.4
2	A	192	TYR	2.4
2	h	208	SER	2.4
3	M	217	SER	2.4
3	K	217	SER	2.4
3	i	130	SER	2.4
3	B	152	VAL	2.4
3	M	127	ALA	2.4
2	h	154	LEU	2.4
3	u	125	PRO	2.4
3	f	135	GLY	2.4
3	i	197	ILE	2.4
2	A	155	GLN	2.4
3	H	216	LYS	2.4
3	S	129	SER	2.4
2	t	205	VAL	2.4
3	u	215	PRO	2.4
2	A	117	ILE	2.4
3	u	127	ALA	2.4
3	i	140	LEU	2.4
3	u	191	LEU	2.4
2	A	156	SER	2.4
1	p	216	GLY	2.3
2	R	180	THR	2.3
3	V	191	LEU	2.3
3	B	184	VAL	2.3
3	E	209	VAL	2.3
2	h	135	LEU	2.3
2	O	160	GLN	2.3
2	h	205	VAL	2.3
3	H	135	GLY	2.3

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Mol	Chain	Res	Type	RSRZ
3	P	179	SER	2.3
3	Z	129	SER	2.3
3	o	116	ALA	2.3
3	r	127	ALA	2.3
1	X	146	HIS	2.3
2	h	186	TYR	2.3
3	Z	161	LEU	2.3
3	K	215	PRO	2.3
1	g	216	GLY	2.3
2	A	127	SER	2.3
2	e	125	LEU	2.3
2	O	132	VAL	2.3
2	h	132	VAL	2.3
3	o	120	GLY	2.3
2	q	181	LEU	2.3
2	A	189	HIS	2.3
1	Q	215	SER	2.3
3	H	217	SER	2.3
2	e	128	GLY	2.2
3	o	135	GLY	2.2
2	D	178	THR	2.2
2	R	3	GLN	2.2
2	A	204	PRO	2.2
3	i	204	PRO	2.2
2	h	181	LEU	2.2
3	E	140	LEU	2.2
3	i	118	THR	2.2
1	s	215	SER	2.2
2	t	208	SER	2.2
3	K	115	SER	2.2
3	P	114	SER	2.2
3	B	197	ILE	2.2
3	P	204	PRO	2.2
3	r	187	PRO	2.2
3	u	183	VAL	2.2
3	M	129	SER	2.2
3	i	181	SER	2.2
3	r	181	SER	2.2
2	J	120	PRO	2.2
2	O	184	ALA	2.2
3	B	159	GLY	2.2
3	P	215	PRO	2.2

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Mol	Chain	Res	Type	RSRZ
3	r	192	GLY	2.2
3	u	138	ALA	2.2
3	u	142	CYS	2.2
3	P	63	LYS	2.2
3	P	216	LYS	2.2
2	O	191	VAL	2.2
2	Y	147	GLN	2.2
3	i	217	SER	2.2
3	u	158	SER	2.2
3	u	197	ILE	2.2
3	u	126	LEU	2.2
3	f	62	GLU	2.2
3	M	135	GLY	2.2
2	t	194	CYS	2.2
2	J	100	GLN	2.1
1	a	215	SER	2.1
3	M	130	SER	2.1
3	B	160	ALA	2.1
2	t	181	LEU	2.1
3	V	216	LYS	2.1
3	i	216	LYS	2.1
2	A	184	ALA	2.1
3	B	181	SER	2.1
3	P	190	SER	2.1
2	O	134	CYS	2.1
2	h	129	THR	2.1
2	q	180	THR	2.1
3	f	191	LEU	2.1
3	i	13	LYS	2.1
3	i	191	LEU	2.1
2	D	147	GLN	2.1
2	D	193	ALA	2.1
3	r	125	PRO	2.1
2	D	121	SER	2.1
2	t	196	VAL	2.1
2	Y	145	LYS	2.1
2	O	125	LEU	2.1
3	i	161	LEU	2.1
3	K	185	THR	2.1
3	V	194	GLN	2.1
3	K	136	GLY	2.1
3	u	200	VAL	2.1

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Mol	Chain	Res	Type	RSRZ
3	K	143	LEU	2.1
2	q	140	TYR	2.1
3	Z	196	TYR	2.1
3	f	142	CYS	2.1
2	A	183	LYS	2.0
2	D	145	LYS	2.0
3	u	152	VAL	2.0
1	m	215	SER	2.0
2	U	208	SER	2.0
3	B	163	SER	2.0
3	P	126	LEU	2.0
2	O	180	THR	2.0
2	Y	112	ALA	2.0
2	e	129	THR	2.0
2	k	193	ALA	2.0
2	t	206	THR	2.0
2	h	207	LYS	2.0
2	h	213	GLU	2.0
2	D	132	VAL	2.0
3	S	213	VAL	2.0
3	Z	144	VAL	2.0
2	O	154	LEU	2.0
3	u	161	LEU	2.0
2	t	131	SER	2.0
2	h	184	ALA	2.0
3	f	204	PRO	2.0
3	E	183	VAL	2.0
3	u	213	VAL	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum,

median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	SO4	T	302	5/5	0.65	0.18	100,109,119,126	0
5	SO4	Q	302	5/5	0.68	0.15	95,101,112,119	0
5	SO4	m	302	5/5	0.68	0.13	104,108,115,117	0
5	SO4	X	302	5/5	0.70	0.19	101,119,123,127	0
5	SO4	s	302	5/5	0.71	0.17	84,106,112,120	0
5	SO4	v	302	5/5	0.73	0.13	80,101,107,112	0
5	SO4	j	302	5/5	0.74	0.18	91,114,118,122	0
5	SO4	W	302	5/5	0.75	0.17	96,102,115,117	0
5	SO4	g	302	5/5	0.76	0.15	104,105,120,121	0
4	GOL	m	301	6/6	0.77	0.26	78,86,97,102	0
5	SO4	p	302	5/5	0.80	0.12	100,107,115,122	0
4	GOL	C	301	6/6	0.81	0.21	40,59,62,64	0
5	SO4	C	302	5/5	0.82	0.14	75,80,94,104	0
4	GOL	v	301	6/6	0.82	0.22	56,66,70,72	0
4	GOL	I	301	6/6	0.84	0.22	57,81,88,97	0
4	GOL	j	301	6/6	0.86	0.23	57,87,91,104	0
4	GOL	F	301	6/6	0.86	0.17	46,73,76,78	0
4	GOL	W	301	6/6	0.87	0.23	28,55,64,64	0
4	GOL	X	301	6/6	0.88	0.20	51,67,92,94	0
4	GOL	g	301	6/6	0.88	0.19	47,67,76,77	0
4	GOL	s	301	6/6	0.88	0.21	46,65,80,80	0
5	SO4	N	302	5/5	0.89	0.09	74,99,101,104	0
4	GOL	T	301	6/6	0.89	0.23	65,68,75,79	0
4	GOL	d	301	6/6	0.90	0.16	39,59,63,66	0
4	GOL	p	301	6/6	0.90	0.17	56,67,85,88	0
4	GOL	Q	301	6/6	0.91	0.13	38,66,82,83	0
4	GOL	N	301	6/6	0.91	0.14	35,53,71,73	0
4	GOL	a	301	6/6	0.93	0.14	35,63,69,72	0

6.5 Other polymers ⓘ

There are no such residues in this entry.