



# Full wwPDB X-ray Structure Validation Report ⓘ

Oct 11, 2023 – 04:18 PM EDT

PDB ID : 7S11  
Title : Crystal structure of Fab in complex with mouse CD96 monomer  
Authors : Lee, P.S.; Chau, B.; Strop, P.  
Deposited on : 2021-08-31  
Resolution : 2.58 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

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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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 : 1.8.5 (274361), CSD as541be (2020)  
Xtrriage (Phenix) : 1.13  
EDS : 2.35.1  
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) : 2.35.1

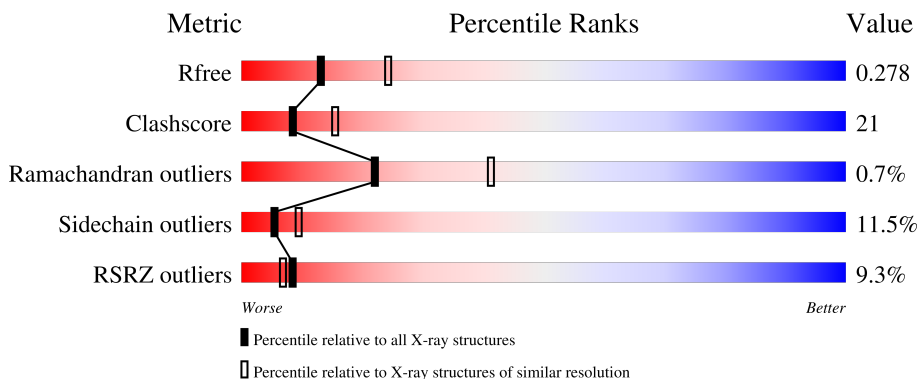
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.58 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	3676 (2.60-2.56)
Clashscore	141614	4049 (2.60-2.56)
Ramachandran outliers	138981	3979 (2.60-2.56)
Sidechain outliers	138945	3979 (2.60-2.56)
RSRZ outliers	127900	3614 (2.60-2.56)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	C	122	
1	D	122	
1	E	122	
1	F	122	
2	H	229	

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Mol	Chain	Length	Quality of chain
2	I	229	
2	J	229	
2	K	229	
3	L	216	
3	M	216	
3	N	216	
3	O	216	

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
3	PCA	M	1	-	-	-	X

## 2 Entry composition i

There are 5 unique types of molecules in this entry. The entry contains 16283 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 T-cell surface protein tactile.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	C	113	897	572	142	177	6	0	0	0
1	D	113	897	572	142	177	6	0	0	0
1	E	95	753	482	119	146	6	0	0	0
1	F	102	810	517	128	159	6	0	0	0

There are 28 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	139	GLY	-	expression tag	UNP Q3U0X8
C	140	HIS	-	expression tag	UNP Q3U0X8
C	141	HIS	-	expression tag	UNP Q3U0X8
C	142	HIS	-	expression tag	UNP Q3U0X8
C	143	HIS	-	expression tag	UNP Q3U0X8
C	144	HIS	-	expression tag	UNP Q3U0X8
C	145	HIS	-	expression tag	UNP Q3U0X8
D	139	GLY	-	expression tag	UNP Q3U0X8
D	140	HIS	-	expression tag	UNP Q3U0X8
D	141	HIS	-	expression tag	UNP Q3U0X8
D	142	HIS	-	expression tag	UNP Q3U0X8
D	143	HIS	-	expression tag	UNP Q3U0X8
D	144	HIS	-	expression tag	UNP Q3U0X8
D	145	HIS	-	expression tag	UNP Q3U0X8
E	139	GLY	-	expression tag	UNP Q3U0X8
E	140	HIS	-	expression tag	UNP Q3U0X8
E	141	HIS	-	expression tag	UNP Q3U0X8
E	142	HIS	-	expression tag	UNP Q3U0X8
E	143	HIS	-	expression tag	UNP Q3U0X8
E	144	HIS	-	expression tag	UNP Q3U0X8
E	145	HIS	-	expression tag	UNP Q3U0X8

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Chain	Residue	Modelled	Actual	Comment	Reference
F	139	GLY	-	expression tag	UNP Q3U0X8
F	140	HIS	-	expression tag	UNP Q3U0X8
F	141	HIS	-	expression tag	UNP Q3U0X8
F	142	HIS	-	expression tag	UNP Q3U0X8
F	143	HIS	-	expression tag	UNP Q3U0X8
F	144	HIS	-	expression tag	UNP Q3U0X8
F	145	HIS	-	expression tag	UNP Q3U0X8

- Molecule 2 is a protein called Fab heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	H	218	Total	C	N	O	S	0	0	0
			1630	1027	273	322	8			
2	I	214	Total	C	N	O	S	0	0	0
			1603	1012	268	315	8			
2	J	219	Total	C	N	O	S	0	0	0
			1636	1030	274	324	8			
2	K	218	Total	C	N	O	S	0	0	0
			1630	1027	273	322	8			

- Molecule 3 is a protein called Fab light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	L	212	Total	C	N	O	S	0	0	0
			1591	996	268	323	4			
3	M	211	Total	C	N	O	S	0	0	0
			1582	991	266	321	4			
3	N	215	Total	C	N	O	S	0	0	0
			1614	1009	272	329	4			
3	O	211	Total	C	N	O	S	0	0	0
			1582	991	267	320	4			

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: C<sub>8</sub>H<sub>15</sub>NO<sub>6</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	
			Total	C	N			O
4	C	1	14	8	1	5	0	0
4	D	1	14	8	1	5	0	0

- Molecule 5 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf	
			O	S			
5	C	1	5	4	1	0	0
5	L	1	5	4	1	0	0

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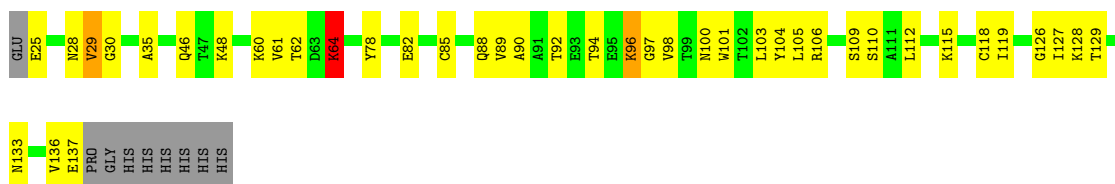
<b>Mol</b>	<b>Chain</b>	<b>Residues</b>	<b>Atoms</b>			<b>ZeroOcc</b>	<b>AltConf</b>
5	D	1	Total	O	S	0	0
			5	4	1		
5	D	1	Total	O	S	0	0
			5	4	1		
5	N	1	Total	O	S	0	0
			5	4	1		
5	K	1	Total	O	S	0	0
			5	4	1		

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

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

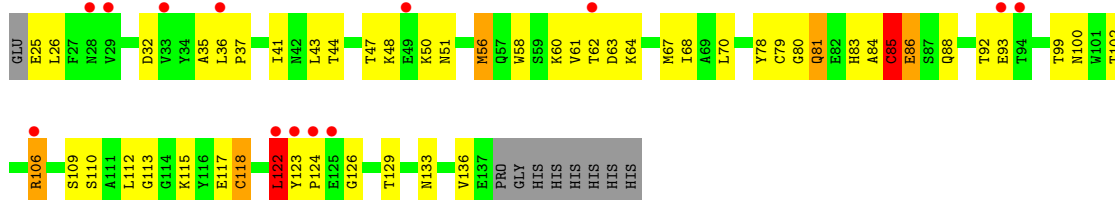
- Molecule 1: T-cell surface protein tactile

Chain C:  59% 31% 7%



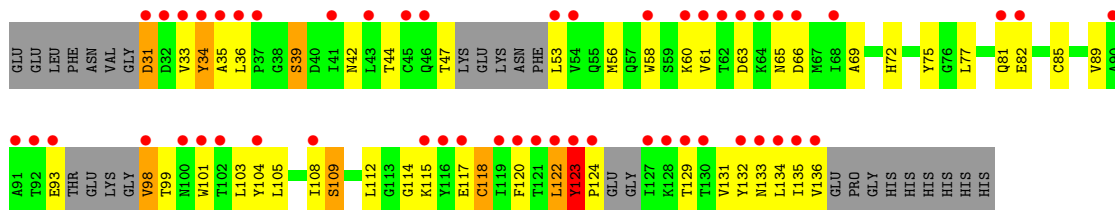
- Molecule 1: T-cell surface protein tactile

Chain D:  11% 50% 37% 7%



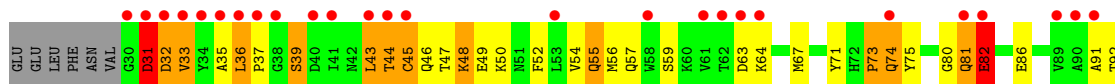
- Molecule 1: T-cell surface protein tactile

Chain E:  43% 37% 34% 6% 22%



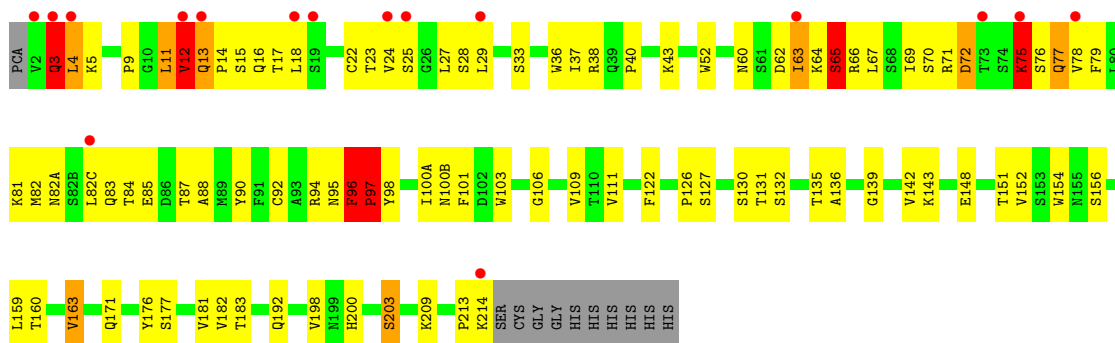
- Molecule 1: T-cell surface protein tactile

Chain F:  40% 35% 30% 14% 16%

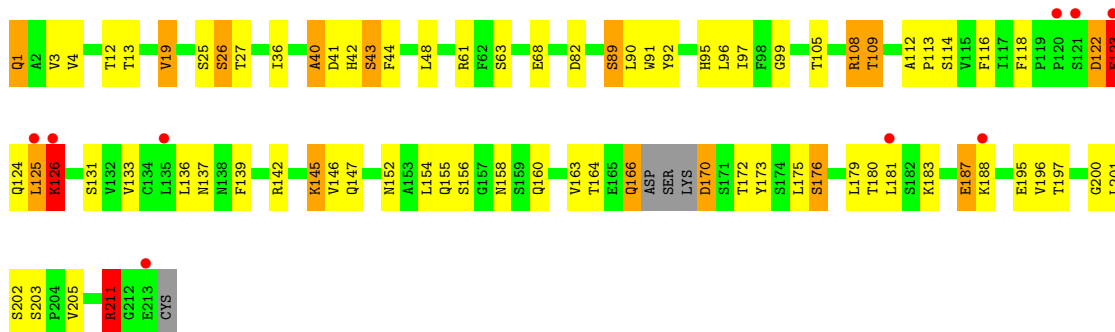




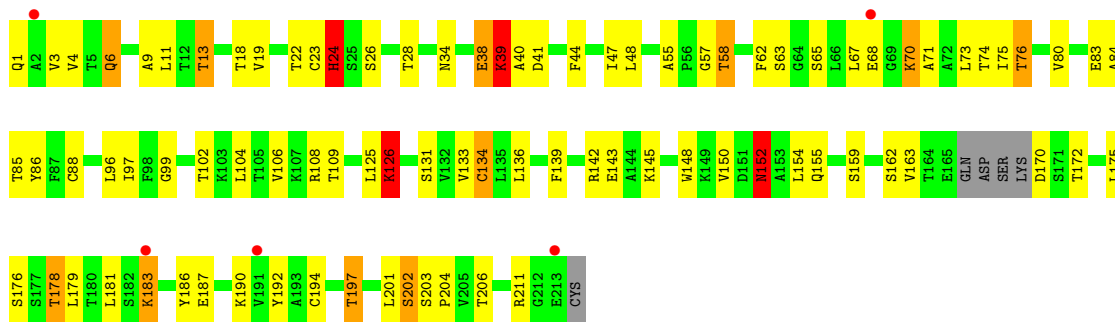




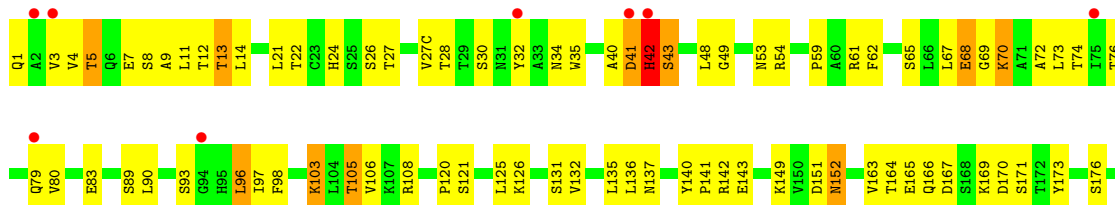
• Molecule 3: Fab light chain



• Molecule 3: Fab light chain

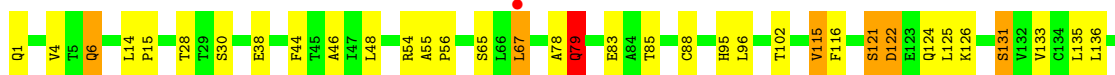


• Molecule 3: Fab light chain





- Molecule 3: Fab light chain



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	124.93Å 154.89Å 306.00Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	61.20 – 2.58 61.20 – 2.58	Depositor EDS
% Data completeness (in resolution range)	63.8 (61.20-2.58) 63.8 (61.20-2.58)	Depositor EDS
$R_{merge}$	0.20	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.49 (at 2.58Å)	Xtrriage
Refinement program	PHENIX 1.19.1_4122	Depositor
R, $R_{free}$	0.226 , 0.279 0.227 , 0.278	Depositor DCC
$R_{free}$ test set	2923 reflections (4.90%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	55.2	Xtrriage
Anisotropy	0.064	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 35.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	16283	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	50.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.03% 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 i

### 5.1 Standard geometry i

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	C	0.65	0/916	0.77	0/1245
1	D	0.71	3/916 (0.3%)	1.23	6/1245 (0.5%)
1	E	0.43	0/767	0.66	0/1043
1	F	0.71	3/827 (0.4%)	2.11	26/1123 (2.3%)
2	H	0.66	0/1669	1.07	13/2276 (0.6%)
2	I	0.67	0/1641	1.01	14/2238 (0.6%)
2	J	0.57	0/1675	0.98	10/2284 (0.4%)
2	K	0.70	4/1669 (0.2%)	1.07	14/2276 (0.6%)
3	L	0.77	6/1616 (0.4%)	1.05	13/2201 (0.6%)
3	M	0.82	5/1607 (0.3%)	1.13	15/2189 (0.7%)
3	N	0.63	3/1640 (0.2%)	1.05	10/2234 (0.4%)
3	O	0.56	0/1607	0.92	10/2189 (0.5%)
All	All	0.67	24/16550 (0.1%)	1.10	131/22543 (0.6%)

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	C	0	1
1	D	0	2
1	E	0	2
1	F	1	4
2	H	0	3
2	I	0	3
2	J	0	2
2	K	0	4
3	L	0	3
3	M	0	4
3	N	0	2

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Mol	Chain	#Chirality outliers	#Planarity outliers
3	O	0	1
All	All	1	31

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	M	126	LYS	CD-CE	11.07	1.78	1.51
3	L	126	LYS	CE-NZ	9.79	1.73	1.49
3	M	68	GLU	CD-OE2	9.41	1.36	1.25
2	K	77	GLN	CA-CB	8.80	1.73	1.53
3	L	123	GLU	CG-CD	8.40	1.64	1.51
2	K	75	LYS	CG-CD	-8.03	1.25	1.52
3	M	68	GLU	CG-CD	-7.67	1.40	1.51
3	N	126	LYS	CB-CG	6.89	1.71	1.52
3	L	123	GLU	CD-OE2	6.63	1.32	1.25
3	M	126	LYS	CE-NZ	6.33	1.64	1.49
3	L	123	GLU	CB-CG	-6.08	1.40	1.52
3	N	68	GLU	CB-CG	5.79	1.63	1.52
1	D	106	ARG	CG-CD	5.68	1.66	1.51
2	K	3	GLN	CB-CG	5.61	1.67	1.52
1	F	82	GLU	CD-OE2	5.58	1.31	1.25
3	L	145	LYS	CB-CG	-5.56	1.37	1.52
3	M	68	GLU	CB-CG	-5.45	1.41	1.52
3	L	19	VAL	CB-CG1	-5.44	1.41	1.52
3	N	103	LYS	CD-CE	5.39	1.64	1.51
1	F	82	GLU	CB-CG	5.38	1.62	1.52
1	D	85	CYS	CB-SG	-5.30	1.73	1.81
1	F	125	GLU	CD-OE1	5.19	1.31	1.25
1	D	79	CYS	CB-SG	-5.06	1.73	1.81
2	K	65	SER	CB-OG	5.00	1.48	1.42

All (131) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	31	ASP	CB-CG-OD2	-34.56	87.20	118.30
1	F	31	ASP	CB-CG-OD1	30.47	145.72	118.30
1	D	106	ARG	CB-CG-CD	-22.50	53.10	111.60
3	N	68	GLU	OE1-CD-OE2	-22.01	96.88	123.30
3	M	68	GLU	CA-CB-CG	-20.94	67.33	113.40
2	H	195	ILE	CG1-CB-CG2	-19.98	67.43	111.40
1	F	136	VAL	CG1-CB-CG2	-16.23	84.94	110.90
3	N	68	GLU	CG-CD-OE1	15.28	148.87	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	K	3	GLN	CA-CB-CG	13.77	143.69	113.40
2	K	75	LYS	CB-CA-C	-13.53	83.34	110.40
3	L	126	LYS	CB-CG-CD	-13.36	76.86	111.60
2	J	3	GLN	CA-CB-CG	-12.62	85.63	113.40
3	M	68	GLU	CG-CD-OE1	-12.39	93.52	118.30
1	F	82	GLU	OE1-CD-OE2	-12.36	108.47	123.30
1	D	106	ARG	CG-CD-NE	12.25	137.53	111.80
3	O	79	GLN	CA-CB-CG	-11.87	87.29	113.40
1	F	31	ASP	OD1-CG-OD2	-11.69	101.08	123.30
1	F	49	GLU	CA-CB-CG	-11.66	87.75	113.40
3	L	123	GLU	CB-CA-C	11.31	133.01	110.40
3	N	68	GLU	CG-CD-OE2	-10.98	96.34	118.30
1	F	82	GLU	CG-CD-OE1	10.86	140.03	118.30
2	J	43	LYS	CB-CG-CD	10.78	139.64	111.60
2	J	43	LYS	CD-CE-NZ	10.78	136.49	111.70
2	J	5	LYS	CA-CB-CG	-10.68	89.91	113.40
3	L	188	LYS	CA-CB-CG	10.38	136.24	113.40
1	F	74	GLN	CA-CB-CG	10.23	135.92	113.40
1	D	106	ARG	CA-CB-CG	10.10	135.62	113.40
1	D	122	LEU	CA-CB-CG	10.06	138.43	115.30
3	L	123	GLU	CA-CB-CG	10.04	135.50	113.40
3	L	126	LYS	N-CA-CB	-9.87	92.83	110.60
1	F	82	GLU	CG-CD-OE2	-9.78	98.74	118.30
2	I	210	ARG	CG-CD-NE	9.44	131.63	111.80
2	I	96	PHE	C-N-CD	-9.44	99.83	120.60
3	O	190	LYS	CD-CE-NZ	-9.39	90.10	111.70
2	K	12	VAL	C-N-CA	9.32	145.00	121.70
3	O	188	LYS	CB-CG-CD	9.29	135.75	111.60
2	H	201	LYS	CB-CG-CD	-9.13	87.86	111.60
3	M	68	GLU	OE1-CD-OE2	8.97	134.07	123.30
2	I	105	GLN	N-CA-CB	-8.80	94.76	110.60
3	M	126	LYS	CG-CD-CE	-8.63	86.00	111.90
2	I	206	LYS	CA-CB-CG	8.25	131.54	113.40
1	F	73	PRO	C-N-CA	-8.24	101.09	121.70
1	F	125	GLU	CA-CB-CG	8.14	131.32	113.40
2	K	96	PHE	C-N-CD	-8.14	102.69	120.60
2	I	210	ARG	CA-CB-CG	8.13	131.28	113.40
1	F	74	GLN	CB-CG-CD	8.09	132.63	111.60
2	J	5	LYS	CB-CG-CD	8.08	132.60	111.60
2	H	85	GLU	CB-CA-C	-8.02	94.36	110.40
2	K	75	LYS	CB-CG-CD	7.85	132.02	111.60
1	F	125	GLU	CB-CA-C	7.67	125.75	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	K	75	LYS	CA-CB-CG	7.61	130.15	113.40
3	N	70	LYS	CG-CD-CE	-7.59	89.12	111.90
2	I	210	ARG	NE-CZ-NH2	-7.49	116.56	120.30
3	M	24	HIS	CB-CA-C	-7.40	95.60	110.40
3	L	123	GLU	N-CA-CB	-7.29	97.48	110.60
3	N	70	LYS	CD-CE-NZ	7.21	128.28	111.70
2	H	27	LEU	CA-CB-CG	7.17	131.80	115.30
1	F	43	LEU	CB-CG-CD2	-7.14	98.86	111.00
2	H	164	HIS	N-CA-CB	7.11	123.40	110.60
2	K	3	GLN	CB-CA-C	-7.08	96.23	110.40
1	F	31	ASP	N-CA-C	-6.86	92.47	111.00
3	M	68	GLU	CG-CD-OE2	6.81	131.92	118.30
2	I	210	ARG	CD-NE-CZ	6.80	133.13	123.60
1	D	106	ARG	NE-CZ-NH1	6.79	123.69	120.30
3	O	188	LYS	CD-CE-NZ	-6.76	96.14	111.70
3	M	183	LYS	CB-CG-CD	-6.75	94.04	111.60
2	I	206	LYS	CB-CG-CD	6.61	128.79	111.60
2	H	201	LYS	CG-CD-CE	6.61	131.73	111.90
2	K	43	LYS	CD-CE-NZ	-6.54	96.67	111.70
3	M	70	LYS	CB-CG-CD	-6.45	94.82	111.60
3	M	48	LEU	CA-CB-CG	6.40	130.01	115.30
2	H	187	SER	CB-CA-C	-6.39	97.97	110.10
2	J	96	PHE	C-N-CD	-6.38	106.56	120.60
1	F	82	GLU	CA-CB-CG	6.38	127.44	113.40
2	K	11	LEU	CA-CB-CG	6.37	129.96	115.30
2	K	64	LYS	C-N-CA	-6.34	105.86	121.70
1	F	81	GLN	C-N-CA	6.29	137.43	121.70
3	O	67	LEU	CA-CB-CG	6.28	129.75	115.30
1	F	125	GLU	N-CA-CB	-6.26	99.33	110.60
1	F	33	VAL	CG1-CB-CG2	-6.25	100.89	110.90
3	O	188	LYS	CA-CB-CG	-6.25	99.64	113.40
2	I	206	LYS	CB-CA-C	-6.24	97.93	110.40
3	L	145	LYS	CA-CB-CG	-6.23	99.70	113.40
2	H	83	GLN	CA-CB-CG	6.22	127.09	113.40
2	K	4	LEU	CA-CB-CG	6.20	129.55	115.30
3	M	57	GLY	C-N-CA	-6.19	106.23	121.70
2	K	43	LYS	CA-CB-CG	-6.18	99.79	113.40
3	N	103	LYS	N-CA-CB	-6.15	99.54	110.60
3	O	154	LEU	CA-CB-CG	6.10	129.33	115.30
1	F	121	THR	CA-CB-CG2	6.09	120.93	112.40
2	I	105	GLN	CB-CG-CD	-6.09	95.76	111.60
3	L	188	LYS	CB-CG-CD	-6.08	95.80	111.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L	126	LYS	CA-CB-CG	6.06	126.74	113.40
3	L	48	LEU	CA-CB-CG	6.06	129.23	115.30
2	I	210	ARG	NE-CZ-NH1	5.90	123.25	120.30
1	F	106	ARG	CG-CD-NE	5.87	124.12	111.80
1	F	121	THR	OG1-CB-CG2	5.78	123.29	110.00
3	L	145	LYS	CD-CE-NZ	-5.77	98.42	111.70
2	I	5	LYS	CA-CB-CG	-5.74	100.78	113.40
1	F	74	GLN	N-CA-CB	5.73	120.91	110.60
2	I	185	PRO	C-N-CA	-5.63	107.62	121.70
3	N	136	LEU	CA-CB-CG	5.62	128.24	115.30
2	H	201	LYS	CD-CE-NZ	5.62	124.62	111.70
3	M	126	LYS	CB-CA-C	5.61	121.62	110.40
2	I	5	LYS	CB-CG-CD	5.60	126.17	111.60
1	F	136	VAL	CA-CB-CG2	-5.59	102.51	110.90
2	J	43	LYS	CA-CB-CG	-5.55	101.18	113.40
3	M	38	GLU	C-N-CA	-5.54	107.86	121.70
2	K	3	GLN	CB-CG-CD	5.52	125.94	111.60
3	N	126	LYS	CA-CB-CG	5.48	125.46	113.40
1	F	129	THR	CA-CB-CG2	-5.48	104.73	112.40
3	M	67	LEU	CA-CB-CG	5.47	127.88	115.30
3	O	181	LEU	CB-CG-CD2	-5.47	101.70	111.00
2	K	65	SER	N-CA-CB	5.44	118.66	110.50
3	L	68	GLU	C-N-CA	-5.42	110.92	122.30
1	F	122	LEU	C-N-CA	5.28	134.90	121.70
3	O	190	LYS	CB-CG-CD	-5.26	97.92	111.60
2	H	183	THR	OG1-CB-CG2	5.23	122.03	110.00
3	M	70	LYS	CA-CB-CG	5.22	124.89	113.40
2	H	192	GLN	CB-CA-C	-5.21	99.97	110.40
3	M	152	ASN	N-CA-CB	5.21	119.99	110.60
2	J	2	VAL	C-N-CA	-5.18	108.75	121.70
2	J	5	LYS	N-CA-CB	5.14	119.85	110.60
2	H	85	GLU	N-CA-CB	5.13	119.83	110.60
3	O	48	LEU	CA-CB-CG	5.12	127.09	115.30
3	N	126	LYS	CD-CE-NZ	5.12	123.48	111.70
1	D	93	GLU	CA-CB-CG	5.12	124.66	113.40
2	H	25	SER	CB-CA-C	-5.10	100.40	110.10
2	J	43	LYS	CG-CD-CE	-5.07	96.69	111.90
3	N	103	LYS	CD-CE-NZ	5.07	123.35	111.70
3	L	188	LYS	CB-CA-C	-5.06	100.28	110.40

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	F	121	THR	CB

All (31) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	64	LYS	Peptide
1	D	106	ARG	Sidechain
1	D	122	LEU	Peptide
1	E	123	TYR	Peptide
1	E	98	VAL	Peptide
1	F	106	ARG	Sidechain
1	F	31	ASP	Sidechain,Peptide
1	F	82	GLU	Sidechain
2	H	147	PRO	Peptide
2	H	164	HIS	Sidechain
2	H	25	SER	Peptide
2	I	205	THR	Peptide
2	I	210	ARG	Sidechain
2	I	96	PHE	Peptide
2	J	210	ARG	Sidechain
2	J	96	PHE	Peptide
2	K	12	VAL	Peptide
2	K	3	GLN	Peptide
2	K	75	LYS	Peptide
2	K	96	PHE	Peptide
3	L	123	GLU	Sidechain
3	L	125	LEU	Peptide
3	L	40	ALA	Peptide
3	M	126	LYS	Mainchain
3	M	24	HIS	Sidechain
3	M	39	LYS	Peptide
3	M	40	ALA	Peptide
3	N	42	HIS	Sidechain
3	N	68	GLU	Sidechain
3	O	79	GLN	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	C	897	0	862	30	0
1	D	897	0	862	35	0
1	E	753	0	725	37	0
1	F	810	0	777	53	0
2	H	1630	0	1613	78	0
2	I	1603	0	1584	51	0
2	J	1636	0	1618	78	0
2	K	1630	0	1612	107	0
3	L	1591	0	1544	80	0
3	M	1582	0	1536	61	0
3	N	1614	0	1567	72	0
3	O	1582	0	1538	40	0
4	C	14	0	13	0	0
4	D	14	0	13	0	0
5	C	5	0	0	1	0
5	D	10	0	0	0	0
5	K	5	0	0	1	0
5	L	5	0	0	1	0
5	N	5	0	0	0	0
All	All	16283	0	15864	667	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 21.

All (667) 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)
3:M:126:LYS:CE	3:M:126:LYS:CD	1.78	1.59
3:L:126:LYS:NZ	3:L:126:LYS:CE	1.73	1.50
3:M:126:LYS:CE	3:M:126:LYS:CG	2.21	1.19
2:K:75:LYS:NZ	2:K:77:GLN:O	1.75	1.17
2:K:75:LYS:CD	2:K:77:GLN:HE21	1.60	1.13
2:K:75:LYS:CD	2:K:77:GLN:HB2	1.80	1.09
2:K:75:LYS:HD2	2:K:77:GLN:CB	1.82	1.09
1:F:43:LEU:HD23	1:F:132:TYR:HD2	1.11	1.08
3:N:24:HIS:HD2	3:N:70:LYS:HE2	1.15	1.04
2:K:75:LYS:HD2	2:K:77:GLN:HB2	1.06	1.04
3:M:126:LYS:CE	3:M:126:LYS:HG3	1.85	1.04
2:K:3:GLN:OE1	2:K:25:SER:HB3	1.62	1.00
2:K:72:ASP:HB3	2:K:75:LYS:HE3	1.41	0.98
3:O:78:ALA:C	3:O:79:GLN:HG2	1.84	0.97
3:L:122:ASP:O	3:L:126:LYS:HG3	1.64	0.97

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:189:LEU:HD12	2:I:213:PRO:HG3	1.44	0.97
2:J:89:MET:HE3	3:N:42:HIS:CD2	2.01	0.95
2:K:87:THR:HG22	2:K:111:VAL:H	1.29	0.94
2:K:97:PRO:HG3	3:O:96:LEU:HD13	1.46	0.94
2:K:75:LYS:CD	2:K:77:GLN:NE2	2.31	0.93
2:J:2:VAL:HG23	2:J:27:LEU:HD23	1.50	0.93
2:J:89:MET:HB2	3:N:42:HIS:HD2	1.34	0.92
1:F:43:LEU:HD23	1:F:132:TYR:CD2	2.04	0.91
2:K:75:LYS:HZ3	2:K:77:GLN:N	1.69	0.89
2:K:75:LYS:HD2	2:K:77:GLN:HE21	1.38	0.89
2:H:195:ILE:HG13	2:H:210:ARG:HA	1.50	0.89
3:L:108:ARG:HH21	3:L:109:THR:HG23	1.35	0.89
3:N:24:HIS:CD2	3:N:70:LYS:HE2	2.07	0.88
2:K:75:LYS:HZ3	2:K:77:GLN:H	1.20	0.88
3:L:145:LYS:HG2	3:L:146:VAL:N	1.85	0.88
2:K:75:LYS:HD2	2:K:77:GLN:NE2	1.90	0.86
2:I:97:PRO:HG3	3:M:96:LEU:HD13	1.57	0.86
2:J:3:GLN:HG2	2:J:4:LEU:H	1.40	0.84
1:D:63:ASP:HB2	1:D:64:LYS:NZ	1.92	0.84
1:E:82:GLU:HG3	2:K:83:GLN:HG2	1.60	0.84
3:N:5:THR:HG23	3:N:24:HIS:HB3	1.60	0.83
2:J:40:PRO:HG2	2:J:43:LYS:HB2	1.60	0.82
2:J:185:PRO:O	2:J:188:SER:OG	1.96	0.82
1:D:62:THR:HG23	1:D:63:ASP:H	1.46	0.81
2:J:143:LYS:HA	2:J:177:SER:HB2	1.62	0.81
2:J:89:MET:HB2	3:N:42:HIS:CD2	2.17	0.80
2:K:17:THR:HG22	2:K:82(A):ASN:HA	1.64	0.79
3:L:145:LYS:HE2	3:L:197:THR:H	1.46	0.79
2:K:13:GLN:O	2:K:16:GLN:HB2	1.83	0.79
1:F:32:ASP:HB3	1:F:133:ASN:HB2	1.64	0.79
3:N:41:ASP:C	3:N:42:HIS:HD1	1.86	0.79
2:J:87:THR:HG22	2:J:111:VAL:H	1.48	0.78
1:D:61:VAL:HG23	1:D:115:LYS:HB3	1.66	0.77
2:H:87:THR:HB	2:H:111:VAL:H	1.50	0.77
3:L:123:GLU:HA	3:L:126:LYS:NZ	2.00	0.76
2:I:67:LEU:HD23	2:I:82:MET:HG3	1.67	0.76
2:H:123:PRO:HD3	3:L:123:GLU:OE1	1.85	0.76
2:J:18:LEU:HB2	2:J:82(C):LEU:HD11	1.65	0.76
2:K:126:PRO:HD2	2:K:213:PRO:HA	1.67	0.76
1:F:104:TYR:HE2	1:F:106:ARG:HH11	1.31	0.76
2:J:192:GLN:HB2	1:F:125:GLU:CG	2.15	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:M:126:LYS:HG3	3:M:126:LYS:HE3	1.66	0.75
2:H:2:VAL:HG13	2:H:94:ARG:HH12	1.51	0.75
3:N:61:ARG:CZ	3:N:79:GLN:OE1	2.35	0.75
3:L:158:ASN:HD22	3:L:179:LEU:HD11	1.52	0.75
3:L:145:LYS:HD2	3:L:147:GLN:CG	2.17	0.74
2:I:5:LYS:HG3	2:I:6:GLU:N	2.02	0.74
1:D:63:ASP:HB2	1:D:64:LYS:HZ1	1.51	0.74
2:K:72:ASP:CB	2:K:75:LYS:HE3	2.16	0.74
3:M:38:GLU:O	3:M:39:LYS:NZ	2.20	0.73
3:L:158:ASN:ND2	3:L:179:LEU:HD11	2.03	0.73
3:N:201:LEU:HD13	3:N:205:VAL:HG23	1.70	0.73
1:E:109:SER:H	1:E:112:LEU:HD13	1.54	0.73
2:J:84:THR:O	2:J:87:THR:HG23	1.89	0.73
3:M:150:VAL:HB	3:M:155:GLN:NE2	2.04	0.72
2:K:75:LYS:HD2	2:K:77:GLN:CG	2.19	0.72
1:C:82:GLU:O	1:C:82:GLU:HG2	1.89	0.72
3:L:145:LYS:HD2	3:L:147:GLN:HG3	1.71	0.72
2:I:11:LEU:HD23	2:I:116:THR:HG22	1.72	0.72
2:I:39:GLN:HB2	2:I:45:LEU:HD23	1.72	0.72
3:O:78:ALA:O	3:O:79:GLN:HG2	1.90	0.72
1:F:45:CYS:SG	1:F:130:THR:OG1	2.48	0.72
3:M:84:ALA:HB3	3:M:86:TYR:CE1	2.25	0.71
2:K:75:LYS:CG	2:K:77:GLN:HE21	2.01	0.71
1:F:35:ALA:HB2	1:F:134:LEU:HD11	1.71	0.71
2:H:62:ASP:O	2:H:63:ILE:HD13	1.91	0.71
2:K:75:LYS:HD3	2:K:77:GLN:NE2	2.06	0.71
2:I:87:THR:HG22	2:I:111:VAL:H	1.56	0.70
2:K:75:LYS:CE	2:K:77:GLN:HB2	2.21	0.70
3:O:185:ASP:HA	3:O:188:LYS:HD3	1.73	0.70
2:K:75:LYS:HZ3	2:K:77:GLN:CA	2.02	0.70
2:J:89:MET:CB	3:N:42:HIS:HD2	2.04	0.70
3:N:169:LYS:HG3	3:N:170:ASP:H	1.57	0.70
3:L:145:LYS:HE2	3:L:197:THR:N	2.07	0.69
2:I:87:THR:CG2	2:I:111:VAL:H	2.06	0.69
2:J:191:THR:HB	1:F:125:GLU:OE2	1.92	0.69
2:K:3:GLN:HB2	2:K:25:SER:OG	1.92	0.69
3:M:39:LYS:HE3	3:M:83:GLU:O	1.93	0.69
2:J:89:MET:HE1	2:J:108:MET:SD	2.32	0.69
2:J:97:PRO:HG3	3:N:96:LEU:HD13	1.74	0.69
2:K:75:LYS:NZ	2:K:77:GLN:C	2.46	0.69
2:H:138:LEU:HB2	2:H:211:VAL:HG11	1.75	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:29:LEU:O	2:I:71:ARG:NH1	2.25	0.68
2:I:4:LEU:HD21	2:I:94:ARG:HB2	1.75	0.68
3:M:39:LYS:HZ1	3:M:84:ALA:HA	1.57	0.68
1:C:133:ASN:ND2	5:C:202:SO4:O2	2.26	0.68
2:H:203:SER:OG	2:H:205:THR:OG1	2.12	0.68
2:I:84:THR:O	2:I:87:THR:HG23	1.94	0.68
3:O:125:LEU:O	3:O:183:LYS:HD2	1.94	0.68
1:F:55:GLN:NE2	2:K:98:TYR:OH	2.26	0.68
3:L:122:ASP:O	3:L:126:LYS:CG	2.42	0.68
3:N:62:PHE:HD2	3:N:73:LEU:HD21	1.59	0.68
3:M:74:THR:HG22	3:M:76:THR:HG22	1.75	0.67
2:J:192:GLN:HB2	1:F:125:GLU:HG2	1.74	0.67
2:K:3:GLN:O	2:K:4:LEU:HD22	1.95	0.67
2:K:75:LYS:HD3	2:K:77:GLN:HE21	1.55	0.67
2:K:94:ARG:HH21	2:K:100(B):ASN:HB3	1.60	0.67
3:M:22:THR:HB	3:M:70:LYS:HD2	1.75	0.67
1:F:67:MET:HE1	2:K:100(A):ILE:HD12	1.75	0.67
1:E:108:ILE:HD11	1:E:134:LEU:HD21	1.77	0.66
3:N:61:ARG:NH1	3:N:79:GLN:HE22	1.94	0.66
3:O:122:ASP:OD1	3:O:122:ASP:N	2.27	0.66
1:F:44:THR:OG1	1:F:102:THR:HG23	1.97	0.65
2:H:195:ILE:HG13	2:H:210:ARG:CA	2.23	0.65
1:E:103:LEU:HD23	1:E:104:TYR:N	2.11	0.65
2:J:184:VAL:HG13	2:J:185:PRO:HD2	1.78	0.65
3:L:123:GLU:HA	3:L:126:LYS:HZ2	1.61	0.65
1:D:25:GLU:HG3	1:D:26:LEU:H	1.61	0.65
2:J:87:THR:CG2	2:J:111:VAL:H	2.08	0.65
3:N:40:ALA:HB3	3:N:43:SER:HB3	1.77	0.65
2:J:63:ILE:HG13	2:J:67:LEU:HD21	1.77	0.65
1:C:110:SER:HA	1:C:136:VAL:HG21	1.78	0.65
2:H:17:THR:HG22	2:H:82(A):ASN:HA	1.78	0.65
1:F:33:VAL:N	1:F:133:ASN:O	2.30	0.65
3:L:145:LYS:HE3	3:L:195:GLU:O	1.97	0.64
3:N:151:ASP:O	3:N:152:ASN:ND2	2.31	0.64
2:J:96:PHE:CD2	2:J:97:PRO:HD3	2.31	0.64
2:J:100(A):ILE:HG23	2:J:100(B):ASN:H	1.62	0.64
2:I:67:LEU:CD2	2:I:82:MET:HG3	2.27	0.64
2:J:139:GLY:HA3	2:J:181:VAL:HG12	1.80	0.64
3:L:61:ARG:NH1	3:L:82:ASP:OD1	2.30	0.64
3:O:190:LYS:O	3:O:210:ASN:HA	1.99	0.63
2:J:3:GLN:CG	2:J:4:LEU:H	2.12	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:127:SER:HB2	2:K:214:LYS:HE3	1.81	0.63
3:N:41:ASP:O	3:N:42:HIS:ND1	2.29	0.63
3:L:108:ARG:HH11	3:L:172:THR:HG22	1.64	0.62
1:D:85:CYS:O	1:D:88:GLN:N	2.28	0.62
2:H:84:THR:O	2:H:87:THR:HG22	2.00	0.62
3:M:154:LEU:HB2	3:N:14:LEU:HD21	1.80	0.62
2:I:87:THR:HB	2:I:110:THR:HA	1.81	0.62
3:M:9:ALA:O	3:M:11:LEU:HD23	1.99	0.62
1:E:69:ALA:HB2	1:E:85:CYS:HB2	1.81	0.62
1:F:82:GLU:O	1:F:82:GLU:HG2	1.99	0.62
3:O:38:GLU:HB2	3:O:44:PHE:CE1	2.35	0.62
2:J:199:ASN:HD22	2:J:206:LYS:HG2	1.65	0.62
1:F:108:ILE:HD11	1:F:134:LEU:HD21	1.80	0.62
3:O:124:GLN:NE2	3:O:131:SER:OG	2.28	0.62
2:I:11:LEU:HB2	2:I:147:PRO:HG3	1.82	0.62
2:K:71:ARG:NE	5:K:301:SO4:O4	2.33	0.62
1:F:48:LYS:HE3	1:F:48:LYS:H	1.65	0.62
1:F:91:ALA:HB2	1:F:101:TRP:HA	1.81	0.62
2:K:75:LYS:NZ	2:K:77:GLN:H	1.97	0.62
3:L:4:VAL:HG22	3:L:90:LEU:HD12	1.82	0.62
2:J:24:VAL:HG11	2:J:27:LEU:HD11	1.81	0.62
3:N:59:PRO:HG2	3:N:61:ARG:NH2	2.15	0.62
3:L:187:GLU:HG3	3:L:211:ARG:NH1	2.15	0.61
2:J:89:MET:CE	3:N:42:HIS:CD2	2.80	0.61
2:I:5:LYS:HE3	2:I:6:GLU:O	2.00	0.61
2:J:194:TYR:O	2:J:195:ILE:HD13	2.00	0.61
1:C:89:VAL:HG22	1:C:103:LEU:HD12	1.82	0.61
2:K:84:THR:HG22	2:K:85:GLU:OE2	2.01	0.61
3:O:147:GLN:NE2	3:O:155:GLN:O	2.34	0.61
1:F:43:LEU:CD2	1:F:132:TYR:HD2	2.02	0.61
1:F:92:THR:HG22	1:F:93:GLU:H	1.65	0.61
2:K:24:VAL:HB	2:K:27:LEU:HD21	1.83	0.61
2:H:169:VAL:HG21	3:L:160:GLN:HB3	1.82	0.60
2:K:36:TRP:HE1	2:K:78:VAL:HG12	1.66	0.60
3:N:83:GLU:HG3	3:N:105:THR:HA	1.83	0.60
2:I:17:THR:HG22	2:I:82(A):ASN:HA	1.84	0.60
2:H:2:VAL:HG22	2:H:27:LEU:HD21	1.82	0.60
2:J:3:GLN:CG	2:J:4:LEU:N	2.65	0.60
2:J:97:PRO:HG3	3:N:96:LEU:CD1	2.31	0.60
1:C:60:LYS:HE2	1:C:62:THR:CG2	2.33	0.59
2:K:72:ASP:H	2:K:75:LYS:NZ	2.00	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:18:LEU:HD11	2:H:20:LEU:HD21	1.83	0.59
1:F:31:ASP:OD2	1:F:32:ASP:C	2.40	0.59
2:I:96:PHE:CD2	2:I:97:PRO:HD3	2.37	0.59
2:K:37:ILE:HD13	2:K:103:TRP:CH2	2.38	0.59
1:D:67:MET:HE1	1:D:70:LEU:HB2	1.85	0.58
2:K:9:PRO:HG2	2:K:12:VAL:HG11	1.84	0.58
2:I:96:PHE:CE1	3:M:34:ASN:ND2	2.71	0.58
2:I:102:ASP:OD1	2:I:103:TRP:N	2.35	0.58
3:M:163:VAL:HG22	3:M:175:LEU:HD12	1.84	0.58
2:K:63:ILE:HB	2:K:67:LEU:HD22	1.85	0.58
2:H:200:HIS:NE2	2:H:202:PRO:HG2	2.19	0.58
2:J:3:GLN:HG2	2:J:4:LEU:N	2.14	0.58
1:C:61:VAL:HA	1:C:64:LYS:O	2.03	0.58
1:C:94:THR:HB	1:C:98:VAL:HG22	1.86	0.58
2:J:89:MET:CE	2:J:108:MET:SD	2.91	0.58
3:L:170:ASP:HB2	3:L:172:THR:HG23	1.85	0.57
2:J:40:PRO:HA	2:J:88:ALA:HA	1.85	0.57
3:L:123:GLU:HA	3:L:126:LYS:HZ3	1.70	0.57
2:H:89:MET:HG2	2:H:91:PHE:CZ	2.40	0.57
2:H:126:PRO:HD2	2:H:213:PRO:HA	1.87	0.56
2:H:97:PRO:HG3	3:L:96:LEU:HD13	1.87	0.56
1:E:122:LEU:HD23	1:E:122:LEU:H	1.70	0.56
3:M:170:ASP:OD1	3:M:172:THR:HG23	2.05	0.56
3:O:146:VAL:HG22	3:O:196:VAL:HG22	1.88	0.56
2:J:27:LEU:HD22	2:J:94:ARG:NH1	2.20	0.56
2:H:171:GLN:HA	3:L:160:GLN:NE2	2.21	0.56
3:L:152:ASN:HD22	3:L:152:ASN:N	2.03	0.56
2:J:6:GLU:HA	2:J:22:CYS:HA	1.88	0.56
2:J:24:VAL:CG1	2:J:27:LEU:HD11	2.35	0.56
2:J:165:THR:HG23	2:J:180:SER:HB2	1.86	0.56
1:E:69:ALA:HB3	1:E:89:VAL:HG11	1.87	0.56
2:K:84:THR:O	2:K:87:THR:HG23	2.05	0.56
2:H:164:HIS:NE2	3:L:166:GLN:HB2	2.22	0.55
2:K:3:GLN:CB	2:K:25:SER:H	2.19	0.55
3:L:158:ASN:N	3:L:158:ASN:OD1	2.39	0.55
3:M:62:PHE:HD2	3:M:73:LEU:HD11	1.70	0.55
1:D:67:MET:CE	1:D:70:LEU:HB2	2.36	0.55
1:C:94:THR:HG22	1:C:96:LYS:H	1.71	0.55
2:I:18:LEU:HD11	2:I:20:LEU:HD21	1.87	0.55
2:H:52:TRP:CZ3	2:H:98:TYR:HB3	2.41	0.55
2:K:75:LYS:HD2	2:K:77:GLN:CD	2.27	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:60:LYS:HE2	1:C:62:THR:HG21	1.88	0.55
1:E:115:LYS:HG2	1:E:133:ASN:ND2	2.22	0.55
3:O:183:LYS:O	3:O:187:GLU:HG3	2.07	0.55
1:C:82:GLU:O	1:C:82:GLU:CG	2.54	0.55
1:E:31:ASP:OD1	1:E:31:ASP:N	2.39	0.55
1:D:63:ASP:CB	1:D:64:LYS:NZ	2.69	0.55
3:N:120:PRO:HD3	3:N:132:VAL:HG22	1.88	0.55
3:M:150:VAL:HB	3:M:155:GLN:HE21	1.70	0.54
1:C:94:THR:HB	1:C:98:VAL:CG2	2.37	0.54
2:H:121:VAL:O	2:H:209:LYS:HG3	2.08	0.54
1:D:48:LYS:H	1:D:48:LYS:HD2	1.69	0.54
1:D:60:LYS:NZ	1:D:113:GLY:O	2.38	0.54
2:H:89:MET:HE3	3:L:42:HIS:CD2	2.43	0.54
2:J:161:SER:HB3	1:F:123:TYR:CE1	2.43	0.54
2:J:185:PRO:HD3	1:F:52:PHE:CD1	2.43	0.54
2:H:141:LEU:HD13	3:L:133:VAL:HG21	1.89	0.54
1:E:34:TYR:HA	1:E:135:ILE:HG23	1.88	0.54
2:K:33:SER:OG	2:K:95:ASN:HA	2.08	0.54
3:L:108:ARG:NH1	3:L:172:THR:HG22	2.23	0.54
3:M:39:LYS:HZ1	3:M:84:ALA:CA	2.20	0.54
3:O:6:GLN:OE1	3:O:88:CYS:N	2.39	0.54
3:O:167:ASP:OD1	3:O:167:ASP:N	2.40	0.54
3:L:36:ILE:HD12	3:L:44:PHE:CD1	2.43	0.54
3:M:34:ASN:N	3:M:34:ASN:OD1	2.38	0.54
3:N:209:PHE:C	3:N:210:ASN:HD22	2.12	0.54
2:I:2:VAL:CG1	2:I:27:LEU:HD23	2.38	0.53
1:D:68:ILE:HG12	1:D:83:HIS:CE1	2.43	0.53
1:E:53:LEU:HD21	1:E:120:PHE:HD2	1.73	0.53
2:H:100(A):ILE:O	2:H:100(B):ASN:HB2	2.09	0.53
3:L:145:LYS:HD2	3:L:147:GLN:HG2	1.89	0.53
3:N:89:SER:HB2	3:N:96:LEU:HD21	1.89	0.53
1:F:67:MET:CE	2:K:100(A):ILE:HD12	2.39	0.53
1:D:117:GLU:OE1	1:D:129:THR:HG21	2.09	0.53
3:M:4:VAL:HG13	3:M:99:GLY:HA2	1.91	0.53
3:M:13:THR:HG23	3:M:106:VAL:HG12	1.91	0.53
2:K:63:ILE:HB	2:K:67:LEU:CD2	2.39	0.53
3:O:142:ARG:HG2	3:O:142:ARG:O	2.09	0.53
1:E:56:MET:HB3	1:E:101:TRP:CD1	2.43	0.53
1:E:58:TRP:CZ3	1:E:118:CYS:HB2	2.44	0.53
3:N:149:LYS:NZ	3:N:195:GLU:OE1	2.38	0.53
1:D:109:SER:H	1:D:112:LEU:HD12	1.74	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:5:LYS:CG	2:J:6:GLU:N	2.71	0.53
2:H:35:SER:HG	2:H:47:TRP:HE1	1.57	0.52
2:K:75:LYS:HB2	2:K:76:SER:C	2.29	0.52
2:I:27:LEU:HD22	2:I:94:ARG:NE	2.24	0.52
1:F:74:GLN:O	1:F:74:GLN:HG2	2.08	0.52
2:I:2:VAL:HG12	2:I:27:LEU:HD23	1.91	0.52
3:M:6:GLN:HB3	3:M:22:THR:O	2.10	0.52
1:F:46:GLN:HG3	1:F:47:THR:N	2.25	0.52
2:K:3:GLN:HB3	2:K:25:SER:H	1.73	0.52
2:H:144:ASP:HA	2:H:175:LEU:HB3	1.91	0.52
2:K:75:LYS:HB3	2:K:77:GLN:HE21	1.75	0.52
3:O:14:LEU:HD23	3:O:15:PRO:HD2	1.92	0.52
3:L:201:LEU:HD13	3:L:205:VAL:HG23	1.92	0.52
3:M:55:ALA:O	3:M:58:THR:HG23	2.10	0.52
2:J:90:TYR:O	2:J:106:GLY:HA2	2.10	0.52
2:K:72:ASP:O	2:K:75:LYS:HG3	2.10	0.52
2:J:183:THR:HG21	3:N:137:ASN:ND2	2.24	0.51
2:K:9:PRO:CG	2:K:12:VAL:HG11	2.40	0.51
1:E:72:HIS:HB3	1:E:75:TYR:HB2	1.93	0.51
3:N:9:ALA:O	3:N:11:LEU:HD23	2.10	0.51
2:H:11:LEU:HB2	2:H:147:PRO:HG3	1.92	0.51
1:E:35:ALA:O	1:E:136:VAL:HA	2.11	0.51
2:J:12:VAL:HG11	2:J:82(C):LEU:HD13	1.92	0.51
2:H:9:PRO:HD2	2:H:20:LEU:HD23	1.93	0.51
2:H:205:THR:HG22	2:H:207:VAL:HG23	1.92	0.51
1:E:61:VAL:HG23	1:E:65:ASN:HA	1.92	0.51
1:E:115:LYS:HG2	1:E:133:ASN:HD21	1.76	0.51
2:H:132:SER:HB2	3:L:116:PHE:HE1	1.75	0.51
1:D:122:LEU:HG	1:D:126:GLY:N	2.25	0.51
3:L:25:SER:OG	3:L:27:THR:HG22	2.10	0.51
3:M:13:THR:O	3:M:106:VAL:HA	2.11	0.51
3:N:74:THR:HG22	3:N:76:THR:HG22	1.92	0.51
2:J:94:ARG:NH2	2:J:100(B):ASN:HB3	2.26	0.51
1:C:94:THR:HG22	1:C:96:LYS:N	2.25	0.51
3:M:197:THR:HG22	3:M:204:PRO:HB3	1.93	0.51
3:N:13:THR:HG23	3:N:106:VAL:HG22	1.93	0.51
2:K:75:LYS:HZ3	2:K:77:GLN:C	2.12	0.51
1:D:84:ALA:O	1:D:86:GLU:N	2.44	0.51
2:I:138:LEU:HD23	2:I:182:VAL:O	2.11	0.50
3:N:169:LYS:HG3	3:N:170:ASP:N	2.23	0.50
2:K:4:LEU:HD12	2:K:92:CYS:SG	2.52	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:145:LYS:CE	3:L:197:THR:N	2.74	0.50
2:I:145:TYR:CE1	2:I:150:VAL:HG13	2.46	0.50
2:H:62:ASP:C	2:H:63:ILE:HD13	2.32	0.50
3:O:83:GLU:OE2	3:O:173:TYR:OH	2.22	0.50
1:E:42:ASN:HB2	1:E:103:LEU:O	2.12	0.50
2:K:63:ILE:HG22	2:K:66:ARG:HD3	1.94	0.50
2:H:130:SER:OG	3:L:118:PHE:HE1	1.94	0.50
2:K:52:TRP:CZ3	2:K:98:TYR:HB3	2.47	0.50
2:K:90:TYR:O	2:K:106:GLY:HA2	2.11	0.50
2:K:131:THR:HG22	2:K:136:ALA:HB2	1.94	0.50
1:F:93:GLU:O	1:F:94:THR:OG1	2.29	0.50
2:K:67:LEU:HA	2:K:81:LYS:O	2.11	0.50
1:E:103:LEU:HD23	1:E:104:TYR:H	1.77	0.50
2:J:87:THR:HB	2:J:110:THR:HA	1.94	0.49
3:N:183:LYS:NZ	3:N:187:GLU:OE2	2.40	0.49
2:H:136:ALA:N	2:H:186:SER:HB3	2.27	0.49
3:L:125:LEU:O	3:L:183:LYS:HD3	2.12	0.49
3:L:155:GLN:HB3	3:L:158:ASN:HD21	1.77	0.49
3:L:142:ARG:NH2	5:L:301:SO4:O2	2.45	0.49
1:E:115:LYS:HA	1:E:133:ASN:ND2	2.27	0.49
3:O:115:VAL:HA	3:O:135:LEU:O	2.11	0.49
2:J:192:GLN:HB2	1:F:125:GLU:HG3	1.92	0.49
1:F:104:TYR:HE2	1:F:106:ARG:NH1	2.05	0.49
1:F:128:LYS:HE2	1:F:130:THR:HG23	1.94	0.49
2:I:100(A):ILE:HG23	2:I:100(B):ASN:HD22	1.76	0.49
1:D:56:MET:O	1:D:70:LEU:HD12	2.13	0.49
3:N:7:GLU:OE2	3:N:22:THR:HG23	2.12	0.49
2:H:145:TYR:O	2:H:175:LEU:HD12	2.13	0.49
1:E:103:LEU:HD22	1:E:105:LEU:CD1	2.43	0.49
2:I:19:SER:HA	2:I:80:LEU:O	2.12	0.48
2:J:181:VAL:HG21	3:N:135:LEU:HD22	1.95	0.48
3:N:80:VAL:HG21	3:N:108:ARG:HB3	1.94	0.48
3:O:136:LEU:HD22	3:O:175:LEU:HD22	1.95	0.48
2:H:13:GLN:C	2:H:15:SER:H	2.16	0.48
2:H:200:HIS:CD2	2:H:202:PRO:HG2	2.48	0.48
3:O:179:LEU:HD21	3:O:181:LEU:HD11	1.96	0.48
2:H:18:LEU:HB2	2:H:82(C):LEU:HD11	1.95	0.48
1:D:62:THR:HG23	1:D:63:ASP:N	2.23	0.48
1:E:47:THR:OG1	1:E:98:VAL:HG22	2.13	0.48
2:H:16:GLN:NE2	2:H:17:THR:O	2.47	0.48
2:J:5:LYS:HG2	2:J:6:GLU:N	2.26	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:12:THR:HG23	3:L:105:THR:OG1	2.13	0.48
1:E:36:LEU:O	1:E:39:SER:OG	2.31	0.48
2:J:194:TYR:C	2:J:195:ILE:HD13	2.34	0.48
3:N:62:PHE:CD2	3:N:73:LEU:HD21	2.45	0.48
2:K:23:THR:HG23	2:K:77:GLN:HG2	1.95	0.48
1:C:29:VAL:HG23	1:C:30:GLY:N	2.29	0.48
2:H:82(C):LEU:HA	2:H:82(C):LEU:HD23	1.63	0.48
2:H:123:PRO:CD	3:L:123:GLU:OE1	2.60	0.48
1:D:36:LEU:HD12	1:D:37:PRO:O	2.14	0.48
3:N:8:SER:O	3:N:103:LYS:HG3	2.14	0.48
3:N:61:ARG:NE	3:N:79:GLN:OE1	2.47	0.48
2:K:29:LEU:HD23	2:K:29:LEU:HA	1.69	0.48
1:F:123:TYR:HA	1:F:124:PRO:HA	1.39	0.48
2:K:126:PRO:HG2	2:K:213:PRO:HB3	1.96	0.48
1:D:122:LEU:HG	1:D:126:GLY:H	1.79	0.47
2:I:4:LEU:HD21	2:I:94:ARG:CB	2.41	0.47
3:M:133:VAL:HG22	3:M:178:THR:HB	1.96	0.47
2:J:2:VAL:HG22	2:J:2:VAL:O	2.13	0.47
3:L:89:SER:OG	3:L:96:LEU:HD11	2.14	0.47
1:F:36:LEU:H	1:F:36:LEU:HG	1.56	0.47
2:K:96:PHE:CD2	2:K:97:PRO:HD3	2.48	0.47
1:C:46:GLN:HG2	1:C:100:ASN:OD1	2.14	0.47
2:K:69:ILE:HA	2:K:79:PHE:O	2.14	0.47
2:K:143:LYS:HA	2:K:177:SER:HB2	1.96	0.47
3:O:133:VAL:HG22	3:O:178:THR:HG23	1.96	0.47
2:H:39:GLN:HB2	2:H:45:LEU:HD23	1.97	0.47
2:J:87:THR:HG22	2:J:111:VAL:N	2.23	0.47
2:J:96:PHE:CE1	3:N:34:ASN:ND2	2.82	0.47
3:N:142:ARG:HB2	3:N:173:TYR:CE1	2.48	0.47
2:K:11:LEU:HG	2:K:13:GLN:NE2	2.29	0.47
2:H:26:GLY:O	2:H:27:LEU:HD23	2.14	0.47
1:D:41:ILE:HG22	1:D:43:LEU:HD13	1.96	0.47
3:M:125:LEU:HD23	3:M:183:LYS:HG3	1.95	0.47
1:C:29:VAL:HG23	1:C:30:GLY:H	1.78	0.47
3:M:139:PHE:O	3:M:172:THR:HB	2.14	0.47
1:C:78:TYR:CE2	2:H:53:SER:HB3	2.50	0.47
1:C:104:TYR:HE2	1:C:106:ARG:HG2	1.79	0.47
3:M:38:GLU:HB2	3:M:44:PHE:CE2	2.50	0.47
2:J:27:LEU:HD22	2:J:94:ARG:HH11	1.79	0.47
3:N:27(C):VAL:HG22	3:N:69:GLY:O	2.14	0.47
2:I:195:ILE:HD13	2:I:210:ARG:HA	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:M:75:ILE:HD12	3:M:75:ILE:H	1.79	0.47
2:J:87:THR:HG22	2:J:111:VAL:HB	1.96	0.47
1:F:108:ILE:HA	1:F:112:LEU:HD22	1.96	0.47
1:F:119:ILE:HG12	1:F:129:THR:HG22	1.96	0.47
3:M:23:CYS:HB3	3:M:71:ALA:HB3	1.96	0.47
3:N:140:TYR:CG	3:N:141:PRO:HA	2.50	0.47
1:C:112:LEU:HD23	1:C:112:LEU:HA	1.73	0.46
3:N:76:THR:O	3:N:76:THR:OG1	2.31	0.46
2:H:124:LEU:HB3	3:L:118:PHE:CD2	2.50	0.46
2:I:72:ASP:OD1	2:I:74:SER:HB2	2.16	0.46
3:N:96:LEU:C	3:N:97:ILE:HD12	2.36	0.46
2:K:40:PRO:HA	2:K:88:ALA:HA	1.96	0.46
2:H:35:SER:HB2	2:H:96:PHE:O	2.16	0.46
2:H:171:GLN:HA	3:L:160:GLN:HE22	1.79	0.46
2:I:47:TRP:HZ2	2:I:50:VAL:HG12	1.80	0.46
2:I:51:ILE:HD13	2:I:71:ARG:HD3	1.97	0.46
2:K:159:LEU:CD2	2:K:182:VAL:HG21	2.46	0.46
3:M:187:GLU:HG2	3:M:211:ARG:NH1	2.31	0.46
1:E:44:THR:O	1:E:132:TYR:OH	2.18	0.46
1:E:123:TYR:HD1	1:E:123:TYR:HA	1.51	0.46
2:K:160:THR:O	2:K:163:VAL:HG13	2.16	0.46
1:C:89:VAL:HG11	1:C:101:TRP:CH2	2.51	0.46
1:D:110:SER:HA	1:D:136:VAL:HG11	1.98	0.46
3:M:19:VAL:HG11	3:M:104:LEU:HD11	1.98	0.46
2:J:63:ILE:O	2:J:67:LEU:HD23	2.16	0.46
1:D:25:GLU:OE2	1:D:126:GLY:HA3	2.16	0.46
2:K:72:ASP:H	2:K:75:LYS:HZ2	1.63	0.46
3:O:54:ARG:NH1	3:O:54:ARG:HG3	2.29	0.46
2:H:87:THR:OG1	2:H:110:THR:HA	2.15	0.46
2:H:164:HIS:CE1	3:L:166:GLN:HB2	2.51	0.46
2:I:40:PRO:HG2	2:I:43:LYS:HB2	1.98	0.46
2:J:18:LEU:HD11	2:J:20:LEU:HD21	1.97	0.46
3:N:61:ARG:HH11	3:N:79:GLN:HE22	1.64	0.46
2:K:159:LEU:HD21	2:K:182:VAL:HG21	1.97	0.46
2:H:13:GLN:O	2:H:15:SER:N	2.49	0.46
3:L:40:ALA:O	3:L:43:SER:HB3	2.15	0.46
1:F:92:THR:HG22	1:F:93:GLU:N	2.28	0.46
2:H:40:PRO:HG2	2:H:43:LYS:HB2	1.98	0.46
1:D:47:THR:HG22	1:D:99:THR:OG1	2.15	0.46
1:E:33:VAL:HG13	1:E:134:LEU:HA	1.98	0.46
2:J:95:ASN:HD22	2:J:100(B):ASN:HB2	1.81	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:66:ARG:O	2:K:82:MET:HA	2.15	0.46
2:K:181:VAL:HG21	3:O:135:LEU:HD13	1.98	0.46
2:H:20:LEU:HD21	2:H:109:VAL:HG21	1.98	0.45
2:H:154:TRP:HB2	2:H:159:LEU:HB3	1.98	0.45
3:M:126:LYS:CD	3:M:126:LYS:NZ	2.74	0.45
1:E:81:GLN:O	1:E:82:GLU:HB2	2.16	0.45
3:N:61:ARG:HD3	3:N:79:GLN:NE2	2.31	0.45
3:O:166:GLN:O	3:O:171:SER:HA	2.16	0.45
3:O:191:VAL:HG22	3:O:210:ASN:HD21	1.81	0.45
3:L:3:VAL:HG12	3:L:26:SER:CB	2.46	0.45
2:K:4:LEU:HD13	2:K:24:VAL:HG12	1.98	0.45
2:H:139:GLY:HA2	2:H:154:TRP:CZ2	2.51	0.45
3:M:136:LEU:HD22	3:M:175:LEU:HD22	1.98	0.45
3:M:154:LEU:HB2	3:N:14:LEU:CD2	2.47	0.45
1:E:56:MET:HB3	1:E:101:TRP:CG	2.52	0.45
1:E:123:TYR:CD1	1:E:124:PRO:HD3	2.52	0.45
2:H:12:VAL:HG13	2:H:111:VAL:HG22	1.98	0.45
3:L:175:LEU:HD23	3:L:176:SER:N	2.32	0.45
2:J:171:GLN:HB2	2:J:175:LEU:O	2.17	0.45
2:I:36:TRP:HE1	2:I:78:VAL:HG12	1.82	0.45
3:N:210:ASN:HD22	3:N:210:ASN:N	2.15	0.45
3:M:13:THR:CG2	3:M:106:VAL:HG12	2.46	0.45
3:M:80:VAL:HA	3:M:106:VAL:CG2	2.47	0.45
2:H:189:LEU:HG	2:H:213:PRO:HG3	1.99	0.45
2:K:11:LEU:HG	2:K:13:GLN:HE21	1.81	0.45
3:L:152:ASN:N	3:L:152:ASN:ND2	2.65	0.45
1:D:44:THR:OG1	1:D:102:THR:HG22	2.17	0.45
2:I:203:SER:O	2:I:205:THR:HG23	2.17	0.45
1:C:103:LEU:HD21	1:C:105:LEU:HD21	1.98	0.45
2:H:124:LEU:HD13	3:L:133:VAL:HG11	1.98	0.45
3:L:1:PCA:HG2	3:L:97:ILE:HD11	1.99	0.45
2:I:52:TRP:CZ3	2:I:98:TYR:HB3	2.52	0.45
3:M:186:TYR:O	3:M:192:TYR:OH	2.28	0.45
3:N:27:THR:HG22	3:N:27:THR:O	2.17	0.45
3:O:161:GLU:OE1	3:O:175:LEU:HD11	2.17	0.45
2:H:19:SER:HA	2:H:80:LEU:O	2.17	0.45
2:J:6:GLU:CD	2:J:6:GLU:H	2.19	0.45
3:N:40:ALA:N	3:N:165:GLU:OE2	2.50	0.45
2:K:9:PRO:HB2	2:K:12:VAL:CG1	2.47	0.45
3:L:118:PHE:HB2	3:L:133:VAL:HB	1.98	0.44
3:L:166:GLN:HG3	3:L:170:ASP:OD1	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:M:201:LEU:HD23	3:M:201:LEU:HA	1.73	0.44
2:J:192:GLN:CB	1:F:125:GLU:HG3	2.47	0.44
2:K:12:VAL:HG23	2:K:82(C):LEU:CD1	2.47	0.44
3:M:3:VAL:N	3:M:26:SER:OG	2.41	0.44
3:N:166:GLN:NE2	3:N:171:SER:HB2	2.32	0.44
2:H:98:TYR:CD1	2:H:99:PRO:HA	2.51	0.44
3:L:142:ARG:HB2	3:L:173:TYR:CE1	2.53	0.44
3:N:108:ARG:NH1	3:N:170:ASP:O	2.49	0.44
2:H:175:LEU:HD13	2:H:175:LEU:HA	1.71	0.44
2:K:75:LYS:CB	2:K:77:GLN:HE21	2.30	0.44
1:D:115:LYS:HE2	1:D:115:LYS:HB2	1.75	0.44
2:I:18:LEU:HD13	2:I:109:VAL:HG11	2.00	0.44
1:E:123:TYR:CG	1:E:124:PRO:HD3	2.52	0.44
2:J:6:GLU:OE1	2:J:106:GLY:N	2.33	0.44
2:J:89:MET:CG	3:N:42:HIS:HD2	2.30	0.44
3:N:4:VAL:HG22	3:N:90:LEU:HD12	1.98	0.44
2:H:146:PHE:HB2	2:H:175:LEU:CD1	2.48	0.44
3:L:61:ARG:NH1	3:L:82:ASP:OD2	2.51	0.44
3:M:4:VAL:HG12	3:M:97:ILE:HG22	2.00	0.44
2:K:139:GLY:HA2	2:K:154:TRP:CH2	2.53	0.44
2:I:126:PRO:HG3	2:I:189:LEU:HD11	2.00	0.44
3:M:142:ARG:O	3:M:142:ARG:HG2	2.17	0.44
2:J:6:GLU:OE1	2:J:105:GLN:N	2.51	0.44
2:J:51:ILE:HD13	2:J:71:ARG:HB3	2.00	0.44
2:K:5:LYS:HA	2:K:5:LYS:HD3	1.45	0.44
2:H:98:TYR:CG	2:H:99:PRO:HA	2.53	0.44
3:M:47:ILE:HA	3:M:58:THR:HG21	1.98	0.44
2:J:99:PRO:HG2	2:J:100(A):ILE:HG22	2.00	0.44
1:F:67:MET:O	1:F:80:GLY:HA3	2.17	0.44
2:H:63:ILE:HG22	2:H:63:ILE:O	2.18	0.43
2:H:184:VAL:HG11	2:H:194:TYR:CE2	2.52	0.43
1:E:60:LYS:HE2	1:E:114:GLY:HA3	2.00	0.43
1:F:136:VAL:H	1:F:136:VAL:HG23	1.56	0.43
3:L:36:ILE:HD12	3:L:44:PHE:HD1	1.83	0.43
1:D:35:ALA:O	1:D:136:VAL:HA	2.19	0.43
2:I:34:VAL:HB	2:I:78:VAL:HG21	1.99	0.43
3:L:108:ARG:NH2	3:L:109:THR:HG23	2.18	0.43
1:D:123:TYR:HA	1:D:124:PRO:HA	1.44	0.43
1:F:56:MET:HE2	1:F:71:TYR:CD2	2.53	0.43
1:F:56:MET:HE2	1:F:71:TYR:HD2	1.82	0.43
3:N:8:SER:O	3:N:103:LYS:HB2	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:121:SER:O	3:N:125:LEU:HG	2.18	0.43
1:C:89:VAL:HG12	1:C:90:ALA:N	2.33	0.43
3:M:202:SER:HB2	3:N:197:THR:HG21	1.99	0.43
1:E:53:LEU:HD23	1:E:56:MET:CE	2.48	0.43
3:N:35:TRP:CG	3:N:73:LEU:HD12	2.54	0.43
3:N:131:SER:HA	3:N:179:LEU:O	2.18	0.43
2:I:138:LEU:CD2	2:I:182:VAL:HG13	2.49	0.43
3:M:108:ARG:NH1	3:M:109:THR:O	2.52	0.43
2:K:72:ASP:H	2:K:75:LYS:CE	2.32	0.43
1:D:78:TYR:CZ	2:I:53:SER:HB2	2.54	0.43
3:N:40:ALA:HB2	3:N:165:GLU:OE2	2.18	0.43
1:F:36:LEU:HD12	1:F:39:SER:CB	2.48	0.43
2:K:12:VAL:HG23	2:K:12:VAL:O	2.19	0.43
2:K:60:ASN:HB3	2:K:63:ILE:HD11	2.01	0.43
3:O:186:TYR:CZ	3:O:211:ARG:HG3	2.54	0.43
1:C:103:LEU:CD2	1:C:105:LEU:HD21	2.49	0.43
3:M:134:CYS:HB3	3:M:148:TRP:CZ2	2.53	0.43
2:J:153:SER:O	2:J:197:ASN:N	2.36	0.43
3:N:89:SER:HB3	3:N:98:PHE:CD1	2.54	0.43
3:N:140:TYR:CD1	3:N:141:PRO:HA	2.54	0.43
1:F:37:PRO:HA	1:F:108:ILE:HG22	2.01	0.43
2:H:149:PRO:HG2	2:H:202:PRO:HG3	2.00	0.43
3:L:27:THR:HG21	3:L:92:TYR:HE1	1.84	0.43
3:M:170:ASP:OD1	3:M:172:THR:N	2.49	0.43
1:E:93:GLU:HA	1:E:99:THR:HA	2.01	0.43
2:J:2:VAL:HG23	2:J:27:LEU:CD2	2.36	0.43
2:K:122:PHE:CE2	3:O:124:GLN:HG3	2.54	0.43
2:H:83:GLN:HB3	2:H:85:GLU:OE1	2.19	0.43
2:J:98:TYR:HD2	3:N:32:TYR:CZ	2.37	0.43
3:N:5:THR:CG2	3:N:24:HIS:HB3	2.38	0.43
1:F:92:THR:CG2	1:F:93:GLU:H	2.31	0.43
3:O:188:LYS:H	3:O:188:LYS:HG3	1.60	0.43
3:L:3:VAL:HG12	3:L:26:SER:HB3	2.00	0.42
2:I:75:LYS:O	2:I:77:GLN:HG3	2.19	0.42
2:I:87:THR:HG22	2:I:111:VAL:HB	2.01	0.42
2:J:89:MET:HG2	2:J:91:PHE:CZ	2.54	0.42
2:K:3:GLN:HG2	2:K:25:SER:N	2.34	0.42
1:C:119:ILE:HG12	1:C:129:THR:HG22	2.00	0.42
2:K:122:PHE:HB3	3:O:121:SER:OG	2.19	0.42
3:L:3:VAL:H	3:L:26:SER:HB3	1.84	0.42
1:D:92:THR:OG1	1:D:100:ASN:HB2	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:75:TYR:O	2:K:52:TRP:HB3	2.20	0.42
2:K:72:ASP:CA	2:K:75:LYS:HE3	2.48	0.42
2:K:152:VAL:HG22	2:K:198:VAL:HG22	2.01	0.42
3:L:61:ARG:NH1	3:L:82:ASP:CG	2.72	0.42
3:M:18:THR:HG23	3:M:76:THR:HA	2.01	0.42
3:O:55:ALA:HB1	3:O:56:PRO:HD2	2.02	0.42
1:C:126:GLY:O	1:C:127:ILE:HD12	2.19	0.42
3:L:145:LYS:HE2	3:L:145:LYS:HB3	1.61	0.42
3:M:39:LYS:NZ	3:M:84:ALA:HA	2.28	0.42
2:J:4:LEU:HD22	2:J:24:VAL:HG22	2.02	0.42
3:N:9:ALA:HA	3:N:103:LYS:HB2	2.02	0.42
3:L:112:ALA:HB2	3:L:200:GLY:O	2.20	0.42
1:F:103:LEU:HG	1:F:105:LEU:CD1	2.50	0.42
1:C:28:ASN:ND2	1:C:128:LYS:HE2	2.35	0.42
1:C:48:LYS:HZ1	1:C:97:GLY:HA3	1.84	0.42
1:C:126:GLY:C	1:C:127:ILE:HD12	2.40	0.42
2:H:40:PRO:HA	2:H:88:ALA:HA	2.01	0.42
3:L:142:ARG:CZ	3:L:163:VAL:HG21	2.49	0.42
1:D:67:MET:HE3	2:I:100(A):ILE:HD13	2.00	0.42
1:E:133:ASN:HD22	1:E:133:ASN:HA	1.59	0.42
2:J:5:LYS:HG3	2:J:6:GLU:N	2.33	0.42
2:K:75:LYS:HB3	2:K:77:GLN:NE2	2.34	0.42
3:O:161:GLU:HG2	3:O:177:SER:HB2	2.02	0.42
2:H:2:VAL:HG13	2:H:94:ARG:NH1	2.25	0.42
2:H:126:PRO:HD3	2:H:211:VAL:HG13	2.01	0.42
3:L:131:SER:HA	3:L:179:LEU:O	2.20	0.42
1:E:82:GLU:HG3	2:K:83:GLN:CG	2.39	0.42
1:C:85:CYS:HA	1:C:88:GLN:HG2	2.00	0.42
3:M:85:THR:HA	3:M:102:THR:O	2.20	0.42
3:N:49:GLY:O	3:N:53:ASN:HB2	2.20	0.42
2:K:37:ILE:HD11	2:K:96:PHE:CD2	2.55	0.42
2:K:171:GLN:HE21	2:K:171:GLN:HB2	1.69	0.42
3:O:54:ARG:HG3	3:O:54:ARG:HH11	1.84	0.42
3:N:163:VAL:HG12	3:N:164:THR:O	2.19	0.42
1:F:55:GLN:NE2	2:K:98:TYR:CE2	2.88	0.42
2:K:18:LEU:HB2	2:K:82(C):LEU:HD11	2.00	0.42
2:K:72:ASP:HB3	2:K:75:LYS:CE	2.30	0.42
2:H:18:LEU:O	2:H:81:LYS:HA	2.19	0.41
3:L:4:VAL:O	3:L:99:GLY:HA2	2.20	0.41
3:L:136:LEU:HD11	3:L:196:VAL:HG22	2.02	0.41
3:L:145:LYS:NZ	3:L:195:GLU:HG2	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:57:GLN:C	1:F:101:TRP:HE1	2.24	0.41
1:C:61:VAL:HG13	1:C:115:LYS:HB3	2.01	0.41
2:H:139:GLY:HA2	2:H:154:TRP:HZ2	1.84	0.41
3:L:13:THR:CG2	3:L:19:VAL:HG13	2.50	0.41
3:L:154:LEU:HA	3:L:154:LEU:HD23	1.77	0.41
3:M:38:GLU:O	3:M:39:LYS:HG2	2.20	0.41
2:H:95:ASN:CB	2:H:99:PRO:HD2	2.51	0.41
3:O:85:THR:HA	3:O:102:THR:O	2.20	0.41
1:D:67:MET:O	1:D:80:GLY:HA3	2.20	0.41
3:M:55:ALA:HB3	3:M:58:THR:CG2	2.50	0.41
1:F:31:ASP:OD1	1:F:33:VAL:HG23	2.20	0.41
2:K:18:LEU:HD13	2:K:109:VAL:HG11	2.01	0.41
3:O:38:GLU:HB2	3:O:44:PHE:CD1	2.55	0.41
3:L:145:LYS:CE	3:L:197:THR:H	2.25	0.41
1:D:32:ASP:OD1	1:D:133:ASN:HB2	2.20	0.41
3:N:48:LEU:HD23	3:N:54:ARG:HA	2.01	0.41
1:F:54:VAL:O	1:F:73:PRO:HD2	2.20	0.41
2:K:65:SER:O	2:K:65:SER:OG	2.38	0.41
2:H:171:GLN:H	2:H:171:GLN:HG3	1.73	0.41
3:L:124:GLN:HE21	3:L:124:GLN:HB2	1.59	0.41
3:L:180:THR:C	3:L:181:LEU:HD22	2.41	0.41
2:I:6:GLU:OE1	2:I:104:GLY:HA3	2.20	0.41
1:F:33:VAL:O	1:F:134:LEU:HD12	2.18	0.41
1:C:35:ALA:O	1:C:136:VAL:HA	2.21	0.41
3:L:12:THR:HA	3:L:105:THR:O	2.20	0.41
2:J:201:LYS:N	2:J:202:PRO:CD	2.84	0.41
1:F:31:ASP:HB2	1:F:32:ASP:H	1.44	0.41
3:O:147:GLN:HE21	3:O:148:TRP:N	2.19	0.41
2:H:13:GLN:C	2:H:15:SER:N	2.74	0.41
2:H:54:ASN:OD1	2:H:54:ASN:C	2.59	0.41
2:I:98:TYR:CD1	2:I:99:PRO:HA	2.56	0.41
2:J:70:SER:OG	2:J:71:ARG:N	2.53	0.41
3:N:21:LEU:O	3:N:72:ALA:HA	2.20	0.41
3:N:143:GLU:O	3:N:198:HIS:HD2	2.04	0.41
2:H:122:PHE:CZ	3:L:124:GLN:HG3	2.56	0.41
3:L:114:SER:OG	3:L:137:ASN:HB3	2.20	0.41
1:D:58:TRP:CH2	1:D:118:CYS:HB2	2.56	0.41
2:I:98:TYR:CG	2:I:99:PRO:HA	2.56	0.41
3:O:210:ASN:O	3:O:212:GLY:N	2.54	0.41
2:H:5:LYS:HE3	2:H:6:GLU:O	2.20	0.41
3:L:112:ALA:HB2	3:L:200:GLY:C	2.41	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:113:PRO:HB3	3:L:139:PHE:CD1	2.56	0.41
3:M:75:ILE:HD12	3:M:75:ILE:N	2.35	0.41
2:J:95:ASN:HB3	2:J:99:PRO:HD2	2.03	0.41
1:F:64:LYS:HD2	1:F:64:LYS:HA	1.76	0.41
1:F:131:VAL:O	1:F:132:TYR:HD1	2.04	0.41
2:K:200:HIS:CE1	2:K:203:SER:HB3	2.56	0.41
2:H:200:HIS:ND1	2:H:203:SER:HB3	2.36	0.40
2:I:59:TYR:HB2	2:I:64:LYS:HG3	2.03	0.40
1:E:53:LEU:HD12	1:E:122:LEU:HA	2.02	0.40
2:J:90:TYR:HB2	2:J:107:VAL:HG23	2.03	0.40
2:H:97:PRO:HG2	3:L:91:TRP:CE3	2.57	0.40
2:I:27:LEU:HD13	2:I:32:ASN:CG	2.41	0.40
1:F:32:ASP:CB	1:F:133:ASN:HB2	2.45	0.40
2:K:52:TRP:HZ3	2:K:98:TYR:HB3	1.85	0.40
2:K:82(C):LEU:HD23	2:K:82(C):LEU:HA	1.60	0.40
2:K:101:PHE:CD2	3:O:46:ALA:HB1	2.57	0.40
3:O:14:LEU:CD2	3:O:15:PRO:HD2	2.51	0.40
1:D:70:LEU:O	1:D:78:TYR:N	2.46	0.40
3:M:76:THR:O	3:M:76:THR:OG1	2.38	0.40
3:M:150:VAL:HG22	3:M:192:TYR:CD2	2.57	0.40
2:J:192:GLN:HG3	2:J:193:THR:N	2.35	0.40
2:K:14:PRO:C	2:K:16:GLN:H	2.24	0.40
3:O:116:PHE:CD2	3:O:135:LEU:HD23	2.56	0.40
2:I:5:LYS:HA	2:I:105:GLN:OE1	2.21	0.40
2:I:67:LEU:HD22	2:I:80:LEU:HD11	2.03	0.40
2:J:82(A):ASN:OD1	2:J:82(A):ASN:C	2.60	0.40
3:M:22:THR:CB	3:M:70:LYS:HD2	2.46	0.40
3:M:23:CYS:O	3:M:70:LYS:HB3	2.22	0.40
3:M:39:LYS:HE2	3:M:84:ALA:HB2	2.02	0.40
1:E:117:GLU:HB3	1:E:131:VAL:HG22	2.03	0.40
2:J:200:HIS:CD2	2:J:202:PRO:HD2	2.57	0.40
3:N:12:THR:HG22	3:N:105:THR:HG23	2.02	0.40
3:N:61:ARG:NH1	3:N:79:GLN:NE2	2.68	0.40
2:K:27:LEU:HD13	2:K:94:ARG:HD2	2.04	0.40
2:K:63:ILE:O	2:K:67:LEU:HD23	2.21	0.40
2:K:126:PRO:HA	2:K:130:SER:OG	2.22	0.40
2:K:148:GLU:HG3	2:K:176:TYR:CE2	2.57	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	C	111/122 (91%)	103 (93%)	7 (6%)	1 (1%)	17	34
1	D	111/122 (91%)	103 (93%)	6 (5%)	2 (2%)	8	16
1	E	87/122 (71%)	77 (88%)	10 (12%)	0	100	100
1	F	98/122 (80%)	90 (92%)	6 (6%)	2 (2%)	7	13
2	H	216/229 (94%)	207 (96%)	7 (3%)	2 (1%)	17	34
2	I	210/229 (92%)	204 (97%)	5 (2%)	1 (0%)	29	50
2	J	217/229 (95%)	205 (94%)	11 (5%)	1 (0%)	29	50
2	K	216/229 (94%)	208 (96%)	7 (3%)	1 (0%)	29	50
3	L	208/216 (96%)	194 (93%)	12 (6%)	2 (1%)	15	31
3	M	207/216 (96%)	196 (95%)	9 (4%)	2 (1%)	15	31
3	N	213/216 (99%)	198 (93%)	15 (7%)	0	100	100
3	O	207/216 (96%)	197 (95%)	9 (4%)	1 (0%)	29	50
All	All	2101/2268 (93%)	1982 (94%)	104 (5%)	15 (1%)	22	41

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	L	126	LYS
1	D	81	GLN
1	D	85	CYS
2	I	97	PRO
3	M	41	ASP
2	J	97	PRO
2	K	97	PRO
3	O	211	ARG
1	F	81	GLN
1	C	29	VAL
1	F	50	LYS
2	H	16	GLN

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Mol	Chain	Res	Type
3	M	152	ASN
3	L	211	ARG
2	H	14	PRO

### 5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	99/107 (92%)	92 (93%)	7 (7%)	14	28
1	D	99/107 (92%)	92 (93%)	7 (7%)	14	28
1	E	84/107 (78%)	73 (87%)	11 (13%)	4	7
1	F	89/107 (83%)	69 (78%)	20 (22%)	1	1
2	H	191/199 (96%)	167 (87%)	24 (13%)	4	8
2	I	187/199 (94%)	169 (90%)	18 (10%)	8	15
2	J	192/199 (96%)	174 (91%)	18 (9%)	8	16
2	K	191/199 (96%)	170 (89%)	21 (11%)	6	10
3	L	175/179 (98%)	156 (89%)	19 (11%)	6	11
3	M	174/179 (97%)	147 (84%)	27 (16%)	2	4
3	N	178/179 (99%)	160 (90%)	18 (10%)	7	13
3	O	174/179 (97%)	154 (88%)	20 (12%)	5	9
All	All	1833/1940 (94%)	1623 (88%)	210 (12%)	5	9

All (210) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	25	GLU
1	C	64	LYS
1	C	92	THR
1	C	96	LYS
1	C	109	SER
1	C	118	CYS
1	C	137	GLU

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
2	H	15	SER
2	H	16	GLN
2	H	21	THR
2	H	28	SER
2	H	61	SER
2	H	73	THR
2	H	84	THR
2	H	101	PHE
2	H	107	VAL
2	H	110	THR
2	H	112	SER
2	H	113	SER
2	H	127	SER
2	H	129	LYS
2	H	130	SER
2	H	132	SER
2	H	153	SER
2	H	156	SER
2	H	161	SER
2	H	179	SER
2	H	183	THR
2	H	187	SER
2	H	188	SER
2	H	203	SER
3	L	26	SER
3	L	41	ASP
3	L	43	SER
3	L	63	SER
3	L	89	SER
3	L	95	HIS
3	L	108	ARG
3	L	109	THR
3	L	122	ASP
3	L	126	LYS
3	L	156	SER
3	L	164	THR
3	L	166	GLN
3	L	170	ASP
3	L	176	SER
3	L	187	GLU
3	L	202	SER
3	L	203	SER

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
3	L	211	ARG
1	D	50	LYS
1	D	51	ASN
1	D	56	MET
1	D	81	GLN
1	D	86	GLU
1	D	118	CYS
1	D	122	LEU
2	I	2	VAL
2	I	12	VAL
2	I	21	THR
2	I	28	SER
2	I	35	SER
2	I	38	ARG
2	I	82(A)	ASN
2	I	87	THR
2	I	89	MET
2	I	112	SER
2	I	113	SER
2	I	115	SER
2	I	132	SER
2	I	135	THR
2	I	160	THR
2	I	161	SER
2	I	180	SER
2	I	197	ASN
3	M	6	GLN
3	M	13	THR
3	M	24	HIS
3	M	28	THR
3	M	39	LYS
3	M	58	THR
3	M	63	SER
3	M	65	SER
3	M	76	THR
3	M	88	CYS
3	M	131	SER
3	M	134	CYS
3	M	143	GLU
3	M	145	LYS
3	M	152	ASN
3	M	159	SER

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
3	M	162	SER
3	M	176	SER
3	M	178	THR
3	M	179	LEU
3	M	181	LEU
3	M	190	LYS
3	M	194	CYS
3	M	197	THR
3	M	202	SER
3	M	203	SER
3	M	206	THR
1	E	31	ASP
1	E	34	TYR
1	E	39	SER
1	E	63	ASP
1	E	66	ASP
1	E	77	LEU
1	E	109	SER
1	E	118	CYS
1	E	122	LEU
1	E	123	TYR
1	E	129	THR
2	J	4	LEU
2	J	22	CYS
2	J	66	ARG
2	J	67	LEU
2	J	70	SER
2	J	76	SER
2	J	87	THR
2	J	107	VAL
2	J	130	SER
2	J	135	THR
2	J	151	THR
2	J	153	SER
2	J	156	SER
2	J	180	SER
2	J	183	THR
2	J	186	SER
2	J	187	SER
2	J	191	THR
3	N	3	VAL
3	N	5	THR

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
3	N	13	THR
3	N	26	SER
3	N	28	THR
3	N	30	SER
3	N	41	ASP
3	N	42	HIS
3	N	43	SER
3	N	65	SER
3	N	67	LEU
3	N	93	SER
3	N	96	LEU
3	N	105	THR
3	N	152	ASN
3	N	167	ASP
3	N	176	SER
3	N	185	ASP
1	F	31	ASP
1	F	32	ASP
1	F	36	LEU
1	F	39	SER
1	F	44	THR
1	F	45	CYS
1	F	48	LYS
1	F	55	GLN
1	F	59	SER
1	F	63	ASP
1	F	82	GLU
1	F	86	GLU
1	F	102	THR
1	F	106	ARG
1	F	108	ILE
1	F	118	CYS
1	F	122	LEU
1	F	128	LYS
1	F	129	THR
1	F	136	VAL
2	K	13	GLN
2	K	15	SER
2	K	22	CYS
2	K	28	SER
2	K	38	ARG
2	K	62	ASP

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
2	K	63	ILE
2	K	65	SER
2	K	70	SER
2	K	72	ASP
2	K	97	PRO
2	K	132	SER
2	K	135	THR
2	K	142	VAL
2	K	151	THR
2	K	156	SER
2	K	163	VAL
2	K	183	THR
2	K	192	GLN
2	K	203	SER
2	K	209	LYS
3	O	4	VAL
3	O	6	GLN
3	O	28	THR
3	O	30	SER
3	O	65	SER
3	O	67	LEU
3	O	95	HIS
3	O	115	VAL
3	O	121	SER
3	O	122	ASP
3	O	126	LYS
3	O	131	SER
3	O	159	SER
3	O	162	SER
3	O	171	SER
3	O	176	SER
3	O	177	SER
3	O	178	THR
3	O	202	SER
3	O	203	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	C	88	GLN
2	H	83	GLN
2	H	197	ASN

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Mol	Chain	Res	Type
3	L	42	HIS
3	L	152	ASN
3	L	160	GLN
3	L	210	ASN
1	D	81	GLN
1	D	83	HIS
2	I	16	GLN
1	E	133	ASN
2	J	3	GLN
2	J	171	GLN
2	J	199	ASN
3	N	24	HIS
3	N	42	HIS
3	N	210	ASN
1	F	55	GLN
1	F	133	ASN
2	K	13	GLN
2	K	77	GLN
3	O	147	GLN
3	O	210	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

4 non-standard protein/DNA/RNA residues 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
3	PCA	N	1	3	7,8,9	1.81	1 (14%)	9,10,12	1.86	4 (44%)
3	PCA	L	1	3	7,8,9	1.79	1 (14%)	9,10,12	1.97	4 (44%)
3	PCA	O	1	3	7,8,9	1.92	1 (14%)	9,10,12	1.99	4 (44%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	PCA	M	1	3	7,8,9	2.10	1 (14%)	9,10,12	1.97	4 (44%)

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
3	PCA	N	1	3	-	0/0/11/13	0/1/1/1
3	PCA	L	1	3	-	0/0/11/13	0/1/1/1
3	PCA	O	1	3	-	0/0/11/13	0/1/1/1
3	PCA	M	1	3	-	0/0/11/13	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	M	1	PCA	CD-N	5.29	1.48	1.34
3	O	1	PCA	CD-N	4.85	1.47	1.34
3	N	1	PCA	CD-N	4.57	1.46	1.34
3	L	1	PCA	CD-N	4.55	1.46	1.34

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	M	1	PCA	OE-CD-CG	-3.51	120.64	126.76
3	N	1	PCA	CB-CA-N	3.08	112.13	103.30
3	O	1	PCA	CB-CA-N	3.03	112.01	103.30
3	O	1	PCA	CA-N-CD	-2.95	103.48	113.58
3	N	1	PCA	CA-N-CD	-2.84	103.86	113.58
3	L	1	PCA	CA-N-CD	-2.80	103.98	113.58
3	L	1	PCA	CB-CA-N	2.75	111.20	103.30
3	M	1	PCA	CA-N-CD	-2.56	104.82	113.58
3	O	1	PCA	CG-CD-N	2.49	114.84	108.39
3	L	1	PCA	OE-CD-CG	-2.48	122.43	126.76
3	L	1	PCA	CG-CD-N	2.46	114.77	108.39
3	M	1	PCA	CG-CD-N	2.28	114.31	108.39
3	M	1	PCA	CB-CA-N	2.28	109.84	103.30
3	N	1	PCA	CG-CD-N	2.25	114.20	108.39
3	N	1	PCA	OE-CD-CG	-2.07	123.16	126.76
3	O	1	PCA	OE-CD-CG	-2.04	123.20	126.76

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
3	L	1	PCA	1	0

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

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	NAG	D	201	1	14,14,15	0.39	0	17,19,21	0.59	0
5	SO4	D	203	-	4,4,4	0.23	0	6,6,6	0.50	0
5	SO4	D	202	-	4,4,4	0.32	0	6,6,6	0.16	0
5	SO4	L	301	-	4,4,4	0.23	0	6,6,6	0.19	0
5	SO4	C	202	-	4,4,4	0.25	0	6,6,6	0.39	0
5	SO4	K	301	-	4,4,4	0.27	0	6,6,6	0.25	0
4	NAG	C	201	1	14,14,15	0.42	0	17,19,21	0.48	0
5	SO4	N	301	-	4,4,4	0.09	0	6,6,6	0.45	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	C	201	1	-	0/6/23/26	0/1/1/1
4	NAG	D	201	1	-	0/6/23/26	0/1/1/1

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.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	L	301	SO4	1	0
5	C	202	SO4	1	0
5	K	301	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	C	113/122 (92%)	0.43	0 <b>100</b> <b>100</b>	31, 40, 53, 59	0
1	D	113/122 (92%)	0.76	13 (11%) <b>4</b> <b>3</b>	37, 50, 73, 77	0
1	E	95/122 (77%)	2.48	52 (54%) <b>0</b> <b>0</b>	60, 82, 91, 95	0
1	F	102/122 (83%)	2.46	49 (48%) <b>0</b> <b>0</b>	58, 80, 97, 102	0
2	H	218/229 (95%)	0.88	36 (16%) <b>1</b> <b>1</b>	33, 55, 83, 90	0
2	I	214/229 (93%)	0.38	4 (1%) <b>66</b> <b>64</b>	29, 37, 57, 64	0
2	J	219/229 (95%)	0.34	5 (2%) <b>60</b> <b>57</b>	31, 48, 59, 62	0
2	K	218/229 (95%)	0.47	16 (7%) <b>15</b> <b>12</b>	36, 54, 71, 77	0
3	L	211/216 (97%)	0.50	9 (4%) <b>35</b> <b>31</b>	33, 46, 68, 77	0
3	M	210/216 (97%)	0.38	5 (2%) <b>59</b> <b>55</b>	33, 41, 54, 61	0
3	N	214/216 (99%)	0.42	8 (3%) <b>41</b> <b>37</b>	30, 49, 68, 76	0
3	O	210/216 (97%)	0.35	2 (0%) <b>82</b> <b>81</b>	37, 44, 55, 66	0
All	All	2137/2268 (94%)	0.66	199 (9%) <b>8</b> <b>7</b>	29, 47, 82, 102	0

All (199) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	104	TYR	8.5
1	F	36	LEU	7.7
1	E	53	LEU	7.4
1	F	132	TYR	7.3
1	F	108	ILE	6.9
1	E	123	TYR	6.8
1	E	127	ILE	6.3
1	F	33	VAL	6.1
1	F	137	GLU	6.1
1	F	32	ASP	6.0
2	H	132	SER	6.0

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	F	136	VAL	6.0
1	F	43	LEU	5.6
1	F	35	ALA	5.5
1	E	34	TYR	5.4
1	E	136	VAL	5.4
1	F	34	TYR	5.4
1	F	41	ILE	5.3
1	F	110	SER	5.1
2	H	189	LEU	5.1
1	E	36	LEU	5.0
1	E	35	ALA	4.9
2	H	187	SER	4.9
1	F	103	LEU	4.9
1	E	33	VAL	4.8
1	E	46	GLN	4.7
1	E	134	LEU	4.7
1	E	101	TRP	4.7
1	E	132	TYR	4.6
1	E	122	LEU	4.6
3	O	67	LEU	4.6
1	E	37	PRO	4.5
1	F	106	ARG	4.5
1	E	43	LEU	4.5
1	E	98	VAL	4.4
2	K	12	VAL	4.4
1	F	112	LEU	4.3
2	I	131	THR	4.3
1	F	135	ILE	4.2
1	F	45	CYS	4.2
2	H	211	VAL	4.2
1	F	125	GLU	4.2
2	K	13	GLN	4.2
3	L	213	GLU	4.1
2	H	194	TYR	4.1
3	N	41	ASP	4.0
2	H	188	SER	4.0
1	E	119	ILE	4.0
1	E	92	THR	3.9
1	E	120	PHE	3.9
1	F	63	ASP	3.9
2	K	3	GLN	3.9
2	H	159	LEU	3.9

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	F	89	VAL	3.8
1	E	64	LYS	3.8
1	F	105	LEU	3.8
1	F	116	TYR	3.7
2	H	135	THR	3.7
1	E	32	ASP	3.7
1	E	117	GLU	3.7
1	E	116	TYR	3.7
1	F	82	GLU	3.6
2	H	131	THR	3.6
2	H	191	THR	3.6
2	K	63	ILE	3.6
3	L	125	LEU	3.6
1	E	58	TRP	3.5
1	D	122	LEU	3.5
1	F	31	ASP	3.5
2	H	185	PRO	3.5
1	E	54	VAL	3.5
3	O	190	LYS	3.5
1	E	82	GLU	3.4
1	F	62	THR	3.4
1	F	115	LYS	3.4
2	H	214	LYS	3.4
1	F	107	ASN	3.3
1	E	135	ILE	3.3
1	E	115	LYS	3.3
1	E	62	THR	3.3
3	L	126	LYS	3.3
2	J	131	THR	3.3
1	D	28	ASN	3.3
3	L	123	GLU	3.2
3	N	94	GLY	3.2
1	E	63	ASP	3.2
1	E	124	PRO	3.2
1	F	134	LEU	3.1
1	E	31	ASP	3.1
1	D	94	THR	3.1
1	E	108	ILE	3.1
2	J	100(A)	ILE	3.1
2	H	192	GLN	3.0
1	F	133	ASN	3.0
2	K	2	VAL	3.0

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	E	93	GLU	3.0
1	F	44	THR	3.0
2	J	189	LEU	3.0
1	D	93	GLU	3.0
3	N	42	HIS	2.9
1	D	106	ARG	2.9
1	F	53	LEU	2.9
2	H	152	VAL	2.9
2	K	82(C)	LEU	2.9
2	H	2	VAL	2.9
1	F	61	VAL	2.9
1	E	104	TYR	2.9
1	E	41	ILE	2.8
2	K	214	LYS	2.8
1	F	64	LYS	2.8
3	M	183	LYS	2.8
1	D	36	LEU	2.8
1	F	111	ALA	2.8
1	E	133	ASN	2.8
2	H	85	GLU	2.8
1	E	128	LYS	2.8
3	N	79	GLN	2.8
1	D	29	VAL	2.7
1	E	100	ASN	2.7
2	H	129	LYS	2.7
3	L	181	LEU	2.7
2	J	215	SER	2.7
2	H	184	VAL	2.7
2	H	195	ILE	2.6
1	D	125	GLU	2.6
2	I	210	ARG	2.6
2	H	125	ALA	2.6
2	K	78	VAL	2.6
1	F	130	THR	2.6
2	K	19	SER	2.6
1	E	121	THR	2.5
2	H	163	VAL	2.5
2	I	189	LEU	2.5
3	L	121	SER	2.5
2	J	3	GLN	2.5
2	K	18	LEU	2.5
3	M	191	VAL	2.5

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	D	123	TYR	2.5
2	H	137	ALA	2.5
2	H	193	THR	2.5
2	H	164	HIS	2.5
3	N	3	VAL	2.5
1	E	45	CYS	2.4
1	E	81	GLN	2.4
3	N	32	TYR	2.4
3	M	2	ALA	2.4
3	L	188	LYS	2.4
3	L	135	LEU	2.4
1	F	122	LEU	2.4
1	F	40	ASP	2.4
1	F	91	ALA	2.4
1	D	33	VAL	2.4
1	F	127	ILE	2.4
2	H	126	PRO	2.3
2	H	147	PRO	2.3
2	H	209	LYS	2.3
1	F	58	TRP	2.3
2	H	122	PHE	2.3
2	H	186	SER	2.3
2	I	132	SER	2.3
3	N	2	ALA	2.3
1	F	37	PRO	2.3
2	K	73	THR	2.3
1	E	61	VAL	2.3
1	F	74	GLN	2.3
2	H	12	VAL	2.2
1	E	91	ALA	2.2
1	F	119	ILE	2.2
1	F	81	GLN	2.2
1	E	60	LYS	2.2
1	E	90	ALA	2.2
3	N	75	ILE	2.2
2	K	75	LYS	2.2
2	H	109	VAL	2.2
2	K	25	SER	2.2
1	F	118	CYS	2.2
2	K	24	VAL	2.1
1	E	65	ASN	2.1
1	F	90	ALA	2.1

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Mol	Chain	Res	Type	RSRZ
1	D	124	PRO	2.1
1	D	49	GLU	2.1
1	E	129	THR	2.1
1	E	130	THR	2.1
2	K	29	LEU	2.1
3	M	68	GLU	2.1
1	F	30	GLY	2.1
1	E	66	ASP	2.1
3	M	213	GLU	2.1
1	D	62	THR	2.1
3	L	120	PRO	2.1
2	H	15	SER	2.1
2	H	127	SER	2.1
1	F	38	GLY	2.1
2	H	158	ALA	2.0
2	K	4	LEU	2.0
1	E	102	THR	2.0
2	H	213	PRO	2.0
2	H	161	SER	2.0
1	E	68	ILE	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains [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, 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	B-factors(Å <sup>2</sup> )	Q<0.9
3	PCA	M	1	8/9	0.56	0.55	68,73,74,74	0
3	PCA	N	1	8/9	0.74	0.34	82,84,85,85	0
3	PCA	O	1	8/9	0.90	0.24	58,61,64,64	0
3	PCA	L	1	8/9	0.96	0.15	46,49,50,51	0

## 6.3 Carbohydrates [i](#)

There are no monosaccharides 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, 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	B-factors(Å <sup>2</sup> )	Q<0.9
4	NAG	C	201	14/15	0.86	0.27	55,61,64,65	0
5	SO4	L	301	5/5	0.87	0.20	77,81,85,86	0
5	SO4	D	202	5/5	0.89	0.26	76,79,82,86	0
4	NAG	D	201	14/15	0.91	0.29	63,69,73,74	0
5	SO4	K	301	5/5	0.92	0.22	77,77,77,77	0
5	SO4	C	202	5/5	0.97	0.14	45,45,45,47	0
5	SO4	N	301	5/5	0.98	0.15	40,41,42,42	0
5	SO4	D	203	5/5	0.98	0.13	50,54,54,54	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.