



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 04:48 AM UTC

PDB ID : 7S11 / pdb_00007s11
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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

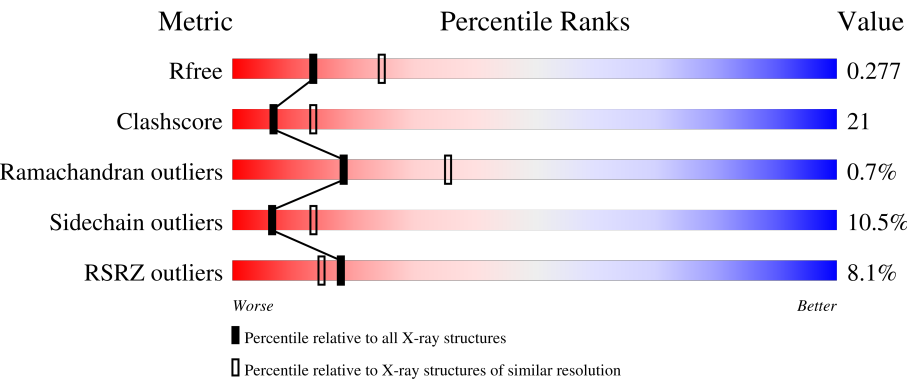
MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry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

1 Overall quality at a glance i

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}	180053	4770 (2.60-2.56)
Clashscore	190562	5124 (2.60-2.56)
Ramachandran outliers	187476	5046 (2.60-2.56)
Sidechain outliers	187428	5046 (2.60-2.56)
RSRZ outliers	180081	4770 (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 ≥ 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	2% 61% 30% 7%
1	D	122	14% 49% 37% 6% 7%
1	E	122	25% 37% 34% 6% 22%
1	F	122	30% 36% 30% 12% 5% 16%
2	H	229	10% 48% 41% 6% 5%

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Mol	Chain	Length	Quality of chain
2	I	229	2% 59% 31% 7%
2	J	229	4% 61% 27% 8%
2	K	229	6% 51% 38% 5%
3	L	216	4% 62% 29% 6%
3	M	216	4% 59% 32% 6%
3	N	216	6% 59% 36%
3	O	216	4% 69% 23% 6%

2 Entry composition

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
1	C	113	Total	C	N	O	S	0	0	0
			897	572	142	177	6			
1	D	113	Total	C	N	O	S	0	0	0
			897	572	142	177	6			
1	E	95	Total	C	N	O	S	0	0	0
			753	482	119	146	6			
1	F	102	Total	C	N	O	S	0	0	0
			810	517	128	159	6			

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

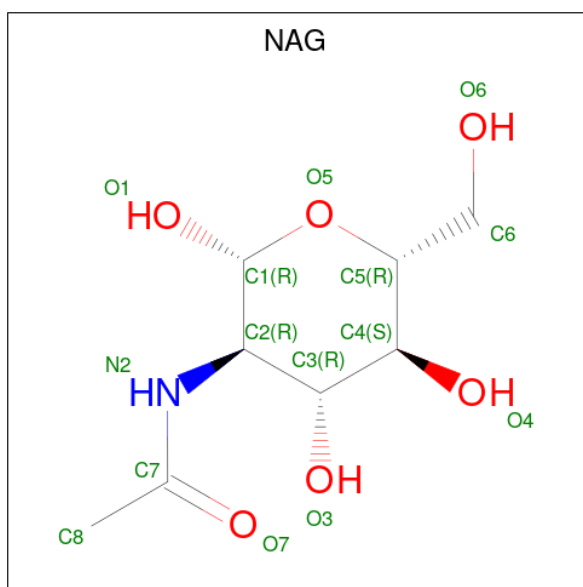
- Molecule 2 is a protein called Fab heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
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.

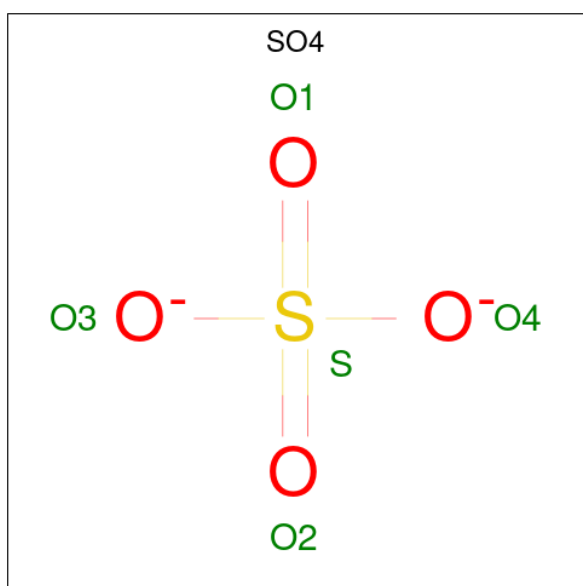
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	L	212	Total	C	N	O	S	0	0	0
			1591	996	268	323	4			
3	M	211	Total	C	N	O	S	0	0	0
			1582	991	266	321	4			
3	N	215	Total	C	N	O	S	0	0	0
			1614	1009	272	329	4			
3	O	211	Total	C	N	O	S	0	0	0
			1582	991	267	320	4			

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).



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

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



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

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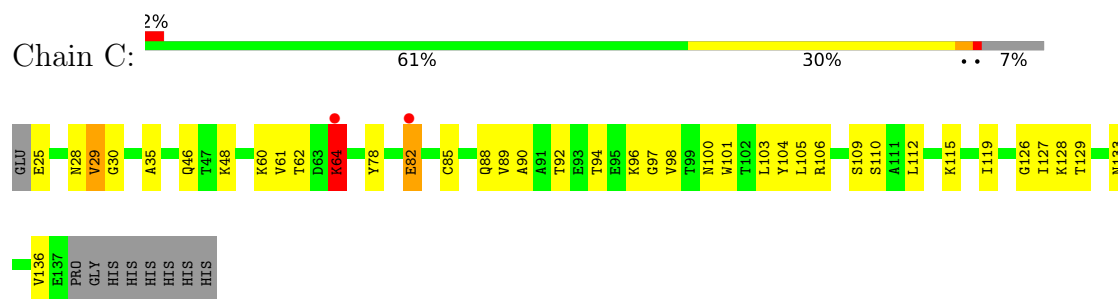
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	D	1	Total	O	S	0	0
			5	4	1		
5	D	1	Total	O	S	0	0
			5	4	1		
5	N	1	Total	O	S	0	0
			5	4	1		
5	K	1	Total	O	S	0	0
			5	4	1		

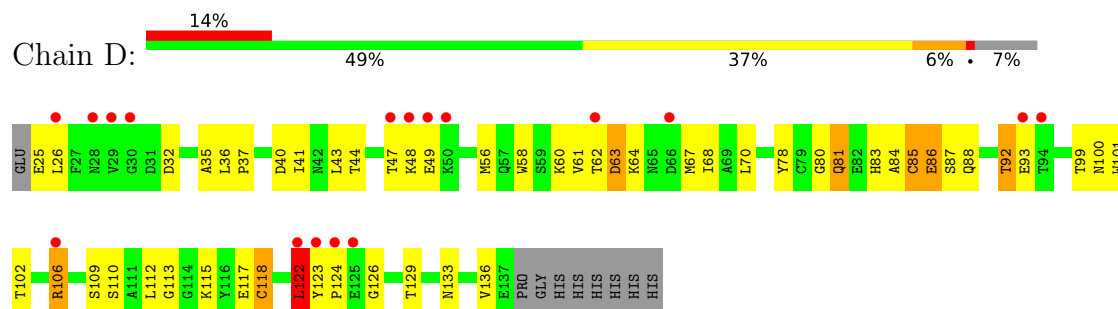
3 Residue-property plots [i](#)

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.

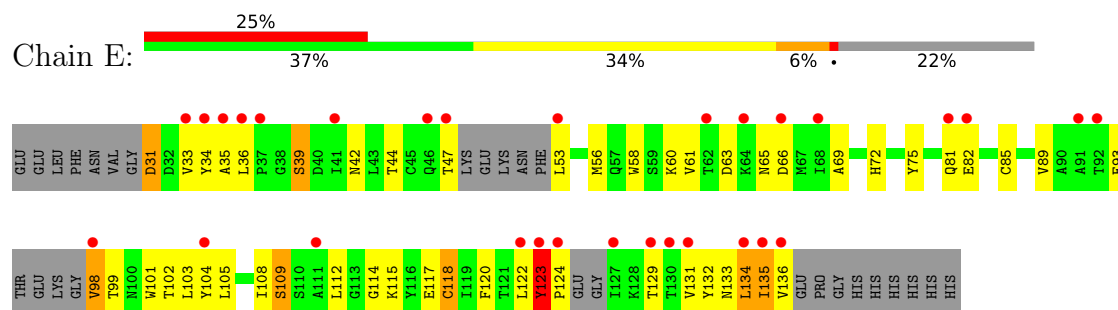
- Molecule 1: T-cell surface protein tactile



- Molecule 1: T-cell surface protein tactile

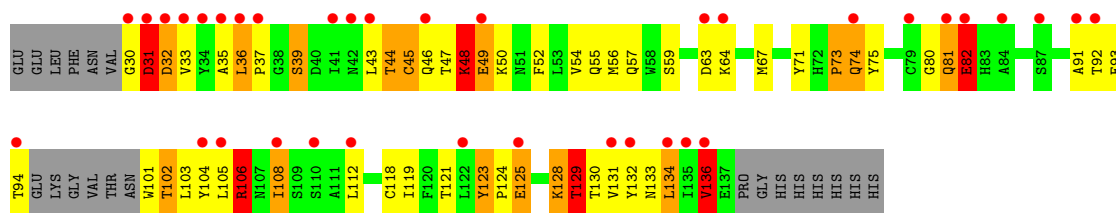


- Molecule 1: T-cell surface protein tactile

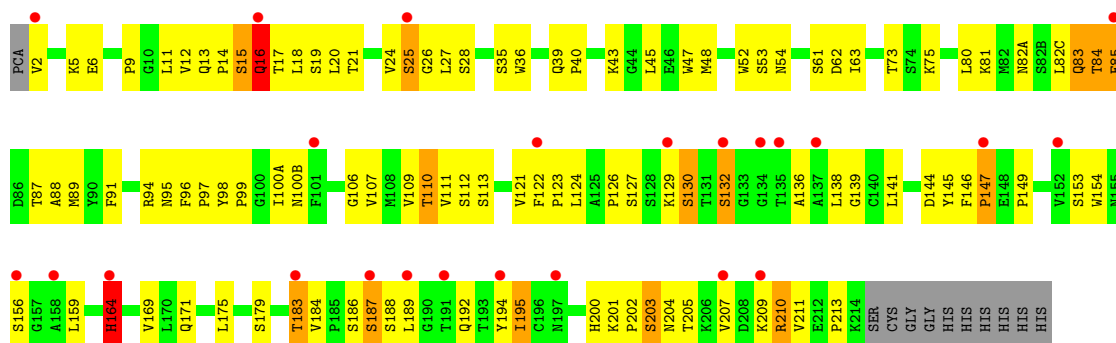


- Molecule 1: T-cell surface protein tactile

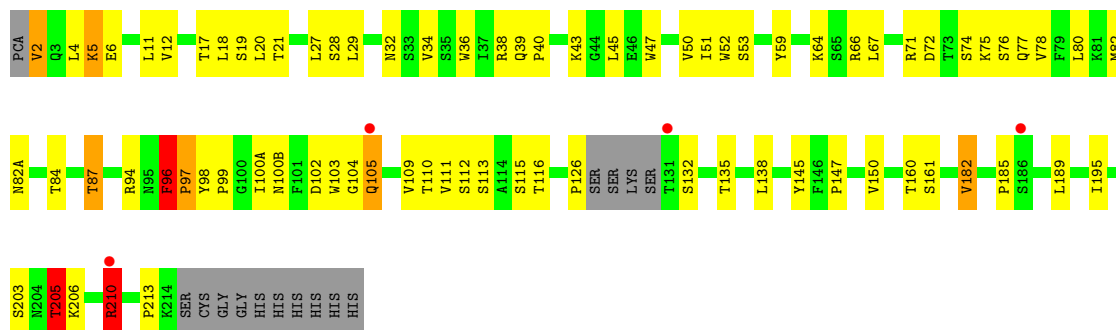




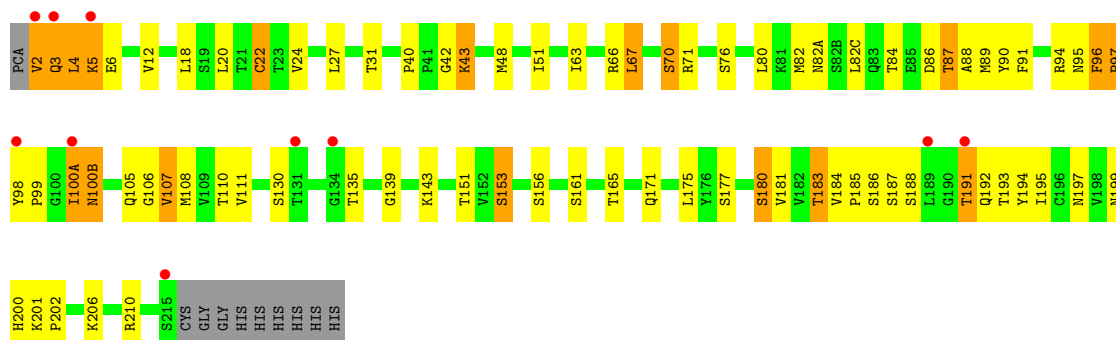
• Molecule 2: Fab heavy chain



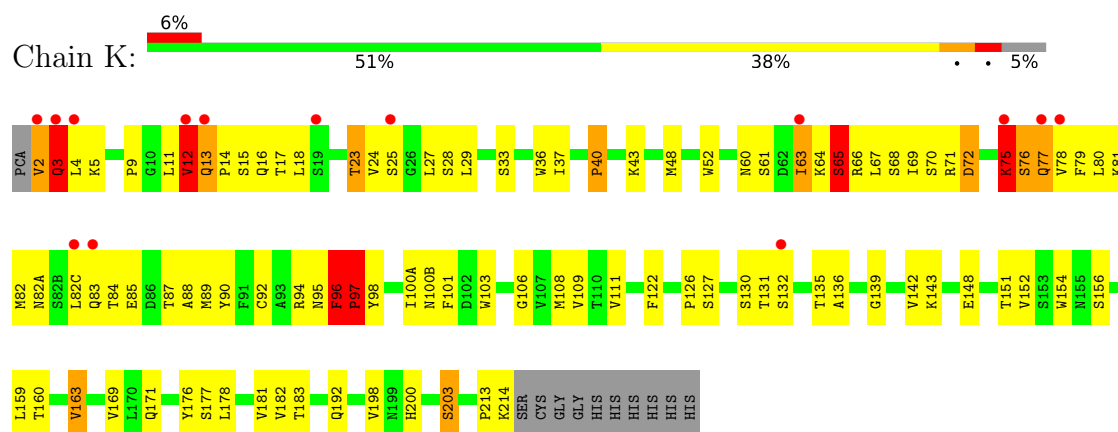
• Molecule 2: Fab heavy chain



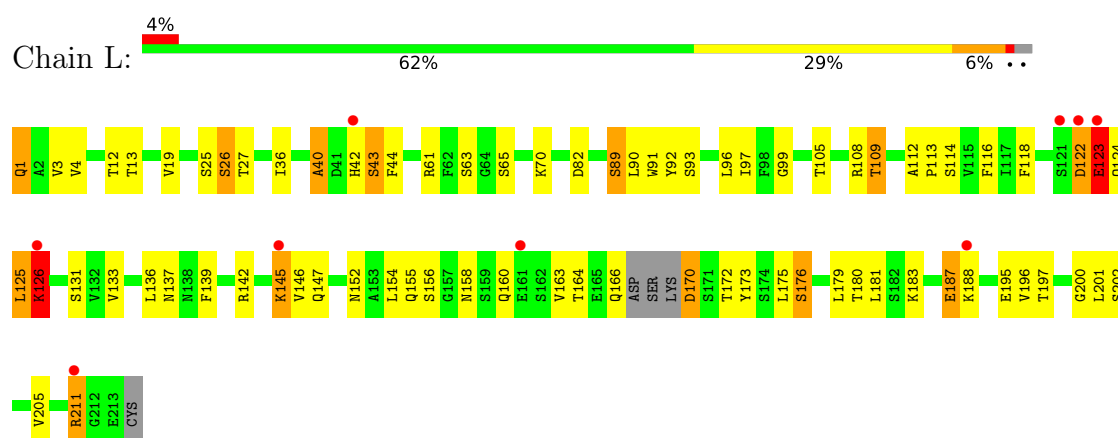
• Molecule 2: Fab heavy chain



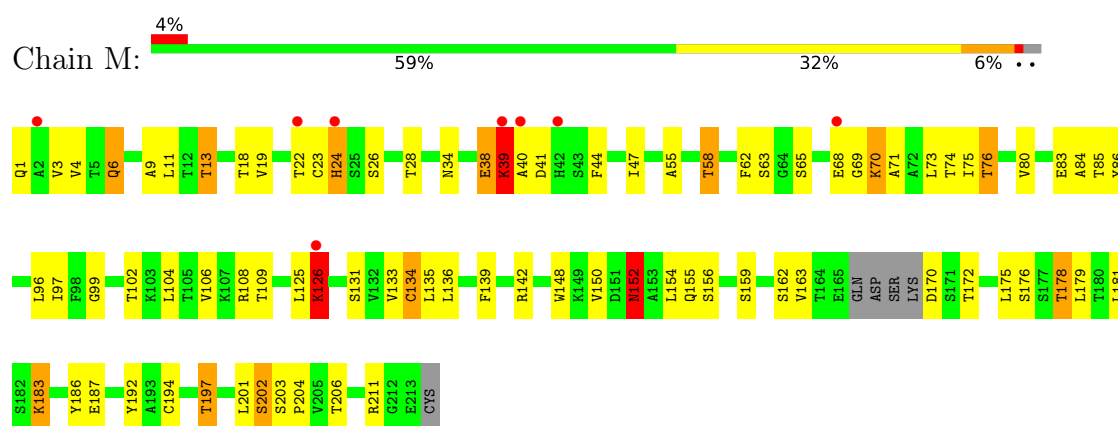
- Molecule 2: Fab heavy chain



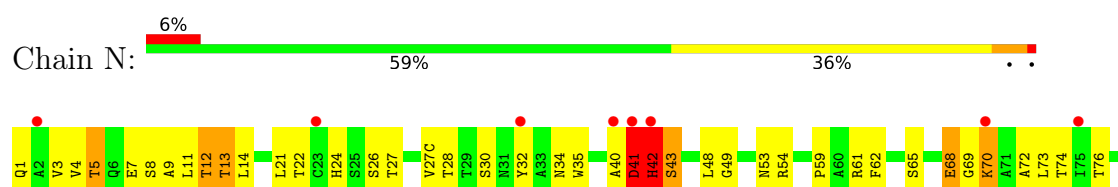
- Molecule 3: Fab light chain

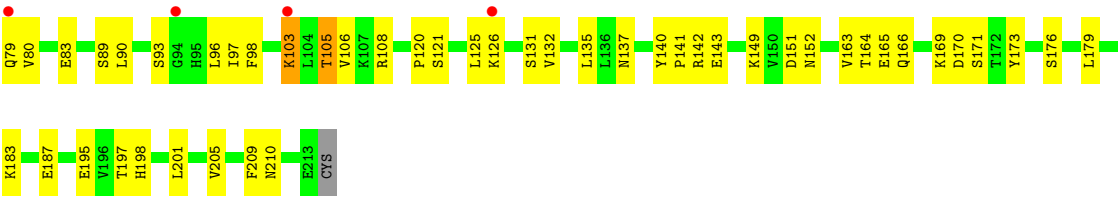


- Molecule 3: Fab light chain

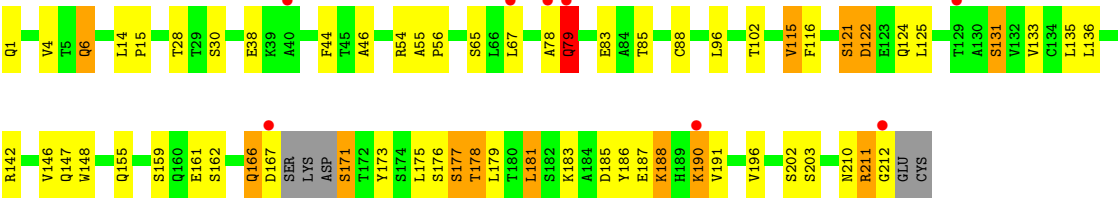


- Molecule 3: Fab light chain





● 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, α , β , γ	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) 63.9 (61.20-2.58)	Depositor EDS
R_{merge}	0.20	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.49 (at 2.58Å)	Xtriage
Refinement program	PHENIX 1.19.1_4122	Depositor
R, R_{free}	0.226 , 0.279 0.226 , 0.277	Depositor DCC
R_{free} test set	2923 reflections (3.12%)	wwPDB-VP
Wilson B-factor (Å ²)	55.2	Xtriage
Anisotropy	0.064	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 39.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	16283	wwPDB-VP
Average B, all atoms (Å ²)	50.0	wwPDB-VP

Xtriage'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.*

¹Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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	0.57	0/916	0.86	2/1245 (0.2%)
1	D	0.63	0/916	1.34	9/1245 (0.7%)
1	E	0.38	0/767	0.63	0/1043
1	F	0.69	0/827	1.88	37/1123 (3.3%)
2	H	0.69	1/1669 (0.1%)	1.13	13/2276 (0.6%)
2	I	0.64	0/1641	1.06	16/2238 (0.7%)
2	J	0.55	0/1675	1.04	13/2284 (0.6%)
2	K	0.78	6/1669 (0.4%)	1.19	20/2276 (0.9%)
3	L	0.71	5/1616 (0.3%)	1.11	11/2201 (0.5%)
3	M	0.72	3/1607 (0.2%)	1.23	17/2189 (0.8%)
3	N	0.58	1/1640 (0.1%)	0.97	11/2234 (0.5%)
3	O	0.50	0/1607	0.93	8/2189 (0.4%)
All	All	0.64	16/16550 (0.1%)	1.13	157/22543 (0.7%)

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 (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	K	77	GLN	CA-CB	11.89	1.73	1.53
2	K	40	PRO	CA-C	-9.89	1.46	1.51
2	K	75	LYS	CG-CD	-9.10	1.25	1.52
3	M	126	LYS	CD-CE	8.83	1.78	1.52
3	L	126	LYS	CE-NZ	8.05	1.73	1.49
3	L	122	ASP	C-N	-6.45	1.24	1.33
3	N	126	LYS	CB-CG	6.23	1.71	1.52
2	K	77	GLN	N-CA	-6.07	1.38	1.46
2	H	210	ARG	N-CA	6.05	1.53	1.46
3	L	122	ASP	CA-C	-5.91	1.45	1.52
3	M	68	GLU	CD-OE2	5.61	1.36	1.25
2	K	76	SER	CA-C	5.41	1.60	1.52
3	L	126	LYS	CG-CD	-5.25	1.36	1.52
3	M	126	LYS	CE-NZ	5.18	1.64	1.49
2	K	3	GLN	CB-CG	5.08	1.67	1.52
3	L	123	GLU	CG-CD	5.00	1.64	1.52

All (157) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	106	ARG	CB-CG-CD	-25.30	53.10	111.30
3	M	68	GLU	CA-CB-CG	-23.39	67.33	114.10
2	K	75	LYS	CB-CA-C	-16.50	83.34	110.74
3	L	126	LYS	CB-CG-CD	-14.97	76.86	111.30
2	K	3	GLN	CA-CB-CG	14.80	143.69	114.10
2	H	195	ILE	CG1-CB-CG2	-14.42	67.43	110.70
2	J	3	GLN	CA-CB-CG	-14.23	85.63	114.10
1	F	31	ASP	CB-CG-OD2	-13.57	87.20	118.40
3	O	79	GLN	CA-CB-CG	-13.41	87.29	114.10
3	N	68	GLU	CG-CD-OE1	13.25	148.87	118.40
1	F	49	GLU	CA-CB-CG	-13.18	87.75	114.10
2	J	43	LYS	CB-CG-CD	12.32	139.64	111.30
2	J	5	LYS	CA-CB-CG	-12.10	89.91	114.10
1	F	31	ASP	CB-CG-OD1	11.88	145.72	118.40
1	F	74	GLN	CB-CG-CD	11.78	132.63	112.60
1	F	136	VAL	CG1-CB-CG2	-11.76	84.94	110.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	73	PRO	CA-C-N	-11.67	101.08	123.13
1	F	73	PRO	C-N-CA	-11.67	101.08	123.13
1	D	106	ARG	CG-CD-NE	11.61	137.53	112.00
3	L	123	GLU	CB-CA-C	11.35	133.01	110.42
3	L	188	LYS	CA-CB-CG	11.07	136.24	114.10
3	M	126	LYS	CG-CD-CE	-11.00	86.00	111.30
1	F	74	GLN	CA-CB-CG	10.91	135.92	114.10
3	N	68	GLU	OE1-CD-OE2	-10.84	96.88	122.90
3	M	68	GLU	CG-CD-OE1	-10.82	93.52	118.40
1	F	31	ASP	N-CA-C	-10.80	92.47	108.34
1	D	106	ARG	CA-CB-CG	10.76	135.62	114.10
3	L	123	GLU	CA-CB-CG	10.70	135.50	114.10
3	O	188	LYS	CB-CG-CD	10.63	135.75	111.30
1	F	31	ASP	CB-CA-C	-10.57	101.11	116.54
3	L	126	LYS	N-CA-CB	-10.45	92.83	110.49
2	H	201	LYS	CB-CG-CD	-10.19	87.86	111.30
2	I	105	GLN	CB-CG-CD	-9.90	95.76	112.60
2	K	64	LYS	CA-C-N	-9.69	105.89	122.56
2	K	64	LYS	C-N-CA	-9.69	105.89	122.56
3	N	70	LYS	CG-CD-CE	-9.64	89.12	111.30
1	F	81	GLN	CA-C-N	9.60	137.43	122.93
1	F	81	GLN	C-N-CA	9.60	137.43	122.93
3	N	68	GLU	CG-CD-OE2	-9.59	96.34	118.40
1	F	82	GLU	CG-CD-OE1	9.40	140.03	118.40
2	I	105	GLN	N-CA-CB	-9.27	94.76	110.51
2	J	5	LYS	CB-CG-CD	9.26	132.60	111.30
1	F	31	ASP	OD1-CG-OD2	-9.09	101.08	122.90
2	K	75	LYS	CB-CG-CD	9.01	132.02	111.30
2	I	210	ARG	CG-CD-NE	8.94	131.67	112.00
2	H	201	LYS	CG-CD-CE	8.88	131.73	111.30
2	I	206	LYS	CA-CB-CG	8.72	131.54	114.10
2	K	2	VAL	CA-C-N	8.72	133.88	121.42
2	K	2	VAL	C-N-CA	8.72	133.88	121.42
1	F	125	GLU	CA-CB-CG	8.61	131.32	114.10
2	I	210	ARG	CA-CB-CG	8.59	131.28	114.10
1	F	82	GLU	CG-CD-OE2	-8.55	98.74	118.40
2	H	85	GLU	CB-CA-C	-8.49	94.36	110.67
1	F	82	GLU	CB-CG-CD	8.43	126.93	112.60
2	J	2	VAL	CA-C-N	-8.32	108.75	122.39
2	J	2	VAL	C-N-CA	-8.32	108.75	122.39
1	F	125	GLU	CB-CG-CD	8.29	126.70	112.60
3	M	24	HIS	CB-CA-C	-8.26	95.60	109.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	164	HIS	N-CA-CB	8.17	123.40	110.65
2	K	75	LYS	CA-CB-CG	8.03	130.15	114.10
3	M	68	GLU	CB-CG-CD	7.91	126.04	112.60
2	K	3	GLN	CB-CA-C	-7.87	96.23	109.53
2	K	3	GLN	CB-CG-CD	7.85	125.94	112.60
1	F	125	GLU	CB-CA-C	7.70	125.75	110.42
3	L	123	GLU	N-CA-CB	-7.70	97.48	110.49
2	J	43	LYS	CD-CE-NZ	7.68	136.49	111.90
2	I	206	LYS	CB-CG-CD	7.61	128.79	111.30
3	M	183	LYS	CB-CG-CD	-7.51	94.04	111.30
1	F	49	GLU	CB-CG-CD	7.44	125.24	112.60
2	K	40	PRO	O-C-N	-7.38	117.92	121.31
1	D	92	THR	CA-C-N	7.26	132.28	122.84
1	D	92	THR	C-N-CA	7.26	132.28	122.84
3	O	188	LYS	CA-CB-CG	-7.23	99.64	114.10
3	L	145	LYS	CA-CB-CG	-7.20	99.70	114.10
3	M	38	GLU	CA-C-N	-7.16	107.86	121.54
3	M	38	GLU	C-N-CA	-7.16	107.86	121.54
3	M	70	LYS	CB-CG-CD	-7.16	94.82	111.30
2	K	43	LYS	CA-CB-CG	-7.15	99.79	114.10
1	F	121	THR	OG1-CB-CG2	6.99	123.29	109.30
2	K	12	VAL	CA-C-N	6.98	145.00	121.27
2	K	12	VAL	C-N-CA	6.98	145.00	121.27
2	I	206	LYS	CB-CA-C	-6.87	97.93	109.53
2	I	185	PRO	CA-C-N	-6.85	107.62	121.18
2	I	185	PRO	C-N-CA	-6.85	107.62	121.18
1	C	82	GLU	CA-C-N	-6.83	111.96	122.62
1	C	82	GLU	C-N-CA	-6.83	111.96	122.62
3	O	190	LYS	CD-CE-NZ	-6.81	90.10	111.90
3	M	183	LYS	CG-CD-CE	6.77	126.87	111.30
3	L	188	LYS	CB-CG-CD	-6.74	95.80	111.30
1	F	136	VAL	N-CA-C	6.70	116.83	110.53
1	F	82	GLU	CA-CB-CG	6.67	127.44	114.10
2	I	5	LYS	CA-CB-CG	-6.66	100.78	114.10
1	F	125	GLU	N-CA-CB	-6.60	99.33	110.49
2	H	83	GLN	CA-CB-CG	6.50	127.09	114.10
2	I	5	LYS	CB-CG-CD	6.46	126.17	111.30
2	J	43	LYS	CA-CB-CG	-6.46	101.18	114.10
2	J	42	GLY	CA-C-N	-6.39	111.63	123.01
2	J	42	GLY	C-N-CA	-6.39	111.63	123.01
2	H	183	THR	OG1-CB-CG2	6.37	122.03	109.30
2	J	43	LYS	CG-CD-CE	-6.35	96.69	111.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	74	GLN	N-CA-CB	6.33	120.88	111.51
1	D	122	LEU	CA-CB-CG	6.32	138.43	116.30
3	L	126	LYS	CA-CB-CG	6.32	126.74	114.10
2	H	195	ILE	CB-CG1-CD1	-6.32	100.53	113.80
3	O	79	GLN	CB-CG-CD	6.28	123.28	112.60
3	L	123	GLU	CB-CG-CD	-6.28	101.93	112.60
3	N	41	ASP	CA-C-N	-6.26	113.46	122.67
3	N	41	ASP	C-N-CA	-6.26	113.46	122.67
2	I	210	ARG	CD-NE-CZ	6.23	133.12	124.40
2	H	85	GLU	N-CA-CB	6.16	119.83	110.28
2	I	96	PHE	C-N-CD	-6.14	99.83	125.00
1	F	121	THR	CA-CB-CG2	6.14	120.93	110.50
1	F	74	GLN	CG-CD-NE2	-6.09	107.26	116.40
1	F	82	GLU	OE1-CD-OE2	-6.01	108.47	122.90
2	K	75	LYS	CG-CD-CE	-5.92	97.69	111.30
3	M	68	GLU	CG-CD-OE2	5.88	131.92	118.40
2	K	13	GLN	N-CA-CB	-5.82	101.70	110.32
3	O	190	LYS	CB-CG-CD	-5.82	97.92	111.30
3	M	39	LYS	CG-CD-CE	-5.80	97.96	111.30
2	K	13	GLN	CA-CB-CG	-5.80	102.51	114.10
2	J	5	LYS	N-CA-CB	5.78	119.85	110.77
3	N	42	HIS	CA-CB-CG	5.78	119.58	113.80
1	F	30	GLY	CA-C-N	-5.74	113.69	121.84
1	F	30	GLY	C-N-CA	-5.74	113.69	121.84
2	K	65	SER	N-CA-CB	5.69	118.71	110.47
3	N	126	LYS	CA-CB-CG	5.68	125.46	114.10
3	N	70	LYS	CA-CB-CG	-5.65	102.79	114.10
3	M	152	ASN	N-CA-CB	5.62	119.99	110.49
2	H	25	SER	CB-CA-C	-5.61	100.40	109.72
2	H	187	SER	CB-CA-C	-5.59	97.97	110.21
2	I	206	LYS	N-CA-CB	5.54	118.42	110.06
1	F	106	ARG	CG-CD-NE	5.51	124.12	112.00
1	F	82	GLU	N-CA-C	-5.47	104.51	110.91
2	H	192	GLN	N-CA-CB	5.46	118.03	110.17
2	K	96	PHE	C-N-CD	-5.44	102.69	125.00
1	D	49	GLU	N-CA-C	5.43	117.25	108.34
2	I	205	THR	CA-C-N	5.43	129.18	121.42
2	I	205	THR	C-N-CA	5.43	129.18	121.42
3	M	70	LYS	CA-CB-CG	5.40	124.89	114.10
2	K	43	LYS	CB-CG-CD	-5.36	98.97	111.30
3	M	126	LYS	CB-CA-C	5.35	121.62	110.32
1	F	129	THR	OG1-CB-CG2	-5.31	98.68	109.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	93	GLU	CA-CB-CG	5.28	124.66	114.10
2	J	43	LYS	N-CA-C	-5.21	101.78	109.18
2	H	192	GLN	CB-CA-C	-5.20	99.97	109.54
1	F	48	LYS	CA-C-N	-5.19	115.83	122.79
1	F	48	LYS	C-N-CA	-5.19	115.83	122.79
3	M	69	GLY	CA-C-N	-5.18	113.58	123.32
3	M	69	GLY	C-N-CA	-5.18	113.58	123.32
1	D	63	ASP	N-CA-C	-5.14	107.68	114.31
3	N	70	LYS	CD-CE-NZ	5.12	128.28	111.90
3	O	181	LEU	CD1-CG-CD2	-5.12	99.55	110.80
3	O	188	LYS	CG-CD-CE	5.05	122.91	111.30
1	F	123	TYR	CA-C-N	-5.03	114.93	127.00
1	F	123	TYR	C-N-CA	-5.03	114.93	127.00
3	L	188	LYS	N-CA-CB	5.01	118.84	110.41
3	N	103	LYS	N-CA-CB	-5.00	99.54	110.29

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	Peptide,Sidechain
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

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Mol	Chain	Res	Type	Group
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	37	0
1	E	753	0	725	38	0
1	F	810	0	777	55	0
2	H	1630	0	1613	83	0
2	I	1603	0	1584	52	0
2	J	1636	0	1618	82	0
2	K	1630	0	1612	112	0
3	L	1591	0	1544	83	0
3	M	1582	0	1536	61	0
3	N	1614	0	1567	74	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	689	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 (689) 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:J:89:MET:HE3	3:N:42:HIS:CD2	1.93	1.04
3:O:78:ALA:C	3:O:79:GLN:HG2	1.84	1.02
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:L:122:ASP:O	3:L:126:LYS:HG3	1.64	0.97
2:I:189:LEU:HD12	2:I:213:PRO:HG3	1.44	0.97
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:HD2	2:K:77:GLN:HE21	1.38	0.89
2:K:75:LYS:HZ3	2:K:77:GLN:N	1.69	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
3:L:145:LYS:HG2	3:L:146:VAL:N	1.85	0.88
2:K:75:LYS:HZ3	2:K:77:GLN:H	1.20	0.87
1:E:53:LEU:HD23	1:E:56:MET:HE3	1.55	0.87
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:41:ASP:C	3:N:42:HIS:HD1	1.86	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
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
2:K:75:LYS:NZ	2:K:77:GLN:C	2.46	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:45:CYS:SG	1:F:130:THR:OG1	2.48	0.72
2:K:75:LYS:HZ3	2:K:77:GLN:CA	2.01	0.71
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: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:97:PRO:HG3	3:N:96:LEU:HD13	1.74	0.69
2:H:138:LEU:HB2	2:H:211:VAL:HG11	1.75	0.69
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
2:H:130:SER:HG	3:L:118:PHE:HE1	1.42	0.67
3:M:22:THR:HB	3:M:70:LYS:HD2	1.75	0.67
1:E:108:ILE:HD11	1:E:134:LEU:HD21	1.77	0.66
1:F:56:MET:HE2	1:F:71:TYR:HD2	1.60	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:F:56:MET:HE2	1:F:71:TYR:CD2	2.32	0.64
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
1:F:31:ASP:OD2	1:F:32:ASP:C	2.40	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
1:F:67:MET:HE1	2:K:100(A):ILE:HD12	1.80	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
2:K:75:LYS:HD2	2:K:77:GLN:CD	2.27	0.59
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
2:H:18:LEU:HD11	2:H:20:LEU:HD21	1.83	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
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:N:209:PHE:C	3:N:210:ASN:HD22	2.12	0.58
3:M:163:VAL:HG22	3:M:175:LEU:HD12	1.84	0.58
2:J:89:MET:CE	2:J:108:MET:SD	2.91	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:K:75:LYS:HZ3	2:K:77:GLN:C	2.11	0.58
3:L:170:ASP:HB2	3:L:172:THR:HG23	1.85	0.57
2:K:75:LYS:HB2	2:K:76:SER:C	2.29	0.57
2:H:89:MET:HE3	3:L:42:HIS:CG	2.40	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:40:PRO:HA	2:J:88:ALA:HA	1.85	0.57
2:K:88:ALA:C	2:K:108:MET:HE3	2.30	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
3:N:149:LYS:NZ	3:N:195:GLU:OE1	2.38	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
2:J:89:MET:HE2	2:J:108:MET:SD	2.46	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:H:62:ASP:C	2:H:63:ILE:HD13	2.32	0.55
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
2:J:48:MET:HE1	2:J:80:LEU:HD21	1.88	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:H:13:GLN:C	2:H:15:SER:H	2.16	0.53
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
2:K:48:MET:HE1	2:K:80:LEU:HD22	1.90	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
1:D:109:SER:H	1:D:112:LEU:HD12	1.74	0.53
2:J:5:LYS:CG	2:J:6:GLU:N	2.71	0.53
2:J:89:MET:CE	3:N:42:HIS:CD2	2.80	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
2:J:194:TYR:C	2:J:195:ILE:HD13	2.34	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:D:67:MET:HE3	2:I:100(A):ILE:HD13	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:N:96:LEU:C	3:N:97:ILE:HD12	2.36	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
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
2:J:6:GLU:CD	2:J:6:GLU:H	2.19	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
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:J:89:MET:HE1	2:J:108:MET:SD	2.50	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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:C:48:LYS:HZ3	1:C:97:GLY:C	2.20	0.49
2:H:130:SER:OG	3:L:118:PHE:HE1	1.94	0.49
2:H:89:MET:HE3	3:L:42:HIS:CD2	2.48	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
3:O:83:GLU:OE2	3:O:173:TYR:OH	2.22	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: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
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
3:L:61:ARG:NH1	3:L:82:ASP:CG	2.72	0.47
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
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
1:D:67:MET:HE1	1:D:70:LEU:HB2	1.98	0.46
2:I:72:ASP:OD1	2:I:74:SER:HB2	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:F:57:GLN:C	1:F:101:TRP:HE1	2.24	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
2:J:89:MET:HE3	3:N:42:HIS:HD2	1.69	0.46
1:C:126:GLY:C	1:C:127:ILE:HD12	2.40	0.46
1:D:25:GLU:OE2	1:D:126:GLY:HA3	2.16	0.46
3:L:180:THR:C	3:L:181:LEU:HD22	2.41	0.46
2:K:89:MET:HB2	2:K:89:MET:HE2	1.70	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
1:F:93:GLU:O	1:F:94:THR:OG1	2.29	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
2:H:54:ASN:OD1	2:H:54:ASN:C	2.59	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:H:13:GLN:C	2:H:15:SER:N	2.74	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:27:LEU:HD13	2:I:32:ASN:CG	2.41	0.45
2:I:36:TRP:HE1	2:I:78:VAL:HG12	1.82	0.45
2:H:89:MET:HB2	2:H:89:MET:HE2	1.61	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
1:F:67:MET:HE3	1:F:67:MET:HB3	1.76	0.45
2:K:14:PRO:C	2:K:16:GLN:H	2.24	0.45
2:H:189:LEU:HG	2:H:213:PRO:HG3	1.99	0.45
2:J:82(A):ASN:OD1	2:J:82(A):ASN:C	2.60	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
2:K:88:ALA:O	2:K:108:MET:HE3	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:N:27:THR:HG22	3:N:27:THR:O	2.17	0.45
2:K:72:ASP:H	2:K:75:LYS:HZ2	1.65	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
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:112:ALA:HB2	3:L:200:GLY:C	2.41	0.44
3:L:118:PHE:HB2	3:L:133:VAL:HB	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:166:GLN:HG3	3:L:170:ASP:OD1	2.17	0.44
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
3:M:186:TYR:O	3:M:192:TYR:OH	2.28	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:82:MET:HE2	2:J:86:ASP:OD2	2.18	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:35:SER:OG	2:H:47:TRP:NE1	2.45	0.43
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:123:TYR:HA	1:D:124:PRO:HA	1.44	0.43
3:N:8:SER:O	3:N:103:LYS:HB2	2.19	0.43
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:56:MET:HE2	1:E:99:THR:HG21	2.00	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
3:N:210:ASN:HD22	3:N:210:ASN:N	2.15	0.43
2:H:36:TRP:HB3	2:H:48:MET:HE3	2.00	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:56:MET:HE2	1:D:101:TRP:CE3	2.54	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
2:H:6:GLU:CD	2:H:106:GLY:H	2.25	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:36:TRP:C	2:K:37:ILE:HG13	2.42	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
3:N:41:ASP:C	3:N:42:HIS:ND1	2.66	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
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: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
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:F:48:LYS:C	1:F:49:GLU:CG	2.93	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
1:D:40:ASP:C	1:D:41:ILE:HD13	2.46	0.41
2:I:75:LYS:O	2:I:76:SER:C	2.63	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:92:TYR:O	3:L:93:SER:C	2.63	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
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
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
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
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%)	14	29
1	D	111/122 (91%)	103 (93%)	6 (5%)	2 (2%)	6	13
1	E	87/122 (71%)	77 (88%)	10 (12%)	0	100	100
1	F	98/122 (80%)	90 (92%)	6 (6%)	2 (2%)	6	11
2	H	216/229 (94%)	207 (96%)	7 (3%)	2 (1%)	14	29
2	I	210/229 (92%)	204 (97%)	5 (2%)	1 (0%)	24	44
2	J	217/229 (95%)	205 (94%)	11 (5%)	1 (0%)	24	44
2	K	216/229 (94%)	208 (96%)	7 (3%)	1 (0%)	24	44
3	L	208/216 (96%)	194 (93%)	12 (6%)	2 (1%)	12	26
3	M	207/216 (96%)	196 (95%)	9 (4%)	2 (1%)	12	26
3	N	213/216 (99%)	198 (93%)	15 (7%)	0	100	100
3	O	207/216 (96%)	197 (95%)	9 (4%)	1 (0%)	24	44
All	All	2101/2268 (93%)	1982 (94%)	104 (5%)	15 (1%)	18	36

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 ⓘ

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%)	95 (96%)	4 (4%)	28	52
1	D	99/107 (92%)	94 (95%)	5 (5%)	21	43
1	E	84/107 (78%)	73 (87%)	11 (13%)	4	7
1	F	89/107 (83%)	71 (80%)	18 (20%)	1	2
2	H	191/199 (96%)	166 (87%)	25 (13%)	4	7
2	I	187/199 (94%)	172 (92%)	15 (8%)	11	24
2	J	192/199 (96%)	171 (89%)	21 (11%)	6	12
2	K	191/199 (96%)	168 (88%)	23 (12%)	5	9
3	L	175/179 (98%)	162 (93%)	13 (7%)	13	27
3	M	174/179 (97%)	150 (86%)	24 (14%)	3	6
3	N	178/179 (99%)	164 (92%)	14 (8%)	11	24
3	O	174/179 (97%)	155 (89%)	19 (11%)	6	12
All	All	1833/1940 (94%)	1641 (90%)	192 (10%)	6	13

All (192) 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	109	SER
2	H	15	SER
2	H	16	GLN
2	H	21	THR

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Mol	Chain	Res	Type
2	H	24	VAL
2	H	28	SER
2	H	61	SER
2	H	73	THR
2	H	75	LYS
2	H	84	THR
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	179	SER
2	H	183	THR
2	H	187	SER
2	H	188	SER
2	H	203	SER
2	H	204	ASN
3	L	26	SER
3	L	43	SER
3	L	63	SER
3	L	65	SER
3	L	70	LYS
3	L	89	SER
3	L	109	THR
3	L	156	SER
3	L	164	THR
3	L	170	ASP
3	L	176	SER
3	L	187	GLU
3	L	202	SER
1	D	81	GLN
1	D	86	GLU
1	D	87	SER
1	D	118	CYS
1	D	122	LEU
2	I	2	VAL
2	I	12	VAL

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Mol	Chain	Res	Type
2	I	21	THR
2	I	28	SER
2	I	38	ARG
2	I	66	ARG
2	I	87	THR
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	182	VAL
3	M	6	GLN
3	M	13	THR
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	131	SER
3	M	134	CYS
3	M	135	LEU
3	M	152	ASN
3	M	156	SER
3	M	159	SER
3	M	162	SER
3	M	176	SER
3	M	178	THR
3	M	179	LEU
3	M	181	LEU
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	39	SER
1	E	63	ASP
1	E	66	ASP
1	E	102	THR

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Mol	Chain	Res	Type
1	E	109	SER
1	E	118	CYS
1	E	123	TYR
1	E	129	THR
1	E	134	LEU
1	E	135	ILE
2	J	4	LEU
2	J	22	CYS
2	J	31	THR
2	J	66	ARG
2	J	67	LEU
2	J	70	SER
2	J	76	SER
2	J	87	THR
2	J	100(A)	ILE
2	J	100(B)	ASN
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
3	N	12	THR
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	93	SER
3	N	105	THR
3	N	176	SER
1	F	31	ASP

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Mol	Chain	Res	Type
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	59	SER
1	F	63	ASP
1	F	82	GLU
1	F	102	THR
1	F	106	ARG
1	F	108	ILE
1	F	118	CYS
1	F	128	LYS
1	F	129	THR
1	F	134	LEU
1	F	136	VAL
2	K	2	VAL
2	K	12	VAL
2	K	15	SER
2	K	23	THR
2	K	28	SER
2	K	61	SER
2	K	63	ILE
2	K	65	SER
2	K	68	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	169	VAL
2	K	178	LEU
2	K	183	THR
2	K	192	GLN
2	K	203	SER
3	O	4	VAL
3	O	6	GLN

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Mol	Chain	Res	Type
3	O	28	THR
3	O	30	SER
3	O	65	SER
3	O	67	LEU
3	O	115	VAL
3	O	121	SER
3	O	122	ASP
3	O	131	SER
3	O	159	SER
3	O	162	SER
3	O	166	GLN
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 (32) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	88	GLN
2	H	39	GLN
2	H	83	GLN
2	H	171	GLN
2	H	197	ASN
3	L	37	GLN
3	L	42	HIS
3	L	152	ASN
3	L	158	ASN
3	L	189	HIS
1	D	81	GLN
1	D	88	GLN
2	I	16	GLN
2	I	77	GLN
2	J	164	HIS
2	J	171	GLN
2	J	199	ASN
3	N	24	HIS
3	N	137	ASN
3	N	138	ASN
3	N	210	ASN

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Mol	Chain	Res	Type
1	F	42	ASN
1	F	55	GLN
1	F	133	ASN
2	K	13	GLN
2	K	16	GLN
2	K	60	ASN
2	K	77	GLN
2	K	82(A)	ASN
3	O	37	GLN
3	O	147	GLN
3	O	210	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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	1.92	1 (14%)	9,10,12	1.91	3 (33%)
3	PCA	M	1	3	7,8,9	2.24	1 (14%)	9,10,12	1.99	4 (44%)
3	PCA	L	1	3	7,8,9	1.91	1 (14%)	9,10,12	2.01	4 (44%)
3	PCA	O	1	3	7,8,9	2.04	1 (14%)	9,10,12	2.05	3 (33%)

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	M	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

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	M	1	PCA	CD-N	5.65	1.48	1.34
3	O	1	PCA	CD-N	5.18	1.47	1.34
3	N	1	PCA	CD-N	4.88	1.46	1.34
3	L	1	PCA	CD-N	4.86	1.46	1.34

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	M	1	PCA	OE-CD-CG	-3.41	120.64	126.72
3	N	1	PCA	CB-CA-N	3.23	112.13	103.24
3	O	1	PCA	CB-CA-N	3.19	112.01	103.24
3	O	1	PCA	CA-N-CD	-2.95	103.48	113.58
3	L	1	PCA	CB-CA-N	2.89	111.20	103.24
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	O	1	PCA	CG-CD-N	2.64	114.84	108.39
3	L	1	PCA	CG-CD-N	2.61	114.77	108.39
3	M	1	PCA	CA-N-CD	-2.56	104.82	113.58
3	M	1	PCA	CG-CD-N	2.42	114.31	108.39
3	L	1	PCA	OE-CD-CG	-2.40	122.43	126.72
3	M	1	PCA	CB-CA-N	2.40	109.84	103.24
3	N	1	PCA	CG-CD-N	2.38	114.20	108.39

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 oligosaccharides 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	$\# Z > 2$
5	SO4	L	301	-	4,4,4	0.35	0	6,6,6	0.23	0
5	SO4	K	301	-	4,4,4	0.38	0	6,6,6	0.22	0
5	SO4	D	202	-	4,4,4	0.42	0	6,6,6	0.18	0
4	NAG	D	201	1	14,14,15	0.37	0	17,19,21	0.61	0
5	SO4	C	202	-	4,4,4	0.36	0	6,6,6	0.38	0
5	SO4	N	301	-	4,4,4	0.20	0	6,6,6	0.42	0
4	NAG	C	201	1	14,14,15	0.45	0	17,19,21	0.48	0
5	SO4	D	203	-	4,4,4	0.34	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	K	301	SO4	1	0
5	C	202	SO4	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	C	113/122 (92%)	0.41	2 (1%) 67 64	31, 40, 53, 59	0
1	D	113/122 (92%)	0.99	17 (15%) 5 4	37, 50, 73, 77	0
1	E	95/122 (77%)	1.83	30 (31%) 1 1	60, 82, 91, 95	0
1	F	102/122 (83%)	1.81	36 (35%) 1 1	58, 80, 97, 102	0
2	H	218/229 (95%)	0.86	24 (11%) 10 8	33, 55, 83, 90	0
2	I	214/229 (93%)	0.22	4 (1%) 66 62	29, 37, 57, 64	0
2	J	219/229 (95%)	0.40	10 (4%) 37 33	31, 48, 59, 62	0
2	K	218/229 (95%)	0.70	14 (6%) 25 21	36, 54, 71, 77	0
3	L	211/216 (97%)	0.53	9 (4%) 40 35	33, 46, 68, 77	0
3	M	210/216 (97%)	0.40	8 (3%) 44 39	33, 41, 54, 61	0
3	N	214/216 (99%)	0.60	12 (5%) 30 25	30, 49, 68, 76	0
3	O	210/216 (97%)	0.38	8 (3%) 44 39	37, 44, 55, 66	0
All	All	2137/2268 (94%)	0.65	174 (8%) 18 15	29, 47, 82, 102	0

All (174) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	122	LEU	5.7
2	K	13	GLN	5.3
1	E	41	ILE	5.0
1	F	36	LEU	4.9
1	E	47	THR	4.9
1	E	123	TYR	4.9
2	K	2	VAL	4.9
1	E	36	LEU	4.9
3	N	41	ASP	4.7
1	F	104	TYR	4.7
2	K	12	VAL	4.6

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Mol	Chain	Res	Type	RSRZ
1	D	94	THR	4.6
3	O	67	LEU	4.4
1	F	132	TYR	4.3
3	N	94	GLY	4.2
1	F	94	THR	4.2
1	E	122	LEU	4.2
3	N	79	GLN	4.1
2	K	3	GLN	4.0
1	F	33	VAL	4.0
1	E	98	VAL	3.9
1	F	125	GLU	3.9
1	D	62	THR	3.8
1	D	29	VAL	3.8
2	H	135	THR	3.8
1	F	135	ILE	3.8
2	K	63	ILE	3.7
3	N	42	HIS	3.7
3	M	68	GLU	3.7
1	E	34	TYR	3.7
2	I	105	GLN	3.6
1	F	92	THR	3.6
1	D	28	ASN	3.6
1	E	136	VAL	3.6
3	L	123	GLU	3.5
2	J	100(A)	ILE	3.5
1	F	64	LYS	3.5
2	H	85	GLU	3.5
1	E	66	ASP	3.4
2	H	16	GLN	3.3
1	F	108	ILE	3.3
1	F	31	ASP	3.3
2	H	2	VAL	3.3
2	H	164	HIS	3.3
1	F	37	PRO	3.3
2	J	2	VAL	3.3
3	O	212	GLY	3.3
1	E	127	ILE	3.3
1	E	124	PRO	3.3
1	F	49	GLU	3.3
3	O	40	ALA	3.2
1	F	32	ASP	3.2
3	O	190	LYS	3.2

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Mol	Chain	Res	Type	RSRZ
2	J	3	GLN	3.2
1	D	125	GLU	3.1
1	E	129	THR	3.1
2	J	131	THR	3.1
3	M	39	LYS	3.1
1	E	135	ILE	3.0
1	E	53	LEU	3.0
1	E	130	THR	3.0
3	O	78	ALA	3.0
3	L	145	LYS	3.0
1	F	43	LEU	2.9
1	D	123	TYR	2.9
2	H	191	THR	2.9
2	I	210	ARG	2.8
2	K	75	LYS	2.8
3	M	42	HIS	2.8
2	K	82(C)	LEU	2.8
1	D	93	GLU	2.8
2	H	152	VAL	2.8
2	H	132	SER	2.8
1	E	33	VAL	2.8
1	F	35	ALA	2.8
1	F	110	SER	2.7
3	L	126	LYS	2.7
1	D	124	PRO	2.7
1	E	131	VAL	2.7
1	E	35	ALA	2.7
1	E	104	TYR	2.7
1	E	82	GLU	2.6
2	K	77	GLN	2.6
1	D	48	LYS	2.6
1	F	74	GLN	2.6
3	N	40	ALA	2.6
1	F	34	TYR	2.6
1	E	64	LYS	2.6
1	F	41	ILE	2.6
1	E	37	PRO	2.5
3	O	167	ASP	2.5
2	H	129	LYS	2.5
2	H	209	LYS	2.5
1	F	87	SER	2.5
1	F	30	GLY	2.5

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Mol	Chain	Res	Type	RSRZ
3	N	75	ILE	2.5
1	F	46	GLN	2.5
3	N	2	ALA	2.5
2	J	191	THR	2.5
2	K	19	SER	2.5
1	D	66	ASP	2.4
2	H	194	TYR	2.4
3	L	122	ASP	2.4
3	L	188	LYS	2.4
2	H	101	PHE	2.4
2	H	25	SER	2.4
1	C	82	GLU	2.4
2	J	215	SER	2.4
1	E	68	ILE	2.4
1	D	26	LEU	2.4
3	O	79	GLN	2.4
2	H	207	VAL	2.4
1	E	111	ALA	2.4
1	C	64	LYS	2.4
2	K	132	SER	2.4
1	D	30	GLY	2.4
1	D	106	ARG	2.4
3	M	24	HIS	2.4
3	O	129	THR	2.3
2	H	134	GLY	2.3
1	F	79	CYS	2.3
1	E	91	ALA	2.3
1	F	134	LEU	2.3
1	F	84	ALA	2.3
2	H	158	ALA	2.3
2	H	147	PRO	2.3
3	N	32	TYR	2.3
1	D	47	THR	2.2
3	M	22	THR	2.2
1	E	134	LEU	2.2
3	L	121	SER	2.2
1	F	82	GLU	2.2
3	L	211	ARG	2.2
1	E	92	THR	2.2
3	N	126	LYS	2.2
1	F	105	LEU	2.2
1	F	112	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
2	K	78	VAL	2.2
1	E	81	GLN	2.2
3	N	70	LYS	2.2
2	H	189	LEU	2.2
2	I	186	SER	2.2
2	H	187	SER	2.2
2	H	122	PHE	2.2
3	M	126	LYS	2.2
1	F	136	VAL	2.1
2	H	137	ALA	2.1
1	E	62	THR	2.1
2	H	183	THR	2.1
3	N	23	CYS	2.1
1	F	81	GLN	2.1
1	F	91	ALA	2.1
3	L	161	GLU	2.1
2	J	5	LYS	2.1
1	E	46	GLN	2.1
1	F	122	LEU	2.1
2	I	131	THR	2.1
2	J	98	TYR	2.1
1	F	63	ASP	2.1
2	H	156	SER	2.1
2	H	197	ASN	2.1
2	J	189	LEU	2.1
3	N	103	LYS	2.1
1	F	42	ASN	2.0
2	K	4	LEU	2.0
1	D	49	GLU	2.0
2	J	134	GLY	2.0
3	L	42	HIS	2.0
2	K	83	GLN	2.0
1	F	131	VAL	2.0
3	M	2	ALA	2.0
3	M	40	ALA	2.0
1	D	50	LYS	2.0
2	K	25	SER	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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	PCA	N	1	8/9	0.44	0.21	82,84,85,85	0
3	PCA	M	1	8/9	0.56	0.27	68,73,74,74	0
3	PCA	O	1	8/9	0.80	0.16	58,61,64,64	0
3	PCA	L	1	8/9	0.87	0.12	46,49,50,51	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	SO4	D	202	5/5	0.68	0.21	76,79,82,86	0
4	NAG	C	201	14/15	0.74	0.14	55,61,64,65	0
5	SO4	L	301	5/5	0.78	0.17	77,81,85,86	0
4	NAG	D	201	14/15	0.79	0.13	63,69,73,74	0
5	SO4	K	301	5/5	0.84	0.18	77,77,77,77	0
5	SO4	N	301	5/5	0.94	0.07	40,41,42,42	0
5	SO4	D	203	5/5	0.96	0.08	50,54,54,54	0
5	SO4	C	202	5/5	0.97	0.06	45,45,45,47	0

6.5 Other polymers [i](#)

There are no such residues in this entry.