



Full wwPDB X-ray Structure Validation Report ⓘ

May 22, 2020 – 04:39 pm BST

PDB ID : 4Z5R
Title : Rontalizumab Fab bound to Interferon- α 2
Authors : Eigenbrot, C.; Maurer, B.; Bosanac, I.
Deposited on : 2015-04-02
Resolution : 3.00 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 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 : 2.11
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

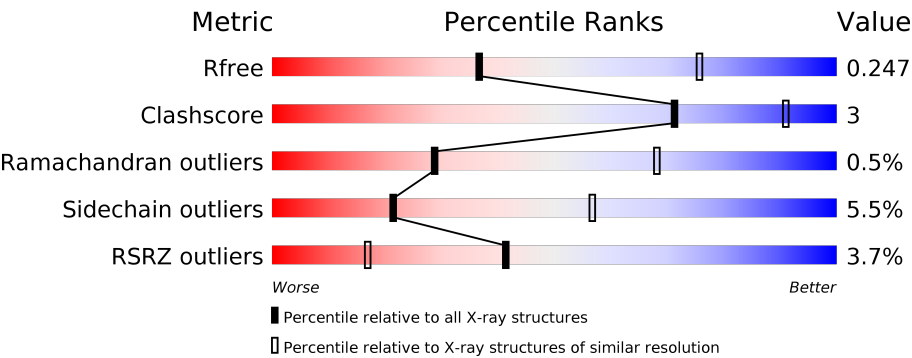
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (3.00-3.00)

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 on 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	D	165	<div><div>2%</div><div></div><div>69%</div><div>13%</div><div>•</div><div>15%</div></div>
1	E	165	<div><div>%</div><div></div><div>70%</div><div>12%</div><div>•</div><div>15%</div></div>
1	F	165	<div><div>2%</div><div></div><div>64%</div><div>16%</div><div>5%</div><div>15%</div></div>
1	G	165	<div><div>%</div><div></div><div>68%</div><div>13%</div><div>•</div><div>17%</div></div>
1	H	165	<div><div>2%</div><div></div><div>73%</div><div>9%</div><div>•</div><div>16%</div></div>
1	I	165	<div><div>2%</div><div></div><div>67%</div><div>13%</div><div>•</div><div>17%</div></div>

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Mol	Chain	Length	Quality of chain
1	N	165	
1	X	165	
2	A	218	
2	J	218	
2	L	218	
2	P	218	
2	R	218	
2	T	218	
2	V	218	
2	Y	218	
3	B	225	
3	K	225	
3	M	225	
3	Q	225	
3	S	225	
3	U	225	
3	W	225	
3	Z	225	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 34056 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 Interferon alpha-2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	D	141	Total	C	N	O	S	0	0	0
			1165	748	195	214	8			
1	E	141	Total	C	N	O	S	0	0	0
			1165	748	195	214	8			
1	F	140	Total	C	N	O	S	0	0	0
			1156	745	192	211	8			
1	G	137	Total	C	N	O	S	0	0	0
			1121	719	187	208	7			
1	H	139	Total	C	N	O	S	0	0	0
			1145	734	192	211	8			
1	I	137	Total	C	N	O	S	0	0	0
			1127	723	188	208	8			
1	X	137	Total	C	N	O	S	0	0	0
			1133	728	189	208	8			
1	N	145	Total	C	N	O	S	0	0	0
			1198	768	200	222	8			

- Molecule 2 is a protein called anti-IFN-a antibody rontalizumab light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	J	217	Total	C	N	O	S	0	0	0
			1669	1041	282	340	6			
2	L	217	Total	C	N	O	S	0	0	0
			1669	1041	282	340	6			
2	V	217	Total	C	N	O	S	0	0	0
			1669	1041	282	340	6			
2	P	217	Total	C	N	O	S	0	0	0
			1669	1041	282	340	6			
2	R	217	Total	C	N	O	S	0	0	0
			1669	1041	282	340	6			
2	T	217	Total	C	N	O	S	0	0	0
			1669	1041	282	340	6			

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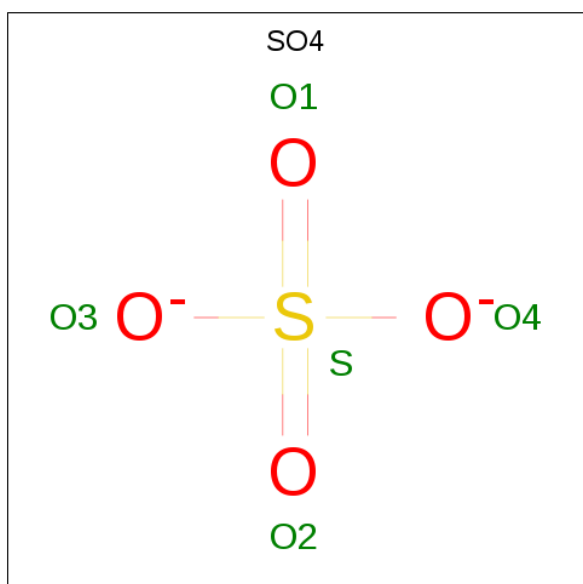
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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	Y	110	Total	C	N	O	S	0	0	0
			840	525	141	170	4			
2	A	217	Total	C	N	O	S	0	0	0
			1669	1041	282	340	6			

- Molecule 3 is a protein called anti-IFN-a antibody rontalizumab heavy chain modules VH and CH1 (Fab).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	K	213	Total	C	N	O	S	0	0	0
			1622	1033	268	316	5			
3	M	213	Total	C	N	O	S	0	0	0
			1622	1033	268	316	5			
3	W	213	Total	C	N	O	S	0	0	0
			1622	1033	268	316	5			
3	Q	213	Total	C	N	O	S	0	0	0
			1622	1033	268	316	5			
3	S	213	Total	C	N	O	S	0	0	0
			1622	1033	268	316	5			
3	U	213	Total	C	N	O	S	0	0	0
			1622	1033	268	316	5			
3	Z	117	Total	C	N	O	S	0	0	0
			929	593	155	178	3			
3	B	213	Total	C	N	O	S	0	0	0
			1622	1033	268	316	5			

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



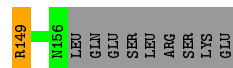
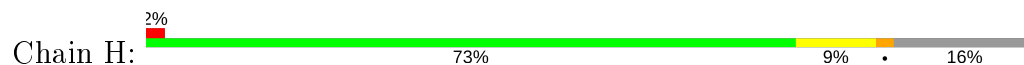
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	J	1	Total	O	S	0	0
			5	4	1		
4	J	1	Total	O	S	0	0
			5	4	1		
4	L	1	Total	O	S	0	0
			5	4	1		
4	F	1	Total	O	S	0	0
			5	4	1		
4	V	1	Total	O	S	0	0
			5	4	1		
4	V	1	Total	O	S	0	0
			5	4	1		
4	G	1	Total	O	S	0	0
			5	4	1		
4	P	1	Total	O	S	0	0
			5	4	1		

- Molecule 1: Interferon alpha-2

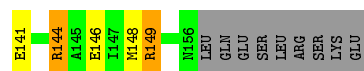




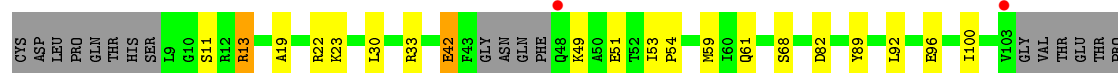
- Molecule 1: Interferon alpha-2



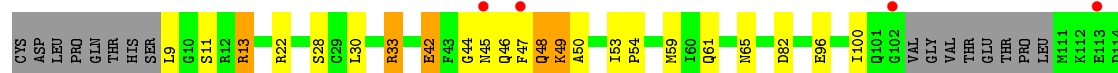
- Molecule 1: Interferon alpha-2



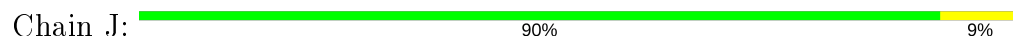
- Molecule 1: Interferon alpha-2



- Molecule 1: Interferon alpha-2



- Molecule 2: anti-IFN-a antibody rontalizumab light chain





- Molecule 2: anti-IFN-a antibody rontalizumab light chain

Chain L: 88% 11%



- Molecule 2: anti-IFN-a antibody rontalizumab light chain

Chain V: 89% 11%



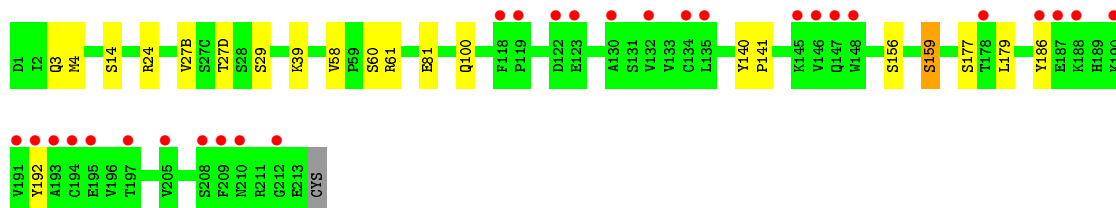
- Molecule 2: anti-IFN-a antibody rontalizumab light chain

Chain P: 89% 9%



- Molecule 2: anti-IFN-a antibody rontalizumab light chain

Chain R: 13% 90% 9%



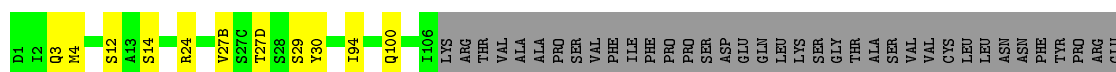
- Molecule 2: anti-IFN-a antibody rontalizumab light chain

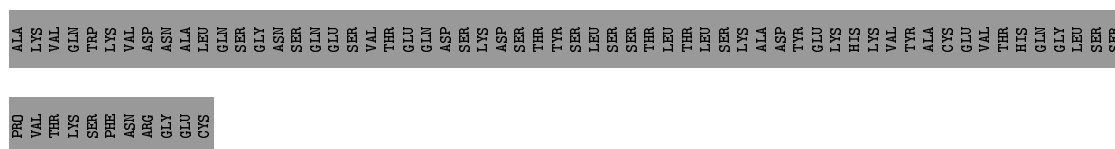
Chain T: 87% 11%



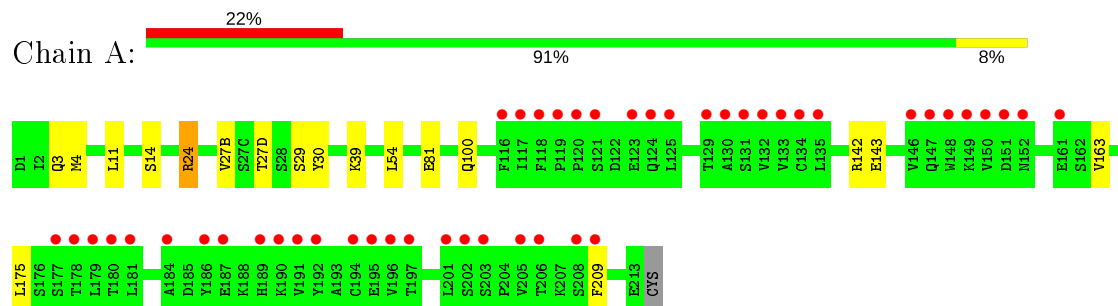
- Molecule 2: anti-IFN-a antibody rontalizumab light chain

Chain Y: 45% 5% 50%

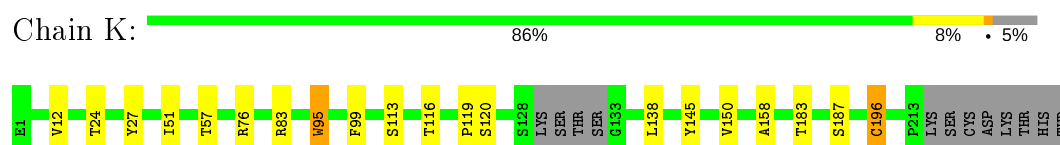




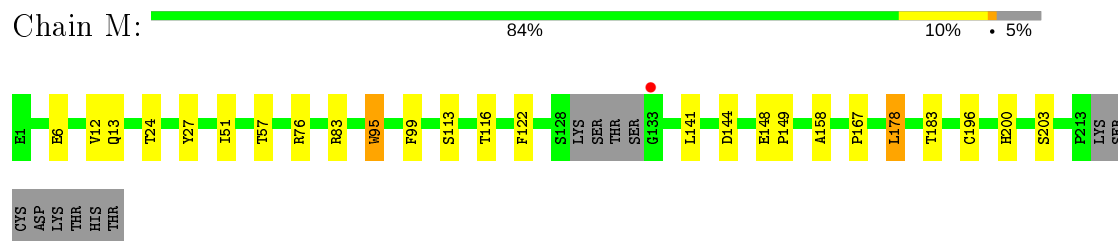
- Molecule 2: anti-IFN- α antibody rontalizumab light chain



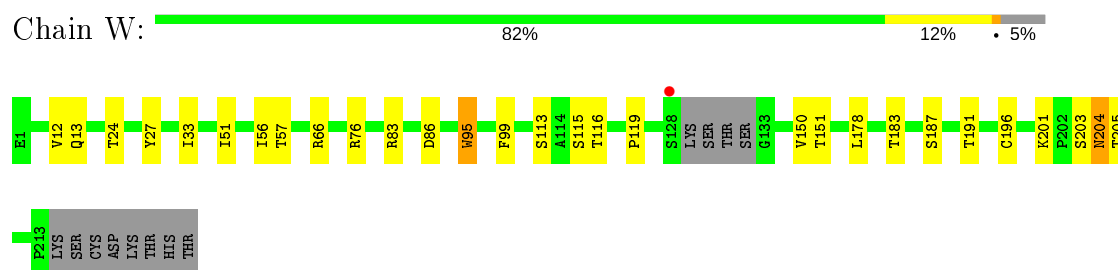
- Molecule 3: anti-IFN- α antibody rontalizumab heavy chain modules VH and CH1 (Fab)



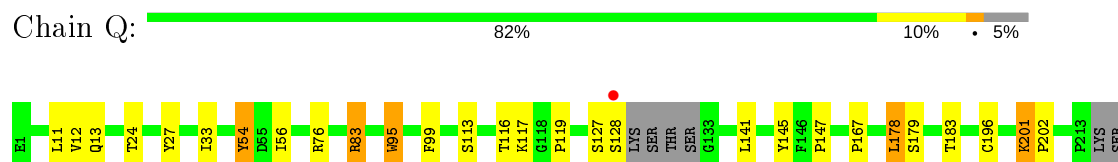
- Molecule 3: anti-IFN- α antibody rontalizumab heavy chain modules VH and CH1 (Fab)



- Molecule 3: anti-IFN- α antibody rontalizumab heavy chain modules VH and CH1 (Fab)



- Molecule 3: anti-IFN- α antibody rontalizumab heavy chain modules VH and CH1 (Fab)



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	90.83 Å 331.86 Å 98.14 Å 90.00° 111.28° 90.00°	Depositor
Resolution (Å)	48.21 – 3.00 48.21 – 3.00	Depositor EDS
% Data completeness (in resolution range)	94.8 (48.21-3.00) 94.9 (48.21-3.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.10	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.70 (at 3.01 Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, R_{free}	0.223 , 0.251 0.215 , 0.247	Depositor DCC
R_{free} test set	2285 reflections (2.24%)	wwPDB-VP
Wilson B-factor (Å ²)	65.6	Xtriage
Anisotropy	0.726	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 36.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	34056	wwPDB-VP
Average B, all atoms (Å ²)	75.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 14.73% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 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

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	D	0.48	0/1187	0.85	5/1594 (0.3%)
1	E	0.46	0/1187	0.87	5/1594 (0.3%)
1	F	0.47	0/1177	0.86	6/1579 (0.4%)
1	G	0.52	0/1141	0.90	5/1534 (0.3%)
1	H	0.43	0/1165	0.85	4/1563 (0.3%)
1	I	0.54	1/1147 (0.1%)	0.85	5/1540 (0.3%)
1	N	0.44	0/1220	0.88	7/1638 (0.4%)
1	X	0.42	0/1153	0.83	4/1547 (0.3%)
2	A	0.40	0/1707	0.65	1/2317 (0.0%)
2	J	0.54	0/1707	0.77	1/2317 (0.0%)
2	L	0.58	0/1707	0.80	1/2317 (0.0%)
2	P	0.55	0/1707	0.77	1/2317 (0.0%)
2	R	0.43	0/1707	0.68	1/2317 (0.0%)
2	T	0.49	1/1707 (0.1%)	0.70	1/2317 (0.0%)
2	V	0.54	0/1707	0.76	1/2317 (0.0%)
2	Y	0.45	0/861	0.76	1/1169 (0.1%)
3	B	0.42	0/1664	0.78	6/2270 (0.3%)
3	K	0.57	0/1664	0.82	3/2270 (0.1%)
3	M	0.62	1/1664 (0.1%)	0.84	3/2270 (0.1%)
3	Q	0.62	1/1664 (0.1%)	0.82	3/2270 (0.1%)
3	S	0.44	0/1664	0.74	3/2270 (0.1%)
3	U	0.46	0/1664	0.79	5/2270 (0.2%)
3	W	0.57	1/1664 (0.1%)	0.80	4/2270 (0.2%)
3	Z	0.47	0/953	0.81	5/1295 (0.4%)
All	All	0.51	5/34788 (0.0%)	0.79	81/47162 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	D	0	1
1	E	0	1
1	F	0	1
1	G	0	1
1	H	0	1
1	I	0	1
1	N	0	3
1	X	0	1
3	Q	0	1
3	Z	0	1
All	All	0	12

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	I	45	ASN	C-O	9.76	1.41	1.23
3	W	13	GLN	CD-OE1	-9.44	1.03	1.24
3	Q	13	GLN	CD-OE1	-8.69	1.04	1.24
3	M	13	GLN	CD-OE1	-7.85	1.06	1.24
2	T	27(B)	VAL	CB-CG1	-6.99	1.38	1.52

All (81) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	13	ARG	NE-CZ-NH2	-15.87	112.37	120.30
1	D	13	ARG	NE-CZ-NH2	-15.57	112.51	120.30
1	E	13	ARG	NE-CZ-NH2	-15.57	112.52	120.30
1	I	13	ARG	NE-CZ-NH2	-15.50	112.55	120.30
1	N	13	ARG	NE-CZ-NH2	-15.49	112.56	120.30
1	F	13	ARG	NE-CZ-NH2	-15.39	112.61	120.30
1	X	13	ARG	NE-CZ-NH2	-15.29	112.65	120.30
1	H	13	ARG	NE-CZ-NH2	-14.99	112.80	120.30
3	B	83	ARG	NE-CZ-NH2	-14.51	113.04	120.30
3	M	83	ARG	NE-CZ-NH2	-14.42	113.09	120.30
3	K	83	ARG	NE-CZ-NH2	-14.40	113.10	120.30
3	U	83	ARG	NE-CZ-NH2	-14.23	113.18	120.30
3	W	83	ARG	NE-CZ-NH2	-14.13	113.23	120.30
3	S	83	ARG	NE-CZ-NH2	-14.07	113.26	120.30
3	Q	83	ARG	NE-CZ-NH2	-13.87	113.37	120.30
3	B	83	ARG	NE-CZ-NH1	13.78	127.19	120.30
1	E	13	ARG	NE-CZ-NH1	13.54	127.07	120.30
1	G	13	ARG	NE-CZ-NH1	13.43	127.02	120.30
3	M	83	ARG	NE-CZ-NH1	13.37	126.98	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	K	83	ARG	NE-CZ-NH1	13.32	126.96	120.30
1	N	13	ARG	NE-CZ-NH1	13.31	126.96	120.30
3	U	83	ARG	NE-CZ-NH1	13.28	126.94	120.30
3	Q	83	ARG	NE-CZ-NH1	13.20	126.90	120.30
3	W	83	ARG	NE-CZ-NH1	13.14	126.87	120.30
3	S	83	ARG	NE-CZ-NH1	13.11	126.85	120.30
1	D	13	ARG	NE-CZ-NH1	12.98	126.79	120.30
1	I	13	ARG	NE-CZ-NH1	12.91	126.75	120.30
1	H	13	ARG	NE-CZ-NH1	12.88	126.74	120.30
1	F	13	ARG	NE-CZ-NH1	12.66	126.63	120.30
1	X	13	ARG	NE-CZ-NH1	12.38	126.49	120.30
3	Z	13	GLN	CA-CB-CG	9.90	135.19	113.40
3	B	13	GLN	CA-CB-CG	9.74	134.83	113.40
3	U	13	GLN	CA-CB-CG	9.50	134.29	113.40
1	E	13	ARG	CG-CD-NE	-9.19	92.49	111.80
1	I	13	ARG	CG-CD-NE	-9.18	92.53	111.80
2	Y	27(B)	VAL	CG1-CB-CG2	-9.13	96.28	110.90
3	Z	83	ARG	CD-NE-CZ	9.11	136.36	123.60
1	D	13	ARG	CG-CD-NE	-9.10	92.69	111.80
1	G	13	ARG	CG-CD-NE	-9.08	92.72	111.80
1	N	13	ARG	CG-CD-NE	-9.02	92.86	111.80
1	F	13	ARG	CG-CD-NE	-8.96	92.98	111.80
2	J	27(B)	VAL	CG1-CB-CG2	-8.95	96.58	110.90
1	X	13	ARG	CG-CD-NE	-8.95	93.01	111.80
2	R	27(B)	VAL	CG1-CB-CG2	-8.86	96.72	110.90
1	H	13	ARG	CG-CD-NE	-8.86	93.20	111.80
2	L	27(B)	VAL	CG1-CB-CG2	-8.83	96.77	110.90
2	V	27(B)	VAL	CG1-CB-CG2	-8.80	96.82	110.90
2	P	27(B)	VAL	CG1-CB-CG2	-8.74	96.92	110.90
2	A	27(B)	VAL	CG1-CB-CG2	-8.65	97.06	110.90
3	Z	83	ARG	NE-CZ-NH2	-8.60	116.00	120.30
2	T	27(B)	VAL	CG1-CB-CG2	-7.87	98.31	110.90
1	N	13	ARG	CD-NE-CZ	7.01	133.42	123.60
1	H	13	ARG	CD-NE-CZ	6.93	133.31	123.60
1	F	13	ARG	CD-NE-CZ	6.91	133.27	123.60
1	G	13	ARG	CD-NE-CZ	6.82	133.15	123.60
1	X	13	ARG	CD-NE-CZ	6.69	132.97	123.60
3	U	13	GLN	CB-CG-CD	6.68	128.97	111.60
1	I	13	ARG	CD-NE-CZ	6.62	132.86	123.60
1	D	13	ARG	CD-NE-CZ	6.60	132.84	123.60
1	E	13	ARG	CD-NE-CZ	6.54	132.76	123.60
3	Z	83	ARG	NE-CZ-NH1	-6.31	117.15	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	13	GLN	CB-CG-CD	6.27	127.90	111.60
3	Z	13	GLN	CB-CG-CD	6.18	127.66	111.60
1	N	45	ASN	N-CA-C	5.98	127.14	111.00
1	G	33	ARG	NE-CZ-NH1	5.85	123.23	120.30
1	N	33	ARG	NE-CZ-NH1	5.77	123.19	120.30
3	B	83	ARG	CD-NE-CZ	5.75	131.64	123.60
3	Q	83	ARG	CD-NE-CZ	5.74	131.64	123.60
3	S	83	ARG	CD-NE-CZ	5.73	131.62	123.60
3	W	83	ARG	CD-NE-CZ	5.69	131.56	123.60
1	N	33	ARG	NE-CZ-NH2	-5.67	117.46	120.30
3	U	83	ARG	CD-NE-CZ	5.66	131.53	123.60
3	K	83	ARG	CD-NE-CZ	5.60	131.44	123.60
3	M	83	ARG	CD-NE-CZ	5.49	131.29	123.60
1	I	33	ARG	NE-CZ-NH1	5.49	123.04	120.30
3	B	13	GLN	CG-CD-NE2	-5.45	103.61	116.70
3	W	13	GLN	CG-CD-OE1	5.41	132.43	121.60
1	F	33	ARG	NE-CZ-NH2	-5.35	117.63	120.30
1	E	33	ARG	NE-CZ-NH1	5.16	122.88	120.30
1	D	33	ARG	NE-CZ-NH1	5.15	122.87	120.30
1	F	33	ARG	NE-CZ-NH1	5.12	122.86	120.30

There are no chirality outliers.

All (12) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	13	ARG	Sidechain
1	E	13	ARG	Sidechain
1	F	13	ARG	Sidechain
1	G	13	ARG	Sidechain
1	H	13	ARG	Sidechain
1	I	13	ARG	Sidechain
1	N	13	ARG	Sidechain
1	N	44	GLY	Peptide
1	N	49	LYS	Peptide
3	Q	83	ARG	Sidechain
1	X	13	ARG	Sidechain
3	Z	83	ARG	Sidechain

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	1165	0	1163	11	1
1	E	1165	0	1163	8	0
1	F	1156	0	1159	24	0
1	G	1121	0	1114	10	2
1	H	1145	0	1145	10	0
1	I	1127	0	1124	9	2
1	N	1198	0	1195	18	1
1	X	1133	0	1136	24	1
2	A	1669	0	1611	10	0
2	J	1669	0	1611	5	1
2	L	1669	0	1611	8	0
2	P	1669	0	1611	9	0
2	R	1669	0	1611	12	0
2	T	1669	0	1611	16	0
2	V	1669	0	1611	11	0
2	Y	840	0	804	8	0
3	B	1622	0	1578	6	1
3	K	1622	0	1578	9	0
3	M	1622	0	1578	10	0
3	Q	1622	0	1578	13	0
3	S	1622	0	1578	13	1
3	U	1622	0	1578	18	0
3	W	1622	0	1578	11	0
3	Z	929	0	888	17	0
4	F	5	0	0	0	0
4	G	5	0	0	0	0
4	J	10	0	0	0	0
4	L	5	0	0	0	0
4	P	5	0	0	0	0
4	V	10	0	0	1	0
All	All	34056	0	33214	235	5

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:V:39:LYS:NZ	4:V:302:SO4:O3	2.03	0.92
1:G:125:ARG:CZ	3:Q:56:ILE:HD11	2.08	0.83
3:B:27:TYR:O	3:B:76:ARG:NH1	2.12	0.82
2:Y:27(D):THR:HG22	2:Y:29:SER:H	1.44	0.82
3:Q:27:TYR:O	3:Q:76:ARG:NH1	2.12	0.82
3:K:27:TYR:O	3:K:76:ARG:NH1	2.14	0.80
3:Z:27:TYR:O	3:Z:76:ARG:NH1	2.15	0.80
3:M:27:TYR:O	3:M:76:ARG:NH1	2.14	0.80
2:A:27(D):THR:HG22	2:A:29:SER:H	1.46	0.79
2:J:27(D):THR:HG22	2:J:29:SER:H	1.48	0.79
3:S:27:TYR:O	3:S:76:ARG:NH1	2.16	0.79
2:P:27(D):THR:HG22	2:P:29:SER:H	1.48	0.78
3:W:27:TYR:O	3:W:76:ARG:NH1	2.16	0.78
3:U:27:TYR:O	3:U:76:ARG:NH1	2.16	0.78
2:T:27(D):THR:HG22	2:T:29:SER:H	1.47	0.77
3:M:158:ALA:HA	1:G:31:LYS:HE3	1.67	0.77
2:R:27(D):THR:HG22	2:R:29:SER:H	1.48	0.76
2:L:27(D):THR:HG22	2:L:29:SER:H	1.51	0.76
2:V:27(D):THR:HG22	2:V:29:SER:H	1.50	0.75
3:K:158:ALA:HA	1:F:31:LYS:HE3	1.70	0.72
2:R:60:SER:OG	3:U:68:THR:OG1	1.83	0.72
1:X:148:MET:HG2	2:Y:27(D):THR:HG21	1.71	0.71
2:R:58:VAL:O	3:U:82(A):ASN:ND2	2.26	0.68
2:V:167:ASP:HB3	2:V:170:ASP:OD1	1.97	0.65
1:X:148:MET:HG2	2:Y:27(D):THR:CG2	2.27	0.65
1:D:23:LYS:O	3:W:187:SER:OG	2.14	0.64
1:E:45:ASN:OD1	1:E:46:GLN:N	2.30	0.64
1:G:141:GLU:OE1	1:G:144:ARG:NH2	2.31	0.63
1:F:125:ARG:CZ	3:W:56:ILE:HD11	2.29	0.63
1:F:68:SER:HB2	1:X:89:TYR:OH	1.98	0.63
3:Z:13:GLN:NE2	1:N:28:SER:O	2.31	0.63
2:J:149:LYS:HA	2:J:153:ALA:O	1.99	0.62
2:R:186:TYR:O	2:R:192:TYR:OH	2.16	0.62
2:T:186:TYR:O	2:T:192:TYR:OH	2.18	0.60
1:D:49:LYS:O	1:D:50:ALA:HB3	2.02	0.60
1:E:141:GLU:OE1	1:E:144:ARG:NH2	2.35	0.60
1:F:89:TYR:OH	1:X:68:SER:HB2	2.02	0.59
1:N:141:GLU:OE1	1:N:144:ARG:NH2	2.36	0.59
1:E:45:ASN:O	1:E:47:PHE:N	2.36	0.58
1:G:125:ARG:HD2	3:Q:54:TYR:CE2	2.38	0.58
3:Z:13:GLN:HE22	1:N:28:SER:C	2.08	0.58
1:X:141:GLU:OE1	1:X:144:ARG:NH2	2.37	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Z:82(A):ASN:OD1	2:A:54:LEU:HD23	2.04	0.57
2:V:209:PHE:HB2	2:V:213:GLU:OE1	2.04	0.57
1:I:148:MET:HG2	2:T:27(D):THR:HG21	1.85	0.57
1:I:141:GLU:OE1	1:I:144:ARG:NH2	2.37	0.57
1:H:125:ARG:CZ	3:S:56:ILE:HD11	2.34	0.57
2:R:60:SER:HG	3:U:68:THR:HG1	0.97	0.56
3:Z:13:GLN:NE2	1:N:28:SER:C	2.59	0.56
3:Z:13:GLN:NE2	1:N:28:SER:HA	2.20	0.56
3:Z:13:GLN:CD	1:N:28:SER:HA	2.26	0.56
1:H:125:ARG:HD2	3:S:54:TYR:CE2	2.40	0.55
1:F:141:GLU:OE1	1:F:144:ARG:NH2	2.39	0.55
2:T:176:SER:O	2:T:176:SER:OG	2.25	0.55
3:K:187:SER:OG	1:F:23:LYS:O	2.17	0.55
1:F:120:ARG:HB3	1:X:100:ILE:HD11	1.88	0.55
2:J:142:ARG:HD2	2:J:163:VAL:HG11	1.89	0.54
3:K:95:TRP:HB2	3:K:99:PHE:O	2.07	0.54
1:I:148:MET:HG2	2:T:27(D):THR:CG2	2.37	0.54
3:U:24:THR:OG1	3:U:76:ARG:NH2	2.41	0.54
1:H:141:GLU:OE1	1:H:144:ARG:NH2	2.40	0.54
3:Z:13:GLN:OE1	1:N:28:SER:HA	2.08	0.54
1:F:102:GLY:O	1:F:103:VAL:C	2.46	0.53
1:D:49:LYS:O	1:D:50:ALA:CB	2.57	0.53
3:Q:95:TRP:HB2	3:Q:99:PHE:O	2.08	0.53
3:M:122:PHE:HB2	3:M:141:LEU:HB3	1.89	0.53
2:R:60:SER:HB2	3:U:68:THR:HB	1.90	0.53
3:Q:24:THR:OG1	3:Q:76:ARG:NH2	2.42	0.53
2:R:159:SER:HB2	2:R:179:LEU:HA	1.91	0.53
1:D:141:GLU:OE1	1:D:144:ARG:NH2	2.42	0.52
2:V:186:TYR:O	2:V:192:TYR:OH	2.27	0.52
3:M:178:LEU:HD23	3:M:178:LEU:C	2.30	0.52
2:R:61:ARG:HA	3:U:68:THR:HG21	1.91	0.52
3:M:95:TRP:HB2	3:M:99:PHE:O	2.10	0.52
3:Q:119:PRO:HB3	3:Q:145:TYR:HB3	1.92	0.52
2:R:60:SER:CB	3:U:68:THR:OG1	2.58	0.52
1:X:49:LYS:O	1:X:51:GLU:N	2.33	0.51
3:S:24:THR:OG1	3:S:76:ARG:NH2	2.44	0.50
3:U:201:LYS:N	3:U:202:PRO:CD	2.74	0.50
3:W:24:THR:OG1	3:W:76:ARG:NH2	2.44	0.50
1:I:96:GLU:O	1:I:100:ILE:HG12	2.12	0.50
1:G:125:ARG:HD2	3:Q:54:TYR:CD2	2.47	0.50
1:F:49:LYS:O	1:F:50:ALA:CB	2.59	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:T:160:GLN:HE22	3:U:171:GLN:HA	1.76	0.50
1:F:65:ASN:O	1:X:89:TYR:OH	2.20	0.49
1:H:31:LYS:HE2	3:U:13:GLN:HG2	1.94	0.49
2:Y:94:ILE:HD13	3:Z:58:ASN:HB3	1.93	0.49
2:L:108:ARG:HD2	2:L:171:SER:HB2	1.93	0.49
1:D:45:ASN:OD1	1:D:46:GLN:N	2.45	0.49
3:Z:24:THR:OG1	3:Z:76:ARG:NH2	2.46	0.49
2:A:163:VAL:HG22	2:A:175:LEU:HD12	1.94	0.49
3:U:95:TRP:HB2	3:U:99:PHE:O	2.12	0.49
3:B:24:THR:OG1	3:B:76:ARG:NH2	2.46	0.49
3:S:197:ASN:ND2	3:S:208:ASP:OD1	2.46	0.48
1:F:111:MET:HB2	1:F:114:ASP:HB2	1.95	0.48
2:T:192:TYR:HB2	2:T:209:PHE:CE1	2.48	0.48
3:W:119:PRO:HD2	3:W:205:THR:HG21	1.96	0.48
1:X:144:ARG:NH1	2:Y:29:SER:OG	2.46	0.48
3:Q:141:LEU:HD12	3:Q:178:LEU:O	2.14	0.48
1:F:100:ILE:HG21	1:X:124:GLN:HE22	1.79	0.47
3:Z:82(A):ASN:HD21	2:A:54:LEU:HD21	1.79	0.47
1:X:96:GLU:O	1:X:100:ILE:HG12	2.15	0.47
1:X:146:GLU:OE1	1:X:149:ARG:NH1	2.47	0.47
1:I:146:GLU:OE1	1:I:149:ARG:NH1	2.47	0.47
2:T:161:GLU:HA	2:T:176:SER:O	2.14	0.47
1:F:89:TYR:OH	1:X:68:SER:CB	2.62	0.47
3:M:24:THR:OG1	3:M:76:ARG:NH2	2.47	0.47
1:G:35:ASP:HB3	3:Q:33:ILE:HD11	1.97	0.47
3:B:95:TRP:HB2	3:B:99:PHE:O	2.15	0.47
3:S:95:TRP:HB2	3:S:99:PHE:O	2.15	0.46
2:T:136:LEU:HD12	2:T:136:LEU:N	2.30	0.46
3:M:148:GLU:OE2	3:M:149:PRO:HA	2.16	0.46
3:W:95:TRP:HB2	3:W:99:PHE:O	2.14	0.46
1:F:68:SER:CB	1:X:89:TYR:OH	2.61	0.46
3:K:95:TRP:CD1	3:K:95:TRP:C	2.89	0.46
2:L:210:ASN:O	2:L:213:GLU:HB2	2.16	0.46
2:T:167:ASP:O	2:T:171:SER:HA	2.15	0.46
1:F:103:VAL:HG12	1:F:103:VAL:O	2.16	0.46
1:H:146:GLU:OE1	1:H:149:ARG:NH1	2.48	0.46
1:N:96:GLU:O	1:N:100:ILE:HG12	2.15	0.46
3:U:95:TRP:CD1	3:U:95:TRP:C	2.89	0.46
2:V:24:ARG:CG	3:S:187:SER:HB2	2.46	0.46
3:K:24:THR:OG1	3:K:76:ARG:NH2	2.49	0.46
3:W:203:SER:O	3:W:204:ASN:C	2.54	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:96:GLU:O	1:H:100:ILE:HG12	2.17	0.45
1:H:125:ARG:HD2	3:S:54:TYR:CZ	2.52	0.45
1:X:22:ARG:HD2	2:Y:30:TYR:OH	2.17	0.45
1:X:53:ILE:N	1:X:54:PRO:HD2	2.31	0.45
3:Z:95:TRP:HB2	3:Z:99:PHE:O	2.17	0.45
1:G:96:GLU:O	1:G:100:ILE:HG12	2.17	0.44
3:K:51:ILE:HG13	3:K:57:THR:HG22	2.00	0.44
2:L:148:TRP:HB2	2:L:155:GLN:HB2	1.99	0.44
1:D:47:PHE:HD1	1:D:51:GLU:OE1	1.99	0.44
3:M:51:ILE:HG13	3:M:57:THR:HG22	2.00	0.44
2:T:136:LEU:HD21	2:T:196:VAL:HG13	1.99	0.44
1:E:146:GLU:OE1	1:E:149:ARG:NH1	2.50	0.44
2:R:60:SER:HB2	3:U:68:THR:CB	2.47	0.44
3:S:95:TRP:CD1	3:S:95:TRP:C	2.91	0.44
1:H:31:LYS:HE2	3:U:13:GLN:CG	2.48	0.44
1:I:42:GLU:HG2	1:I:115:SER:HA	1.99	0.44
1:F:35:ASP:HB3	3:W:33:ILE:HD11	1.99	0.44
3:W:95:TRP:C	3:W:95:TRP:CD1	2.90	0.44
1:X:42:GLU:HG2	1:X:115:SER:HA	2.00	0.44
1:G:119:VAL:O	1:G:122:TYR:HB3	2.17	0.44
3:K:196:CYS:O	3:K:196:CYS:SG	2.75	0.44
1:N:53:ILE:N	1:N:54:PRO:HD2	2.33	0.44
1:F:146:GLU:OE1	1:F:149:ARG:NH1	2.51	0.44
3:Z:95:TRP:C	3:Z:95:TRP:CD1	2.91	0.44
1:F:96:GLU:O	1:F:100:ILE:HG12	2.18	0.43
1:E:53:ILE:N	1:E:54:PRO:HD2	2.33	0.43
2:L:123:GLU:HG3	2:L:124:GLN:N	2.33	0.43
3:Q:11:LEU:HB2	3:Q:147:PRO:HG3	2.00	0.43
1:D:146:GLU:OE1	1:D:149:ARG:NH1	2.52	0.43
2:L:39:LYS:HE2	2:L:81:GLU:O	2.17	0.43
3:B:119:PRO:HB3	3:B:145:TYR:HB3	2.00	0.43
1:D:42:GLU:HG2	1:D:115:SER:HA	2.00	0.43
1:E:124:GLN:O	1:E:128:LEU:HG	2.18	0.43
1:F:48:GLN:O	1:F:49:LYS:C	2.56	0.43
2:P:6:GLN:N	2:P:100:GLN:OE1	2.46	0.43
2:P:39:LYS:HE2	2:P:81:GLU:O	2.19	0.43
3:Q:95:TRP:CD1	3:Q:95:TRP:C	2.91	0.43
3:W:51:ILE:HG13	3:W:57:THR:HG22	2.00	0.43
1:I:43:PHE:O	1:I:44:GLY:C	2.57	0.43
1:G:42:GLU:HG2	1:G:115:SER:HA	1.99	0.43
1:N:146:GLU:OE1	1:N:149:ARG:NH1	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:V:26:SER:HB3	3:S:191:THR:HG22	2.00	0.43
3:B:51:ILE:HG13	3:B:57:THR:HG22	2.01	0.43
2:V:39:LYS:HE2	2:V:81:GLU:O	2.19	0.43
1:X:49:LYS:C	1:X:51:GLU:H	2.20	0.43
3:Z:13:GLN:HE22	1:N:28:SER:HA	1.83	0.43
3:M:95:TRP:CD1	3:M:95:TRP:C	2.91	0.43
2:P:11:LEU:HD23	2:P:11:LEU:C	2.39	0.43
2:T:182:SER:OG	2:T:185:ASP:HB2	2.19	0.43
1:H:42:GLU:HG2	1:H:115:SER:HA	2.00	0.42
1:F:124:GLN:O	1:F:128:LEU:HG	2.19	0.42
2:V:11:LEU:C	2:V:11:LEU:HD23	2.39	0.42
2:V:167:ASP:CB	2:V:170:ASP:OD1	2.66	0.42
3:U:85:GLU:HB3	1:X:134:LYS:HE2	2.02	0.42
1:H:53:ILE:N	1:H:54:PRO:HD2	2.34	0.42
2:L:147:GLN:HB3	2:L:195:GLU:HB3	2.01	0.42
3:M:200:HIS:ND1	3:M:203:SER:OG	2.35	0.42
1:I:30:LEU:O	1:I:33:ARG:HG2	2.19	0.42
1:I:53:ILE:N	1:I:54:PRO:HD2	2.35	0.42
1:N:42:GLU:HG2	1:N:115:SER:HA	2.00	0.42
3:S:51:ILE:HG13	3:S:57:THR:HG22	2.02	0.42
2:P:24:ARG:HB2	2:P:24:ARG:HE	1.76	0.42
3:S:198:VAL:HG12	3:S:199:ASN:N	2.35	0.42
3:U:51:ILE:HG13	3:U:57:THR:HG22	2.02	0.42
1:X:111:MET:HB2	1:X:114:ASP:HB2	2.01	0.42
2:P:149:LYS:HG2	2:P:154:LEU:HD23	2.00	0.42
3:B:95:TRP:CD1	3:B:95:TRP:C	2.92	0.42
1:G:53:ILE:N	1:G:54:PRO:HD2	2.35	0.42
2:V:149:LYS:HE2	2:V:154:LEU:CD2	2.49	0.42
1:X:148:MET:CG	2:Y:27(D):THR:CG2	2.96	0.42
3:Z:51:ILE:HG13	3:Z:57:THR:HG22	2.02	0.42
1:D:53:ILE:N	1:D:54:PRO:HD2	2.35	0.42
3:Z:13:GLN:NE2	1:N:28:SER:CA	2.83	0.42
2:A:24:ARG:HE	2:A:24:ARG:HB2	1.75	0.42
1:F:53:ILE:N	1:F:54:PRO:HD2	2.35	0.42
2:L:11:LEU:C	2:L:11:LEU:HD23	2.40	0.41
2:J:146:VAL:HG12	2:J:147:GLN:N	2.35	0.41
2:P:149:LYS:HA	2:P:153:ALA:O	2.20	0.41
3:Q:201:LYS:N	3:Q:202:PRO:CD	2.83	0.41
3:Z:13:GLN:HE22	1:N:28:SER:CA	2.33	0.41
2:A:209:PHE:C	2:A:209:PHE:CD2	2.94	0.41
1:F:42:GLU:HG2	1:F:115:SER:HA	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:182:SER:OG	2:P:185:ASP:HB2	2.21	0.41
2:T:94:ILE:HD13	3:U:58:ASN:HB3	2.01	0.41
1:N:22:ARG:HD2	2:A:30:TYR:OH	2.21	0.41
1:E:119:VAL:O	1:E:122:TYR:HB3	2.20	0.41
1:X:19:ALA:HA	1:X:148:MET:HE1	2.02	0.41
1:D:96:GLU:O	1:D:100:ILE:HG12	2.20	0.41
3:K:119:PRO:HB3	3:K:145:TYR:HB3	2.03	0.41
1:N:46:GLN:O	1:N:48:GLN:N	2.52	0.41
1:N:30:LEU:O	1:N:33:ARG:HG2	2.21	0.41
2:T:24:ARG:HE	2:T:24:ARG:HB2	1.75	0.41
1:E:42:GLU:HG2	1:E:115:SER:HA	2.02	0.41
1:F:49:LYS:O	1:F:50:ALA:HB2	2.21	0.41
2:R:140:TYR:CG	2:R:141:PRO:HA	2.56	0.41
2:T:145:LYS:HB3	2:T:197:THR:HB	2.03	0.41
2:T:39:LYS:HE2	2:T:81:GLU:O	2.20	0.41
1:X:148:MET:CG	2:Y:27(D):THR:HG23	2.50	0.41
2:A:39:LYS:HE2	2:A:81:GLU:O	2.21	0.41
2:P:142:ARG:HD2	2:P:163:VAL:HG11	2.03	0.41
3:W:66:ARG:NH2	3:W:86:ASP:OD2	2.54	0.41
2:R:39:LYS:HE2	2:R:81:GLU:O	2.21	0.40
2:A:11:LEU:HD23	2:A:11:LEU:C	2.41	0.40
1:N:124:GLN:O	1:N:128:LEU:HG	2.22	0.40
1:F:30:LEU:O	1:F:33:ARG:HG2	2.21	0.40
1:D:124:GLN:O	1:D:128:LEU:HG	2.20	0.40
2:J:39:LYS:HE2	2:J:81:GLU:O	2.21	0.40
3:Q:127:SER:O	3:Q:128:SER:CB	2.70	0.40
2:A:142:ARG:HD2	2:A:163:VAL:HG11	2.04	0.40
3:S:178:LEU:HD23	3:S:178:LEU:C	2.42	0.40
1:X:30:LEU:O	1:X:33:ARG:HG2	2.22	0.40

All (5) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:S:13:GLN:NE2	1:I:27:PHE:CB[1_655]	2.05	0.15
2:J:202:SER:OG	1:G:132:GLU:OE2[1_556]	2.07	0.13
1:D:89:TYR:OH	1:N:65:ASN:O[2_645]	2.15	0.05
1:G:65:ASN:O	1:I:89:TYR:OH[1_554]	2.16	0.04
1:X:23:LYS:O	3:B:113:SER:CB[1_455]	2.18	0.02

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	D	137/165 (83%)	131 (96%)	4 (3%)	2 (2%)	10	42
1	E	137/165 (83%)	131 (96%)	3 (2%)	3 (2%)	6	31
1	F	134/165 (81%)	127 (95%)	4 (3%)	3 (2%)	6	31
1	G	131/165 (79%)	126 (96%)	4 (3%)	1 (1%)	19	57
1	H	133/165 (81%)	128 (96%)	4 (3%)	1 (1%)	19	57
1	I	131/165 (79%)	126 (96%)	5 (4%)	0	100	100
1	N	141/165 (86%)	129 (92%)	8 (6%)	4 (3%)	5	25
1	X	131/165 (79%)	126 (96%)	5 (4%)	0	100	100
2	A	215/218 (99%)	200 (93%)	14 (6%)	1 (0%)	29	68
2	J	215/218 (99%)	207 (96%)	8 (4%)	0	100	100
2	L	215/218 (99%)	204 (95%)	10 (5%)	1 (0%)	29	68
2	P	215/218 (99%)	207 (96%)	8 (4%)	0	100	100
2	R	215/218 (99%)	203 (94%)	11 (5%)	1 (0%)	29	68
2	T	215/218 (99%)	207 (96%)	8 (4%)	0	100	100
2	V	215/218 (99%)	207 (96%)	8 (4%)	0	100	100
2	Y	108/218 (50%)	103 (95%)	5 (5%)	0	100	100
3	B	209/225 (93%)	198 (95%)	9 (4%)	2 (1%)	15	53
3	K	209/225 (93%)	201 (96%)	8 (4%)	0	100	100
3	M	209/225 (93%)	199 (95%)	9 (4%)	1 (0%)	29	68
3	Q	209/225 (93%)	200 (96%)	8 (4%)	1 (0%)	29	68
3	S	209/225 (93%)	198 (95%)	11 (5%)	0	100	100
3	U	209/225 (93%)	198 (95%)	10 (5%)	1 (0%)	29	68
3	W	209/225 (93%)	200 (96%)	8 (4%)	1 (0%)	29	68
3	Z	115/225 (51%)	112 (97%)	3 (3%)	0	100	100
All	All	4266/4864 (88%)	4068 (95%)	175 (4%)	23 (0%)	29	68

All (23) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	46	GLN
3	U	204	ASN
1	N	47	PHE
1	N	48	GLN
1	D	50	ALA
1	E	48	GLN
2	L	128	GLY
3	M	144	ASP
1	F	50	ALA
1	G	102	GLY
2	R	156	SER
1	N	160	SER
3	B	193	THR
1	F	102	GLY
1	D	46	GLN
1	F	48	GLN
3	W	204	ASN
2	A	143	GLU
3	Q	54	TYR
1	H	50	ALA
1	N	50	ALA
1	E	102	GLY
3	B	134	GLY

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	129/152 (85%)	121 (94%)	8 (6%)	18	52
1	E	129/152 (85%)	120 (93%)	9 (7%)	15	47
1	F	128/152 (84%)	120 (94%)	8 (6%)	18	51
1	G	124/152 (82%)	116 (94%)	8 (6%)	17	50
1	H	127/152 (84%)	119 (94%)	8 (6%)	18	51
1	I	125/152 (82%)	115 (92%)	10 (8%)	12	40

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	N	133/152 (88%)	121 (91%)	12 (9%)	9	35
1	X	126/152 (83%)	117 (93%)	9 (7%)	14	46
2	A	192/193 (100%)	187 (97%)	5 (3%)	46	78
2	J	192/193 (100%)	182 (95%)	10 (5%)	23	59
2	L	192/193 (100%)	182 (95%)	10 (5%)	23	59
2	P	192/193 (100%)	181 (94%)	11 (6%)	20	56
2	R	192/193 (100%)	185 (96%)	7 (4%)	35	70
2	T	192/193 (100%)	183 (95%)	9 (5%)	26	63
2	V	192/193 (100%)	183 (95%)	9 (5%)	26	63
2	Y	96/193 (50%)	90 (94%)	6 (6%)	18	51
3	B	181/193 (94%)	175 (97%)	6 (3%)	38	73
3	K	181/193 (94%)	172 (95%)	9 (5%)	24	60
3	M	181/193 (94%)	172 (95%)	9 (5%)	24	60
3	Q	181/193 (94%)	170 (94%)	11 (6%)	18	53
3	S	181/193 (94%)	173 (96%)	8 (4%)	28	65
3	U	181/193 (94%)	171 (94%)	10 (6%)	21	57
3	W	181/193 (94%)	169 (93%)	12 (7%)	16	49
3	Z	99/193 (51%)	94 (95%)	5 (5%)	24	60
All	All	3827/4304 (89%)	3618 (94%)	209 (6%)	21	57

All (209) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	11	SER
1	D	42	GLU
1	D	59	MET
1	D	61	GLN
1	D	82	ASP
1	D	112	LYS
1	D	144	ARG
1	D	149	ARG
2	J	3	GLN
2	J	4	MET
2	J	24	ARG
2	J	100	GLN
2	J	126	LYS

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Mol	Chain	Res	Type
2	J	135	LEU
2	J	142	ARG
2	J	168	SER
2	J	182	SER
2	J	213	GLU
3	K	12	VAL
3	K	95	TRP
3	K	113	SER
3	K	116	THR
3	K	120	SER
3	K	138	LEU
3	K	150	VAL
3	K	183	THR
3	K	196	CYS
1	E	11	SER
1	E	42	GLU
1	E	59	MET
1	E	61	GLN
1	E	82	ASP
1	E	92	LEU
1	E	112	LYS
1	E	144	ARG
1	E	149	ARG
2	L	3	GLN
2	L	4	MET
2	L	24	ARG
2	L	100	GLN
2	L	107	LYS
2	L	108	ARG
2	L	123	GLU
2	L	154	LEU
2	L	159	SER
2	L	197	THR
3	M	6	GLU
3	M	12	VAL
3	M	95	TRP
3	M	113	SER
3	M	116	THR
3	M	167	PRO
3	M	178	LEU
3	M	183	THR
3	M	196	CYS

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Mol	Chain	Res	Type
1	F	11	SER
1	F	42	GLU
1	F	59	MET
1	F	61	GLN
1	F	82	ASP
1	F	112	LYS
1	F	144	ARG
1	F	149	ARG
2	V	3	GLN
2	V	4	MET
2	V	12	SER
2	V	14	SER
2	V	24	ARG
2	V	100	GLN
2	V	114	SER
2	V	123	GLU
2	V	129	THR
3	W	12	VAL
3	W	95	TRP
3	W	113	SER
3	W	115	SER
3	W	116	THR
3	W	150	VAL
3	W	151	THR
3	W	178	LEU
3	W	183	THR
3	W	191	THR
3	W	196	CYS
3	W	201	LYS
1	G	9	LEU
1	G	11	SER
1	G	42	GLU
1	G	59	MET
1	G	61	GLN
1	G	82	ASP
1	G	144	ARG
1	G	149	ARG
2	P	3	GLN
2	P	4	MET
2	P	14	SER
2	P	24	ARG
2	P	29	SER

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Mol	Chain	Res	Type
2	P	100	GLN
2	P	114	SER
2	P	142	ARG
2	P	152	ASN
2	P	197	THR
2	P	213	GLU
3	Q	12	VAL
3	Q	95	TRP
3	Q	113	SER
3	Q	116	THR
3	Q	117	LYS
3	Q	167	PRO
3	Q	178	LEU
3	Q	179	SER
3	Q	183	THR
3	Q	196	CYS
3	Q	201	LYS
1	H	11	SER
1	H	42	GLU
1	H	59	MET
1	H	61	GLN
1	H	82	ASP
1	H	103	VAL
1	H	144	ARG
1	H	149	ARG
2	R	3	GLN
2	R	4	MET
2	R	14	SER
2	R	24	ARG
2	R	100	GLN
2	R	159	SER
2	R	177	SER
3	S	12	VAL
3	S	95	TRP
3	S	113	SER
3	S	135	THR
3	S	161	SER
3	S	178	LEU
3	S	191	THR
3	S	201	LYS
1	I	11	SER
1	I	42	GLU

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Mol	Chain	Res	Type
1	I	59	MET
1	I	61	GLN
1	I	82	ASP
1	I	92	LEU
1	I	103	VAL
1	I	112	LYS
1	I	144	ARG
1	I	149	ARG
2	T	3	GLN
2	T	4	MET
2	T	24	ARG
2	T	100	GLN
2	T	123	GLU
2	T	142	ARG
2	T	154	LEU
2	T	176	SER
2	T	182	SER
3	U	12	VAL
3	U	13	GLN
3	U	95	TRP
3	U	113	SER
3	U	116	THR
3	U	150	VAL
3	U	178	LEU
3	U	186	SER
3	U	192	GLN
3	U	196	CYS
1	X	11	SER
1	X	42	GLU
1	X	59	MET
1	X	61	GLN
1	X	82	ASP
1	X	92	LEU
1	X	144	ARG
1	X	148	MET
1	X	149	ARG
2	Y	3	GLN
2	Y	4	MET
2	Y	12	SER
2	Y	14	SER
2	Y	24	ARG
2	Y	100	GLN

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Mol	Chain	Res	Type
3	Z	12	VAL
3	Z	13	GLN
3	Z	83	ARG
3	Z	95	TRP
3	Z	113	SER
1	N	9	LEU
1	N	11	SER
1	N	42	GLU
1	N	49	LYS
1	N	59	MET
1	N	61	GLN
1	N	82	ASP
1	N	144	ARG
1	N	148	MET
1	N	149	ARG
1	N	157	LEU
1	N	158	GLN
2	A	3	GLN
2	A	4	MET
2	A	14	SER
2	A	24	ARG
2	A	100	GLN
3	B	12	VAL
3	B	13	GLN
3	B	95	TRP
3	B	113	SER
3	B	155	ASN
3	B	201	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
2	J	124	GLN
2	L	124	GLN
2	L	152	ASN
2	L	199	GLN
2	V	147	GLN
3	Q	199	ASN
2	R	124	GLN
1	X	124	GLN
2	Y	79	GLN
1	N	158	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

8 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
4	SO4	J	302	-	4,4,4	0.62	0	6,6,6	0.32	0
4	SO4	L	301	-	4,4,4	0.57	0	6,6,6	0.34	0
4	SO4	F	201	-	4,4,4	0.43	0	6,6,6	0.20	0
4	SO4	V	302	-	4,4,4	0.53	0	6,6,6	0.41	0
4	SO4	G	501	-	4,4,4	0.52	0	6,6,6	0.26	0
4	SO4	P	301	-	4,4,4	0.70	0	6,6,6	0.63	0
4	SO4	V	301	-	4,4,4	0.67	0	6,6,6	0.71	0
4	SO4	J	301	-	4,4,4	0.54	0	6,6,6	0.33	0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	V	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 ⓘ

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	D	141/165 (85%)	-0.01	4 (2%) 53 25	48, 70, 120, 167	0
1	E	141/165 (85%)	-0.08	2 (1%) 75 49	50, 71, 122, 180	0
1	F	140/165 (84%)	-0.06	4 (2%) 51 23	49, 70, 121, 152	0
1	G	137/165 (83%)	-0.03	2 (1%) 73 46	41, 61, 103, 133	1 (0%)
1	H	139/165 (84%)	-0.05	4 (2%) 51 23	61, 80, 121, 161	0
1	I	137/165 (83%)	0.01	4 (2%) 51 23	57, 74, 104, 140	0
1	N	145/165 (87%)	0.07	7 (4%) 30 11	59, 83, 144, 186	0
1	X	137/165 (83%)	0.06	3 (2%) 62 33	64, 82, 115, 139	0
2	A	217/218 (99%)	0.85	47 (21%) 0 0	65, 96, 158, 172	3 (1%)
2	J	217/218 (99%)	-0.30	0 100 100	41, 54, 74, 104	1 (0%)
2	L	217/218 (99%)	-0.36	0 100 100	41, 52, 71, 94	0
2	P	217/218 (99%)	-0.36	0 100 100	37, 53, 73, 96	0
2	R	217/218 (99%)	0.44	28 (12%) 3 1	57, 84, 136, 149	0
2	T	217/218 (99%)	0.05	1 (0%) 91 75	70, 86, 110, 125	0
2	V	217/218 (99%)	-0.30	0 100 100	45, 57, 78, 98	0
2	Y	110/218 (50%)	-0.03	0 100 100	65, 80, 102, 113	0
3	B	213/225 (94%)	0.49	20 (9%) 8 3	64, 100, 159, 167	0
3	K	213/225 (94%)	-0.36	0 100 100	40, 54, 79, 101	0
3	M	213/225 (94%)	-0.32	1 (0%) 91 75	40, 57, 84, 101	0
3	Q	213/225 (94%)	-0.20	1 (0%) 91 75	38, 54, 81, 110	0
3	S	213/225 (94%)	0.21	12 (5%) 24 8	60, 85, 136, 155	0
3	U	213/225 (94%)	0.45	22 (10%) 6 2	65, 85, 134, 152	0
3	W	213/225 (94%)	-0.29	1 (0%) 91 75	43, 58, 85, 114	0
3	Z	117/225 (52%)	0.00	0 100 100	66, 82, 105, 116	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å ²)	Q<0.9
All	All	4354/4864 (89%)	-0.00	163 (3%)	41	17	37, 71, 131, 186	5 (0%)

All (163) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	B	128	SER	6.1
2	A	194	CYS	6.1
2	A	195	GLU	5.6
3	U	128	SER	5.4
2	R	194	CYS	5.3
2	A	196	VAL	5.0
2	A	209	PHE	4.9
1	N	159	GLU	4.9
2	A	181	LEU	4.8
2	R	134	CYS	4.8
3	S	128	SER	4.8
1	D	103	VAL	4.7
3	B	127	SER	4.7
1	E	47	PHE	4.7
2	A	119	PRO	4.6
2	A	131	SER	4.6
2	A	133	VAL	4.6
3	U	183	THR	4.5
1	F	111	MET	4.5
3	B	133	GLY	4.3
2	A	206	THR	4.2
3	B	208	ASP	4.1
1	F	113	GLU	4.1
2	A	205	VAL	4.0
3	B	138	LEU	4.0
1	I	45	ASN	4.0
2	R	193	ALA	4.0
2	A	192	TYR	4.0
2	R	192	TYR	3.9
1	H	45	ASN	3.9
2	A	150	VAL	3.8
1	F	47	PHE	3.7
2	A	148	TRP	3.7
2	A	147	GLN	3.7
1	D	46	GLN	3.6
2	A	177	SER	3.6
2	R	212	GLY	3.6

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Mol	Chain	Res	Type	RSRZ
3	U	194	TYR	3.6
1	D	47	PHE	3.6
3	U	191	THR	3.6
3	U	157	GLY	3.5
2	A	132	VAL	3.5
1	X	103	VAL	3.5
1	N	47	PHE	3.4
2	A	208	SER	3.4
1	N	158	GLN	3.4
3	B	139	GLY	3.4
1	H	103	VAL	3.4
1	D	102	GLY	3.3
3	U	211	VAL	3.3
1	G	103	VAL	3.3
2	A	129	THR	3.3
2	A	130	ALA	3.3
3	U	193	THR	3.3
2	R	208	SER	3.2
3	B	123	PRO	3.2
3	U	212	GLU	3.2
3	U	197	ASN	3.2
3	B	126	PRO	3.1
1	I	103	VAL	3.1
2	A	179	LEU	3.1
2	R	209	PHE	3.0
3	B	125	ALA	3.0
3	U	123	PRO	3.0
2	A	203	SER	3.0
3	Q	128	SER	3.0
1	F	112	LYS	3.0
2	A	134	CYS	3.0
3	U	208	ASP	3.0
2	A	201	LEU	3.0
3	B	122	PHE	2.9
3	U	182	VAL	2.9
3	B	191	THR	2.9
3	B	193	THR	2.9
2	A	180	THR	2.8
3	U	196	CYS	2.8
2	A	124	GLN	2.8
3	S	193	THR	2.8
3	B	194	TYR	2.8

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Mol	Chain	Res	Type	RSRZ
3	S	212	GLU	2.8
3	B	212	GLU	2.8
2	A	161	GLU	2.8
2	A	116	PHE	2.8
1	N	113	GLU	2.7
2	A	187	GLU	2.7
2	A	184	ALA	2.7
3	S	182	VAL	2.7
3	B	211	VAL	2.7
2	A	186	TYR	2.7
2	R	122	ASP	2.6
2	R	178	THR	2.6
3	S	137	ALA	2.6
2	R	118	PHE	2.6
2	R	123	GLU	2.6
2	A	118	PHE	2.6
3	S	123	PRO	2.6
3	U	158	ALA	2.6
3	U	137	ALA	2.6
2	R	195	GLU	2.6
1	H	48	GLN	2.5
1	E	46	GLN	2.5
3	S	194	TYR	2.5
3	M	133	GLY	2.5
3	U	138	LEU	2.5
2	A	149	LYS	2.5
2	A	191	VAL	2.5
2	A	151	ASP	2.5
3	S	126	PRO	2.5
3	S	127	SER	2.5
1	X	48	GLN	2.5
1	N	45	ASN	2.5
2	A	197	THR	2.5
2	R	132	VAL	2.5
2	R	119	PRO	2.5
2	R	147	GLN	2.5
3	S	192	GLN	2.5
3	B	210	LYS	2.5
2	A	125	LEU	2.4
1	H	113	GLU	2.4
3	B	13	GLN	2.4
2	A	152	ASN	2.4

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Mol	Chain	Res	Type	RSRZ
2	R	187	GLU	2.4
1	N	102	GLY	2.4
2	R	145	LYS	2.4
1	I	44	GLY	2.4
2	T	210	ASN	2.4
3	U	181	VAL	2.3
3	U	156	SER	2.3
2	R	186	TYR	2.3
1	X	111	MET	2.3
3	S	122	PHE	2.3
3	U	160	THR	2.3
2	R	205	VAL	2.3
3	U	136	ALA	2.3
2	R	135	LEU	2.3
2	A	146	VAL	2.3
2	A	178	THR	2.3
2	R	188	LYS	2.3
1	G	45	ASN	2.3
2	R	191	VAL	2.2
3	B	137	ALA	2.2
2	A	189	HIS	2.2
3	U	125	ALA	2.2
2	A	123	GLU	2.2
2	R	148	TRP	2.1
3	U	126	PRO	2.1
2	A	190	LYS	2.1
3	B	177	SER	2.1
1	I	111	MET	2.1
2	R	190	LYS	2.1
2	A	120	PRO	2.1
2	A	121	SER	2.1
2	A	202	SER	2.1
1	N	161	LEU	2.1
2	R	130	ALA	2.1
2	R	210	ASN	2.1
3	B	18	LEU	2.1
2	R	197	THR	2.1
2	R	146	VAL	2.0
2	A	117	ILE	2.0
2	A	135	LEU	2.0
3	S	64	LYS	2.0
3	W	128	SER	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 carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. 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(\AA^2)	Q<0.9
4	SO4	J	302	5/5	0.86	0.36	74,86,93,97	0
4	SO4	P	301	5/5	0.89	0.26	66,70,78,81	0
4	SO4	J	301	5/5	0.90	0.28	74,76,85,87	0
4	SO4	F	201	5/5	0.91	0.28	96,97,109,111	0
4	SO4	V	301	5/5	0.92	0.24	69,74,85,96	0
4	SO4	G	501	5/5	0.93	0.24	79,86,97,103	0
4	SO4	L	301	5/5	0.94	0.41	68,69,81,84	0
4	SO4	V	302	5/5	0.94	0.14	78,80,93,94	0

6.5 Other polymers [i](#)

There are no such residues in this entry.