



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 26, 2018 – 06:25 PM EST

PDB ID : 5NJD  
Title : Structure of Interleukin 23 in complex with Briakinumab FAb  
Authors : Bloch, Y.; Savvides, S.N.  
Deposited on : 2017-03-28  
Resolution : 3.90 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](mailto:validation@mail.wwpdb.org)

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20030736  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : rb-20030736

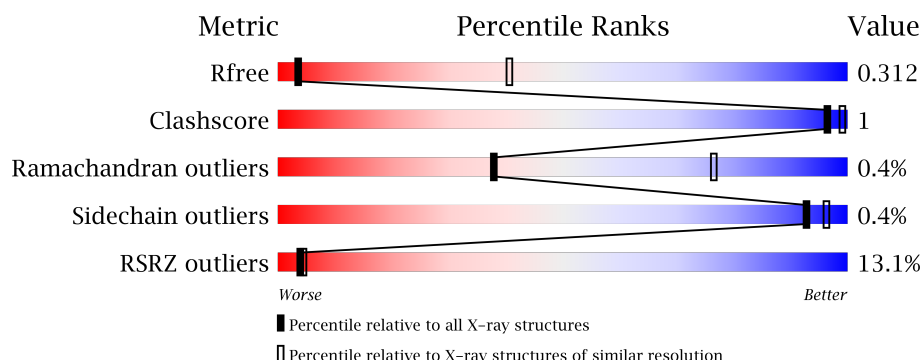
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 3.90 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))
$R_{free}$	100719	1007 (4.20-3.60)
Clashscore	112137	1103 (4.20-3.60)
Ramachandran outliers	110173	1062 (4.20-3.60)
Sidechain outliers	110143	1053 (4.20-3.60)
RSRZ outliers	101464	1020 (4.20-3.60)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . 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	A	328	<div> <div>8%</div> <div>88%</div> <div>9%</div> </div>
1	C	328	<div> <div>8%</div> <div>86%</div> <div>10%</div> </div>
1	E	328	<div> <div>13%</div> <div>87%</div> <div>10%</div> </div>
1	G	328	<div> <div>12%</div> <div>88%</div> <div>11%</div> </div>
1	I	328	<div> <div>12%</div> <div>85%</div> <div>11%</div> </div>

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Mol	Chain	Length	Quality of chain
1	K	328	
2	B	198	
2	D	198	
2	F	198	
2	H	198	
2	J	198	
2	L	198	
3	M	245	
3	O	245	
3	Q	245	
3	S	245	
3	U	245	
3	W	245	
4	N	289	
4	P	289	
4	R	289	
4	T	289	
4	V	289	
4	X	289	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
8	SO4	O	302	-	-	-	X

## 2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 39445 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Interleukin-12 subunit beta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	298	Total	C	N	O	S	0	0	0
			2313	1467	373	461	12			
1	C	294	Total	C	N	O	S	0	0	0
			2304	1461	372	459	12			
1	E	294	Total	C	N	O	S	0	0	0
			2309	1465	373	459	12			
1	G	293	Total	C	N	O	S	0	0	0
			2301	1461	372	456	12			
1	I	292	Total	C	N	O	S	0	0	0
			2288	1453	367	456	12			
1	K	297	Total	C	N	O	S	0	0	0
			2326	1475	377	462	12			

- Molecule 2 is a protein called Interleukin-23 subunit alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	144	Total	C	N	O	S	0	0	0
			1056	681	185	185	5			
2	D	146	Total	C	N	O	S	0	0	0
			1080	694	190	191	5			
2	F	146	Total	C	N	O	S	0	0	0
			1058	681	187	185	5			
2	H	139	Total	C	N	O	S	0	0	0
			1036	669	183	179	5			
2	J	141	Total	C	N	O	S	0	0	0
			1031	666	180	180	5			
2	L	139	Total	C	N	O	S	0	0	0
			1029	665	181	178	5			

There are 54 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	190	GLY	-	expression tag	UNP Q9NPF7

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Chain	Residue	Modelled	Actual	Comment	Reference
B	191	THR	-	expression tag	UNP Q9NPF7
B	192	LYS	-	expression tag	UNP Q9NPF7
B	193	HIS	-	expression tag	UNP Q9NPF7
B	194	HIS	-	expression tag	UNP Q9NPF7
B	195	HIS	-	expression tag	UNP Q9NPF7
B	196	HIS	-	expression tag	UNP Q9NPF7
B	197	HIS	-	expression tag	UNP Q9NPF7
B	198	HIS	-	expression tag	UNP Q9NPF7
D	190	GLY	-	expression tag	UNP Q9NPF7
D	191	THR	-	expression tag	UNP Q9NPF7
D	192	LYS	-	expression tag	UNP Q9NPF7
D	193	HIS	-	expression tag	UNP Q9NPF7
D	194	HIS	-	expression tag	UNP Q9NPF7
D	195	HIS	-	expression tag	UNP Q9NPF7
D	196	HIS	-	expression tag	UNP Q9NPF7
D	197	HIS	-	expression tag	UNP Q9NPF7
D	198	HIS	-	expression tag	UNP Q9NPF7
F	190	GLY	-	expression tag	UNP Q9NPF7
F	191	THR	-	expression tag	UNP Q9NPF7
F	192	LYS	-	expression tag	UNP Q9NPF7
F	193	HIS	-	expression tag	UNP Q9NPF7
F	194	HIS	-	expression tag	UNP Q9NPF7
F	195	HIS	-	expression tag	UNP Q9NPF7
F	196	HIS	-	expression tag	UNP Q9NPF7
F	197	HIS	-	expression tag	UNP Q9NPF7
F	198	HIS	-	expression tag	UNP Q9NPF7
H	190	GLY	-	expression tag	UNP Q9NPF7
H	191	THR	-	expression tag	UNP Q9NPF7
H	192	LYS	-	expression tag	UNP Q9NPF7
H	193	HIS	-	expression tag	UNP Q9NPF7
H	194	HIS	-	expression tag	UNP Q9NPF7
H	195	HIS	-	expression tag	UNP Q9NPF7
H	196	HIS	-	expression tag	UNP Q9NPF7
H	197	HIS	-	expression tag	UNP Q9NPF7
H	198	HIS	-	expression tag	UNP Q9NPF7
J	190	GLY	-	expression tag	UNP Q9NPF7
J	191	THR	-	expression tag	UNP Q9NPF7
J	192	LYS	-	expression tag	UNP Q9NPF7
J	193	HIS	-	expression tag	UNP Q9NPF7
J	194	HIS	-	expression tag	UNP Q9NPF7
J	195	HIS	-	expression tag	UNP Q9NPF7
J	196	HIS	-	expression tag	UNP Q9NPF7

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Chain	Residue	Modelled	Actual	Comment	Reference
J	197	HIS	-	expression tag	UNP Q9NPF7
J	198	HIS	-	expression tag	UNP Q9NPF7
L	190	GLY	-	expression tag	UNP Q9NPF7
L	191	THR	-	expression tag	UNP Q9NPF7
L	192	LYS	-	expression tag	UNP Q9NPF7
L	193	HIS	-	expression tag	UNP Q9NPF7
L	194	HIS	-	expression tag	UNP Q9NPF7
L	195	HIS	-	expression tag	UNP Q9NPF7
L	196	HIS	-	expression tag	UNP Q9NPF7
L	197	HIS	-	expression tag	UNP Q9NPF7
L	198	HIS	-	expression tag	UNP Q9NPF7

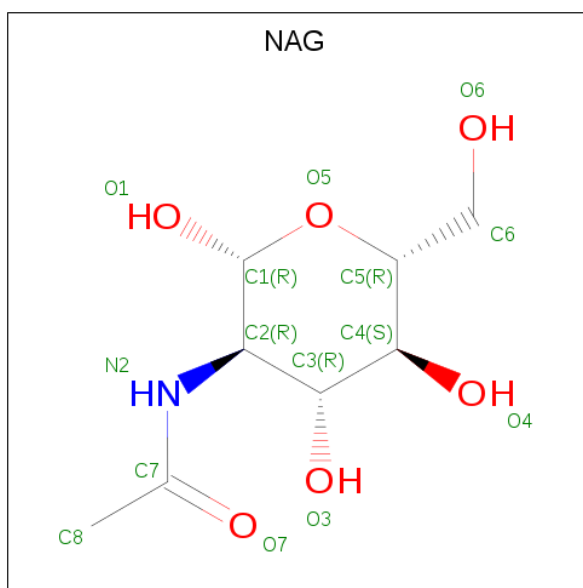
- Molecule 3 is a protein called Briakinumab FAb Light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	M	213	Total	C	N	O	S	0	0	0
			1592	997	268	323	4			
3	O	213	Total	C	N	O	S	0	0	0
			1596	1000	270	322	4			
3	Q	213	Total	C	N	O	S	0	0	0
			1589	997	270	318	4			
3	S	214	Total	C	N	O	S	0	0	0
			1590	995	268	323	4			
3	U	215	Total	C	N	O	S	0	0	0
			1601	1004	269	324	4			
3	W	214	Total	C	N	O	S	0	0	0
			1590	995	270	321	4			

- Molecule 4 is a protein called Briakinumab FAb Heavy chain.

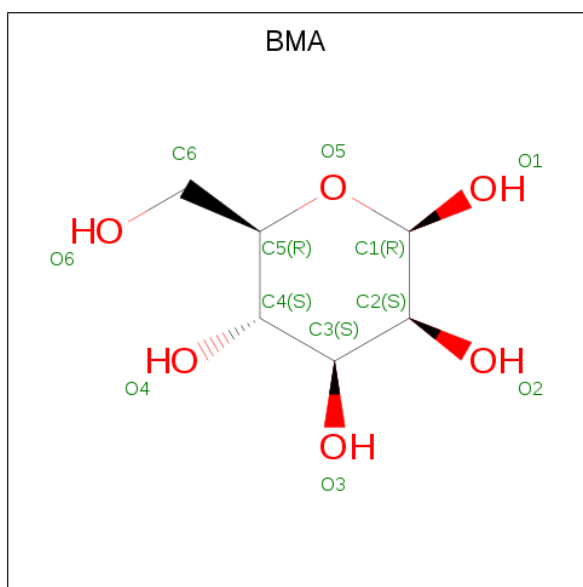
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	N	207	Total	C	N	O	S	0	0	0
			1561	984	269	301	7			
4	P	207	Total	C	N	O	S	0	0	0
			1558	981	268	302	7			
4	R	208	Total	C	N	O	S	0	0	0
			1556	980	268	301	7			
4	T	208	Total	C	N	O	S	0	0	0
			1560	985	267	301	7			
4	V	205	Total	C	N	O	S	0	0	0
			1538	968	265	298	7			
4	X	206	Total	C	N	O	S	0	0	0
			1552	978	267	300	7			

- Molecule 5 is N-ACETYL-D-GLUCOSAMINE (three-letter code: NAG) (formula:  $C_8H_{15}NO_6$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	N	O	0	0
			14	8	1	5		
5	A	1	Total	C	N	O	0	0
			14	8	1	5		
5	C	1	Total	C	N	O	0	0
			14	8	1	5		
5	C	1	Total	C	N	O	0	0
			14	8	1	5		
5	E	1	Total	C	N	O	0	0
			14	8	1	5		
5	E	1	Total	C	N	O	0	0
			14	8	1	5		
5	G	1	Total	C	N	O	0	0
			14	8	1	5		
5	G	1	Total	C	N	O	0	0
			14	8	1	5		
5	I	1	Total	C	N	O	0	0
			14	8	1	5		
5	I	1	Total	C	N	O	0	0
			14	8	1	5		
5	K	1	Total	C	N	O	0	0
			14	8	1	5		
5	K	1	Total	C	N	O	0	0
			14	8	1	5		

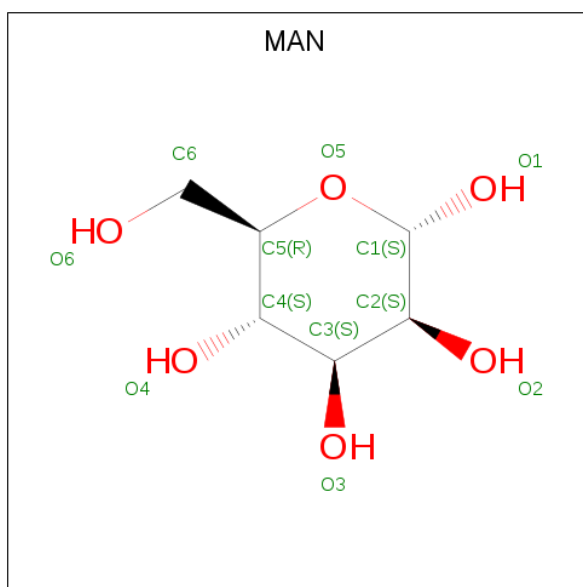
- Molecule 6 is BETA-D-MANNOSE (three-letter code: BMA) (formula:  $C_6H_{12}O_6$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			11	6	5		
6	C	1	Total	C	O	0	0
			11	6	5		
6	E	1	Total	C	O	0	0
			11	6	5		
6	G	1	Total	C	O	0	0
			11	6	5		
6	I	1	Total	C	O	0	0
			11	6	5		
6	K	1	Total	C	O	0	0
			11	6	5		

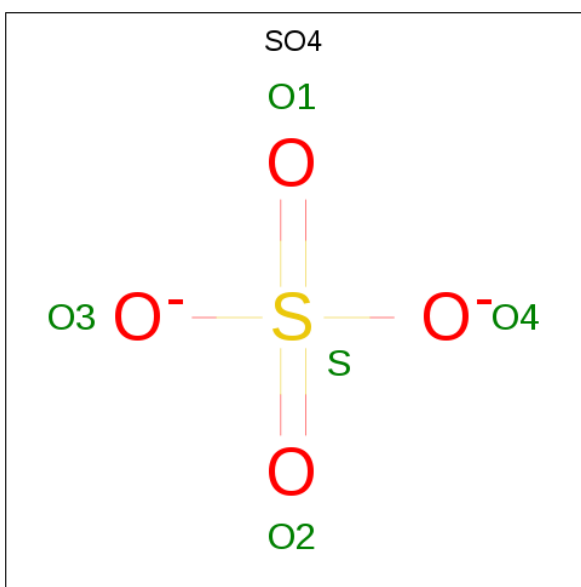
- Molecule 7 is ALPHA-D-MANNOSE (three-letter code: MAN) (formula: C<sub>6</sub>H<sub>12</sub>O<sub>6</sub>).





Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	C	O	0	0
			11	6	5		
7	A	1	Total	C	O	0	0
			11	6	5		
7	C	1	Total	C	O	0	0
			11	6	5		
7	C	1	Total	C	O	0	0
			11	6	5		
7	E	1	Total	C	O	0	0
			11	6	5		
7	E	1	Total	C	O	0	0
			11	6	5		
7	G	1	Total	C	O	0	0
			11	6	5		
7	G	1	Total	C	O	0	0
			11	6	5		
7	I	1	Total	C	O	0	0
			11	6	5		
7	I	1	Total	C	O	0	0
			11	6	5		
7	K	1	Total	C	O	0	0
			11	6	5		
7	K	1	Total	C	O	0	0
			11	6	5		

- Molecule 8 is SULFATE ION (three-letter code: SO<sub>4</sub>) (formula: O<sub>4</sub>S).

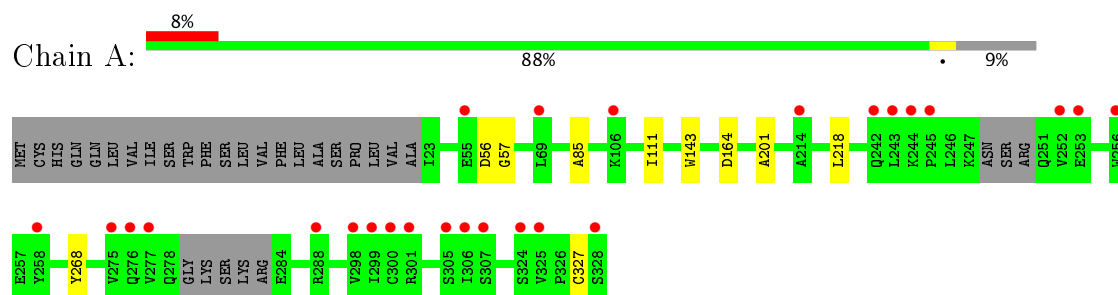


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	M	1	Total	O	S	0	0
			5	4	1		
8	M	1	Total	O	S	0	0
			5	4	1		
8	O	1	Total	O	S	0	0
			5	4	1		
8	O	1	Total	O	S	0	0
			5	4	1		
8	Q	1	Total	O	S	0	0
			5	4	1		
8	R	1	Total	O	S	0	0
			5	4	1		
8	S	1	Total	O	S	0	0
			5	4	1		
8	S	1	Total	O	S	0	0
			5	4	1		
8	S	1	Total	O	S	0	0
			5	4	1		
8	U	1	Total	O	S	0	0
			5	4	1		
8	U	1	Total	O	S	0	0
			5	4	1		
8	W	1	Total	O	S	0	0
			5	4	1		
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			5	4	1		

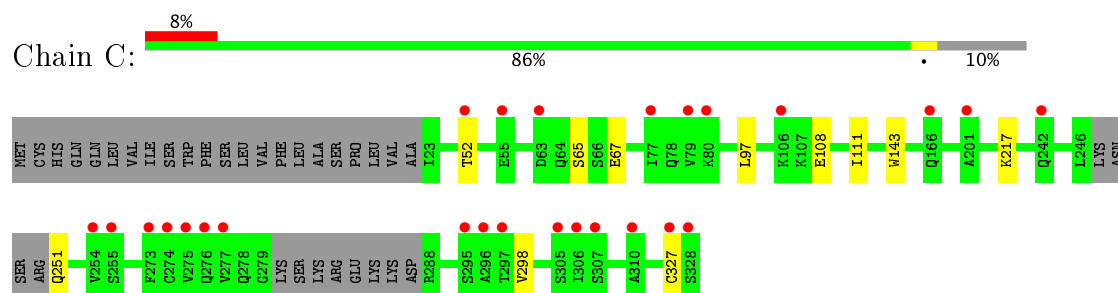
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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.

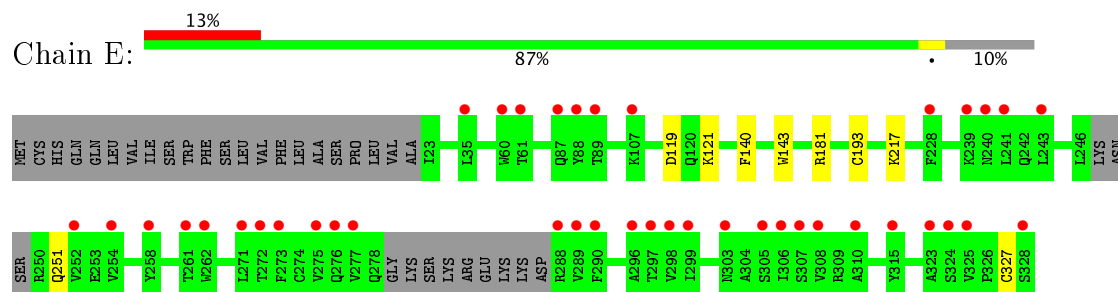
#### • Molecule 1: Interleukin-12 subunit beta



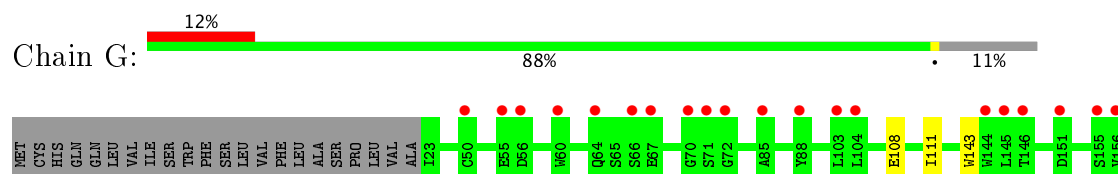
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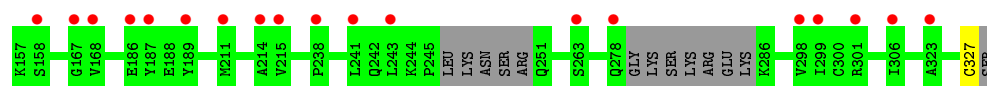


#### • Molecule 1: Interleukin-12 subunit beta

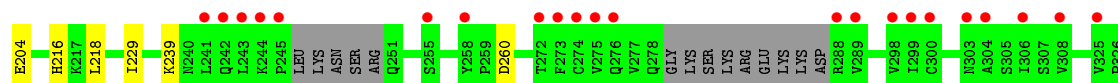
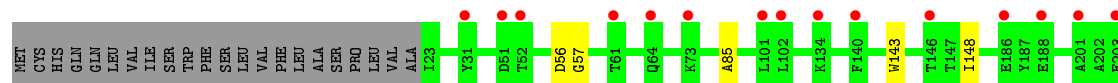
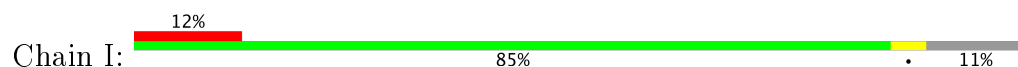


#### • Molecule 1: Interleukin-12 subunit beta

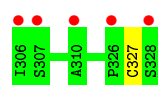
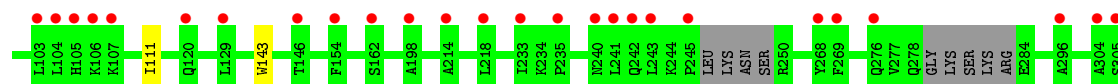
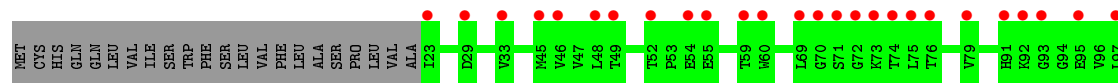




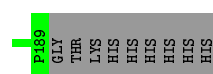
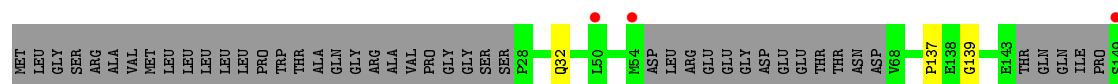
• Molecule 1: Interleukin-12 subunit beta



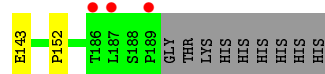
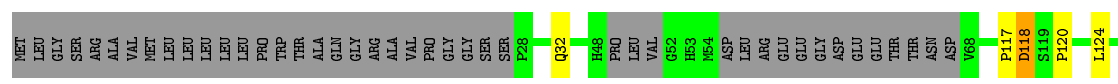
• Molecule 1: Interleukin-12 subunit beta



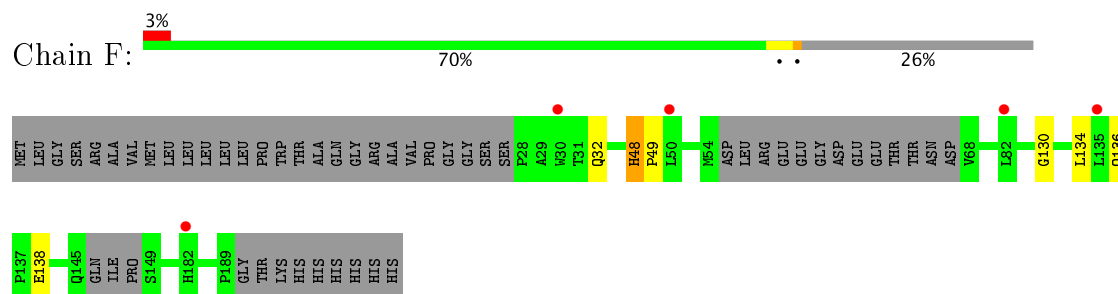
• Molecule 2: Interleukin-23 subunit alpha



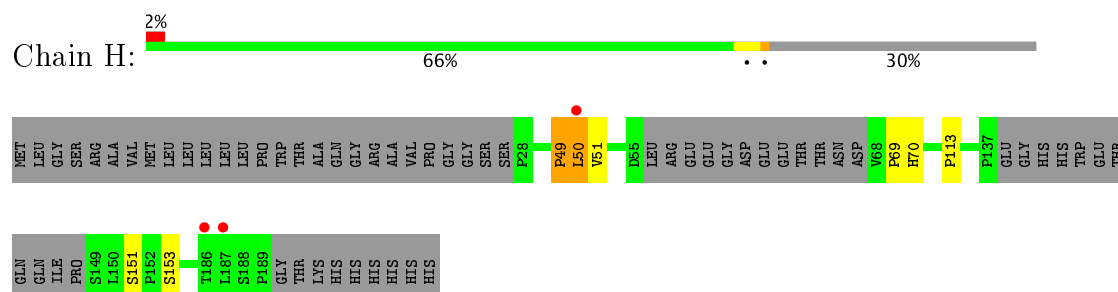
• Molecule 2: Interleukin-23 subunit alpha



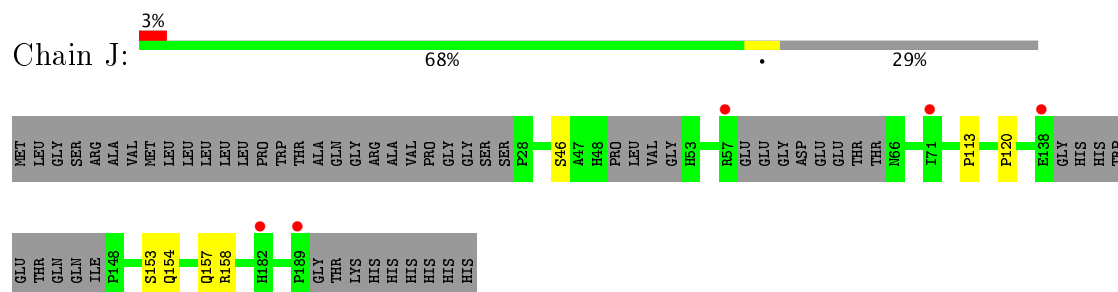
- Molecule 2: Interleukin-23 subunit alpha



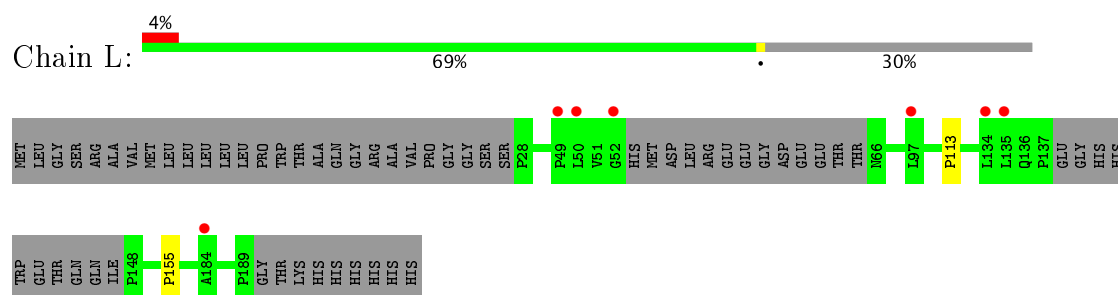
- Molecule 2: Interleukin-23 subunit alpha



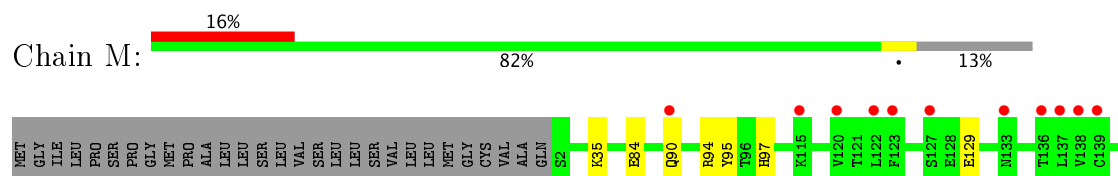
- Molecule 2: Interleukin-23 subunit alpha

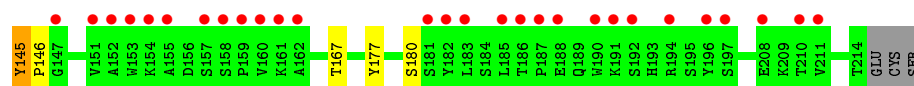


- Molecule 2: Interleukin-23 subunit alpha

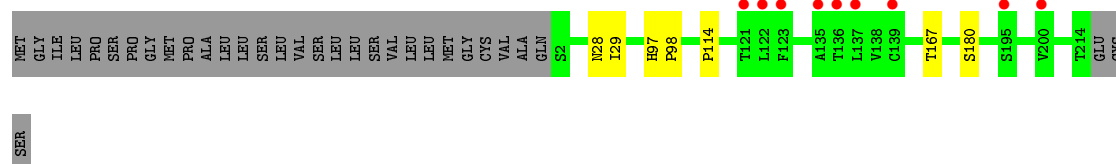
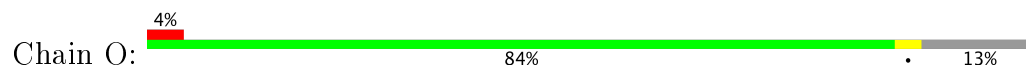


- Molecule 3: Briakinumab Fab Light chain

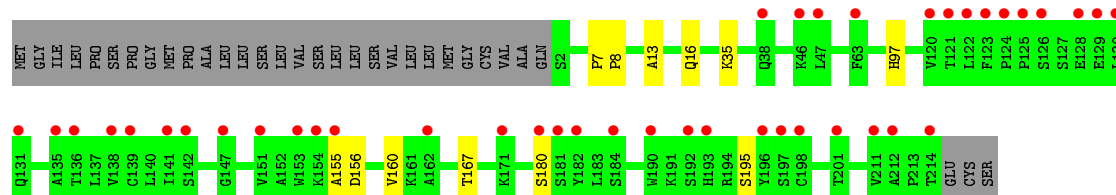
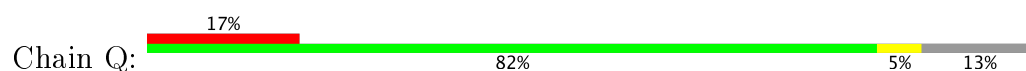




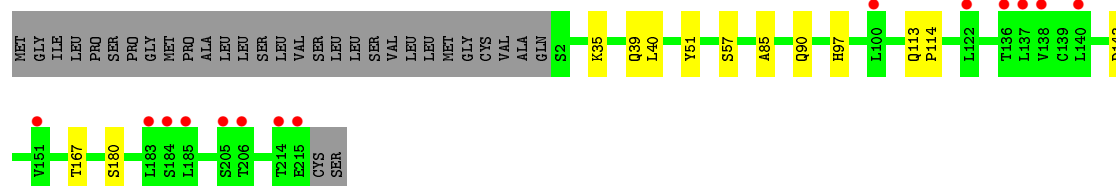
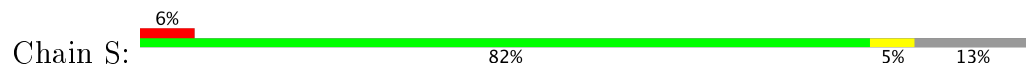
• Molecule 3: Briakinumab FAb Light chain



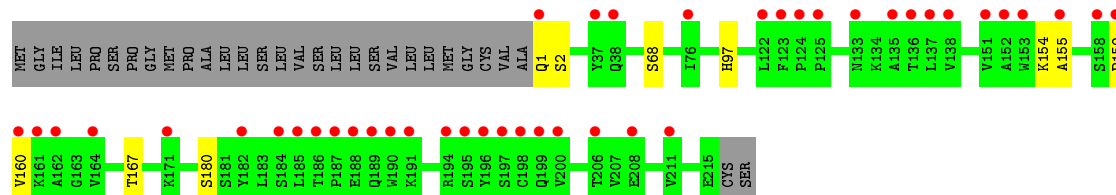
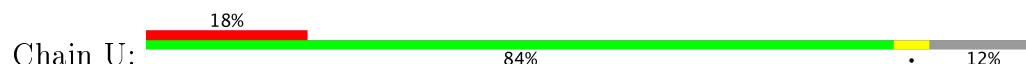
• Molecule 3: Briakinumab FAb Light chain



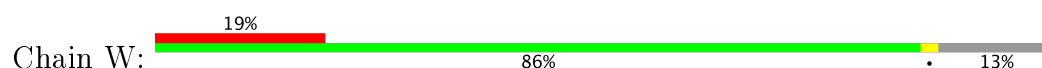
• Molecule 3: Briakinumab FAb Light chain

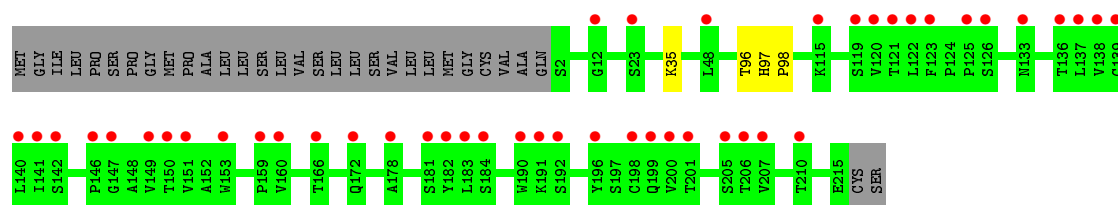


• Molecule 3: Briakinumab FAb Light chain

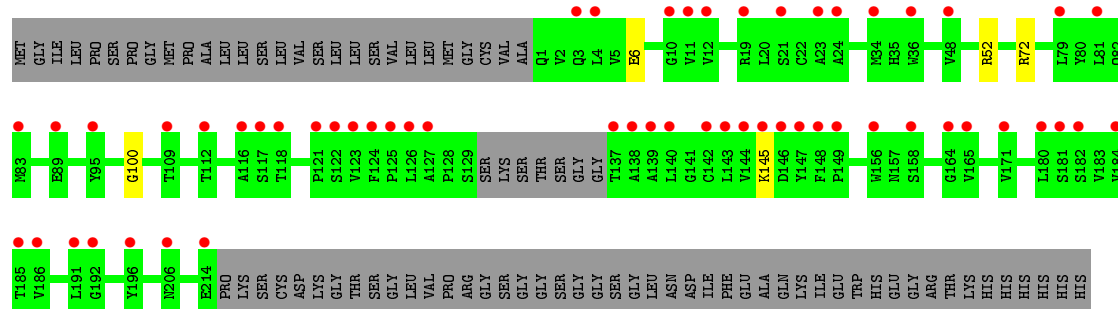


• Molecule 3: Briakinumab FAb Light chain

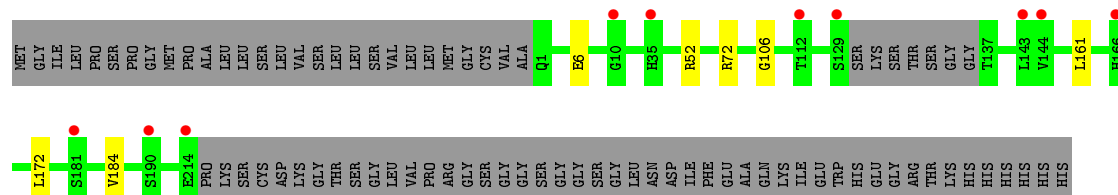




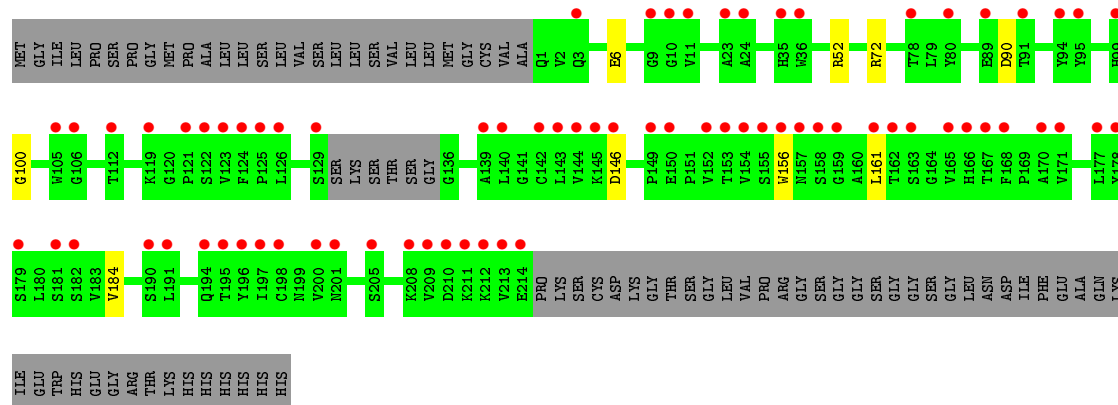
• Molecule 4: Briakinumab Fab Heavy chain



• Molecule 4: Briakinumab Fab Heavy chain

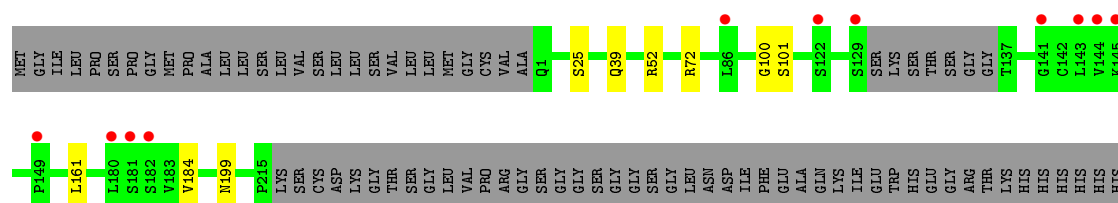


• Molecule 4: Briakinumab Fab Heavy chain

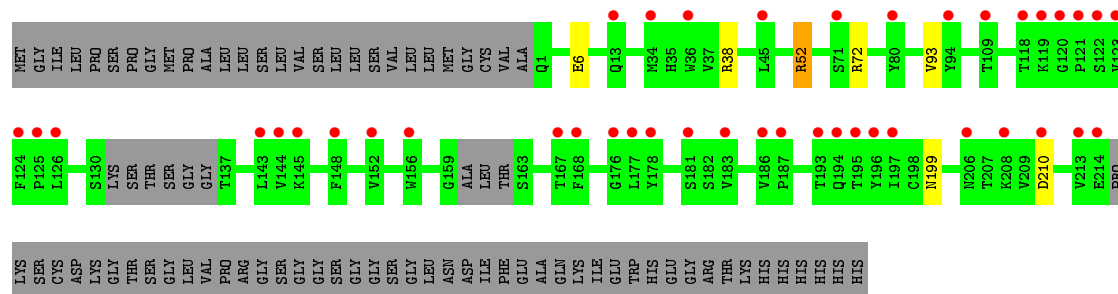


• Molecule 4: Briakinumab Fab Heavy chain

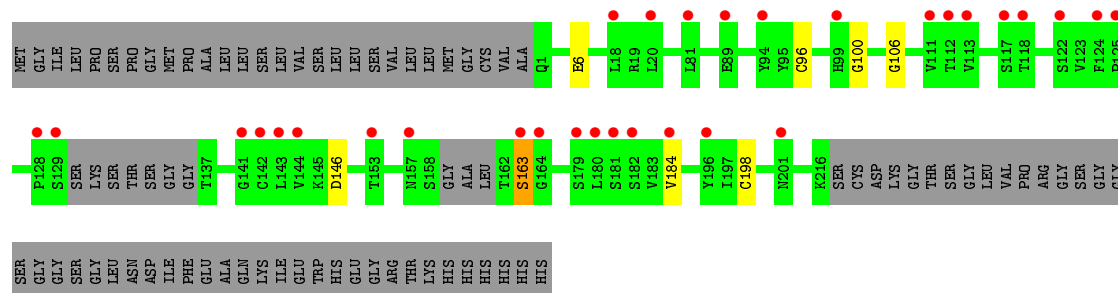




• Molecule 4: Briakinumab FAb Heavy chain



• Molecule 4: Briakinumab FAb Heavy chain





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	191.61Å 191.61Å 519.11Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	95.80 – 3.90 95.80 – 3.90	Depositor EDS
% Data completeness (in resolution range)	97.6 (95.80-3.90) 97.7 (95.80-3.90)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.12 (at 3.89Å)	Xtriage
Refinement program	PHENIX (1.12_2829: ???)	Depositor
R, $R_{free}$	0.272 , 0.312 0.271 , 0.312	Depositor DCC
$R_{free}$ test set	1834 reflections (2.12%)	DCC
Wilson B-factor (Å <sup>2</sup> )	105.6	Xtriage
Anisotropy	0.492	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 92.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.38$ , $\langle L^2 \rangle = 0.20$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.84	EDS
Total number of atoms	39445	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	120.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.93% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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, BMA, NAG, MAN

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	0.28	0/2370	0.46	0/3229
1	C	0.29	0/2361	0.47	0/3213
1	E	0.27	0/2366	0.45	0/3219
1	G	0.28	0/2358	0.46	0/3210
1	I	0.27	0/2345	0.46	0/3192
1	K	0.27	0/2383	0.46	0/3242
2	B	0.28	0/1082	0.38	0/1476
2	D	0.27	0/1107	0.39	0/1509
2	F	0.26	0/1084	0.38	0/1480
2	H	0.28	0/1062	0.43	0/1448
2	J	0.27	0/1056	0.39	0/1440
2	L	0.26	0/1056	0.39	0/1441
3	M	0.29	0/1632	0.47	0/2233
3	O	0.29	0/1636	0.46	0/2236
3	Q	0.29	0/1629	0.47	0/2227
3	S	0.29	0/1629	0.46	0/2228
3	U	0.28	0/1641	0.46	0/2245
3	W	0.27	0/1629	0.45	0/2228
4	N	0.27	0/1599	0.44	0/2176
4	P	0.29	0/1596	0.46	0/2173
4	R	0.27	0/1594	0.45	0/2170
4	T	0.30	0/1599	0.46	0/2178
4	V	0.28	0/1575	0.46	0/2143
4	X	0.27	0/1590	0.45	0/2165
All	All	0.28	0/39979	0.45	0/54501

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2313	0	2156	5	0
1	C	2304	0	2168	5	0
1	E	2309	0	2178	3	0
1	G	2301	0	2171	2	0
1	I	2288	0	2155	6	0
1	K	2326	0	2191	1	0
2	B	1056	0	1016	3	0
2	D	1080	0	1029	4	0
2	F	1058	0	996	5	0
2	H	1036	0	1006	2	0
2	J	1031	0	971	3	0
2	L	1029	0	990	0	0
3	M	1592	0	1540	8	0
3	O	1596	0	1553	3	0
3	Q	1589	0	1547	7	0
3	S	1590	0	1542	8	0
3	U	1601	0	1551	6	0
3	W	1590	0	1542	3	0
4	N	1561	0	1510	4	0
4	P	1558	0	1502	6	0
4	R	1556	0	1500	5	0
4	T	1560	0	1507	7	0
4	V	1538	0	1472	4	0
4	X	1552	0	1488	4	0
5	A	28	0	24	0	0
5	C	28	0	24	0	0
5	E	28	0	24	0	0
5	G	28	0	24	0	0
5	I	28	0	24	0	0
5	K	28	0	24	0	0
6	A	11	0	8	0	0
6	C	11	0	8	0	0
6	E	11	0	8	0	0
6	G	11	0	8	0	0
6	I	11	0	8	0	0
6	K	11	0	8	0	0
7	A	22	0	20	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	C	22	0	20	0	0
7	E	22	0	20	0	0
7	G	22	0	20	0	0
7	I	22	0	20	0	0
7	K	22	0	20	0	0
8	M	10	0	0	0	0
8	O	10	0	0	0	0
8	Q	5	0	0	0	0
8	R	5	0	0	0	0
8	S	15	0	0	1	0
8	U	10	0	0	0	0
8	W	10	0	0	0	0
All	All	39445	0	37593	89	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 1.

All (89) 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:F:130:GLY:O	2:F:134:LEU:HD13	1.89	0.73
1:I:148:ILE:HG21	1:I:216:HIS:CD2	2.24	0.72
2:J:153:SER:O	2:J:158:ARG:NH1	2.23	0.71
4:X:6:GLU:OE1	4:X:6:GLU:N	2.24	0.70
3:Q:13:ALA:N	3:Q:16:GLN:OE1	2.28	0.60
4:T:161:LEU:HD21	4:T:184:VAL:HG21	1.84	0.60
4:R:161:LEU:HD21	4:R:184:VAL:HG21	1.84	0.58
4:P:161:LEU:HD21	4:P:184:VAL:HG21	1.85	0.57
4:R:6:GLU:N	4:R:6:GLU:OE1	2.37	0.57
4:R:52:ARG:O	4:R:72:ARG:NH1	2.38	0.57
2:D:143:GLU:OE1	2:D:143:GLU:N	2.37	0.57
3:M:84:GLU:OE2	3:M:177:TYR:OH	2.17	0.56
2:B:32:GLN:OE1	2:B:32:GLN:N	2.38	0.55
1:E:251:GLN:OE1	1:E:251:GLN:N	2.38	0.55
4:N:52:ARG:O	4:N:72:ARG:NH1	2.40	0.55
1:A:56:ASP:OD1	1:A:57:GLY:N	2.40	0.54
1:E:119:ASP:OD1	1:E:121:LYS:N	2.39	0.54
3:U:1:GLN:O	3:U:2:SER:OG	2.24	0.54
1:A:85:ALA:HB3	1:A:218:LEU:HD13	1.91	0.53
2:F:130:GLY:O	2:F:134:LEU:CD1	2.56	0.53
2:F:32:GLN:OE1	2:F:32:GLN:N	2.39	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:136:GLN:O	2:F:138:GLU:N	2.43	0.51
2:J:46:SER:O	2:J:120:PRO:HG3	2.10	0.51
1:I:85:ALA:HB3	1:I:218:LEU:HD13	1.92	0.51
1:I:239:LYS:NZ	1:I:260:ASP:OD1	2.37	0.51
1:K:111:ILE:HG21	3:M:97:HIS:NE2	2.26	0.50
1:C:251:GLN:N	1:C:298:VAL:O	2.44	0.50
2:D:32:GLN:N	2:D:32:GLN:OE1	2.39	0.50
3:S:51:TYR:HH	4:T:101:SER:HG	1.57	0.50
4:V:199:ASN:ND2	4:V:210:ASP:OD2	2.45	0.50
4:V:6:GLU:OE1	4:V:6:GLU:N	2.43	0.50
1:C:111:ILE:HG21	3:Q:97:HIS:NE2	2.28	0.49
1:C:52:THR:HG21	1:C:97:LEU:HD23	1.95	0.48
3:O:97:HIS:HB3	3:O:98:PRO:HD3	1.94	0.48
2:B:137:PRO:HG2	4:P:172:LEU:HD21	1.95	0.48
4:P:6:GLU:OE1	4:P:6:GLU:N	2.47	0.47
3:S:57:SER:N	8:S:302:SO4:O2	2.48	0.47
2:D:117:PRO:O	2:D:118:ASP:CB	2.63	0.47
3:M:129:GLU:OE2	4:N:145:LYS:NZ	2.48	0.46
4:V:38:ARG:HA	4:V:93:VAL:O	2.15	0.46
3:Q:35:LYS:NZ	4:R:100:GLY:O	2.45	0.46
3:M:35:LYS:NZ	4:N:100:GLY:O	2.47	0.45
4:N:6:GLU:OE1	4:N:6:GLU:N	2.48	0.45
1:C:108:GLU:N	1:C:111:ILE:O	2.43	0.45
2:H:49:PRO:O	2:H:50:LEU:HB2	2.18	0.44
3:M:145:TYR:CD1	3:M:146:PRO:HA	2.53	0.44
3:O:167:THR:HG22	3:O:180:SER:H	1.82	0.44
4:T:25:SER:CB	3:U:68:SER:HB3	2.47	0.44
3:S:113:GLN:OE1	3:S:113:GLN:N	2.51	0.43
3:W:97:HIS:HB3	3:W:98:PRO:HD3	2.00	0.43
2:B:137:PRO:HG2	4:P:172:LEU:CD2	2.49	0.43
2:J:154:GLN:HB2	2:J:157:GLN:CG	2.49	0.43
3:U:167:THR:HG22	3:U:180:SER:H	1.81	0.43
1:C:65:SER:OG	1:C:67:GLU:OE1	2.36	0.43
1:I:148:ILE:HG21	1:I:216:HIS:NE2	2.33	0.43
1:I:56:ASP:OD1	1:I:57:GLY:N	2.50	0.43
3:M:35:LYS:HD2	3:M:90:GLN:OE1	2.19	0.43
3:M:94:ARG:NH1	3:M:95:TYR:OH	2.51	0.43
3:Q:167:THR:HG22	3:Q:180:SER:H	1.84	0.43
3:S:167:THR:HG22	3:S:180:SER:H	1.83	0.43
1:G:111:ILE:HG21	3:S:97:HIS:NE2	2.34	0.43
3:S:40:LEU:HD23	3:S:85:ALA:HB2	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Q:156:ASP:OD1	3:Q:195:SER:N	2.52	0.42
2:H:69:PRO:O	2:H:70:HIS:ND1	2.52	0.42
4:R:156:TRP:HB3	4:R:161:LEU:HD23	2.00	0.42
3:M:167:THR:HG22	3:M:180:SER:H	1.84	0.42
4:P:52:ARG:O	4:P:72:ARG:NH1	2.52	0.42
3:U:155:ALA:N	3:U:160:VAL:HG23	2.32	0.42
3:S:39:GLN:NE2	4:T:39:GLN:OE1	2.50	0.42
2:F:48:HIS:H	2:F:49:PRO:CD	2.32	0.42
3:W:35:LYS:NZ	4:X:100:GLY:O	2.47	0.42
1:I:204:GLU:OE2	1:I:229:ILE:HB	2.20	0.42
3:O:28:ASN:OD1	3:O:29:ILE:N	2.51	0.42
4:V:52:ARG:O	4:V:72:ARG:NH1	2.52	0.42
1:A:164:ASP:OD2	4:T:199:ASN:ND2	2.53	0.41
2:D:120:PRO:O	2:D:124:LEU:N	2.41	0.41
3:S:35:LYS:NZ	4:T:100:GLY:O	2.48	0.41
1:G:108:GLU:N	1:G:111:ILE:O	2.46	0.41
3:Q:155:ALA:N	3:Q:160:VAL:CG2	2.84	0.41
3:U:154:LYS:HD3	3:U:159:PRO:HA	2.03	0.41
4:X:6:GLU:OE2	4:X:106:GLY:HA3	2.21	0.41
3:W:96:THR:O	3:W:96:THR:HG23	2.21	0.41
1:A:201:ALA:HB1	1:A:268:TYR:OH	2.21	0.41
4:T:52:ARG:O	4:T:72:ARG:NH1	2.52	0.41
4:X:163:SER:OG	4:X:184:VAL:CG2	2.69	0.41
1:A:111:ILE:HG21	3:U:97:HIS:NE2	2.36	0.40
1:E:140:PHE:CZ	1:E:193:CYS:HB2	2.56	0.40
4:P:6:GLU:OE2	4:P:106:GLY:HA3	2.22	0.40
3:Q:7:PRO:HA	3:Q:8:PRO:HD3	1.99	0.40

There are no symmetry-related clashes.

## 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	A	292/328 (89%)	283 (97%)	9 (3%)	0	100	100
1	C	288/328 (88%)	279 (97%)	8 (3%)	1 (0%)	44	80
1	E	288/328 (88%)	277 (96%)	10 (4%)	1 (0%)	44	80
1	G	287/328 (88%)	280 (98%)	7 (2%)	0	100	100
1	I	286/328 (87%)	278 (97%)	8 (3%)	0	100	100
1	K	291/328 (89%)	283 (97%)	8 (3%)	0	100	100
2	B	138/198 (70%)	127 (92%)	10 (7%)	1 (1%)	25	67
2	D	140/198 (71%)	129 (92%)	9 (6%)	2 (1%)	13	55
2	F	140/198 (71%)	124 (89%)	15 (11%)	1 (1%)	25	67
2	H	133/198 (67%)	119 (90%)	8 (6%)	6 (4%)	3	31
2	J	133/198 (67%)	123 (92%)	9 (7%)	1 (1%)	22	65
2	L	133/198 (67%)	124 (93%)	7 (5%)	2 (2%)	12	54
3	M	211/245 (86%)	194 (92%)	17 (8%)	0	100	100
3	O	211/245 (86%)	192 (91%)	18 (8%)	1 (0%)	32	73
3	Q	211/245 (86%)	194 (92%)	17 (8%)	0	100	100
3	S	212/245 (86%)	199 (94%)	11 (5%)	2 (1%)	20	63
3	U	213/245 (87%)	197 (92%)	16 (8%)	0	100	100
3	W	212/245 (86%)	191 (90%)	21 (10%)	0	100	100
4	N	203/289 (70%)	190 (94%)	13 (6%)	0	100	100
4	P	203/289 (70%)	191 (94%)	12 (6%)	0	100	100
4	R	204/289 (71%)	191 (94%)	12 (6%)	1 (0%)	32	73
4	T	204/289 (71%)	193 (95%)	11 (5%)	0	100	100
4	V	199/289 (69%)	185 (93%)	14 (7%)	0	100	100
4	X	200/289 (69%)	185 (92%)	13 (6%)	2 (1%)	18	61
All	All	5032/6360 (79%)	4728 (94%)	283 (6%)	21 (0%)	38	76

All (21) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	H	51	VAL
2	D	118	ASP
1	E	217	LYS
2	F	48	HIS
2	H	151	SER
3	O	114	PRO

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Mol	Chain	Res	Type
4	X	163	SER
2	H	50	LEU
4	X	146	ASP
1	C	217	LYS
2	D	152	PRO
4	R	146	ASP
3	S	114	PRO
3	S	143	ASP
2	H	153	SER
2	H	49	PRO
2	L	155	PRO
2	B	139	GLY
2	H	113	PRO
2	L	113	PRO
2	J	113	PRO

### 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	A	252/297 (85%)	250 (99%)	2 (1%)	85	93
1	C	254/297 (86%)	252 (99%)	2 (1%)	85	93
1	E	255/297 (86%)	252 (99%)	3 (1%)	75	89
1	G	254/297 (86%)	252 (99%)	2 (1%)	85	93
1	I	253/297 (85%)	251 (99%)	2 (1%)	85	93
1	K	256/297 (86%)	254 (99%)	2 (1%)	85	93
2	B	106/167 (64%)	106 (100%)	0	100	100
2	D	108/167 (65%)	108 (100%)	0	100	100
2	F	102/167 (61%)	102 (100%)	0	100	100
2	H	105/167 (63%)	105 (100%)	0	100	100
2	J	100/167 (60%)	100 (100%)	0	100	100
2	L	103/167 (62%)	103 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	M	178/207 (86%)	177 (99%)	1 (1%)	89	95
3	O	179/207 (86%)	179 (100%)	0	100	100
3	Q	177/207 (86%)	177 (100%)	0	100	100
3	S	178/207 (86%)	177 (99%)	1 (1%)	89	95
3	U	178/207 (86%)	178 (100%)	0	100	100
3	W	177/207 (86%)	177 (100%)	0	100	100
4	N	172/240 (72%)	172 (100%)	0	100	100
4	P	172/240 (72%)	172 (100%)	0	100	100
4	R	171/240 (71%)	170 (99%)	1 (1%)	89	95
4	T	172/240 (72%)	172 (100%)	0	100	100
4	V	169/240 (70%)	168 (99%)	1 (1%)	89	95
4	X	171/240 (71%)	169 (99%)	2 (1%)	75	89
All	All	4242/5466 (78%)	4223 (100%)	19 (0%)	93	96

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	143	TRP
1	A	327	CYS
1	C	143	TRP
1	C	327	CYS
1	E	143	TRP
1	E	181	ARG
1	E	327	CYS
1	G	143	TRP
1	G	327	CYS
1	I	143	TRP
1	I	327	CYS
1	K	143	TRP
1	K	327	CYS
3	M	145	TYR
4	R	90	ASP
3	S	90	GLN
4	V	52	ARG
4	X	96	CYS
4	X	198	CYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no

such sidechains identified.

### 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 ⓘ

43 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z  > 2$	Counts	RMSZ	# $ Z  > 2$
5	NAG	A	401	1,5	14,14,15	0.22	0	15,19,21	0.54	0
5	NAG	A	402	5,6	14,14,15	0.14	0	15,19,21	0.64	0
6	BMA	A	403	5,7	11,11,12	0.69	0	13,15,17	0.78	0
7	MAN	A	404	6	11,11,12	1.06	1 (9%)	13,15,17	1.11	2 (15%)
7	MAN	A	405	6	11,11,12	0.97	0	13,15,17	1.05	2 (15%)
5	NAG	C	401	1,5	14,14,15	0.22	0	15,19,21	0.43	0
5	NAG	C	402	5,6	14,14,15	0.25	0	15,19,21	0.73	1 (6%)
6	BMA	C	403	5,7	11,11,12	1.34	2 (18%)	13,15,17	0.88	0
7	MAN	C	404	6	11,11,12	1.49	2 (18%)	13,15,17	1.15	1 (7%)
7	MAN	C	405	6	11,11,12	1.36	2 (18%)	13,15,17	1.07	1 (7%)
5	NAG	E	401	1,5	14,14,15	0.22	0	15,19,21	0.43	0
5	NAG	E	402	5,6	14,14,15	0.15	0	15,19,21	0.56	0
6	BMA	E	403	5,7	11,11,12	0.61	0	13,15,17	0.71	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
7	MAN	E	404	6	11,11,12	1.04	1 (9%)	13,15,17	1.09	1 (7%)
7	MAN	E	405	6	11,11,12	1.29	2 (18%)	13,15,17	1.10	1 (7%)
5	NAG	G	401	1,5	14,14,15	0.16	0	15,19,21	0.41	0
5	NAG	G	402	5,6	14,14,15	0.20	0	15,19,21	0.62	0
6	BMA	G	403	5,7	11,11,12	0.74	0	13,15,17	0.79	0
7	MAN	G	404	6	11,11,12	1.39	2 (18%)	13,15,17	1.09	1 (7%)
7	MAN	G	405	6	11,11,12	1.19	1 (9%)	13,15,17	1.11	2 (15%)
5	NAG	I	401	1,5	14,14,15	0.19	0	15,19,21	0.51	0
5	NAG	I	402	5,6	14,14,15	0.24	0	15,19,21	0.74	0
6	BMA	I	403	5,7	11,11,12	0.72	0	13,15,17	0.87	0
7	MAN	I	404	6	11,11,12	1.36	2 (18%)	13,15,17	1.08	0
7	MAN	I	405	6	11,11,12	1.36	1 (9%)	13,15,17	1.06	1 (7%)
5	NAG	K	401	1,5	14,14,15	0.22	0	15,19,21	0.55	0
5	NAG	K	402	5,6	14,14,15	0.19	0	15,19,21	0.56	0
6	BMA	K	403	5,7	11,11,12	0.43	0	13,15,17	0.76	0
7	MAN	K	404	6	11,11,12	1.21	2 (18%)	13,15,17	1.17	1 (7%)
7	MAN	K	405	6	11,11,12	1.45	2 (18%)	13,15,17	1.32	2 (15%)
8	SO4	M	301	-	4,4,4	0.12	0	6,6,6	0.15	0
8	SO4	M	302	-	4,4,4	0.14	0	6,6,6	0.10	0
8	SO4	O	301	-	4,4,4	0.14	0	6,6,6	0.10	0
8	SO4	O	302	-	4,4,4	0.14	0	6,6,6	0.11	0
8	SO4	Q	301	-	4,4,4	0.13	0	6,6,6	0.09	0
8	SO4	R	301	-	4,4,4	0.14	0	6,6,6	0.08	0
8	SO4	S	301	-	4,4,4	0.13	0	6,6,6	0.11	0
8	SO4	S	302	-	4,4,4	0.12	0	6,6,6	0.08	0
8	SO4	S	303	-	4,4,4	0.15	0	6,6,6	0.14	0
8	SO4	U	301	-	4,4,4	0.13	0	6,6,6	0.08	0
8	SO4	U	302	-	4,4,4	0.14	0	6,6,6	0.10	0
8	SO4	W	301	-	4,4,4	0.14	0	6,6,6	0.11	0
8	SO4	W	302	-	4,4,4	0.13	0	6,6,6	0.06	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
5	NAG	A	401	1,5	-	0/6/23/26	0/1/1/1
5	NAG	A	402	5,6	-	0/6/23/26	0/1/1/1
6	BMA	A	403	5,7	-	0/2/19/22	0/1/1/1
7	MAN	A	404	6	-	0/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	MAN	A	405	6	-	0/2/19/22	0/1/1/1
5	NAG	C	401	1,5	-	0/6/23/26	0/1/1/1
5	NAG	C	402	5,6	-	0/6/23/26	0/1/1/1
6	BMA	C	403	5,7	-	0/2/19/22	0/1/1/1
7	MAN	C	404	6	-	0/2/19/22	0/1/1/1
7	MAN	C	405	6	-	0/2/19/22	0/1/1/1
5	NAG	E	401	1,5	-	0/6/23/26	0/1/1/1
5	NAG	E	402	5,6	-	0/6/23/26	0/1/1/1
6	BMA	E	403	5,7	-	0/2/19/22	0/1/1/1
7	MAN	E	404	6	-	0/2/19/22	0/1/1/1
7	MAN	E	405	6	-	0/2/19/22	0/1/1/1
5	NAG	G	401	1,5	-	0/6/23/26	0/1/1/1
5	NAG	G	402	5,6	-	0/6/23/26	0/1/1/1
6	BMA	G	403	5,7	-	0/2/19/22	0/1/1/1
7	MAN	G	404	6	-	0/2/19/22	0/1/1/1
7	MAN	G	405	6	-	0/2/19/22	0/1/1/1
5	NAG	I	401	1,5	-	0/6/23/26	0/1/1/1
5	NAG	I	402	5,6	-	0/6/23/26	0/1/1/1
6	BMA	I	403	5,7	-	0/2/19/22	0/1/1/1
7	MAN	I	404	6	-	0/2/19/22	0/1/1/1
7	MAN	I	405	6	-	0/2/19/22	0/1/1/1
5	NAG	K	401	1,5	-	0/6/23/26	0/1/1/1
5	NAG	K	402	5,6	-	0/6/23/26	0/1/1/1
6	BMA	K	403	5,7	-	0/2/19/22	0/1/1/1
7	MAN	K	404	6	-	0/2/19/22	0/1/1/1
7	MAN	K	405	6	-	0/2/19/22	0/1/1/1
8	SO4	M	301	-	-	0/0/0/0	0/0/0/0
8	SO4	M	302	-	-	0/0/0/0	0/0/0/0
8	SO4	O	301	-	-	0/0/0/0	0/0/0/0
8	SO4	O	302	-	-	0/0/0/0	0/0/0/0
8	SO4	Q	301	-	-	0/0/0/0	0/0/0/0
8	SO4	R	301	-	-	0/0/0/0	0/0/0/0
8	SO4	S	301	-	-	0/0/0/0	0/0/0/0
8	SO4	S	302	-	-	0/0/0/0	0/0/0/0
8	SO4	S	303	-	-	0/0/0/0	0/0/0/0
8	SO4	U	301	-	-	0/0/0/0	0/0/0/0
8	SO4	U	302	-	-	0/0/0/0	0/0/0/0
8	SO4	W	301	-	-	0/0/0/0	0/0/0/0
8	SO4	W	302	-	-	0/0/0/0	0/0/0/0

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	C	404	MAN	O5-C1	-2.47	1.39	1.43
7	G	405	MAN	C1-C2	2.16	1.57	1.52
7	G	404	MAN	C2-C3	2.19	1.55	1.52
7	E	405	MAN	C1-C2	2.20	1.57	1.52
6	C	403	BMA	C4-C3	2.22	1.58	1.52
7	C	405	MAN	C2-C3	2.23	1.55	1.52
7	I	404	MAN	C2-C3	2.34	1.55	1.52
7	A	404	MAN	C1-C2	2.40	1.57	1.52
7	K	404	MAN	C2-C3	2.43	1.55	1.52
7	E	405	MAN	C2-C3	2.47	1.55	1.52
7	K	404	MAN	C1-C2	2.49	1.58	1.52
7	E	404	MAN	C1-C2	2.51	1.58	1.52
7	C	405	MAN	C1-C2	2.59	1.58	1.52
7	K	405	MAN	C1-C2	2.59	1.58	1.52
6	C	403	BMA	O5-C5	2.77	1.49	1.43
7	C	404	MAN	C1-C2	2.78	1.58	1.52
7	I	405	MAN	C2-C3	2.83	1.56	1.52
7	I	404	MAN	C1-C2	2.90	1.59	1.52
7	G	404	MAN	C1-C2	3.40	1.60	1.52
7	K	405	MAN	C2-C3	3.61	1.57	1.52

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	C	404	MAN	O2-C2-C3	-2.46	105.35	110.17
7	C	405	MAN	O2-C2-C3	-2.34	105.57	110.17
7	A	405	MAN	O2-C2-C3	-2.20	105.86	110.17
7	K	405	MAN	O2-C2-C3	-2.19	105.87	110.17
7	G	404	MAN	O2-C2-C3	-2.17	105.92	110.17
7	E	404	MAN	O2-C2-C3	-2.16	105.93	110.17
7	A	404	MAN	O2-C2-C3	-2.04	106.17	110.17
7	G	405	MAN	O2-C2-C3	-2.03	106.19	110.17
7	K	405	MAN	C1-C2-C3	2.15	112.38	109.65
5	C	402	NAG	C1-O5-C5	2.18	115.17	112.17
7	I	405	MAN	C1-O5-C5	2.21	115.21	112.17
7	G	405	MAN	C1-O5-C5	2.25	115.27	112.17
7	A	404	MAN	C1-O5-C5	2.26	115.28	112.17
7	A	405	MAN	C1-O5-C5	2.30	115.33	112.17
7	K	404	MAN	C1-O5-C5	2.46	115.56	112.17
7	E	405	MAN	C1-O5-C5	2.52	115.64	112.17

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
8	S	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 [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	298/328 (90%)	0.65	26 (8%) 11 9	86, 106, 151, 189	0
1	C	294/328 (89%)	0.79	26 (8%) 11 9	86, 111, 155, 188	0
1	E	294/328 (89%)	0.93	41 (13%) 3 4	90, 115, 154, 183	0
1	G	293/328 (89%)	0.91	39 (13%) 4 4	94, 125, 168, 190	0
1	I	292/328 (89%)	0.94	39 (13%) 4 4	100, 122, 159, 195	0
1	K	297/328 (90%)	1.09	57 (19%) 1 2	101, 129, 185, 208	0
2	B	144/198 (72%)	0.29	3 (2%) 64 54	72, 99, 126, 140	0
2	D	146/198 (73%)	0.46	3 (2%) 64 54	83, 117, 156, 168	0
2	F	146/198 (73%)	0.41	5 (3%) 46 36	89, 107, 136, 155	0
2	H	139/198 (70%)	0.46	3 (2%) 62 53	90, 116, 141, 168	0
2	J	141/198 (71%)	0.47	5 (3%) 44 35	91, 116, 149, 159	0
2	L	139/198 (70%)	0.60	7 (5%) 30 24	94, 114, 147, 165	0
3	M	213/245 (86%)	0.98	39 (18%) 1 2	84, 118, 205, 218	0
3	O	213/245 (86%)	0.40	9 (4%) 37 29	80, 106, 139, 149	0
3	Q	213/245 (86%)	0.99	42 (19%) 1 2	86, 117, 154, 177	0
3	S	214/245 (87%)	0.56	14 (6%) 20 14	76, 103, 151, 170	0
3	U	215/245 (87%)	1.04	43 (20%) 1 2	88, 123, 190, 208	0
3	W	214/245 (87%)	1.12	46 (21%) 1 2	93, 134, 180, 195	0
4	N	207/289 (71%)	1.34	57 (27%) 1 1	90, 142, 213, 233	0
4	P	207/289 (71%)	0.54	10 (4%) 31 25	75, 105, 129, 143	0
4	R	208/289 (71%)	1.57	74 (35%) 0 1	95, 125, 189, 214	0
4	T	208/289 (71%)	0.60	11 (5%) 27 22	82, 96, 109, 113	0
4	V	205/289 (70%)	1.17	42 (20%) 1 2	89, 124, 167, 185	0
4	X	206/289 (71%)	0.89	31 (15%) 3 3	83, 118, 146, 158	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
All	All	5146/6360 (80%)	0.83	672 (13%) 4 4	72, 116, 174, 233	0

All (672) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	M	153	TRP	10.6
1	C	328	SER	8.1
3	W	137	LEU	6.5
4	R	10	GLY	6.4
4	N	139	ALA	6.3
3	U	153	TRP	6.2
4	N	138	ALA	6.1
3	W	184	SER	6.1
4	V	213	VAL	5.8
1	A	244	LYS	5.7
1	A	245	PRO	5.6
3	W	200	VAL	5.5
1	K	73	LYS	5.5
4	X	180	LEU	5.5
4	N	10	GLY	5.4
3	W	183	LEU	5.3
3	W	120	VAL	5.2
3	W	138	VAL	5.2
3	S	137	LEU	5.1
1	K	92	LYS	5.1
3	W	199	GLN	4.9
1	I	243	LEU	4.9
4	R	156	TRP	4.9
4	R	196	TYR	4.8
4	N	11	VAL	4.8
4	R	121	PRO	4.7
1	I	303	ASN	4.7
1	A	299	ILE	4.7
1	G	71	SER	4.7
3	U	190	TRP	4.7
4	X	143	LEU	4.7
3	M	138	VAL	4.6
4	X	181	SER	4.6
1	A	300	CYS	4.6
4	X	122	SER	4.6
3	W	206	THR	4.6
3	M	122	LEU	4.6

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Mol	Chain	Res	Type	RSRZ
1	K	305	SER	4.6
3	U	187	PRO	4.6
3	M	188	GLU	4.5
3	U	125	PRO	4.5
3	W	151	VAL	4.5
4	N	181	SER	4.5
4	V	122	SER	4.5
4	V	121	PRO	4.5
4	R	213	VAL	4.4
3	U	1	GLN	4.4
1	I	52	THR	4.3
4	N	23	ALA	4.3
3	W	201	THR	4.3
3	W	121	THR	4.3
4	R	212	LYS	4.3
4	R	163	SER	4.3
4	N	143	LEU	4.3
1	E	289	VAL	4.3
1	A	306	ILE	4.3
3	M	190	TRP	4.2
4	R	122	SER	4.2
1	K	95	GLU	4.2
4	X	18	LEU	4.2
2	J	182	HIS	4.2
4	N	123	VAL	4.2
1	K	328	SER	4.2
3	W	182	TYR	4.2
3	W	181	SER	4.1
4	X	201	ASN	4.1
3	U	159	PRO	4.1
1	G	168	VAL	4.1
1	C	327	CYS	4.1
4	X	118	THR	4.1
1	E	61	THR	4.0
3	M	123	PHE	4.0
1	C	295	SER	4.0
4	N	144	VAL	4.0
3	W	119	SER	4.0
4	N	124	PHE	4.0
3	U	198	CYS	4.0
4	R	153	THR	4.0
4	R	154	VAL	4.0

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Mol	Chain	Res	Type	RSRZ
1	E	324	SER	4.0
4	R	181	SER	3.9
1	I	300	CYS	3.9
3	M	197	SER	3.9
1	I	146	THR	3.9
4	N	118	THR	3.9
1	G	72	GLY	3.9
4	V	156	TRP	3.9
4	N	191	LEU	3.9
3	U	161	LYS	3.8
3	Q	125	PRO	3.8
4	N	126	LEU	3.8
4	R	182	SER	3.8
3	Q	138	VAL	3.8
2	L	49	PRO	3.8
4	N	121	PRO	3.8
1	A	252	VAL	3.8
3	W	126	SER	3.8
1	A	276	GLN	3.8
4	V	123	VAL	3.7
2	J	57	ARG	3.7
1	C	306	ILE	3.7
4	R	142	CYS	3.7
3	Q	153	TRP	3.7
1	E	243	LEU	3.7
3	M	182	TYR	3.7
4	R	9	GLY	3.7
1	A	328	SER	3.7
4	X	179	SER	3.6
4	N	24	ALA	3.6
3	U	182	TYR	3.6
1	E	303	ASN	3.6
3	W	150	THR	3.6
1	C	254	VAL	3.6
3	Q	131	GLN	3.6
1	I	241	LEU	3.6
1	G	214	ALA	3.6
1	E	241	LEU	3.6
1	I	299	ILE	3.6
3	U	137	LEU	3.6
4	R	11	VAL	3.6
2	L	135	LEU	3.6

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Mol	Chain	Res	Type	RSRZ
3	Q	212	ALA	3.6
4	V	143	LEU	3.6
4	V	145	LYS	3.6
4	N	79	LEU	3.5
4	P	181	SER	3.5
4	X	144	VAL	3.5
1	K	74	THR	3.5
4	N	12	VAL	3.5
1	K	97	LEU	3.5
1	I	328	SER	3.5
4	R	171	VAL	3.5
4	N	140	LEU	3.5
3	U	160	VAL	3.5
3	Q	123	PHE	3.5
4	R	124	PHE	3.5
1	I	304	ALA	3.5
3	W	125	PRO	3.5
4	V	125	PRO	3.5
4	R	150	GLU	3.5
1	I	288	ARG	3.5
1	I	186	GLU	3.5
4	R	123	VAL	3.5
1	K	243	LEU	3.4
1	C	166	GLN	3.4
3	M	186	THR	3.4
3	U	185	LEU	3.4
1	K	59	THR	3.4
4	N	185	THR	3.4
4	P	112	THR	3.4
4	V	124	PHE	3.4
4	V	119	LYS	3.4
3	U	162	ALA	3.4
3	Q	180	SER	3.4
4	R	201	ASN	3.4
3	Q	196	TYR	3.4
4	V	196	TYR	3.4
1	K	307	SER	3.4
3	U	184	SER	3.3
1	K	23	ILE	3.3
1	K	72	GLY	3.3
3	U	151	VAL	3.3
1	E	288	ARG	3.3

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
3	M	137	LEU	3.3
3	M	154	LYS	3.3
4	V	148	PHE	3.3
3	U	136	THR	3.3
3	U	189	GLN	3.3
4	R	166	HIS	3.3
4	R	165	VAL	3.3
1	E	88	TYR	3.3
3	M	194	ARG	3.3
1	C	201	ALA	3.3
4	R	125	PRO	3.3
1	I	327	CYS	3.3
3	M	162	ALA	3.3
1	K	242	GLN	3.2
3	M	159	PRO	3.2
3	U	206	THR	3.2
4	N	34	MET	3.2
3	W	207	VAL	3.2
1	I	308	VAL	3.2
1	K	105	HIS	3.2
3	M	210	THR	3.2
1	K	310	ALA	3.2
1	K	79	VAL	3.2
4	R	194	GLN	3.2
3	M	139	CYS	3.2
4	T	122	SER	3.2
3	O	121	THR	3.2
1	G	64	GLN	3.2
1	A	275	VAL	3.2
1	I	73	LYS	3.2
1	I	245	PRO	3.1
4	N	117	SER	3.1
3	M	181	SER	3.1
1	C	296	ALA	3.1
4	V	178	TYR	3.1
3	W	115	LYS	3.1
4	N	186	VAL	3.1
1	A	288	ARG	3.1
1	E	298	VAL	3.1
2	B	149	SER	3.1
3	W	12	GLY	3.1
4	V	214	GLU	3.1

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Mol	Chain	Res	Type	RSRZ
1	K	54	GLU	3.1
2	L	50	LEU	3.1
4	N	146	ASP	3.1
1	A	214	ALA	3.1
1	K	306	ILE	3.1
1	K	49	THR	3.1
3	Q	46	LYS	3.1
4	R	112	THR	3.1
1	C	255	SER	3.1
2	H	50	LEU	3.0
3	Q	120	VAL	3.0
4	V	193	THR	3.0
4	N	116	ALA	3.0
4	V	181	SER	3.0
3	Q	47	LEU	3.0
1	I	274	CYS	3.0
3	Q	124	PRO	3.0
3	W	160	VAL	3.0
3	U	158	SER	3.0
4	R	198	CYS	3.0
1	G	146	THR	3.0
1	E	261	THR	3.0
1	I	201	ALA	3.0
4	N	180	LEU	3.0
1	C	79	VAL	3.0
3	U	188	GLU	3.0
4	N	4	LEU	3.0
1	I	31	TYR	3.0
1	I	258	TYR	3.0
2	D	189	PRO	3.0
4	X	112	THR	3.0
4	V	152	VAL	3.0
4	T	129	SER	3.0
3	M	161	LYS	3.0
3	Q	181	SER	2.9
4	P	144	VAL	2.9
3	W	153	TRP	2.9
1	K	276	GLN	2.9
4	N	125	PRO	2.9
1	K	52	THR	2.9
3	S	138	VAL	2.9
4	V	186	VAL	2.9

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Mol	Chain	Res	Type	RSRZ
1	G	55	GLU	2.9
1	C	305	SER	2.9
3	U	37	TYR	2.9
2	L	134	LEU	2.9
4	R	144	VAL	2.9
3	O	137	LEU	2.9
3	O	136	THR	2.9
1	G	67	GLU	2.9
1	K	104	LEU	2.9
4	R	24	ALA	2.9
4	R	143	LEU	2.9
1	C	80	LYS	2.9
1	E	254	VAL	2.9
2	H	186	THR	2.9
4	R	126	LEU	2.9
1	I	325	VAL	2.9
3	Q	211	VAL	2.9
1	K	70	GLY	2.9
4	R	170	ALA	2.9
2	J	189	PRO	2.9
4	V	109	THR	2.9
3	W	149	VAL	2.9
2	J	138	GLU	2.9
3	S	205	SER	2.9
3	S	183	LEU	2.8
1	C	307	SER	2.8
1	E	107	LYS	2.8
4	X	124	PHE	2.8
3	U	124	PRO	2.8
3	M	192	SER	2.8
1	K	245	PRO	2.8
4	R	139	ALA	2.8
3	S	140	LEU	2.8
3	Q	197	SER	2.8
4	V	120	GLY	2.8
1	E	306	ILE	2.8
1	I	134	LYS	2.8
4	N	196	TYR	2.8
4	X	184	VAL	2.8
3	W	139	CYS	2.8
1	K	268	TYR	2.8
4	R	209	VAL	2.8

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Mol	Chain	Res	Type	RSRZ
1	C	276	GLN	2.8
3	U	133	ASN	2.8
1	I	242	GLN	2.8
4	R	36	TRP	2.8
4	N	137	THR	2.8
3	Q	193	HIS	2.8
4	R	200	VAL	2.8
1	G	158	SER	2.8
4	X	111	VAL	2.8
2	F	135	LEU	2.8
1	E	297	THR	2.8
3	W	196	TYR	2.7
3	W	147	GLY	2.7
4	X	182	SER	2.7
1	G	104	LEU	2.7
1	E	305	SER	2.7
3	S	151	VAL	2.7
1	G	211	MET	2.7
1	K	91	HIS	2.7
1	G	189	TYR	2.7
4	X	141	GLY	2.7
3	Q	201	THR	2.7
4	N	112	THR	2.7
1	E	89	THR	2.7
3	W	210	THR	2.7
4	N	95	TYR	2.7
4	V	168	PHE	2.7
1	G	263	SER	2.7
3	Q	184	SER	2.7
3	W	159	PRO	2.7
3	S	215	GLU	2.7
3	Q	190	TRP	2.7
1	G	50	CYS	2.7
4	N	145	LYS	2.7
3	W	133	ASN	2.7
4	N	147	TYR	2.7
1	E	272	THR	2.7
3	U	197	SER	2.7
1	G	88	TYR	2.7
3	Q	141	ILE	2.7
1	K	106	LYS	2.7
1	G	278	GLN	2.7

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Mol	Chain	Res	Type	RSRZ
1	I	255	SER	2.7
4	N	83	MET	2.7
4	R	211	LYS	2.7
4	R	210	ASP	2.6
4	R	161	LEU	2.6
3	Q	126	SER	2.6
3	Q	182	TYR	2.6
3	W	141	ILE	2.6
1	A	55	GLU	2.6
3	M	183	LEU	2.6
4	R	162	THR	2.6
1	K	48	LEU	2.6
3	Q	214	THR	2.6
3	M	155	ALA	2.6
4	X	128	PRO	2.6
4	V	183	VAL	2.6
2	F	82	LEU	2.6
3	U	122	LEU	2.6
1	C	275	VAL	2.6
1	K	235	PRO	2.6
4	R	129	SER	2.6
2	F	182	HIS	2.6
1	E	35	LEU	2.6
4	R	35	HIS	2.6
1	G	145	LEU	2.6
4	R	94	TYR	2.6
4	V	45	LEU	2.6
4	X	117	SER	2.6
3	W	178	ALA	2.6
1	I	203	GLU	2.6
3	U	155	ALA	2.6
4	T	181	SER	2.6
1	K	326	PRO	2.6
3	S	214	THR	2.6
1	K	241	LEU	2.6
3	U	135	ALA	2.6
4	X	157	ASN	2.5
1	E	277	VAL	2.5
4	V	144	VAL	2.5
2	H	187	LEU	2.5
3	Q	171	LYS	2.5
4	R	89	GLU	2.5

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	A	69	LEU	2.5
1	I	102	LEU	2.5
1	I	306	ILE	2.5
3	Q	154	LYS	2.5
1	C	55	GLU	2.5
4	V	195	THR	2.5
1	K	69	LEU	2.5
1	C	277	VAL	2.5
1	E	325	VAL	2.5
3	M	127	SER	2.5
4	V	34	MET	2.5
3	W	136	THR	2.5
4	N	122	SER	2.5
1	A	243	LEU	2.5
1	I	101	LEU	2.5
1	K	218	LEU	2.5
1	K	46	VAL	2.5
4	V	167	THR	2.5
1	K	296	ALA	2.5
4	N	142	CYS	2.5
3	Q	128	GLU	2.5
1	E	307	SER	2.5
1	G	70	GLY	2.5
1	C	77	ILE	2.5
4	R	195	THR	2.5
1	A	256	TRP	2.5
4	T	143	LEU	2.5
4	R	80	TYR	2.5
4	R	99	HIS	2.5
3	M	152	ALA	2.5
3	Q	130	LEU	2.5
4	X	113	VAL	2.5
3	O	123	PHE	2.5
4	X	94	TYR	2.5
4	V	210	ASP	2.5
1	G	299	ILE	2.5
1	G	306	ILE	2.5
1	G	323	ALA	2.5
1	I	298	VAL	2.5
1	E	271	LEU	2.5
1	E	252	VAL	2.5
3	M	151	VAL	2.5

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Mol	Chain	Res	Type	RSRZ
3	W	192	SER	2.5
4	R	159	GLY	2.5
2	F	50	LEU	2.5
1	A	253	GLU	2.5
1	G	238	PRO	2.5
3	M	133	ASN	2.5
1	I	289	VAL	2.5
1	K	214	ALA	2.5
3	M	120	VAL	2.5
3	U	208	GLU	2.4
3	Q	192	SER	2.4
3	U	195	SER	2.4
4	N	182	SER	2.4
3	Q	135	ALA	2.4
3	W	123	PHE	2.4
4	R	105	TRP	2.4
1	K	93	GLY	2.4
3	S	185	LEU	2.4
3	M	191	LYS	2.4
3	Q	136	THR	2.4
4	R	146	ASP	2.4
4	R	158	SER	2.4
3	M	115	LYS	2.4
3	W	122	LEU	2.4
1	C	310	ALA	2.4
3	S	206	THR	2.4
4	N	19	ARG	2.4
3	M	136	THR	2.4
4	N	156	TRP	2.4
3	O	135	ALA	2.4
1	K	269	PHE	2.4
3	Q	139	CYS	2.4
1	A	325	VAL	2.4
1	G	60	TRP	2.4
4	V	206	ASN	2.4
1	G	151	ASP	2.4
4	N	148	PHE	2.4
3	U	152	ALA	2.4
4	V	13	GLN	2.4
3	S	136	THR	2.4
4	R	179	SER	2.4
1	E	273	PHE	2.4

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
4	N	214	GLU	2.4
1	C	63	ASP	2.4
3	M	147	GLY	2.4
1	I	276	GLN	2.4
3	W	198	CYS	2.4
1	G	215	VAL	2.4
1	K	29	ASP	2.4
3	S	122	LEU	2.4
1	E	310	ALA	2.4
1	E	299	ILE	2.4
3	U	76	ILE	2.4
3	W	140	LEU	2.4
1	K	233	ILE	2.3
4	V	176	GLY	2.3
1	G	66	SER	2.3
1	E	87	GLN	2.3
4	T	180	LEU	2.3
1	A	324	SER	2.3
3	M	158	SER	2.3
3	W	142	SER	2.3
1	I	275	VAL	2.3
4	R	152	VAL	2.3
4	T	144	VAL	2.3
3	O	122	LEU	2.3
4	P	10	GLY	2.3
1	A	307	SER	2.3
3	W	48	LEU	2.3
4	R	119	LYS	2.3
3	Q	198	CYS	2.3
1	E	275	VAL	2.3
4	N	36	TRP	2.3
4	T	145	LYS	2.3
4	N	89	GLU	2.3
4	R	140	LEU	2.3
1	K	71	SER	2.3
4	V	36	TRP	2.3
4	R	23	ALA	2.3
1	C	52	THR	2.3
1	I	244	LYS	2.3
4	R	208	LYS	2.3
1	E	328	SER	2.3
3	O	195	SER	2.3

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Mol	Chain	Res	Type	RSRZ
4	N	21	SER	2.3
4	X	163	SER	2.3
4	N	109	THR	2.3
1	C	242	GLN	2.3
3	M	187	PRO	2.3
4	R	167	THR	2.3
1	E	296	ALA	2.3
4	P	166	HIS	2.3
1	A	258	TYR	2.3
3	O	139	CYS	2.3
3	Q	122	LEU	2.3
1	K	146	THR	2.3
4	R	91	THR	2.3
4	V	177	LEU	2.3
4	T	182	SER	2.3
1	E	240	ASN	2.3
3	U	186	THR	2.3
4	R	95	TYR	2.3
3	W	23	SER	2.3
3	Q	38	GLN	2.2
3	U	171	LYS	2.2
4	R	106	GLY	2.2
4	X	129	SER	2.2
1	K	60	TRP	2.2
4	X	81	LEU	2.2
1	E	290	PHE	2.2
3	Q	63	PHE	2.2
3	Q	129	GLU	2.2
4	R	214	GLU	2.2
4	X	89	GLU	2.2
4	R	190	SER	2.2
1	K	75	LEU	2.2
3	Q	155	ALA	2.2
4	N	206	ASN	2.2
4	P	35	HIS	2.2
1	A	298	VAL	2.2
1	G	298	VAL	2.2
4	N	171	VAL	2.2
1	I	272	THR	2.2
4	N	192	GLY	2.2
1	G	85	ALA	2.2
4	P	129	SER	2.2

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Mol	Chain	Res	Type	RSRZ
3	W	191	LYS	2.2
1	K	162	SER	2.2
4	N	158	SER	2.2
2	L	52	GLY	2.2
1	I	64	GLN	2.2
2	B	54	MET	2.2
4	R	3	GLN	2.2
4	V	118	THR	2.2
1	K	107	LYS	2.2
4	R	155	SER	2.2
1	G	144	TRP	2.2
4	X	153	THR	2.2
3	M	208	GLU	2.2
3	Q	162	ALA	2.2
1	E	315	TYR	2.2
1	K	55	GLU	2.2
3	W	205	SER	2.2
4	X	142	CYS	2.2
1	K	120	GLN	2.2
1	E	258	TYR	2.2
1	A	277	VAL	2.2
1	G	167	GLY	2.2
1	G	241	LEU	2.2
3	Q	121	THR	2.2
4	V	126	LEU	2.2
1	C	273	PHE	2.2
3	M	90	GLN	2.2
3	Q	151	VAL	2.2
4	X	99	HIS	2.2
1	E	308	VAL	2.2
2	B	50	LEU	2.2
1	G	301	ARG	2.2
4	V	187	PRO	2.2
1	E	276	GLN	2.2
1	G	156	VAL	2.2
3	U	38	GLN	2.2
3	M	157	SER	2.2
4	P	190	SER	2.2
1	G	243	LEU	2.2
4	N	3	GLN	2.2
4	R	177	LEU	2.2
1	A	305	SER	2.2

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Mol	Chain	Res	Type	RSRZ
1	K	129	LEU	2.2
4	V	94	TYR	2.2
4	P	214	GLU	2.2
4	N	149	PRO	2.1
1	A	301	ARG	2.1
1	G	155	SER	2.1
4	N	184	VAL	2.1
4	P	143	LEU	2.1
4	R	78	THR	2.1
4	X	125	PRO	2.1
3	U	138	VAL	2.1
1	K	240	ASN	2.1
3	W	146	PRO	2.1
1	K	103	LEU	2.1
3	M	196	TYR	2.1
4	V	197	ILE	2.1
1	K	76	THR	2.1
2	J	71	ILE	2.1
4	R	191	LEU	2.1
4	R	197	ILE	2.1
1	A	106	LYS	2.1
1	E	323	ALA	2.1
1	G	56	ASP	2.1
3	U	196	TYR	2.1
1	I	188	GLU	2.1
1	K	198	ALA	2.1
3	S	184	SER	2.1
4	V	194	GLN	2.1
1	G	103	LEU	2.1
1	I	61	THR	2.1
4	V	80	TYR	2.1
4	N	164	GLY	2.1
4	T	86	LEU	2.1
4	R	149	PRO	2.1
1	I	273	PHE	2.1
1	K	154	PHE	2.1
1	A	242	GLN	2.1
4	R	178	TYR	2.1
3	M	211	VAL	2.1
3	Q	147	GLY	2.1
3	W	166	THR	2.1
1	E	228	PHE	2.1

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Mol	Chain	Res	Type	RSRZ
3	U	123	PHE	2.1
1	K	33	VAL	2.1
3	U	211	VAL	2.1
1	I	140	PHE	2.1
4	R	145	LYS	2.1
1	G	186	GLU	2.1
2	D	187	LEU	2.1
4	N	81	LEU	2.1
4	N	165	VAL	2.1
4	X	20	LEU	2.1
3	U	194	ARG	2.1
4	R	205	SER	2.0
4	V	208	LYS	2.0
2	L	184	ALA	2.0
1	I	51	ASP	2.0
1	E	60	TRP	2.0
3	Q	142	SER	2.0
4	V	71	SER	2.0
3	M	185	LEU	2.0
3	U	200	VAL	2.0
4	N	48	VAL	2.0
4	R	168	PHE	2.0
2	F	30	TRP	2.0
1	C	274	CYS	2.0
3	W	172	GLN	2.0
4	T	141	GLY	2.0
4	X	164	GLY	2.0
4	N	127	ALA	2.0
4	R	157	ASN	2.0
1	E	262	TRP	2.0
3	W	190	TRP	2.0
1	E	239	LYS	2.0
3	S	100	LEU	2.0
3	U	164	VAL	2.0
4	T	149	PRO	2.0
1	K	45	MET	2.0
1	K	304	ALA	2.0
1	G	187	TYR	2.0
3	M	160	VAL	2.0
3	O	200	VAL	2.0
4	X	196	TYR	2.0
1	C	297	THR	2.0

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Mol	Chain	Res	Type	RSRZ
2	D	186	THR	2.0
3	U	199	GLN	2.0
1	C	106	LYS	2.0
2	L	97	LEU	2.0
3	U	191	LYS	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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> 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	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
8	SO4	O	302	5/5	0.79	0.44	3.26	180,180,184,184	0
8	SO4	U	302	5/5	0.78	0.36	0.59	174,174,175,177	0
8	SO4	S	302	5/5	0.89	0.29	0.19	152,153,154,155	0
8	SO4	R	301	5/5	0.83	0.30	0.14	178,179,180,180	0
8	SO4	M	301	5/5	0.85	0.29	-0.26	157,158,158,159	0
8	SO4	W	302	5/5	0.82	0.24	-0.50	184,184,185,188	0
5	NAG	C	401	14/15	0.92	0.20	-1.19	65,66,69,69	0
5	NAG	K	401	14/15	0.89	0.23	-1.34	99,101,103,104	0
5	NAG	E	401	14/15	0.91	0.25	-1.35	92,95,101,101	0
5	NAG	I	401	14/15	0.91	0.24	-1.40	74,75,77,78	0
5	NAG	G	401	14/15	0.91	0.24	-1.47	75,77,78,79	0
5	NAG	A	401	14/15	0.95	0.24	-1.47	91,96,99,100	0
7	MAN	I	405	11/12	0.82	0.27	-	88,90,96,97	0
7	MAN	K	404	11/12	0.72	0.28	-	120,123,126,128	0
6	BMA	I	403	11/12	0.86	0.20	-	87,90,96,97	0
6	BMA	K	403	11/12	0.84	0.21	-	113,114,119,120	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
5	NAG	G	402	14/15	0.90	0.14	-	80,81,84,85	0
8	SO4	Q	301	5/5	0.90	0.32	-	188,189,189,190	0
8	SO4	O	301	5/5	0.92	0.39	-	141,141,141,141	0
6	BMA	G	403	11/12	0.85	0.21	-	87,90,93,94	0
5	NAG	A	402	14/15	0.90	0.20	-	98,100,101,103	0
7	MAN	C	405	11/12	0.82	0.25	-	80,83,87,87	0
7	MAN	A	405	11/12	0.77	0.28	-	105,107,108,109	0
6	BMA	A	403	11/12	0.82	0.25	-	101,103,104,104	0
7	MAN	G	404	11/12	0.80	0.24	-	91,97,106,109	0
7	MAN	E	404	11/12	0.80	0.22	-	111,114,122,122	0
8	SO4	W	301	5/5	0.85	0.33	-	179,179,181,182	0
7	MAN	I	404	11/12	0.85	0.25	-	97,100,104,105	0
8	SO4	M	302	5/5	0.79	0.32	-	175,176,176,176	0
5	NAG	C	402	14/15	0.87	0.19	-	69,71,73,75	0
6	BMA	E	403	11/12	0.86	0.23	-	104,107,111,112	0
6	BMA	C	403	11/12	0.83	0.21	-	76,79,81,81	0
5	NAG	E	402	14/15	0.93	0.23	-	98,100,102,103	0
7	MAN	G	405	11/12	0.77	0.32	-	92,93,103,105	0
8	SO4	S	303	5/5	0.90	0.33	-	146,146,147,150	0
7	MAN	E	405	11/12	0.54	0.40	-	110,113,118,119	0
7	MAN	A	404	11/12	0.79	0.29	-	103,105,108,109	0
7	MAN	C	404	11/12	0.78	0.30	-	81,83,87,88	0
5	NAG	K	402	14/15	0.88	0.29	-	103,106,110,112	0
7	MAN	K	405	11/12	0.70	0.27	-	115,117,121,122	0
5	NAG	I	402	14/15	0.91	0.16	-	78,80,83,84	0
8	SO4	S	301	5/5	0.88	0.27	-	146,146,147,147	0
8	SO4	U	301	5/5	0.86	0.42	-	180,181,182,183	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.