



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 20, 2026 – 06:31 AM UTC

PDB ID : 5BOZ / pdb_00005boz
Title : Ricin A chain bound to camelid nanobody (VHH9)(E1)
Authors : Rudolph, M.J.; Mantis, N.
Deposited on : 2015-05-27
Resolution : 3.10 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

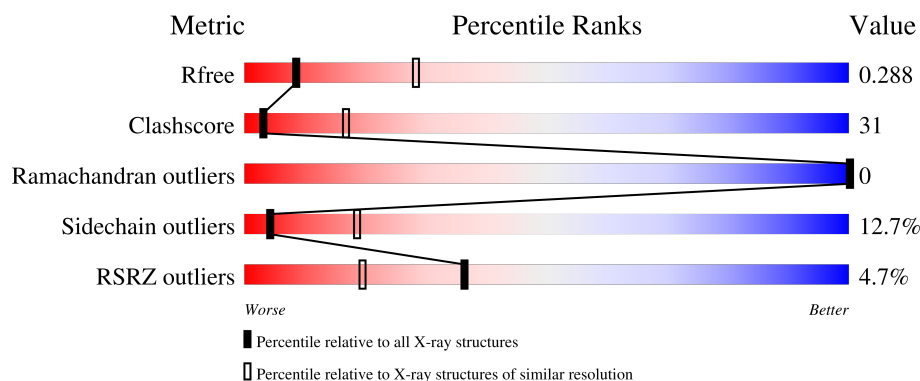
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.10 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	1456 (3.10-3.10)
Clashscore	190562	1539 (3.10-3.10)
Ramachandran outliers	187476	1467 (3.10-3.10)
Sidechain outliers	187428	1467 (3.10-3.10)
RSRZ outliers	180081	1456 (3.10-3.10)

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	A	261	
1	B	261	
1	C	261	
1	D	261	
1	E	261	

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Mol	Chain	Length	Quality of chain
1	F	261	
2	G	127	
2	H	127	
2	I	127	
2	J	127	
2	K	127	
2	L	127	

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	SO4	A	301	-	-	X	-
3	SO4	B	301	-	-	X	-
3	SO4	B	304	-	-	X	-
3	SO4	C	301	-	-	X	-
3	SO4	F	301	-	-	X	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 18136 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.

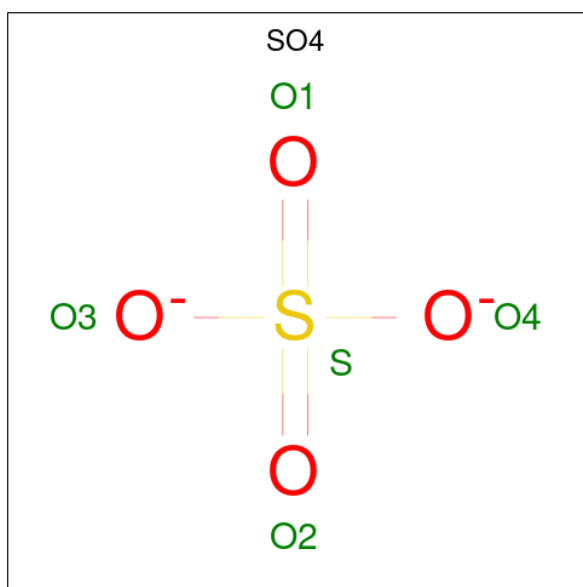
- Molecule 1 is a protein called Ricin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	259	Total	C	N	O	S	0	0	0
			2046	1296	362	383	5			
1	B	260	Total	C	N	O	S	0	0	0
			2052	1299	363	385	5			
1	C	259	Total	C	N	O	S	0	0	0
			2046	1296	362	383	5			
1	D	259	Total	C	N	O	S	0	0	0
			2046	1296	362	383	5			
1	E	259	Total	C	N	O	S	0	2	0
			2068	1308	370	385	5			
1	F	260	Total	C	N	O	S	0	0	0
			2052	1299	363	385	5			

- Molecule 2 is a protein called VHH single chain antibody E1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	G	123	Total	C	N	O	S	0	1	0
			961	601	173	182	5			
2	H	125	Total	C	N	O	S	0	1	0
			973	607	176	185	5			
2	I	118	Total	C	N	O	S	0	0	0
			911	572	160	174	5			
2	J	119	Total	C	N	O	S	0	0	0
			918	576	161	176	5			
2	K	125	Total	C	N	O	S	0	1	0
			973	607	176	185	5			
2	L	123	Total	C	N	O	S	0	1	0
			961	601	173	182	5			

- Molecule 3 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		
3	G	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	C	1	Total	O	S	0	0
			5	4	1		
3	C	1	Total	O	S	0	0
			5	4	1		
3	C	1	Total	O	S	0	0
			5	4	1		
3	I	1	Total	O	S	0	0
			5	4	1		
3	D	1	Total	O	S	0	0
			5	4	1		
3	J	1	Total	O	S	0	0
			5	4	1		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	E	1	Total O S 5 4 1	0	0
3	E	1	Total O S 5 4 1	0	0
3	E	1	Total O S 5 4 1	0	0
3	F	1	Total O S 5 4 1	0	0
3	F	1	Total O S 5 4 1	0	0
3	L	1	Total O S 5 4 1	0	0

- Molecule 4 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	D	1	Total Cl 1 1	0	0
4	E	1	Total Cl 1 1	0	0
4	K	1	Total Cl 1 1	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	G	3	Total O 3 3	0	0
5	B	1	Total O 1 1	0	0
5	H	1	Total O 1 1	0	0
5	C	4	Total O 4 4	0	0
5	I	1	Total O 1 1	0	0
5	D	1	Total O 1 1	0	0
5	E	5	Total O 5 5	0	0
5	K	6	Total O 6 6	0	0

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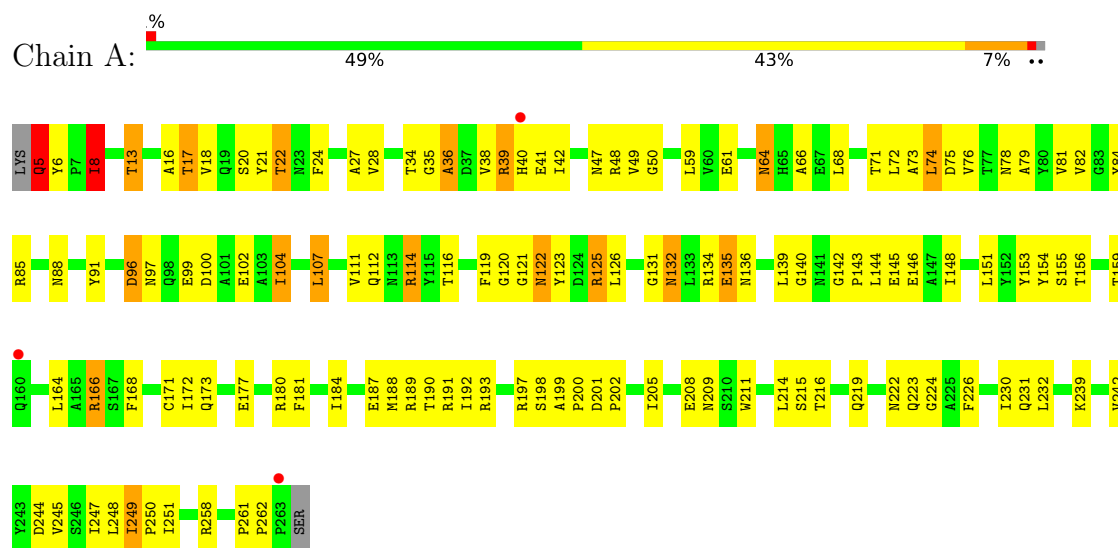
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	F	2	Total	O	0	0
			2	2		
5	L	2	Total	O	0	0
			2	2		

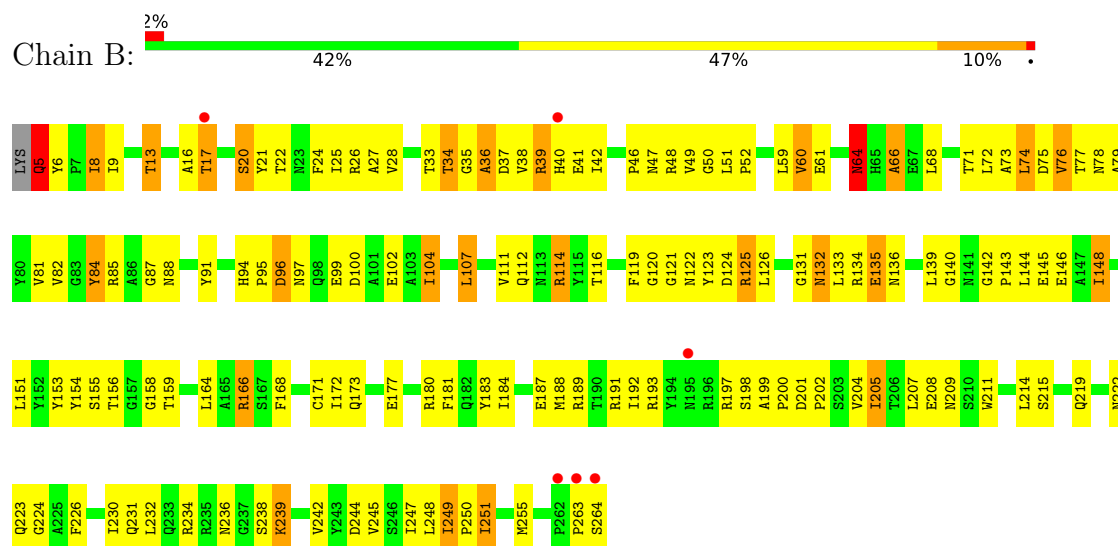
3 Residue-property plots

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: Ricin

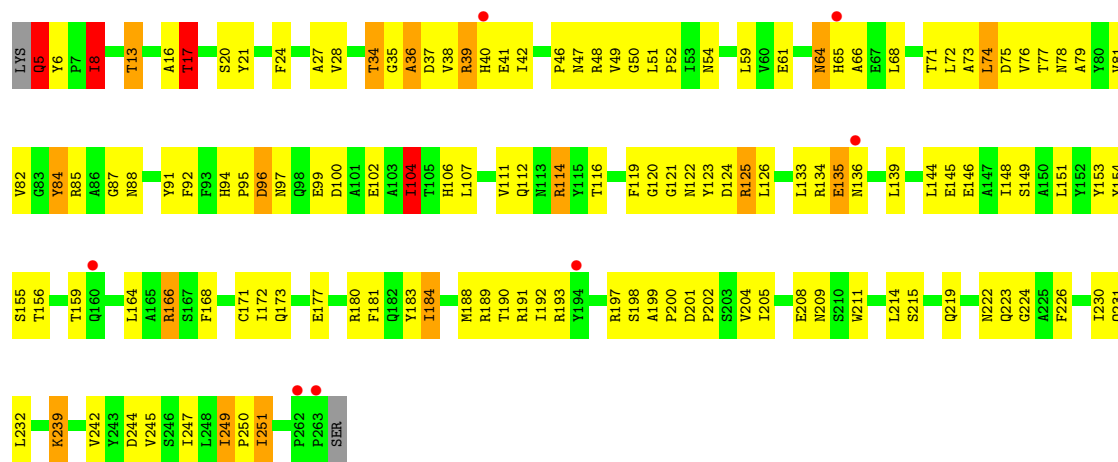


• Molecule 1: Ricin

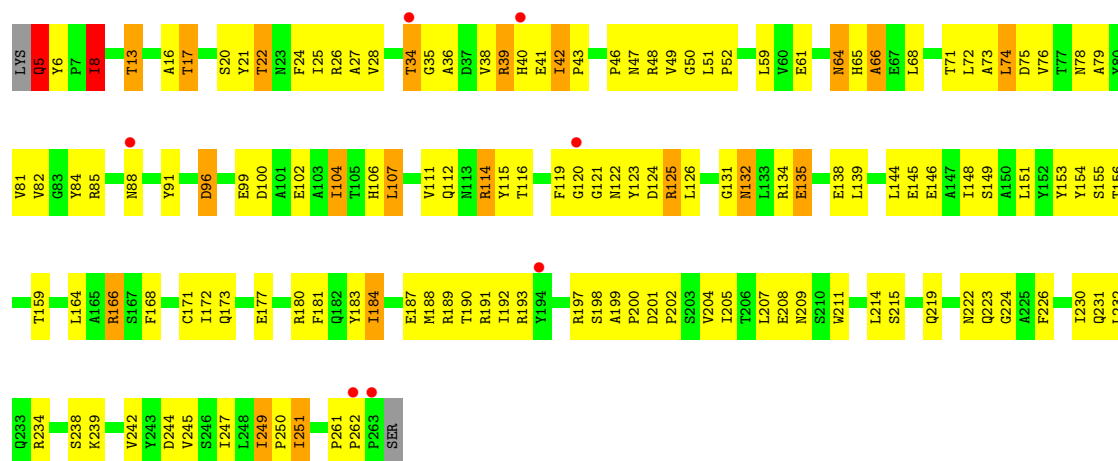


• Molecule 1: Ricin

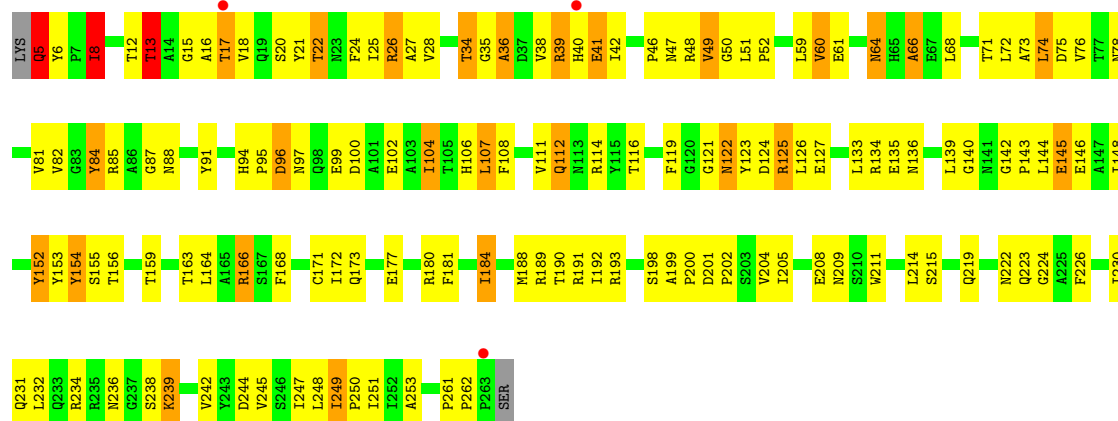
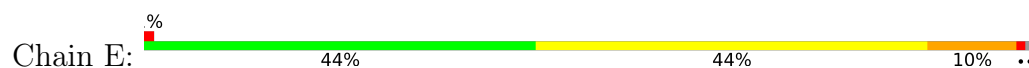




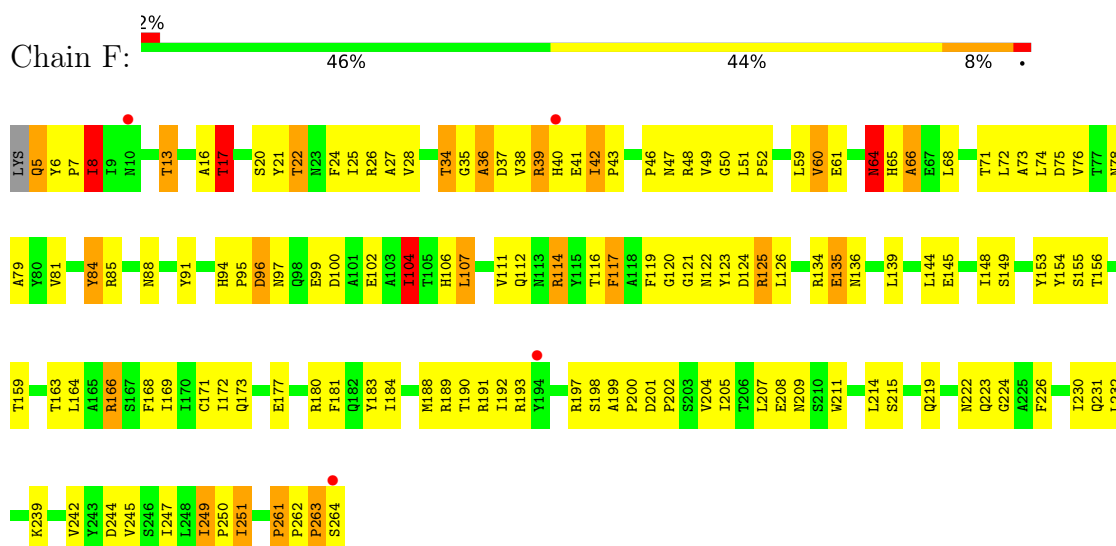
• Molecule 1: Ricin



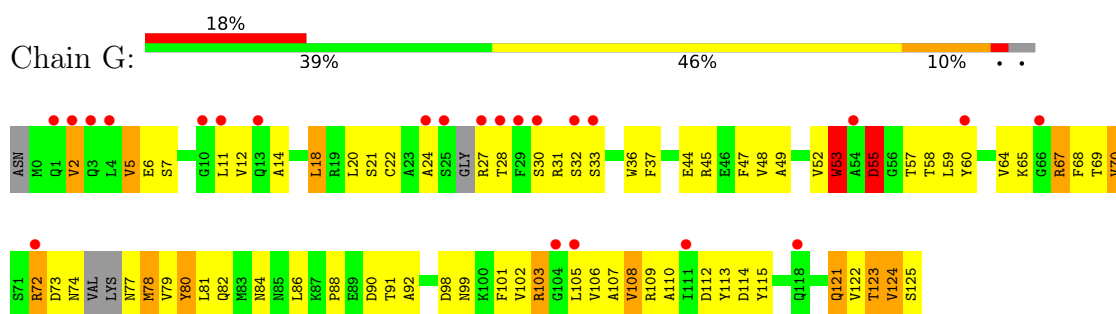
• Molecule 1: Ricin



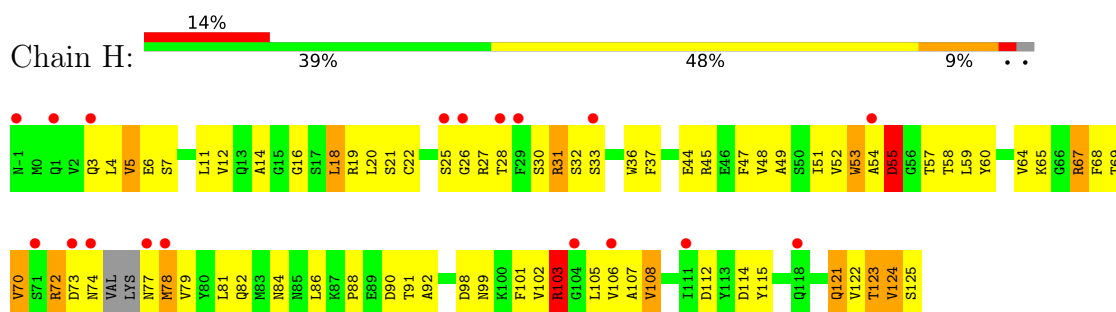
• Molecule 1: Ricin



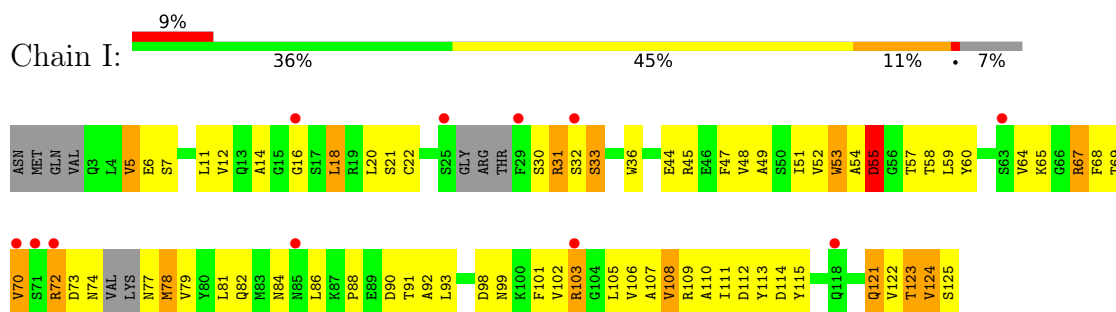
• Molecule 2: VHH single chain antibody E1



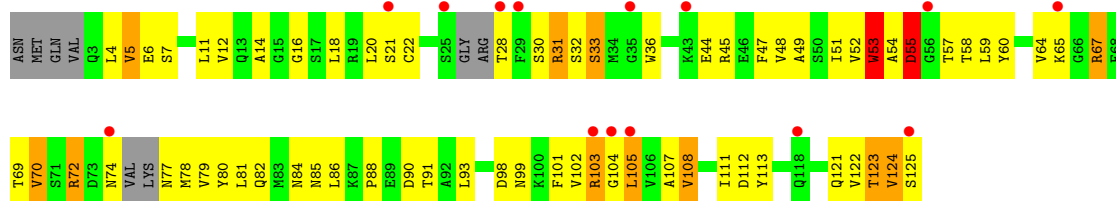
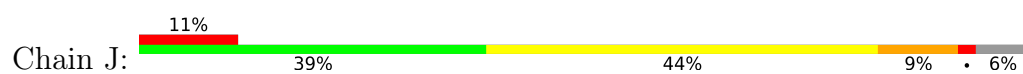
• Molecule 2: VHH single chain antibody E1



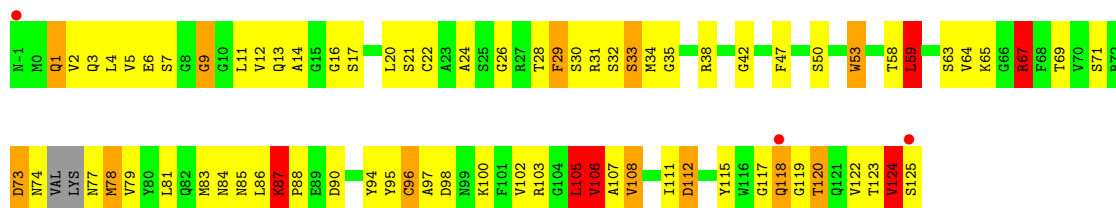
• Molecule 2: VHH single chain antibody E1



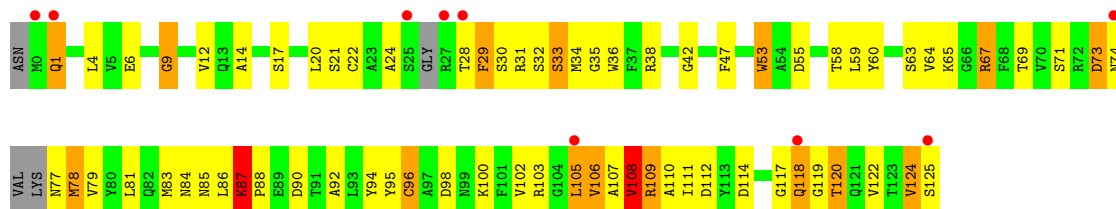
• Molecule 2: VHH single chain antibody E1



• Molecule 2: VHH single chain antibody E1



• Molecule 2: VHH single chain antibody E1



4 Data and refinement statistics

Property	Value	Source
Space group	F 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	239.61Å 242.88Å 355.69Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.68 – 3.10 49.68 – 3.10	Depositor EDS
% Data completeness (in resolution range)	99.8 (49.68-3.10) 99.8 (49.68-3.10)	Depositor EDS
R_{merge}	0.20	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.81 (at 3.12Å)	Xtriage
Refinement program	PHENIX 1.7.1_743	Depositor
R, R_{free}	0.215 , 0.277 0.224 , 0.288	Depositor DCC
R_{free} test set	4702 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	64.8	Xtriage
Anisotropy	0.664	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 102.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	0.000 for -k,-h,-l	Xtriage
Reported twinning fraction	0.017 for -k,-h,-l	Depositor
Outliers	12 of 93146 reflections (0.013%)	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	18136	wwPDB-VP
Average B, all atoms (Å ²)	89.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 64.97 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 7.6203e-06. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CL, 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	A	0.86	0/2091	1.24	21/2847 (0.7%)
1	B	0.92	1/2097 (0.0%)	1.30	24/2855 (0.8%)
1	C	0.88	3/2091 (0.1%)	1.26	22/2847 (0.8%)
1	D	0.81	0/2091	1.22	21/2847 (0.7%)
1	E	1.09	2/2113 (0.1%)	1.43	33/2875 (1.1%)
1	F	0.98	2/2097 (0.1%)	1.31	32/2855 (1.1%)
2	G	0.84	0/977	1.24	10/1317 (0.8%)
2	H	0.92	0/990	1.33	11/1336 (0.8%)
2	I	0.76	0/927	1.16	7/1250 (0.6%)
2	J	0.77	0/934	1.13	6/1260 (0.5%)
2	K	1.41	4/990 (0.4%)	1.61	16/1336 (1.2%)
2	L	1.08	0/977	1.41	17/1317 (1.3%)
All	All	0.95	12/18375 (0.1%)	1.31	220/24942 (0.9%)

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	A	0	2
1	B	0	2
1	C	0	2
1	D	0	2
1	E	0	3
1	F	0	3
2	H	0	1
2	K	0	1
2	L	0	2
All	All	0	18

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	64	ASN	CG-ND2	-10.07	1.12	1.33
1	C	64	ASN	CG-ND2	-9.10	1.14	1.33
1	E	64	ASN	CG-OD1	-8.51	1.07	1.23
1	C	64	ASN	CG-OD1	-8.01	1.08	1.23
2	K	5	VAL	CA-CB	-7.96	1.44	1.54
1	B	251	ILE	CA-CB	-6.08	1.49	1.55
1	F	64	ASN	CG-ND2	-5.80	1.21	1.33
1	F	64	ASN	CG-OD1	-5.50	1.13	1.23
2	K	97	ALA	CA-C	5.30	1.58	1.52
2	K	105	LEU	C-O	-5.15	1.17	1.24
2	K	124	VAL	CA-C	5.07	1.58	1.52
1	C	17	THR	CA-CB	5.06	1.61	1.53

All (220) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	K	108	VAL	N-CA-C	13.25	124.76	112.17
1	E	49	VAL	N-CA-C	10.88	120.85	110.30
2	H	108	VAL	N-CA-C	10.52	122.16	112.17
1	E	107	LEU	CA-C-N	-10.18	108.08	123.14
1	E	107	LEU	C-N-CA	-10.18	108.08	123.14
2	G	108	VAL	N-CA-C	10.05	121.71	112.17
1	E	6	TYR	N-CA-C	9.45	121.64	109.64
1	B	107	LEU	CA-C-N	-9.43	108.89	123.13
1	B	107	LEU	C-N-CA	-9.43	108.89	123.13
1	F	107	LEU	CA-C-N	-9.23	109.19	123.13
1	F	107	LEU	C-N-CA	-9.23	109.19	123.13
2	K	26	GLY	N-CA-C	-9.14	86.79	113.30
1	B	6	TYR	N-CA-C	8.78	120.78	109.64
1	D	6	TYR	N-CA-C	8.69	120.68	109.64
1	C	107	LEU	CA-C-N	-8.66	110.32	123.14
1	C	107	LEU	C-N-CA	-8.66	110.32	123.14
2	L	117	GLY	N-CA-C	-8.50	100.45	112.60
1	A	6	TYR	N-CA-C	8.38	120.28	109.64
1	D	107	LEU	CA-C-N	-8.26	110.92	123.14
1	D	107	LEU	C-N-CA	-8.26	110.92	123.14
1	A	107	LEU	CA-C-N	-8.14	111.10	123.14
1	A	107	LEU	C-N-CA	-8.14	111.10	123.14
1	E	42	ILE	CA-C-N	8.07	128.08	119.76
1	E	42	ILE	C-N-CA	8.07	128.08	119.76
2	H	5	VAL	N-CA-C	7.92	118.81	108.35
1	C	6	TYR	N-CA-C	7.92	119.70	109.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	26	GLY	CA-C-N	-7.79	111.24	122.77
2	H	26	GLY	C-N-CA	-7.79	111.24	122.77
1	C	249	ILE	CA-C-N	7.73	127.40	119.82
1	C	249	ILE	C-N-CA	7.73	127.40	119.82
1	D	42	ILE	CA-C-N	7.63	127.62	119.76
1	D	42	ILE	C-N-CA	7.63	127.62	119.76
2	I	55	ASP	N-CA-C	7.53	120.44	111.33
1	E	249	ILE	CA-C-N	7.50	127.17	119.82
1	E	249	ILE	C-N-CA	7.50	127.17	119.82
1	B	251	ILE	CB-CA-C	-7.49	105.35	111.71
1	F	251	ILE	CB-CA-C	-7.48	105.35	111.71
1	A	42	ILE	CA-C-N	7.43	127.42	119.76
1	A	42	ILE	C-N-CA	7.43	127.42	119.76
1	A	249	ILE	CA-C-N	7.40	127.07	119.82
1	A	249	ILE	C-N-CA	7.40	127.07	119.82
1	E	6	TYR	CA-C-N	7.39	127.81	119.83
1	E	6	TYR	C-N-CA	7.39	127.81	119.83
1	C	251	ILE	CB-CA-C	-7.38	105.44	111.71
1	A	251	ILE	CB-CA-C	-7.37	105.45	111.71
2	G	53	TRP	N-CA-C	-7.36	98.33	109.60
1	B	249	ILE	CA-C-N	7.36	127.03	119.82
1	B	249	ILE	C-N-CA	7.36	127.03	119.82
1	B	16	ALA	N-CA-C	7.32	120.86	109.96
2	I	103	ARG	N-CA-C	-7.31	99.33	110.30
1	D	16	ALA	N-CA-C	7.31	120.99	110.24
1	E	133	LEU	N-CA-C	7.31	120.42	110.55
1	F	6	TYR	N-CA-C	7.27	118.87	109.64
2	G	55	ASP	N-CA-C	7.25	120.11	111.33
2	H	55	ASP	N-CA-C	7.21	120.05	111.33
1	F	42	ILE	CA-C-N	7.18	127.16	119.76
1	F	42	ILE	C-N-CA	7.18	127.16	119.76
1	C	16	ALA	N-CA-C	7.18	120.79	110.10
1	D	192	ILE	CB-CA-C	-7.16	102.81	111.97
2	L	108	VAL	N-CA-CB	-7.15	99.44	111.23
1	F	16	ALA	N-CA-C	7.12	120.70	110.10
1	C	42	ILE	CA-C-N	7.11	127.08	119.76
1	C	42	ILE	C-N-CA	7.11	127.08	119.76
1	F	6	TYR	CA-C-N	7.10	127.50	119.83
1	F	6	TYR	C-N-CA	7.10	127.50	119.83
1	A	104	ILE	CB-CA-C	-7.06	101.74	112.05
1	C	104	ILE	CB-CA-C	-6.98	102.89	112.04
2	H	78	MET	N-CA-C	6.90	119.92	109.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	I	5	VAL	N-CA-C	6.88	117.43	108.35
2	G	5	VAL	N-CA-C	6.87	118.24	108.42
2	J	55	ASP	N-CA-C	6.85	119.62	111.33
2	H	101	PHE	N-CA-C	6.83	121.28	112.12
1	F	249	ILE	CA-C-N	6.74	126.88	119.87
1	F	249	ILE	C-N-CA	6.74	126.88	119.87
1	B	42	ILE	CA-C-N	6.72	127.08	119.83
1	B	42	ILE	C-N-CA	6.72	127.08	119.83
1	C	192	ILE	CB-CA-C	-6.71	103.38	111.97
1	E	192	ILE	CB-CA-C	-6.67	103.44	111.97
2	L	55	ASP	N-CA-C	6.65	120.26	111.75
2	K	67	ARG	N-CA-C	6.63	120.59	112.23
1	D	6	TYR	CA-C-N	6.60	126.96	119.83
1	D	6	TYR	C-N-CA	6.60	126.96	119.83
2	J	5	VAL	N-CA-C	6.58	117.04	108.35
1	B	158	GLY	N-CA-C	-6.52	106.58	114.66
1	A	192	ILE	CB-CA-C	-6.52	103.63	111.97
1	E	84	TYR	N-CA-C	6.51	118.97	109.07
1	F	22	THR	N-CA-C	-6.51	104.19	111.28
1	E	66	ALA	N-CA-C	-6.47	105.14	113.16
1	B	104	ILE	CB-CA-C	-6.46	102.62	112.05
1	E	35	GLY	CA-C-N	-6.46	113.87	122.85
1	E	35	GLY	C-N-CA	-6.46	113.87	122.85
2	K	117	GLY	N-CA-C	-6.45	103.38	112.60
1	F	192	ILE	CB-CA-C	-6.45	103.72	111.97
1	A	22	THR	N-CA-C	-6.44	104.27	111.28
1	B	6	TYR	CA-C-N	6.42	126.76	119.83
1	B	6	TYR	C-N-CA	6.42	126.76	119.83
2	K	53	TRP	N-CA-C	-6.41	102.03	110.43
1	D	104	ILE	CB-CA-C	-6.38	103.69	112.04
1	F	117	PHE	N-CA-C	6.38	118.79	110.43
1	D	251	ILE	CB-CA-C	-6.37	106.29	111.71
1	E	104	ILE	CB-CA-C	-6.36	103.71	112.04
2	L	67	ARG	N-CA-C	6.36	120.24	112.23
1	D	249	ILE	CA-C-N	6.34	126.47	119.87
1	D	249	ILE	C-N-CA	6.34	126.47	119.87
1	A	16	ALA	N-CA-C	6.25	119.43	110.24
1	F	104	ILE	CB-CA-C	-6.25	103.86	112.04
1	F	13	THR	N-CA-C	-6.19	105.22	112.89
1	C	6	TYR	CA-C-N	6.18	126.50	119.83
1	C	6	TYR	C-N-CA	6.18	126.50	119.83
2	K	1	GLN	N-CA-C	6.15	116.36	108.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	192	ILE	CB-CA-C	-6.12	104.14	111.97
1	A	35	GLY	CA-C-N	-6.08	114.39	122.85
1	A	35	GLY	C-N-CA	-6.08	114.39	122.85
1	A	6	TYR	CA-C-N	6.08	126.39	119.83
1	A	6	TYR	C-N-CA	6.08	126.39	119.83
1	F	8	ILE	N-CA-C	6.05	118.17	108.85
2	L	106	VAL	CA-C-N	-6.05	114.45	122.85
2	L	106	VAL	C-N-CA	-6.05	114.45	122.85
1	E	251	ILE	CB-CA-C	-6.01	106.60	111.71
2	I	101	PHE	N-CA-C	5.99	120.14	112.12
2	L	108	VAL	CB-CA-C	-5.97	101.51	111.29
2	L	73	ASP	N-CA-C	5.96	118.47	109.23
1	C	35	GLY	CA-C-N	-5.93	114.60	122.85
1	C	35	GLY	C-N-CA	-5.93	114.60	122.85
2	K	59	LEU	N-CA-C	5.92	118.77	108.76
1	D	13	THR	N-CA-C	-5.90	105.57	112.89
2	L	1	GLN	N-CA-C	5.89	116.02	108.24
1	F	65	HIS	N-CA-C	-5.83	106.13	113.18
2	H	53	TRP	N-CA-C	-5.83	100.69	109.60
1	B	66	ALA	N-CA-C	-5.82	105.95	113.16
1	A	13	THR	N-CA-C	-5.81	105.45	112.54
2	J	101	PHE	N-CA-C	5.80	119.89	112.12
1	E	253	ALA	N-CA-C	5.80	118.82	111.69
1	F	36	ALA	N-CA-C	5.77	118.48	107.75
1	E	97	ASN	N-CA-C	5.75	115.99	107.88
2	K	9	GLY	N-CA-C	-5.73	106.03	112.33
2	K	73	ASP	N-CA-C	5.72	118.10	109.23
1	B	9	ILE	CB-CA-C	-5.70	102.67	110.77
1	F	7	PRO	CA-C-O	-5.69	115.15	121.23
2	J	80	TYR	N-CA-C	5.68	118.04	109.23
1	B	60	VAL	N-CA-C	5.68	116.79	107.24
1	E	49	VAL	CB-CA-C	-5.68	104.71	111.81
1	D	66	ALA	N-CA-C	-5.64	106.37	113.20
2	K	42	GLY	N-CA-C	-5.63	108.37	115.08
2	G	101	PHE	N-CA-C	5.62	119.66	112.12
1	E	16	ALA	N-CA-C	5.60	118.44	110.10
2	K	112	ASP	N-CA-C	-5.59	106.22	113.16
2	I	108	VAL	N-CA-CB	-5.59	102.01	111.23
2	I	78	MET	N-CA-C	5.58	117.75	108.99
1	E	60	VAL	N-CA-C	5.58	116.61	107.24
2	L	87	LYS	CA-C-N	5.57	126.80	119.84
2	L	87	LYS	C-N-CA	5.57	126.80	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	97	ASN	N-CA-C	5.56	116.72	108.60
1	D	65	HIS	N-CA-C	-5.56	106.45	113.18
1	A	18	VAL	N-CA-C	-5.56	105.09	110.42
1	B	148	ILE	CB-CA-C	-5.55	104.59	111.70
2	G	103[A]	ARG	N-CA-C	-5.54	101.99	110.30
2	G	103[B]	ARG	N-CA-C	-5.54	101.99	110.30
1	F	66	ALA	N-CA-C	-5.54	106.29	113.16
1	E	13	THR	N-CA-C	-5.53	106.04	112.89
2	L	114	ASP	N-CA-C	5.52	119.99	112.04
2	J	108	VAL	N-CA-CB	-5.51	102.14	111.23
1	F	97	ASN	N-CA-C	5.50	116.62	108.60
2	I	121	GLN	N-CA-C	5.49	118.60	110.48
1	E	22	THR	N-CA-C	-5.48	105.31	111.28
1	E	152	TYR	N-CA-C	-5.47	105.01	110.97
2	L	53	TRP	N-CA-C	-5.47	103.27	110.43
1	F	261	PRO	CA-C-N	5.46	126.00	120.38
1	F	261	PRO	C-N-CA	5.46	126.00	120.38
1	F	60	VAL	N-CA-C	5.45	116.40	107.24
1	E	26	ARG	N-CA-C	-5.44	104.78	111.75
2	L	9	GLY	N-CA-C	-5.43	104.97	112.25
1	C	8	ILE	N-CA-C	5.42	117.20	108.85
2	L	109	ARG	N-CA-C	-5.42	99.26	110.80
1	C	36	ALA	N-CA-C	5.42	117.82	107.75
2	G	80	TYR	N-CA-C	5.38	117.57	109.23
1	F	35	GLY	CA-C-N	-5.38	115.37	122.85
1	F	35	GLY	C-N-CA	-5.38	115.37	122.85
1	E	112	GLN	N-CA-C	5.36	117.20	111.36
2	G	78	MET	N-CA-C	5.33	117.36	108.99
1	C	84	TYR	N-CA-C	5.32	117.16	109.07
1	D	22	THR	N-CA-C	-5.31	105.49	111.28
1	D	8	ILE	N-CA-C	5.30	117.02	108.85
1	D	84	TYR	N-CA-C	5.30	117.13	109.07
1	B	84	TYR	N-CA-C	5.30	117.12	109.07
2	H	121	GLN	N-CA-C	5.28	118.29	110.48
2	G	121	GLN	N-CA-C	5.27	117.67	110.55
2	L	42	GLY	N-CA-C	-5.26	108.82	115.08
1	E	163	THR	N-CA-C	-5.24	105.65	111.36
1	C	13	THR	N-CA-C	-5.24	106.40	112.89
2	K	87	LYS	CA-C-N	5.24	126.38	119.84
2	K	87	LYS	C-N-CA	5.24	126.38	119.84
2	J	53	TRP	N-CA-C	-5.22	101.61	109.60
1	E	154	TYR	N-CA-C	-5.22	105.26	111.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	8	ILE	N-CA-C	5.19	116.85	108.85
1	B	36	ALA	N-CA-C	5.16	117.34	107.75
1	C	65	HIS	N-CA-C	-5.16	106.94	113.18
1	C	97	ASN	N-CA-C	5.15	116.12	108.60
2	K	106	VAL	CA-C-N	-5.15	115.15	122.77
2	K	106	VAL	C-N-CA	-5.15	115.15	122.77
2	H	19	ARG	N-CA-C	5.14	116.79	108.26
1	F	17	THR	CB-CA-C	-5.12	99.80	110.40
2	L	110	ALA	N-CA-C	-5.12	106.55	112.89
1	A	36	ALA	N-CA-C	5.11	117.26	107.75
1	F	84	TYR	N-CA-C	5.11	116.84	109.07
1	F	37	ASP	N-CA-C	-5.11	98.93	108.02
1	B	37	ASP	N-CA-C	-5.09	98.95	108.02
1	E	8	ILE	N-CA-C	5.09	116.68	108.85
1	F	251	ILE	N-CA-C	5.09	116.26	111.48
1	F	163	THR	N-CA-C	-5.08	105.65	111.14
1	E	251	ILE	N-CA-C	5.08	116.25	111.48
2	K	95	TYR	CB-CA-C	-5.08	100.42	109.71
1	C	37	ASP	N-CA-C	-5.04	99.04	108.02
2	H	103	ARG	N-CA-C	-5.04	102.74	110.30
1	D	35	GLY	CA-C-N	-5.04	115.85	122.85
1	D	35	GLY	C-N-CA	-5.04	115.85	122.85
1	B	205	ILE	N-CA-C	5.03	115.15	110.42
1	E	36	ALA	N-CA-C	5.03	117.11	107.75
1	A	97	ASN	N-CA-C	5.03	115.94	108.60
1	B	64	ASN	N-CA-C	5.01	117.28	109.52

There are no chirality outliers.

All (18) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	36	ALA	Peptide
1	A	5	GLN	Peptide
1	B	36	ALA	Peptide
1	B	5	GLN	Peptide
1	C	36	ALA	Peptide
1	C	5	GLN	Peptide
1	D	36	ALA	Peptide
1	D	5	GLN	Peptide
1	E	15	GLY	Peptide
1	E	36	ALA	Peptide
1	E	5	GLN	Peptide

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Mol	Chain	Res	Type	Group
1	F	263	PRO	Peptide
1	F	36	ALA	Peptide
1	F	5	GLN	Peptide
2	H	25	SER	Peptide
2	K	53	TRP	Peptide
2	L	108	VAL	Mainchain
2	L	53	TRP	Peptide

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2046	0	2014	104	1
1	B	2052	0	2019	133	0
1	C	2046	0	2014	113	0
1	D	2046	0	2014	108	1
1	E	2068	0	2038	149	0
1	F	2052	0	2019	116	1
2	G	961	0	930	78	1
2	H	973	0	940	83	1
2	I	911	0	876	74	0
2	J	918	0	883	73	1
2	K	973	0	940	72	0
2	L	961	0	930	59	0
3	A	10	0	0	3	0
3	B	25	0	0	7	0
3	C	15	0	0	3	0
3	D	5	0	0	0	0
3	E	15	0	0	1	0
3	F	10	0	0	4	0
3	G	5	0	0	0	0
3	I	5	0	0	0	0
3	J	5	0	0	0	0
3	L	5	0	0	0	0
4	D	1	0	0	1	0
4	E	1	0	0	1	0
4	K	1	0	0	0	0
5	B	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	C	4	0	0	1	0
5	D	1	0	0	0	0
5	E	5	0	0	1	0
5	F	2	0	0	1	0
5	G	3	0	0	0	0
5	H	1	0	0	0	0
5	I	1	0	0	0	0
5	K	6	0	0	0	0
5	L	2	0	0	0	0
All	All	18136	0	17617	1120	4

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 31.

All (1120) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:189:ARG:HH21	1:E:193[A]:ARG:NH2	1.20	1.37
1:E:189:ARG:NH2	1:E:193[A]:ARG:HH22	1.45	1.15
1:E:189:ARG:NH2	1:E:193[A]:ARG:NH2	2.00	1.07
2:H:72[A]:ARG:HG2	2:H:72[A]:ARG:HH11	1.28	0.99
2:G:88:PRO:HA	2:G:124:VAL:CG2	1.93	0.99
1:C:197:ARG:NH1	2:I:30:SER:OG	1.96	0.98
3:C:303:SO4:O1	1:D:115:TYR:OH	1.81	0.98
1:E:104:ILE:HG22	1:E:114[B]:ARG:HH21	1.27	0.96
1:E:49:VAL:HG23	1:E:50:GLY:H	1.31	0.96
2:J:88:PRO:HA	2:J:124:VAL:CG2	1.96	0.94
2:K:88:PRO:HA	2:K:124:VAL:CG2	1.98	0.94
2:H:88:PRO:HA	2:H:124:VAL:CG2	1.97	0.94
2:G:44:GLU:HG3	2:G:45:ARG:H	1.33	0.92
1:A:197:ARG:NH1	2:G:30:SER:OG	2.03	0.91
2:K:38:ARG:HH12	2:K:90:ASP:HA	1.35	0.91
2:L:38:ARG:HH12	2:L:90:ASP:HA	1.37	0.89
1:E:189:ARG:HH21	1:E:193[A]:ARG:HH22	0.92	0.89
2:K:9:GLY:H	2:K:120:THR:HG21	1.38	0.88
1:B:125:ARG:NH2	3:B:305:SO4:O1	2.07	0.87
2:K:105:LEU:HD12	2:K:105:LEU:H	1.39	0.87
1:E:104:ILE:CG2	1:E:114[B]:ARG:HH21	1.88	0.87
2:L:88:PRO:HA	2:L:124:VAL:CG2	2.04	0.87
2:I:88:PRO:HA	2:I:124:VAL:CG2	2.05	0.87
1:B:49:VAL:HG23	1:B:50:GLY:H	1.39	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:108:VAL:HG12	2:I:108:VAL:O	1.73	0.87
1:F:39:ARG:HH11	1:F:39:ARG:HG2	1.37	0.86
2:L:9:GLY:H	2:L:120:THR:HG21	1.39	0.86
2:K:108:VAL:HG12	2:K:108:VAL:O	1.73	0.86
2:J:108:VAL:HG12	2:J:108:VAL:O	1.75	0.86
2:G:108:VAL:HG12	2:G:108:VAL:O	1.76	0.85
2:H:108:VAL:HG12	2:H:108:VAL:O	1.75	0.85
1:E:191:ARG:NH1	1:E:198:SER:O	2.10	0.85
1:B:39:ARG:HG2	1:B:39:ARG:HH11	1.40	0.84
1:E:49:VAL:HG23	1:E:50:GLY:N	1.88	0.84
1:C:54:ASN:ND2	5:C:401:HOH:O	2.07	0.84
1:A:49:VAL:HG23	1:A:50:GLY:H	1.43	0.84
2:G:44:GLU:HG3	2:G:45:ARG:N	1.91	0.84
2:G:88:PRO:HA	2:G:124:VAL:HG21	1.59	0.84
1:B:193:ARG:NH1	3:B:304:SO4:O2	2.10	0.83
1:C:8:ILE:HG22	1:C:59:LEU:HB2	1.59	0.83
2:I:47:PHE:CG	2:I:108:VAL:HG13	2.15	0.82
1:E:39:ARG:HG2	1:E:39:ARG:HH11	1.44	0.82
2:K:58:THR:O	2:K:59:LEU:HD23	1.80	0.82
1:B:191:ARG:NH1	1:B:198:SER:O	2.12	0.81
2:H:88:PRO:HA	2:H:124:VAL:HG21	1.64	0.80
1:E:125:ARG:NH2	3:E:303:SO4:O2	2.14	0.80
2:G:88:PRO:HA	2:G:124:VAL:HG23	1.63	0.80
1:D:197:ARG:NH1	2:J:30:SER:OG	2.13	0.80
2:L:108:VAL:HG12	2:L:108:VAL:O	1.79	0.80
1:E:96:ASP:OD1	1:E:96:ASP:N	2.15	0.80
2:J:47:PHE:CG	2:J:108:VAL:HG13	2.17	0.79
1:B:197:ARG:NH1	2:H:30:SER:OG	2.14	0.79
1:D:39:ARG:HG2	1:D:39:ARG:HH11	1.45	0.79
2:J:88:PRO:HA	2:J:124:VAL:HG21	1.64	0.79
1:A:8:ILE:HG22	1:A:59:LEU:HB2	1.64	0.79
1:B:173:GLN:NE2	1:B:208:GLU:OE2	2.15	0.78
2:I:44:GLU:HG3	2:I:45:ARG:H	1.48	0.78
2:J:44:GLU:HG3	2:J:45:ARG:H	1.49	0.78
1:A:191:ARG:NH1	1:A:198:SER:O	2.17	0.78
2:I:44:GLU:HG3	2:I:45:ARG:N	1.98	0.78
2:J:88:PRO:HA	2:J:124:VAL:HG23	1.64	0.78
1:A:5:GLN:OE1	1:A:5:GLN:HA	1.82	0.77
1:A:188:MET:HE2	1:A:188:MET:HA	1.66	0.77
1:B:159:THR:HG22	2:H:115:TYR:CE1	2.19	0.77
1:D:191:ARG:NH1	1:D:198:SER:O	2.18	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:193:ARG:NH1	3:B:304:SO4:S	2.55	0.77
1:F:49:VAL:HG23	1:F:50:GLY:H	1.48	0.77
1:A:39:ARG:HH11	1:A:39:ARG:HG2	1.46	0.77
2:I:58:THR:O	2:I:59:LEU:HD23	1.85	0.77
2:H:67:ARG:NH2	2:H:90:ASP:OD2	2.16	0.77
1:F:96:ASP:N	1:F:96:ASP:OD1	2.16	0.77
2:J:47:PHE:CD1	2:J:108:VAL:HG13	2.19	0.77
1:C:49:VAL:HG23	1:C:50:GLY:H	1.50	0.76
2:J:74:ASN:HB2	2:J:77:ASN:HB3	1.66	0.76
2:G:58:THR:O	2:G:59:LEU:HD23	1.83	0.76
2:G:52:VAL:HG12	2:G:53:TRP:O	1.85	0.76
2:H:44:GLU:HG3	2:H:45:ARG:N	2.01	0.76
2:H:58:THR:O	2:H:59:LEU:HD23	1.86	0.76
2:J:44:GLU:HG3	2:J:45:ARG:N	1.99	0.76
1:B:49:VAL:HG23	1:B:50:GLY:N	1.96	0.76
1:D:49:VAL:HG23	1:D:50:GLY:H	1.49	0.76
1:F:8:ILE:HG22	1:F:59:LEU:HB2	1.66	0.76
1:F:188:MET:HE2	1:F:188:MET:HA	1.67	0.75
1:C:39:ARG:HG2	1:C:39:ARG:HH11	1.50	0.75
1:E:135:GLU:H	1:E:135:GLU:CD	1.94	0.75
1:D:5:GLN:OE1	1:D:5:GLN:HA	1.85	0.75
1:F:125:ARG:NH1	3:F:301:SO4:O4	2.18	0.75
2:G:67:ARG:NH2	2:G:90:ASP:OD2	2.19	0.74
2:I:31:ARG:HG2	2:I:98:ASP:OD1	1.88	0.74
1:A:120:GLY:N	3:A:301:SO4:O4	2.20	0.74
2:I:47:PHE:CD1	2:I:108:VAL:HG13	2.22	0.74
2:H:88:PRO:HA	2:H:124:VAL:HG23	1.68	0.74
1:D:242:VAL:HG13	1:D:247:ILE:HD11	1.69	0.74
1:A:49:VAL:HG23	1:A:50:GLY:N	1.99	0.74
1:A:135:GLU:CD	1:A:135:GLU:H	1.95	0.74
1:B:188:MET:HA	1:B:188:MET:HE2	1.69	0.74
2:I:67:ARG:NH2	2:I:90:ASP:OD2	2.20	0.74
2:K:4:LEU:CD2	2:K:24:ALA:HB2	2.18	0.74
2:K:98:ASP:OD2	2:K:100:LYS:NZ	2.20	0.74
1:A:75:ASP:HB3	1:A:78:ASN:CB	2.18	0.73
1:D:49:VAL:HG23	1:D:50:GLY:N	2.03	0.73
1:E:188:MET:HE2	1:E:188:MET:HA	1.69	0.73
2:L:83:MET:HB3	2:L:86:LEU:HD21	1.70	0.73
1:C:135:GLU:H	1:C:135:GLU:CD	1.96	0.73
1:D:135:GLU:CD	1:D:135:GLU:H	1.95	0.73
2:K:88:PRO:HA	2:K:124:VAL:HG22	1.68	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:5:GLN:OE1	1:C:5:GLN:HA	1.89	0.73
2:L:58:THR:O	2:L:59:LEU:HD23	1.88	0.73
2:H:91:THR:HG23	2:H:123:THR:HG22	1.70	0.73
2:I:74:ASN:HB2	2:I:77:ASN:HB3	1.70	0.73
2:G:74:ASN:HB2	2:G:77:ASN:HB3	1.70	0.73
1:D:222:ASN:C	1:D:223:GLN:HG2	2.14	0.73
2:L:105:LEU:HD12	2:L:105:LEU:H	1.53	0.73
2:J:67:ARG:NH2	2:J:90:ASP:OD2	2.21	0.72
1:A:242:VAL:HG13	1:A:247:ILE:HD11	1.72	0.72
1:F:104:ILE:HG22	1:F:114:ARG:HH21	1.54	0.72
2:H:52:VAL:HG12	2:H:53:TRP:O	1.90	0.72
1:C:188:MET:HE2	1:C:188:MET:HA	1.72	0.72
2:L:88:PRO:HA	2:L:124:VAL:HG22	1.72	0.72
1:D:188:MET:HA	1:D:188:MET:HE2	1.70	0.72
2:K:83:MET:HB3	2:K:86:LEU:HD21	1.71	0.72
1:E:75:ASP:HB3	1:E:78:ASN:CB	2.21	0.71
2:I:88:PRO:HA	2:I:124:VAL:HG23	1.72	0.71
2:J:52:VAL:HG12	2:J:53:TRP:O	1.90	0.71
1:A:17:THR:HB	1:A:20:SER:H	1.55	0.71
2:H:20:LEU:HD12	2:H:81:LEU:HD23	1.71	0.71
1:F:135:GLU:CD	1:F:135:GLU:H	1.97	0.71
1:C:222:ASN:C	1:C:223:GLN:HG2	2.15	0.71
1:F:222:ASN:C	1:F:223:GLN:HG2	2.16	0.71
2:G:31:ARG:HG2	2:G:98:ASP:OD1	1.90	0.70
2:J:58:THR:O	2:J:59:LEU:HD23	1.91	0.70
1:E:72:LEU:N	1:E:72:LEU:HD12	2.04	0.70
2:L:6:GLU:OE1	2:L:118:GLN:O	2.09	0.70
1:F:191:ARG:NH1	1:F:198:SER:O	2.24	0.70
2:H:44:GLU:HG3	2:H:45:ARG:H	1.54	0.70
1:F:75:ASP:HB3	1:F:78:ASN:CB	2.21	0.70
2:G:47:PHE:CD1	2:G:108:VAL:HG13	2.26	0.70
1:C:191:ARG:NH1	1:C:198:SER:O	2.24	0.70
1:F:17:THR:HB	1:F:20:SER:H	1.57	0.70
1:B:75:ASP:HB3	1:B:78:ASN:CB	2.23	0.69
2:J:31:ARG:HG2	2:J:98:ASP:OD1	1.92	0.69
1:D:8:ILE:HG22	1:D:59:LEU:HB2	1.74	0.69
1:B:135:GLU:CD	1:B:135:GLU:H	2.00	0.69
2:I:91:THR:HG23	2:I:123:THR:HG22	1.74	0.69
2:G:47:PHE:CG	2:G:108:VAL:HG13	2.28	0.69
1:D:17:THR:HB	1:D:20:SER:H	1.58	0.69
2:H:74:ASN:HB2	2:H:77:ASN:HB3	1.75	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:242:VAL:HG13	1:F:247:ILE:HD11	1.75	0.69
2:G:20:LEU:HD12	2:G:81:LEU:HD23	1.74	0.69
1:D:119:PHE:HB2	1:D:125:ARG:HD2	1.75	0.69
1:F:49:VAL:HG23	1:F:50:GLY:N	2.07	0.69
2:L:4:LEU:CD2	2:L:24:ALA:HB2	2.23	0.69
1:B:17:THR:HB	1:B:20:SER:H	1.58	0.69
1:E:119:PHE:HB2	1:E:125:ARG:HD2	1.75	0.69
2:I:88:PRO:HA	2:I:124:VAL:HG21	1.75	0.68
2:K:105:LEU:H	2:K:105:LEU:CD1	2.06	0.68
1:D:75:ASP:HB3	1:D:78:ASN:CB	2.23	0.68
1:B:8:ILE:HG22	1:B:59:LEU:HB2	1.75	0.68
1:E:222:ASN:C	1:E:223:GLN:HG2	2.17	0.68
1:B:222:ASN:C	1:B:223:GLN:HG2	2.18	0.68
2:I:52:VAL:HG12	2:I:53:TRP:O	1.94	0.68
1:B:75:ASP:HB3	1:B:78:ASN:HB3	1.76	0.68
2:J:53:TRP:CZ3	2:J:72:ARG:HB2	2.29	0.68
2:J:91:THR:HG23	2:J:123:THR:HG22	1.74	0.68
1:A:96:ASP:OD1	1:A:96:ASP:N	2.26	0.68
1:E:242:VAL:HG13	1:E:247:ILE:HD11	1.76	0.68
1:C:49:VAL:HG23	1:C:50:GLY:N	2.07	0.68
1:A:224:GLY:O	1:A:245:VAL:HG23	1.94	0.67
1:B:231:GLN:O	1:B:232:LEU:HD23	1.93	0.67
2:L:12:VAL:O	2:L:124:VAL:HA	1.94	0.67
1:E:104:ILE:CG2	1:E:114[B]:ARG:NH2	2.57	0.67
1:F:119:PHE:HB2	1:F:125:ARG:HD2	1.77	0.67
1:E:173:GLN:NE2	1:E:208:GLU:OE2	2.22	0.67
2:L:47:PHE:CG	2:L:108:VAL:HG13	2.30	0.67
1:A:75:ASP:HB3	1:A:78:ASN:HB3	1.76	0.67
2:I:20:LEU:HD12	2:I:81:LEU:HD23	1.76	0.67
1:B:125:ARG:NH1	3:B:301:SO4:O1	2.27	0.67
2:K:22:CYS:O	2:K:78:MET:HE3	1.95	0.67
1:F:173:GLN:NE2	1:F:208:GLU:OE2	2.23	0.67
1:B:119:PHE:HB2	1:B:125:ARG:HD2	1.76	0.67
2:K:21:SER:HB3	2:K:78:MET:HE1	1.77	0.67
2:K:88:PRO:CA	2:K:124:VAL:CG2	2.73	0.67
1:F:75:ASP:HB3	1:F:78:ASN:HB3	1.77	0.67
1:E:49:VAL:CG2	1:E:50:GLY:H	2.07	0.66
2:K:67:ARG:NH2	2:K:90:ASP:OD2	2.27	0.66
1:A:125:ARG:NH1	3:A:301:SO4:O2	2.28	0.66
1:F:125:ARG:NH2	3:F:302:SO4:O2	2.28	0.66
1:A:222:ASN:C	1:A:223:GLN:HG2	2.18	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:122:VAL:O	2:H:123:THR:HG23	1.96	0.66
2:I:123:THR:O	2:I:124:VAL:HG13	1.95	0.66
1:B:88:ASN:O	1:B:111:VAL:HG13	1.95	0.66
2:K:6:GLU:OE1	2:K:118:GLN:O	2.14	0.66
1:B:5:GLN:HA	1:B:5:GLN:OE1	1.89	0.66
1:B:244:ASP:OD1	1:C:244:ASP:OD1	2.13	0.66
1:B:224:GLY:O	1:B:245:VAL:HG23	1.95	0.66
1:D:72:LEU:HD12	1:D:72:LEU:N	2.10	0.66
1:A:119:PHE:HB2	1:A:125:ARG:HD2	1.78	0.66
1:C:96:ASP:OD1	1:C:96:ASP:N	2.22	0.66
2:H:47:PHE:CG	2:H:108:VAL:HG13	2.32	0.65
2:H:11:LEU:HD12	2:H:12:VAL:N	2.12	0.65
2:I:53:TRP:CZ3	2:I:72:ARG:HB2	2.31	0.65
1:C:75:ASP:HB3	1:C:78:ASN:CB	2.26	0.65
2:L:31:ARG:O	2:L:32:SER:HB3	1.96	0.65
1:D:231:GLN:O	1:D:232:LEU:HD23	1.95	0.65
1:B:193:ARG:NH1	3:B:304:SO4:O1	2.30	0.65
2:L:67:ARG:NH2	2:L:90:ASP:OD2	2.30	0.65
1:C:242:VAL:HG13	1:C:247:ILE:HD11	1.79	0.65
1:D:249:ILE:N	1:D:250:PRO:HD2	2.11	0.65
1:A:231:GLN:O	1:A:232:LEU:HD23	1.97	0.65
2:G:53:TRP:CZ3	2:G:72:ARG:HB2	2.31	0.65
1:C:249:ILE:N	1:C:250:PRO:HD2	2.12	0.65
1:E:17:THR:HB	1:E:20:SER:H	1.61	0.65
2:G:14:ALA:HB2	2:G:125:SER:HB3	1.79	0.64
2:H:31:ARG:HG2	2:H:98:ASP:OD1	1.97	0.64
2:I:55:ASP:OD1	2:I:57:THR:N	2.30	0.64
1:F:74:LEU:HD11	1:F:81:VAL:HG22	1.79	0.64
2:L:73:ASP:O	2:L:77:ASN:HB3	1.96	0.64
1:A:173:GLN:NE2	1:A:208:GLU:OE2	2.26	0.64
1:A:72:LEU:N	1:A:72:LEU:HD12	2.12	0.64
1:C:231:GLN:O	1:C:232:LEU:HD23	1.98	0.64
2:J:53:TRP:CH2	2:J:72:ARG:HB2	2.32	0.64
2:I:123:THR:C	2:I:124:VAL:HG22	2.23	0.64
1:D:75:ASP:HB3	1:D:78:ASN:HB3	1.80	0.64
2:L:14:ALA:HB2	2:L:125:SER:HB3	1.80	0.64
1:D:74:LEU:HD11	1:D:81:VAL:HG22	1.80	0.64
1:D:104:ILE:HG22	1:D:114:ARG:HH21	1.63	0.64
1:B:96:ASP:OD1	1:B:96:ASP:N	2.25	0.63
1:B:99:GLU:CD	1:B:99:GLU:H	2.06	0.63
1:E:22:THR:OG1	1:E:189:ARG:HD2	1.98	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:75:ASP:HB3	1:E:78:ASN:HB3	1.80	0.63
1:E:190:THR:HG22	1:E:193[A]:ARG:NH1	2.12	0.63
1:E:249:ILE:N	1:E:250:PRO:HD2	2.13	0.63
2:K:108:VAL:O	2:K:108:VAL:CG1	2.46	0.63
2:I:53:TRP:CH2	2:I:72:ARG:HB2	2.33	0.63
2:K:14:ALA:HB2	2:K:125:SER:HB3	1.81	0.63
2:K:67:ARG:HH22	2:K:90:ASP:CG	2.06	0.63
1:B:242:VAL:HG13	1:B:247:ILE:HD11	1.80	0.63
1:C:17:THR:HB	1:C:20:SER:H	1.64	0.63
1:C:119:PHE:HB2	1:C:125:ARG:HD2	1.81	0.63
1:A:249:ILE:N	1:A:250:PRO:HD2	2.14	0.63
2:G:91:THR:HG23	2:G:123:THR:HG22	1.80	0.63
2:H:55:ASP:OD1	2:H:57:THR:N	2.32	0.63
1:C:224:GLY:O	1:C:245:VAL:HG23	1.99	0.63
1:E:39:ARG:HH11	1:E:39:ARG:CG	2.12	0.63
1:B:249:ILE:N	1:B:250:PRO:HD2	2.13	0.63
2:H:47:PHE:CD1	2:H:108:VAL:HG13	2.33	0.62
1:E:189:ARG:HH21	1:E:193[A]:ARG:HH21	1.39	0.62
2:K:20:LEU:HB2	2:K:81:LEU:HB3	1.81	0.62
1:E:119:PHE:HB2	1:E:125:ARG:CD	2.28	0.62
2:K:31:ARG:O	2:K:32:SER:HB3	2.00	0.62
2:G:103[A]:ARG:HH12	2:G:106:VAL:HG21	1.64	0.62
2:H:72[A]:ARG:HG2	2:H:72[A]:ARG:NH1	2.06	0.62
2:H:103:ARG:NH2	2:H:106:VAL:HG21	2.15	0.62
1:C:173:GLN:NE2	1:C:208:GLU:OE2	2.28	0.62
1:C:215:SER:O	1:C:219:GLN:HG3	2.00	0.62
2:J:12:VAL:O	2:J:124:VAL:HA	1.99	0.62
1:E:49:VAL:CG2	1:E:50:GLY:N	2.61	0.62
1:A:181:PHE:CZ	1:A:211:TRP:HD1	2.18	0.62
1:C:104:ILE:HG22	1:C:114:ARG:HH21	1.64	0.62
2:J:20:LEU:HD12	2:J:81:LEU:HD23	1.79	0.62
1:D:224:GLY:O	1:D:245:VAL:HG23	2.00	0.62
2:J:11:LEU:HD12	2:J:12:VAL:N	2.15	0.62
1:F:249:ILE:N	1:F:250:PRO:HD2	2.15	0.62
1:F:231:GLN:O	1:F:232:LEU:HD23	1.98	0.61
1:B:74:LEU:HD11	1:B:81:VAL:HG22	1.80	0.61
1:F:72:LEU:N	1:F:72:LEU:HD12	2.14	0.61
1:B:263:PRO:O	1:B:264:SER:HB3	1.99	0.61
1:E:189:ARG:CZ	1:E:193[A]:ARG:HH22	2.13	0.61
2:J:55:ASP:OD1	2:J:57:THR:N	2.34	0.61
1:E:99:GLU:CD	1:E:99:GLU:H	2.09	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:75:ASP:HB3	1:A:78:ASN:HB2	1.82	0.61
1:B:119:PHE:HB2	1:B:125:ARG:CD	2.30	0.61
2:H:12:VAL:O	2:H:124:VAL:HA	2.00	0.61
1:D:119:PHE:HB2	1:D:125:ARG:CD	2.30	0.61
1:E:75:ASP:HB3	1:E:78:ASN:HB2	1.81	0.61
1:C:121:GLY:HA2	1:C:126:LEU:HD11	1.83	0.61
1:E:231:GLN:O	1:E:232:LEU:HD23	2.01	0.61
1:F:39:ARG:HG2	1:F:39:ARG:NH1	2.11	0.61
1:B:72:LEU:HD12	1:B:72:LEU:N	2.16	0.61
2:I:49:ALA:HB1	2:I:70:VAL:HG21	1.83	0.61
1:E:135:GLU:CD	1:E:135:GLU:N	2.59	0.61
1:E:190:THR:HA	1:E:193[B]:ARG:HB3	1.83	0.61
2:G:12:VAL:O	2:G:124:VAL:HA	2.01	0.61
2:G:123:THR:O	2:G:124:VAL:HG13	2.01	0.61
2:J:14:ALA:HB2	2:J:125:SER:HB3	1.83	0.61
1:E:8:ILE:HG22	1:E:59:LEU:HB2	1.83	0.61
1:E:18:VAL:HG21	1:E:193[B]:ARG:HE	1.66	0.61
1:E:224:GLY:O	1:E:245:VAL:HG23	2.01	0.61
2:L:17:SER:HB3	2:L:84:ASN:OD1	2.01	0.60
2:L:87:LYS:C	2:L:124:VAL:HG21	2.25	0.60
2:H:103:ARG:NH1	2:H:103:ARG:HB3	2.17	0.60
2:J:49:ALA:HB1	2:J:70:VAL:HG21	1.84	0.60
1:A:135:GLU:CD	1:A:135:GLU:N	2.59	0.60
2:G:49:ALA:HB1	2:G:70:VAL:HG21	1.84	0.60
1:B:49:VAL:CG2	1:B:50:GLY:H	2.11	0.60
1:E:247:ILE:HD13	1:F:223:GLN:NE2	2.16	0.60
2:K:12:VAL:O	2:K:124:VAL:HA	2.01	0.60
2:I:11:LEU:HD12	2:I:12:VAL:N	2.16	0.60
1:B:214:LEU:HD21	1:B:230:ILE:HG21	1.84	0.60
2:L:98:ASP:OD2	2:L:100:LYS:NZ	2.35	0.60
2:K:29:PHE:CD1	2:K:29:PHE:N	2.70	0.60
1:C:75:ASP:HB3	1:C:78:ASN:HB3	1.84	0.60
1:E:88:ASN:HD21	1:E:112:GLN:CD	2.10	0.60
1:B:189:ARG:NH2	3:B:304:SO4:O4	2.35	0.60
2:I:14:ALA:HB2	2:I:125:SER:HB3	1.82	0.60
1:D:99:GLU:H	1:D:99:GLU:CD	2.10	0.60
2:H:108:VAL:O	2:H:108:VAL:CG1	2.47	0.59
2:H:60:TYR:HB2	2:H:65:LYS:HG3	1.84	0.59
1:C:119:PHE:HB2	1:C:125:ARG:CD	2.32	0.59
1:E:74:LEU:HD11	1:E:81:VAL:HG22	1.84	0.59
2:K:87:LYS:C	2:K:124:VAL:HG21	2.27	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:119:PHE:HB2	1:A:125:ARG:CD	2.31	0.59
1:A:121:GLY:HA2	1:A:126:LEU:HD11	1.84	0.59
1:B:104:ILE:HG22	1:B:114:ARG:HH21	1.67	0.59
1:C:214:LEU:HD21	1:C:230:ILE:HG21	1.85	0.59
1:E:71:THR:C	1:E:72:LEU:HD12	2.27	0.59
2:K:38:ARG:NH1	2:K:90:ASP:HA	2.13	0.59
1:F:99:GLU:H	1:F:99:GLU:CD	2.10	0.59
1:D:135:GLU:CD	1:D:135:GLU:N	2.61	0.59
1:E:104:ILE:HG22	1:E:114[B]:ARG:NH2	2.09	0.59
1:F:121:GLY:HA2	1:F:126:LEU:HD11	1.85	0.59
2:G:55:ASP:OD1	2:G:57:THR:N	2.35	0.59
1:F:24:PHE:O	1:F:27:ALA:HB3	2.03	0.59
1:F:119:PHE:HB2	1:F:125:ARG:CD	2.32	0.59
1:C:39:ARG:O	1:C:40:HIS:C	2.46	0.59
2:K:17:SER:HB3	2:K:84:ASN:OD1	2.03	0.59
1:E:5:GLN:OE1	1:E:5:GLN:HA	1.97	0.58
1:E:114[B]:ARG:HG2	1:E:114[B]:ARG:HH11	1.68	0.58
1:B:39:ARG:HH11	1:B:39:ARG:CG	2.11	0.58
1:F:224:GLY:O	1:F:245:VAL:HG23	2.03	0.58
2:L:88:PRO:CA	2:L:124:VAL:CG2	2.79	0.58
1:B:159:THR:HG22	2:H:115:TYR:HE1	1.67	0.58
1:D:49:VAL:CG2	1:D:50:GLY:H	2.15	0.58
1:D:214:LEU:HD21	1:D:230:ILE:HG21	1.86	0.58
2:G:122:VAL:O	2:G:123:THR:HG23	2.04	0.58
1:D:73:ALA:O	1:D:74:LEU:HD12	2.04	0.58
1:E:71:THR:O	1:E:84:TYR:HB2	2.02	0.58
1:A:189:ARG:HH21	1:A:193:ARG:HH22	1.52	0.58
1:A:215:SER:O	1:A:219:GLN:HG3	2.04	0.58
2:I:12:VAL:O	2:I:124:VAL:HA	2.03	0.58
2:G:108:VAL:O	2:G:108:VAL:CG1	2.48	0.58
1:C:74:LEU:HD11	1:C:81:VAL:HG22	1.86	0.58
1:D:22:THR:OG1	1:D:189:ARG:HD2	2.04	0.58
1:A:99:GLU:H	1:A:99:GLU:CD	2.12	0.58
1:B:39:ARG:HG2	1:B:39:ARG:NH1	2.14	0.58
1:B:189:ARG:HH21	1:B:193:ARG:HH22	1.52	0.58
1:C:181:PHE:HB2	1:C:184:ILE:HG13	1.86	0.58
1:F:215:SER:O	1:F:219:GLN:HG3	2.04	0.58
1:A:49:VAL:CG2	1:A:50:GLY:H	2.15	0.57
2:G:58:THR:C	2:G:59:LEU:HD23	2.28	0.57
2:L:21:SER:HB3	2:L:78:MET:HE1	1.84	0.57
2:H:123:THR:C	2:H:124:VAL:HG22	2.28	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:181:PHE:CZ	1:B:211:TRP:HD1	2.23	0.57
2:J:36:TRP:O	2:J:48:VAL:HB	2.04	0.57
1:B:135:GLU:CD	1:B:135:GLU:N	2.62	0.57
1:E:51:LEU:HD12	1:E:52:PRO:HD2	1.86	0.57
1:B:39:ARG:CG	1:B:39:ARG:NH1	2.68	0.57
2:H:53:TRP:CH2	2:H:72[B]:ARG:HG3	2.39	0.57
1:E:108:PHE:N	1:E:114[A]:ARG:HH22	2.03	0.57
1:B:121:GLY:HA2	1:B:126:LEU:HD11	1.86	0.57
1:E:125:ARG:NH1	4:E:304:CL:CL	2.75	0.57
1:A:214:LEU:HD21	1:A:230:ILE:HG21	1.85	0.57
2:H:49:ALA:HB1	2:H:70:VAL:HG21	1.87	0.57
1:A:85:ARG:HD3	1:A:111:VAL:CG2	2.35	0.57
2:G:67:ARG:HB3	2:G:84:ASN:O	2.04	0.57
1:B:201:ASP:HB2	1:B:202:PRO:CD	2.34	0.57
1:B:49:VAL:CG2	1:B:50:GLY:N	2.66	0.57
1:C:189:ARG:HH21	1:C:193:ARG:HH22	1.53	0.57
1:D:75:ASP:HB3	1:D:78:ASN:HB2	1.86	0.57
2:J:47:PHE:CG	2:J:108:VAL:CG1	2.87	0.57
2:K:73:ASP:OD1	2:K:74:ASN:N	2.38	0.57
1:F:75:ASP:HB3	1:F:78:ASN:HB2	1.86	0.57
2:L:105:LEU:H	2:L:105:LEU:CD1	2.18	0.57
2:G:53:TRP:CH2	2:G:72:ARG:HB2	2.40	0.56
2:H:12:VAL:HG21	2:H:86:LEU:HD22	1.87	0.56
1:F:39:ARG:NH1	1:F:39:ARG:CG	2.66	0.56
1:A:164:LEU:HG	1:A:168:PHE:CE2	2.40	0.56
2:I:47:PHE:CG	2:I:108:VAL:CG1	2.87	0.56
1:A:159:THR:HG22	2:G:115:TYR:CE1	2.39	0.56
2:G:11:LEU:HD12	2:G:12:VAL:N	2.20	0.56
2:H:67:ARG:HB3	2:H:84:ASN:O	2.06	0.56
2:I:55:ASP:OD1	2:I:57:THR:OG1	2.20	0.56
1:D:181:PHE:HB2	1:D:184:ILE:HG13	1.87	0.56
1:E:214:LEU:HD21	1:E:230:ILE:HG21	1.86	0.56
1:E:215:SER:O	1:E:219:GLN:HG3	2.04	0.56
1:F:214:LEU:HD21	1:F:230:ILE:HG21	1.88	0.56
1:A:104:ILE:HG22	1:A:114:ARG:HH21	1.70	0.56
1:F:135:GLU:CD	1:F:135:GLU:N	2.64	0.56
1:C:34:THR:HG23	1:C:46:PRO:HG3	1.88	0.56
2:J:22:CYS:HB3	2:J:79:VAL:HG12	1.88	0.56
1:B:223:GLN:NE2	1:C:247:ILE:HD13	2.21	0.56
2:H:22:CYS:O	2:H:78:MET:HE3	2.05	0.56
1:A:78:ASN:O	1:A:79:ALA:HB3	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:123:THR:C	2:G:124:VAL:HG22	2.30	0.56
2:L:47:PHE:CD2	2:L:108:VAL:HG13	2.40	0.56
1:E:39:ARG:O	1:E:40:HIS:C	2.48	0.56
2:K:32:SER:O	2:K:33:SER:HB3	2.05	0.56
1:C:75:ASP:HB3	1:C:78:ASN:HB2	1.88	0.56
2:K:73:ASP:O	2:K:77:ASN:HB3	2.05	0.56
1:E:39:ARG:HG2	1:E:39:ARG:NH1	2.19	0.55
1:E:108:PHE:O	1:E:114[A]:ARG:NH1	2.34	0.55
1:B:215:SER:O	1:B:219:GLN:HG3	2.06	0.55
2:H:14:ALA:HB2	2:H:125:SER:HB3	1.88	0.55
1:C:85:ARG:HD3	1:C:111:VAL:CG2	2.36	0.55
2:I:58:THR:C	2:I:59:LEU:HD23	2.30	0.55
2:J:74:ASN:HB2	2:J:77:ASN:CB	2.36	0.55
2:I:121:GLN:NE2	2:I:122:VAL:O	2.39	0.55
1:D:78:ASN:O	1:D:79:ALA:HB3	2.06	0.55
1:D:88:ASN:O	1:D:111:VAL:HG13	2.07	0.55
2:L:38:ARG:NH1	2:L:90:ASP:HA	2.15	0.55
1:A:88:ASN:HD21	1:A:112:GLN:CD	2.14	0.55
1:B:85:ARG:HD3	1:B:111:VAL:CG2	2.36	0.55
1:C:8:ILE:HD12	1:C:61:GLU:HB2	1.88	0.55
2:I:36:TRP:NE1	2:I:81:LEU:HB2	2.22	0.55
1:D:222:ASN:O	1:D:223:GLN:HG2	2.06	0.55
1:E:152:TYR:O	1:E:154:TYR:N	2.39	0.55
2:L:67:ARG:HH22	2:L:90:ASP:CG	2.14	0.55
1:D:173:GLN:NE2	1:D:208:GLU:OE2	2.28	0.55
1:D:189:ARG:HH21	1:D:193:ARG:HH22	1.53	0.55
1:C:24:PHE:O	1:C:27:ALA:HB3	2.06	0.55
1:C:125:ARG:NH1	3:C:301:SO4:O4	2.40	0.55
1:D:139:LEU:HG	1:D:200:PRO:HD3	1.88	0.55
2:J:67:ARG:HB3	2:J:84:ASN:O	2.07	0.55
1:E:152:TYR:C	1:E:154:TYR:H	2.14	0.55
1:E:190:THR:HA	1:E:193[A]:ARG:HB2	1.88	0.55
2:K:83:MET:HE1	2:K:122:VAL:HG21	1.88	0.55
1:A:166:ARG:NH2	2:G:114:ASP:OD1	2.40	0.55
1:C:72:LEU:N	1:C:72:LEU:HD12	2.22	0.55
1:E:154:TYR:HA	1:E:159:THR:OG1	2.07	0.55
1:F:139:LEU:HG	1:F:200:PRO:HD3	1.89	0.55
2:H:6:GLU:HA	2:H:21:SER:O	2.06	0.55
2:H:103:ARG:NH2	2:H:106:VAL:CG2	2.70	0.55
1:F:135:GLU:HG3	1:F:205:ILE:CD1	2.37	0.55
2:G:6:GLU:HA	2:G:21:SER:O	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:177:GLU:OE1	1:B:180:ARG:HD2	2.07	0.54
2:H:58:THR:C	2:H:59:LEU:HD23	2.32	0.54
1:B:75:ASP:HB3	1:B:78:ASN:HB2	1.89	0.54
1:E:144:LEU:O	1:E:148:ILE:HG13	2.07	0.54
2:I:36:TRP:O	2:I:48:VAL:HB	2.08	0.54
1:E:247:ILE:CD1	1:F:223:GLN:NE2	2.70	0.54
1:F:39:ARG:O	1:F:40:HIS:C	2.48	0.54
1:D:88:ASN:HD21	1:D:112:GLN:CD	2.15	0.54
1:D:135:GLU:HG3	1:D:205:ILE:CD1	2.38	0.54
2:H:72[A]:ARG:HH11	2:H:72[A]:ARG:CG	2.10	0.54
2:H:72[B]:ARG:HG2	2:H:73:ASP:N	2.22	0.54
1:C:39:ARG:HG2	1:C:39:ARG:NH1	2.21	0.54
2:K:9:GLY:H	2:K:120:THR:CG2	2.15	0.54
2:I:12:VAL:HG21	2:I:86:LEU:HD22	1.90	0.54
1:D:64:ASN:HB3	1:D:66:ALA:H	1.73	0.54
1:D:166:ARG:NH1	2:J:111:ILE:O	2.38	0.54
2:K:64:VAL:HA	2:K:67:ARG:NH1	2.23	0.54
1:A:49:VAL:CG2	1:A:50:GLY:N	2.70	0.54
1:C:135:GLU:HG3	1:C:205:ILE:CD1	2.38	0.54
1:F:51:LEU:HD12	1:F:52:PRO:HD2	1.88	0.54
1:F:222:ASN:O	1:F:223:GLN:HG2	2.07	0.54
1:D:121:GLY:HA2	1:D:126:LEU:HD11	1.90	0.54
1:F:64:ASN:HB3	1:F:66:ALA:H	1.73	0.54
1:F:188:MET:HE2	1:F:188:MET:CA	2.35	0.54
1:A:181:PHE:CZ	1:A:211:TRP:CD1	2.96	0.54
1:B:247:ILE:HD13	1:C:223:GLN:NE2	2.23	0.54
1:D:39:ARG:HG2	1:D:39:ARG:NH1	2.19	0.54
2:J:58:THR:C	2:J:59:LEU:HD23	2.32	0.54
2:I:108:VAL:O	2:I:108:VAL:CG1	2.45	0.53
1:F:71:THR:O	1:F:84:TYR:HB2	2.08	0.53
1:F:88:ASN:HD21	1:F:112:GLN:CD	2.16	0.53
1:D:215:SER:O	1:D:219:GLN:HG3	2.08	0.53
1:E:39:ARG:CG	1:E:39:ARG:NH1	2.69	0.53
2:H:123:THR:O	2:H:124:VAL:HG13	2.08	0.53
1:C:78:ASN:O	1:C:79:ALA:HB3	2.08	0.53
1:C:99:GLU:CD	1:C:99:GLU:H	2.16	0.53
1:E:64:ASN:HB3	1:E:66:ALA:H	1.73	0.53
1:A:139:LEU:HG	1:A:200:PRO:HD3	1.91	0.53
1:B:164:LEU:HG	1:B:168:PHE:CE2	2.44	0.53
2:I:60:TYR:HB2	2:I:65:LYS:HG3	1.90	0.53
1:F:47:ASN:ND2	1:F:49:VAL:HG22	2.23	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:136:ASN:O	2:L:102:VAL:HA	2.08	0.53
2:G:5:VAL:CG1	2:G:6:GLU:N	2.72	0.53
2:G:22:CYS:O	2:G:78:MET:HE3	2.08	0.53
1:C:139:LEU:HG	1:C:200:PRO:HD3	1.90	0.53
1:E:60:VAL:HG12	1:E:60:VAL:O	2.09	0.53
1:B:74:LEU:CD1	1:B:81:VAL:HG22	2.38	0.53
1:F:123:TYR:O	1:F:124:ASP:C	2.52	0.53
1:E:201:ASP:HB2	1:E:202:PRO:CD	2.38	0.53
1:E:72:LEU:N	1:E:72:LEU:CD1	2.69	0.53
2:H:5:VAL:CG1	2:H:6:GLU:N	2.71	0.53
1:D:39:ARG:HH11	1:D:39:ARG:CG	2.17	0.53
1:D:39:ARG:O	1:D:40:HIS:C	2.51	0.53
1:A:39:ARG:O	1:A:40:HIS:C	2.51	0.52
1:B:247:ILE:CD1	1:C:223:GLN:NE2	2.72	0.52
1:C:190:THR:HG22	1:C:193:ARG:HH11	1.73	0.52
1:E:244:ASP:HB3	1:F:223:GLN:HG3	1.90	0.52
1:A:39:ARG:HG2	1:A:39:ARG:NH1	2.19	0.52
1:B:73:ALA:O	1:B:74:LEU:HD12	2.10	0.52
2:H:72[B]:ARG:CG	2:H:73:ASP:N	2.73	0.52
2:J:60:TYR:HB2	2:J:65:LYS:HG3	1.91	0.52
1:F:125:ARG:HD2	3:F:301:SO4:O4	2.09	0.52
1:C:222:ASN:O	1:C:223:GLN:HG2	2.09	0.52
1:A:201:ASP:HB2	1:A:202:PRO:CD	2.39	0.52
1:B:201:ASP:HB2	1:B:202:PRO:HD2	1.90	0.52
1:D:164:LEU:HG	1:D:168:PHE:CE2	2.44	0.52
1:B:173:GLN:HE21	1:B:208:GLU:CD	2.16	0.52
1:B:199:ALA:HB1	1:B:200:PRO:HD2	1.91	0.52
2:I:22:CYS:HB3	2:I:79:VAL:HG12	1.90	0.52
2:G:88:PRO:CA	2:G:124:VAL:HG21	2.36	0.52
1:F:73:ALA:O	1:F:74:LEU:HD12	2.09	0.52
1:F:78:ASN:O	1:F:79:ALA:HB3	2.09	0.52
1:C:135:GLU:CD	1:C:135:GLU:N	2.63	0.52
1:E:244:ASP:OD1	1:F:244:ASP:OD1	2.26	0.52
2:K:22:CYS:C	2:K:78:MET:HE3	2.35	0.52
1:F:189:ARG:HH21	1:F:193:ARG:HH22	1.56	0.52
1:A:74:LEU:HD11	1:A:81:VAL:HG22	1.91	0.52
1:B:39:ARG:O	1:B:40:HIS:C	2.53	0.52
1:E:21:TYR:O	1:E:24:PHE:HB3	2.10	0.52
1:E:108:PHE:H	1:E:114[A]:ARG:HH22	1.56	0.52
1:E:135:GLU:HG3	1:E:205:ILE:CD1	2.40	0.52
1:E:164:LEU:HG	1:E:168:PHE:CE2	2.45	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:177:GLU:OE1	1:F:180:ARG:HD2	2.10	0.52
1:B:125:ARG:NH1	3:B:301:SO4:S	2.83	0.52
1:E:104:ILE:HG21	1:E:114[B]:ARG:NH2	2.24	0.52
2:K:88:PRO:N	2:K:124:VAL:HG21	2.23	0.52
1:A:24:PHE:O	1:A:27:ALA:HB3	2.10	0.52
1:A:188:MET:HE2	1:A:188:MET:CA	2.39	0.52
1:B:244:ASP:HB3	1:C:223:GLN:HG3	1.91	0.52
1:E:152:TYR:C	1:E:154:TYR:N	2.65	0.52
1:B:24:PHE:O	1:B:27:ALA:HB3	2.10	0.51
1:C:49:VAL:CG2	1:C:50:GLY:H	2.20	0.51
1:D:96:ASP:OD1	1:D:96:ASP:N	2.27	0.51
1:E:108:PHE:H	1:E:114[A]:ARG:NH2	2.08	0.51
2:K:73:ASP:N	2:K:78:MET:O	2.42	0.51
2:L:32:SER:O	2:L:33:SER:HB3	2.10	0.51
1:D:85:ARG:HD3	1:D:111:VAL:CG2	2.40	0.51
2:L:9:GLY:HA3	2:L:120:THR:HB	1.91	0.51
2:L:20:LEU:HB2	2:L:81:LEU:HB3	1.90	0.51
1:A:48:ARG:NH1	1:A:100:ASP:OD1	2.42	0.51
2:H:22:CYS:HB3	2:H:79:VAL:HG12	1.91	0.51
1:E:134:ARG:HH22	1:E:209:ASN:HD21	1.58	0.51
2:G:102:VAL:CG1	2:G:107:ALA:HB2	2.41	0.51
1:B:47:ASN:ND2	1:B:49:VAL:HG22	2.25	0.51
1:C:154:TYR:HA	1:C:159:THR:OG1	2.10	0.51
2:I:122:VAL:O	2:I:123:THR:HG23	2.10	0.51
1:C:177:GLU:OE1	1:C:180:ARG:HD2	2.11	0.51
2:J:103:ARG:HH11	2:J:103:ARG:CG	2.23	0.51
1:C:144:LEU:O	1:C:148:ILE:HG13	2.11	0.51
1:E:85:ARG:HD3	1:E:111:VAL:CG2	2.41	0.51
1:A:135:GLU:HG3	1:A:205:ILE:CD1	2.41	0.51
1:A:177:GLU:OE1	1:A:180:ARG:HD2	2.10	0.51
1:C:146:GLU:OE1	1:C:146:GLU:HA	2.11	0.51
2:J:60:TYR:CD1	2:J:60:TYR:N	2.79	0.51
2:J:123:THR:C	2:J:124:VAL:HG22	2.36	0.51
2:K:58:THR:C	2:K:59:LEU:HD23	2.35	0.51
1:F:49:VAL:CG2	1:F:50:GLY:H	2.18	0.51
2:L:29:PHE:CD1	2:L:29:PHE:N	2.78	0.51
2:L:58:THR:C	2:L:59:LEU:HD23	2.36	0.51
1:B:144:LEU:O	1:B:148:ILE:HG13	2.11	0.51
1:C:201:ASP:HB2	1:C:202:PRO:CD	2.40	0.51
2:I:67:ARG:HB3	2:I:84:ASN:O	2.11	0.51
1:F:85:ARG:HD3	1:F:111:VAL:CG2	2.40	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:12:VAL:HG22	2:L:124:VAL:HG12	1.92	0.51
1:A:144:LEU:O	1:A:148:ILE:HG13	2.10	0.51
2:G:12:VAL:HG21	2:G:86:LEU:HD22	1.93	0.51
1:B:181:PHE:HB2	1:B:184:ILE:HG13	1.93	0.51
1:C:120:GLY:O	1:C:125:ARG:HG2	2.10	0.51
2:L:124:VAL:O	2:L:125:SER:C	2.54	0.51
1:C:73:ALA:O	1:C:74:LEU:HD12	2.11	0.50
1:A:39:ARG:NH1	1:A:39:ARG:CG	2.73	0.50
2:G:124:VAL:O	2:G:125:SER:C	2.54	0.50
1:B:139:LEU:HG	1:B:200:PRO:HD3	1.93	0.50
1:C:159:THR:HG22	2:I:115:TYR:CE1	2.46	0.50
1:E:236:ASN:H	1:E:236:ASN:ND2	2.10	0.50
1:F:166:ARG:NH1	2:L:111:ILE:O	2.43	0.50
1:F:188:MET:HE1	1:F:191:ARG:NE	2.26	0.50
1:A:64:ASN:HB2	1:A:68:LEU:H	1.77	0.50
1:B:140:GLY:C	1:B:143:PRO:HD2	2.37	0.50
1:A:71:THR:C	1:A:72:LEU:HD12	2.35	0.50
1:D:154:TYR:HA	1:D:159:THR:OG1	2.11	0.50
2:I:22:CYS:O	2:I:78:MET:HE3	2.12	0.50
1:E:48:ARG:NH1	1:E:100:ASP:OD1	2.43	0.50
2:G:22:CYS:HB3	2:G:79:VAL:HG12	1.94	0.50
2:I:74:ASN:HB2	2:I:77:ASN:CB	2.39	0.50
1:E:136:ASN:O	2:K:102:VAL:HA	2.11	0.50
1:A:71:THR:O	1:A:84:TYR:HB2	2.11	0.50
2:G:47:PHE:CG	2:G:108:VAL:CG1	2.95	0.50
2:G:52:VAL:C	2:G:53:TRP:O	2.49	0.50
2:H:74:ASN:HB2	2:H:77:ASN:CB	2.42	0.50
1:C:64:ASN:HB3	1:C:66:ALA:H	1.76	0.50
1:B:181:PHE:CZ	1:B:211:TRP:CD1	3.00	0.50
1:C:184:ILE:HD13	1:C:204:VAL:HG13	1.93	0.50
1:E:121:GLY:HA2	1:E:126:LEU:HD11	1.94	0.50
1:F:21:TYR:O	1:F:24:PHE:HB3	2.12	0.50
1:F:125:ARG:NH1	3:F:301:SO4:S	2.85	0.50
2:G:36:TRP:O	2:G:48:VAL:HB	2.11	0.50
2:G:36:TRP:NE1	2:G:81:LEU:HB2	2.27	0.50
1:D:74:LEU:CD1	1:D:81:VAL:HG22	2.42	0.50
2:L:102:VAL:CG1	2:L:107:ALA:HB2	2.42	0.49
2:L:109:ARG:HB2	2:L:112:ASP:OD2	2.12	0.49
1:A:21:TYR:O	1:A:24:PHE:HB3	2.12	0.49
2:G:74:ASN:HB2	2:G:77:ASN:CB	2.40	0.49
1:D:24:PHE:O	1:D:27:ALA:HB3	2.11	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:8:ILE:HD12	1:A:61:GLU:HB2	1.95	0.49
1:A:47:ASN:ND2	1:A:49:VAL:HG22	2.27	0.49
1:C:88:ASN:HD21	1:C:112:GLN:CD	2.21	0.49
1:D:177:GLU:OE1	1:D:180:ARG:HD2	2.12	0.49
1:E:189:ARG:CZ	1:E:193[A]:ARG:NH2	2.71	0.49
2:G:121:GLN:NE2	2:G:122:VAL:O	2.42	0.49
1:B:21:TYR:O	1:B:24:PHE:HB3	2.13	0.49
1:B:78:ASN:O	1:B:79:ALA:HB3	2.13	0.49
1:B:91:TYR:OH	1:B:155:SER:HA	2.11	0.49
1:A:181:PHE:HB2	1:A:184:ILE:HG13	1.95	0.49
1:B:71:THR:C	1:B:72:LEU:HD12	2.38	0.49
1:B:123:TYR:CD1	1:B:134:ARG:HD3	2.47	0.49
2:I:5:VAL:CG1	2:I:6:GLU:N	2.75	0.49
1:B:166:ARG:NH2	2:H:114:ASP:OD1	2.46	0.49
2:I:103:ARG:NH1	2:I:106:VAL:HG21	2.28	0.49
1:D:39:ARG:NH1	1:D:39:ARG:CG	2.73	0.49
1:D:72:LEU:N	1:D:72:LEU:CD1	2.74	0.49
2:L:88:PRO:N	2:L:124:VAL:HG21	2.28	0.49
1:B:135:GLU:HG3	1:B:205:ILE:CD1	2.42	0.49
2:H:16:GLY:O	2:H:86:LEU:HD13	2.12	0.49
1:F:154:TYR:HA	1:F:159:THR:OG1	2.13	0.49
1:A:91:TYR:OH	1:A:155:SER:HA	2.13	0.49
1:D:134:ARG:HH22	1:D:209:ASN:HD21	1.61	0.49
2:J:6:GLU:HA	2:J:21:SER:O	2.13	0.49
1:E:25:ILE:O	1:E:26:ARG:C	2.56	0.49
1:E:248:LEU:N	1:E:248:LEU:HD23	2.28	0.49
2:G:60:TYR:HB2	2:G:65:LYS:HG3	1.95	0.48
1:D:201:ASP:HB2	1:D:202:PRO:CD	2.43	0.48
2:J:123:THR:O	2:J:124:VAL:HG13	2.13	0.48
1:E:153:TYR:HB3	1:E:159:THR:HG23	1.94	0.48
1:F:144:LEU:O	1:F:148:ILE:HG13	2.13	0.48
1:A:72:LEU:N	1:A:72:LEU:CD1	2.76	0.48
1:B:71:THR:O	1:B:84:TYR:HB2	2.13	0.48
1:C:39:ARG:HH11	1:C:39:ARG:CG	2.20	0.48
2:I:73:ASP:O	2:I:74:ASN:O	2.31	0.48
1:B:223:GLN:NE2	1:C:247:ILE:CD1	2.76	0.48
2:H:102:VAL:CG1	2:H:107:ALA:HB2	2.44	0.48
1:D:64:ASN:HB2	1:D:68:LEU:H	1.79	0.48
1:E:12:THR:O	1:E:12:THR:HG23	2.11	0.48
2:K:78:MET:HB3	2:K:78:MET:HE2	1.49	0.48
1:F:13:THR:HG22	1:F:64:ASN:HA	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:9:GLY:H	2:L:120:THR:CG2	2.18	0.48
1:C:136:ASN:O	2:I:102:VAL:HA	2.13	0.48
2:J:55:ASP:OD1	2:J:57:THR:OG1	2.20	0.48
1:E:12:THR:O	1:E:12:THR:CG2	2.61	0.48
1:F:201:ASP:HB2	1:F:202:PRO:CD	2.43	0.48
1:A:125:ARG:NH1	3:A:301:SO4:S	2.86	0.48
1:B:51:LEU:HD12	1:B:52:PRO:HD2	1.95	0.48
1:B:134:ARG:HH22	1:B:209:ASN:HD21	1.62	0.48
1:B:166:ARG:NH2	2:H:112:ASP:O	2.47	0.48
1:C:49:VAL:CG2	1:C:50:GLY:N	2.76	0.48
1:D:47:ASN:ND2	1:D:49:VAL:HG22	2.28	0.48
1:F:123:TYR:CD1	1:F:134:ARG:HD3	2.48	0.48
1:A:190:THR:HG22	1:A:193:ARG:HH11	1.78	0.48
1:F:74:LEU:CD1	1:F:81:VAL:HG22	2.44	0.48
1:C:13:THR:HG22	1:C:64:ASN:HA	1.96	0.48
1:D:64:ASN:HB3	1:D:66:ALA:N	2.29	0.48
2:L:22:CYS:O	2:L:78:MET:HE3	2.13	0.48
2:G:44:GLU:CG	2:G:45:ARG:N	2.73	0.48
1:F:263:PRO:O	1:F:264:SER:C	2.57	0.48
1:B:48:ARG:NH1	1:B:100:ASP:OD1	2.47	0.47
1:E:73:ALA:O	1:E:74:LEU:HD12	2.14	0.47
1:E:159:THR:HG22	2:K:115:TYR:HE2	1.78	0.47
1:E:223:GLN:NE2	1:F:247:ILE:HD13	2.29	0.47
1:F:49:VAL:CG2	1:F:50:GLY:N	2.75	0.47
1:A:73:ALA:O	1:A:74:LEU:HD12	2.14	0.47
1:B:263:PRO:O	1:B:264:SER:CB	2.57	0.47
1:D:181:PHE:CZ	1:D:211:TRP:HD1	2.31	0.47
1:B:154:TYR:HA	1:B:159:THR:OG1	2.13	0.47
2:I:47:PHE:CD2	2:I:108:VAL:HG13	2.49	0.47
1:D:144:LEU:O	1:D:148:ILE:HG13	2.14	0.47
1:C:21:TYR:O	1:C:24:PHE:HB3	2.15	0.47
1:C:47:ASN:ND2	1:C:49:VAL:HG22	2.29	0.47
2:I:6:GLU:HA	2:I:21:SER:O	2.14	0.47
1:D:71:THR:C	1:D:72:LEU:HD12	2.40	0.47
2:L:73:ASP:N	2:L:78:MET:O	2.46	0.47
2:H:51:ILE:HG23	2:H:51:ILE:O	2.15	0.47
2:I:93:LEU:HD12	2:I:93:LEU:HA	1.68	0.47
1:E:26:ARG:NH2	5:E:402:HOH:O	2.46	0.47
1:E:74:LEU:CD1	1:E:81:VAL:HG22	2.44	0.47
1:F:64:ASN:HB3	1:F:66:ALA:N	2.29	0.47
1:F:120:GLY:O	1:F:125:ARG:HG2	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:64:VAL:HA	2:L:67:ARG:NH1	2.30	0.47
2:L:83:MET:HE1	2:L:122:VAL:HG21	1.96	0.47
1:A:64:ASN:HB3	1:A:66:ALA:H	1.80	0.47
1:A:189:ARG:NH2	1:A:193:ARG:HH22	2.11	0.47
1:B:222:ASN:O	1:B:223:GLN:HG2	2.15	0.47
2:H:55:ASP:OD1	2:H:57:THR:OG1	2.23	0.47
1:C:39:ARG:NH1	1:C:39:ARG:CG	2.74	0.47
2:I:102:VAL:HB	2:I:107:ALA:HB2	1.95	0.47
1:D:226:PHE:HE1	1:D:245:VAL:HG22	1.79	0.47
2:J:12:VAL:HG21	2:J:86:LEU:HD22	1.95	0.47
2:J:103:ARG:HH11	2:J:103:ARG:HB2	1.78	0.47
2:K:14:ALA:H	2:K:125:SER:CB	2.28	0.47
2:K:102:VAL:CG1	2:K:107:ALA:HB2	2.45	0.47
1:F:34:THR:HG23	1:F:46:PRO:HG3	1.96	0.47
1:F:71:THR:C	1:F:72:LEU:HD12	2.40	0.47
1:F:226:PHE:HE1	1:F:245:VAL:HG22	1.79	0.47
2:L:78:MET:HB3	2:L:78:MET:HE2	1.61	0.47
1:B:88:ASN:HD21	1:B:112:GLN:CD	2.23	0.47
1:C:188:MET:HE2	1:C:188:MET:CA	2.42	0.47
2:J:122:VAL:O	2:J:123:THR:HG23	2.14	0.47
1:E:68:LEU:HD12	1:E:68:LEU:C	2.40	0.47
1:E:188:MET:HE2	1:E:188:MET:CA	2.44	0.47
2:K:103[A]:ARG:HB3	2:K:106:VAL:CG2	2.45	0.47
1:F:104:ILE:CG2	1:F:114:ARG:HH21	2.25	0.47
2:H:36:TRP:NE1	2:H:81:LEU:HB2	2.30	0.47
2:H:121:GLN:NE2	2:H:122:VAL:O	2.44	0.47
1:D:107:LEU:HA	1:D:107:LEU:HD23	1.57	0.47
2:J:93:LEU:HD12	2:J:93:LEU:HA	1.67	0.47
2:K:9:GLY:HA3	2:K:120:THR:HB	1.96	0.47
2:K:85:ASN:OD1	2:K:85:ASN:C	2.55	0.47
1:F:94:HIS:HA	1:F:95:PRO:HD2	1.81	0.47
2:L:73:ASP:OD1	2:L:74:ASN:N	2.47	0.47
1:D:21:TYR:O	1:D:24:PHE:HB3	2.15	0.47
1:E:139:LEU:HG	1:E:200:PRO:HD3	1.97	0.47
1:E:177:GLU:OE1	1:E:180:ARG:HD2	2.15	0.47
1:F:261:PRO:HA	1:F:262:PRO:HD3	1.69	0.47
1:B:188:MET:HE2	1:B:188:MET:CA	2.43	0.46
1:C:166:ARG:NH2	2:I:114:ASP:OD1	2.48	0.46
2:K:31:ARG:HD3	2:K:34:MET:SD	2.55	0.46
1:F:25:ILE:O	1:F:26:ARG:C	2.58	0.46
1:A:136:ASN:O	2:G:102:VAL:HA	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:36:TRP:O	2:H:48:VAL:HB	2.15	0.46
2:H:52:VAL:C	2:H:53:TRP:O	2.57	0.46
1:C:226:PHE:HE1	1:C:245:VAL:HG22	1.80	0.46
1:E:145:GLU:O	1:E:146:GLU:C	2.58	0.46
2:K:4:LEU:CD2	2:K:24:ALA:CB	2.91	0.46
2:K:77:ASN:HB3	2:K:78:MET:H	1.51	0.46
2:K:94:TYR:O	2:K:119:GLY:HA2	2.15	0.46
1:D:261:PRO:HA	1:D:262:PRO:HD3	1.72	0.46
2:J:102:VAL:HB	2:J:107:ALA:HB2	1.96	0.46
1:F:134:ARG:HH22	1:F:209:ASN:HD21	1.63	0.46
1:A:107:LEU:HD23	1:A:107:LEU:HA	1.64	0.46
1:B:64:ASN:HB2	1:B:68:LEU:H	1.80	0.46
2:H:91:THR:O	2:H:92:ALA:HB2	2.16	0.46
2:J:51:ILE:HG23	2:J:51:ILE:O	2.16	0.46
1:A:261:PRO:HA	1:A:262:PRO:HD3	1.66	0.46
2:H:124:VAL:O	2:H:125:SER:C	2.56	0.46
1:C:74:LEU:CD1	1:C:81:VAL:HG22	2.46	0.46
2:I:60:TYR:N	2:I:60:TYR:CD1	2.82	0.46
1:E:122:ASN:O	1:E:126:LEU:HD13	2.15	0.46
1:E:181:PHE:CZ	1:E:211:TRP:HD1	2.34	0.46
1:F:8:ILE:HD12	1:F:61:GLU:HB2	1.96	0.46
1:F:64:ASN:HB2	1:F:68:LEU:H	1.81	0.46
1:F:245:VAL:O	1:F:245:VAL:HG12	2.14	0.46
2:L:94:TYR:O	2:L:119:GLY:HA2	2.16	0.46
2:G:44:GLU:CG	2:G:45:ARG:H	2.16	0.46
2:H:37:PHE:CD2	2:H:47:PHE:HA	2.51	0.46
2:I:53:TRP:O	2:I:54:ALA:HB3	2.15	0.46
2:G:102:VAL:HB	2:G:107:ALA:HB2	1.98	0.46
1:B:72:LEU:N	1:B:72:LEU:CD1	2.79	0.46
2:I:31:ARG:O	2:I:99:ASN:O	2.34	0.46
2:I:124:VAL:O	2:I:125:SER:C	2.59	0.46
1:E:140:GLY:C	1:E:143:PRO:HD2	2.40	0.46
1:F:204:VAL:O	1:F:208:GLU:HG3	2.16	0.46
1:A:78:ASN:O	1:A:79:ALA:CB	2.64	0.46
1:B:151:LEU:HD23	1:B:164:LEU:CD1	2.46	0.46
1:D:188:MET:HE2	1:D:188:MET:CA	2.40	0.46
1:E:159:THR:HG22	2:K:115:TYR:CE2	2.51	0.46
2:K:103[B]:ARG:HH11	2:K:103[B]:ARG:HG2	1.81	0.46
1:F:17:THR:OG1	1:F:20:SER:HB3	2.16	0.46
1:F:136:ASN:O	2:L:103[B]:ARG:N	2.38	0.46
2:L:74:ASN:HB2	2:L:77:ASN:HB2	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:102:VAL:HB	2:H:107:ALA:HB2	1.98	0.46
1:C:48:ARG:NH1	1:C:100:ASP:OD1	2.49	0.46
1:C:134:ARG:HH22	1:C:209:ASN:HD21	1.63	0.46
2:J:44:GLU:CG	2:J:45:ARG:H	2.26	0.46
1:E:181:PHE:HB2	1:E:184:ILE:HG13	1.98	0.46
2:G:28:THR:HG23	2:G:28:THR:O	2.15	0.45
2:G:31:ARG:O	2:G:99:ASN:O	2.34	0.45
1:B:22:THR:OG1	1:B:189:ARG:HD2	2.16	0.45
1:D:34:THR:HG23	1:D:46:PRO:HG3	1.98	0.45
2:J:64:VAL:O	2:J:65:LYS:C	2.58	0.45
1:A:123:TYR:CD1	1:A:134:ARG:HD3	2.52	0.45
1:A:134:ARG:NH2	1:A:209:ASN:OD1	2.49	0.45
1:A:201:ASP:HB2	1:A:202:PRO:HD2	1.97	0.45
1:B:94:HIS:HA	1:B:95:PRO:HD2	1.81	0.45
1:C:85:ARG:HD2	1:C:87:GLY:O	2.16	0.45
2:J:36:TRP:NE1	2:J:81:LEU:HB2	2.30	0.45
2:J:108:VAL:O	2:J:108:VAL:CG1	2.47	0.45
1:A:120:GLY:O	1:A:125:ARG:HG2	2.16	0.45
1:A:199:ALA:HB1	1:A:200:PRO:HD2	1.99	0.45
1:B:184:ILE:HD13	1:B:204:VAL:HG13	1.98	0.45
1:B:33:THR:O	1:B:35:GLY:N	2.50	0.45
1:E:64:ASN:HB3	1:E:66:ALA:N	2.31	0.45
1:E:166:ARG:NH1	2:K:111:ILE:O	2.49	0.45
1:E:190:THR:HG22	1:E:193[A]:ARG:HH11	1.82	0.45
2:K:47:PHE:CG	2:K:108:VAL:HG13	2.51	0.45
1:B:151:LEU:HD23	1:B:164:LEU:HD12	1.98	0.45
1:C:64:ASN:HB3	1:C:66:ALA:N	2.31	0.45
1:D:8:ILE:HD12	1:D:61:GLU:HB2	1.96	0.45
2:J:22:CYS:O	2:J:78:MET:HE3	2.17	0.45
2:K:14:ALA:CB	2:K:125:SER:HB3	2.45	0.45
1:A:22:THR:OG1	1:A:189:ARG:HD2	2.15	0.45
1:B:142:GLY:N	1:B:143:PRO:CD	2.80	0.45
2:H:107:ALA:HB1	2:H:112:ASP:HB3	1.98	0.45
1:C:153:TYR:HB3	1:C:159:THR:HG23	1.97	0.45
1:F:181:PHE:CZ	1:F:211:TRP:HD1	2.33	0.45
1:A:188:MET:HE1	1:A:191:ARG:NE	2.31	0.45
2:G:91:THR:O	2:G:92:ALA:HB2	2.15	0.45
2:H:53:TRP:O	2:H:54:ALA:HB3	2.17	0.45
1:C:181:PHE:CZ	1:C:211:TRP:HD1	2.35	0.45
2:J:52:VAL:C	2:J:53:TRP:O	2.57	0.45
1:E:114[B]:ARG:HG2	1:E:114[B]:ARG:NH1	2.32	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:102:VAL:HG11	2:G:107:ALA:HB2	1.99	0.45
2:G:109:ARG:O	2:G:110:ALA:C	2.58	0.45
2:H:82:GLN:HA	2:H:82:GLN:OE1	2.15	0.45
2:L:36:TRP:HA	2:L:95:TYR:O	2.16	0.45
1:B:226:PHE:HE1	1:B:245:VAL:HG22	1.82	0.45
1:D:48:ARG:NH1	1:D:100:ASP:OD1	2.50	0.45
1:D:78:ASN:O	1:D:79:ALA:CB	2.65	0.45
2:J:53:TRP:O	2:J:54:ALA:HB3	2.17	0.45
2:K:12:VAL:HG22	2:K:124:VAL:HG12	1.98	0.45
2:G:2:VAL:O	2:G:2:VAL:CG1	2.64	0.45
1:B:239:LYS:HB3	1:B:239:LYS:HE3	1.54	0.45
1:C:68:LEU:HD11	1:C:149:SER:HA	1.99	0.45
1:C:91:TYR:OH	1:C:155:SER:HA	2.17	0.45
1:D:51:LEU:HD12	1:D:52:PRO:HD2	1.98	0.45
2:J:88:PRO:CA	2:J:124:VAL:HG21	2.40	0.45
1:E:8:ILE:HD12	1:E:61:GLU:HB2	1.99	0.45
1:E:91:TYR:OH	1:E:155:SER:HA	2.17	0.45
1:F:48:ARG:NH1	1:F:100:ASP:OD1	2.49	0.45
1:F:72:LEU:N	1:F:72:LEU:CD1	2.79	0.45
1:F:164:LEU:HG	1:F:168:PHE:CE2	2.52	0.45
2:I:67:ARG:HH22	2:I:90:ASP:CG	2.24	0.44
2:J:121:GLN:NE2	2:J:122:VAL:O	2.46	0.44
1:E:104:ILE:C	1:E:106:HIS:N	2.75	0.44
1:A:146:GLU:OE1	1:A:146:GLU:HA	2.17	0.44
1:B:64:ASN:HB3	1:B:66:ALA:H	1.82	0.44
2:H:31:ARG:O	2:H:99:ASN:O	2.34	0.44
1:E:24:PHE:O	1:E:27:ALA:HB3	2.17	0.44
1:E:171:CYS:O	1:E:172:ILE:C	2.58	0.44
2:G:103[A]:ARG:NH1	2:G:106:VAL:HG21	2.32	0.44
2:I:99:ASN:HB2	2:I:113:TYR:CD2	2.52	0.44
2:I:121:GLN:HG3	2:I:122:VAL:N	2.33	0.44
2:J:28:THR:HG23	2:J:28:THR:O	2.17	0.44
2:K:13:GLN:O	2:K:14:ALA:C	2.60	0.44
1:A:134:ARG:HH22	1:A:209:ASN:HD21	1.65	0.44
2:H:88:PRO:CA	2:H:124:VAL:HG21	2.41	0.44
1:C:173:GLN:O	1:C:177:GLU:HB2	2.17	0.44
2:K:102:VAL:HG21	2:K:112:ASP:HB3	1.99	0.44
1:C:164:LEU:HG	1:C:168:PHE:CE2	2.53	0.44
1:D:120:GLY:O	1:D:125:ARG:HG2	2.17	0.44
2:J:5:VAL:CG1	2:J:6:GLU:N	2.79	0.44
1:E:47:ASN:ND2	1:E:49:VAL:HG22	2.33	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:140:GLY:C	1:A:143:PRO:HD2	2.42	0.44
2:G:2:VAL:O	2:G:2:VAL:HG13	2.16	0.44
2:G:18:LEU:HD23	2:G:18:LEU:HA	1.69	0.44
2:G:60:TYR:N	2:G:60:TYR:CD1	2.84	0.44
1:C:64:ASN:HD22	1:C:68:LEU:HD12	1.82	0.44
1:C:94:HIS:HA	1:C:95:PRO:HD2	1.85	0.44
1:D:49:VAL:CG2	1:D:50:GLY:N	2.71	0.44
1:D:123:TYR:CD1	1:D:134:ARG:HD3	2.52	0.44
1:D:189:ARG:NH2	1:D:193:ARG:HH22	2.15	0.44
1:E:123:TYR:CD1	1:E:134:ARG:HD3	2.53	0.44
1:F:232:LEU:HD23	1:F:232:LEU:HA	1.62	0.44
1:A:222:ASN:O	1:A:223:GLN:HG2	2.17	0.44
2:I:51:ILE:HG23	2:I:51:ILE:O	2.18	0.44
2:I:91:THR:O	2:I:92:ALA:HB2	2.18	0.44
1:D:131:GLY:C	1:D:132:ASN:OD1	2.61	0.44
2:J:103:ARG:CG	2:J:103:ARG:NH1	2.81	0.44
2:J:103:ARG:NH1	2:J:103:ARG:HG3	2.31	0.44
2:J:124:VAL:O	2:J:125:SER:C	2.60	0.44
2:K:4:LEU:HD23	2:K:24:ALA:CB	2.48	0.44
1:B:153:TYR:HB3	1:B:159:THR:HG23	1.99	0.44
2:H:103:ARG:HH22	2:H:106:VAL:CG2	2.31	0.44
1:D:190:THR:HG22	1:D:193:ARG:HH11	1.82	0.44
2:L:103[B]:ARG:HG2	2:L:103[B]:ARG:HH11	1.83	0.44
1:A:171:CYS:O	1:A:172:ILE:C	2.59	0.44
1:B:120:GLY:O	1:B:125:ARG:HG2	2.18	0.44
2:I:52:VAL:C	2:I:53:TRP:O	2.60	0.44
1:D:153:TYR:HB3	1:D:159:THR:HG23	1.98	0.44
2:K:83:MET:CB	2:K:86:LEU:HD21	2.44	0.44
1:A:248:LEU:N	1:A:248:LEU:HD23	2.33	0.43
2:G:5:VAL:O	2:G:22:CYS:HA	2.18	0.43
2:G:121:GLN:HG3	2:G:122:VAL:N	2.33	0.43
1:B:33:THR:C	1:B:35:GLY:H	2.26	0.43
1:B:207:LEU:HD23	1:B:207:LEU:HA	1.87	0.43
1:C:71:THR:O	1:C:84:TYR:HB2	2.18	0.43
1:D:201:ASP:HB2	1:D:202:PRO:HD2	1.98	0.43
2:J:99:ASN:HB2	2:J:113:TYR:CD2	2.53	0.43
1:E:222:ASN:O	1:E:223:GLN:HG2	2.17	0.43
2:K:35:GLY:O	2:K:96:CYS:HA	2.18	0.43
1:F:22:THR:OG1	1:F:189:ARG:HD2	2.18	0.43
2:L:85:ASN:C	2:L:85:ASN:OD1	2.60	0.43
1:B:214:LEU:HD23	1:B:214:LEU:HA	1.82	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:17:THR:OG1	1:D:20:SER:HB3	2.18	0.43
1:F:25:ILE:C	1:F:27:ALA:N	2.75	0.43
1:F:91:TYR:OH	1:F:155:SER:HA	2.17	0.43
2:L:22:CYS:C	2:L:78:MET:HE3	2.43	0.43
1:C:64:ASN:HB2	1:C:68:LEU:H	1.83	0.43
1:D:207:LEU:HD23	1:D:207:LEU:HA	1.84	0.43
1:A:64:ASN:HB3	1:A:66:ALA:N	2.33	0.43
1:B:223:GLN:HG3	1:C:244:ASP:HB3	2.00	0.43
2:H:86:LEU:HD12	2:H:86:LEU:N	2.33	0.43
2:I:12:VAL:HG23	2:I:124:VAL:HG12	2.01	0.43
1:E:34:THR:HG23	1:E:46:PRO:HG3	2.00	0.43
2:L:14:ALA:CB	2:L:125:SER:HB3	2.47	0.43
2:I:31:ARG:CG	2:I:98:ASP:OD1	2.64	0.43
1:D:171:CYS:O	1:D:172:ILE:C	2.60	0.43
2:L:35:GLY:O	2:L:96:CYS:HA	2.18	0.43
1:C:64:ASN:HD22	1:C:68:LEU:CD1	2.30	0.43
1:C:239:LYS:HB3	1:C:239:LYS:HE3	1.57	0.43
1:D:183:TYR:HB2	1:D:251:ILE:HG23	2.00	0.43
1:E:134:ARG:HH22	1:E:209:ASN:ND2	2.16	0.43
1:E:204:VAL:O	1:E:208:GLU:HG3	2.19	0.43
1:F:104:ILE:C	1:F:106:HIS:N	2.76	0.43
2:L:60:TYR:CD1	2:L:60:TYR:N	2.87	0.43
1:C:151:LEU:HD23	1:C:164:LEU:CD1	2.49	0.43
2:I:60:TYR:CE2	2:I:70:VAL:HG23	2.53	0.43
1:D:123:TYR:O	1:D:124:ASP:C	2.62	0.43
1:E:199:ALA:HB1	1:E:200:PRO:HD2	2.01	0.43
2:G:86:LEU:HB3	2:G:124:VAL:HG11	2.00	0.43
2:G:107:ALA:HB1	2:G:112:ASP:HB3	2.00	0.43
1:B:34:THR:HG23	1:B:46:PRO:HG3	2.01	0.43
1:B:171:CYS:O	1:B:172:ILE:C	2.61	0.43
1:C:78:ASN:O	1:C:79:ALA:CB	2.66	0.43
2:J:47:PHE:CD2	2:J:108:VAL:HG13	2.53	0.43
2:J:103:ARG:HD3	2:J:105:LEU:HD12	2.00	0.43
1:E:85:ARG:HD2	1:E:87:GLY:O	2.19	0.43
1:E:223:GLN:NE2	1:F:247:ILE:CD1	2.82	0.43
1:E:234:ARG:HD2	1:E:238:SER:OG	2.19	0.43
1:A:104:ILE:O	1:A:107:LEU:HB2	2.19	0.43
1:A:232:LEU:HD23	1:A:232:LEU:HA	1.69	0.43
2:I:44:GLU:CG	2:I:45:ARG:H	2.25	0.43
1:D:166:ARG:NH2	2:J:112:ASP:O	2.52	0.43
1:D:239:LYS:HE3	1:D:239:LYS:HB3	1.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:77:ASN:OD1	2:J:78:MET:HG3	2.19	0.43
2:J:103:ARG:HH11	2:J:103:ARG:CB	2.31	0.43
1:E:201:ASP:HB2	1:E:202:PRO:HD2	1.99	0.43
1:F:107:LEU:HD23	1:F:107:LEU:HA	1.69	0.43
1:B:8:ILE:HD12	1:B:61:GLU:HB2	2.00	0.43
1:B:189:ARG:NH2	1:B:193:ARG:HH22	2.15	0.43
1:B:197:ARG:O	1:B:197:ARG:HG3	2.19	0.43
1:C:189:ARG:NH2	1:C:193:ARG:HH22	2.14	0.43
1:C:204:VAL:O	1:C:208:GLU:HG3	2.19	0.43
1:D:104:ILE:C	1:D:106:HIS:N	2.77	0.43
1:D:184:ILE:O	1:D:188:MET:HG2	2.19	0.43
2:K:103[A]:ARG:HB3	2:K:106:VAL:HG23	2.01	0.43
2:L:14:ALA:H	2:L:125:SER:CB	2.32	0.43
1:A:153:TYR:HB3	1:A:159:THR:HG23	2.00	0.42
1:B:136:ASN:O	2:H:102:VAL:HA	2.19	0.42
1:C:51:LEU:HD12	1:C:52:PRO:HD2	1.99	0.42
1:C:71:THR:C	1:C:72:LEU:HD12	2.44	0.42
1:C:123:TYR:CD1	1:C:134:ARG:HD3	2.53	0.42
1:D:125:ARG:NH1	4:D:302:CL:CL	2.89	0.42
1:D:204:VAL:O	1:D:208:GLU:HG3	2.19	0.42
1:E:190:THR:HA	1:E:193[A]:ARG:CB	2.47	0.42
2:K:47:PHE:CD2	2:K:108:VAL:HG13	2.55	0.42
1:F:60:VAL:O	1:F:60:VAL:HG12	2.19	0.42
1:B:131:GLY:C	1:B:132:ASN:OD1	2.62	0.42
1:C:183:TYR:HB2	1:C:251:ILE:HG23	2.00	0.42
2:I:33:SER:HB3	2:I:99:ASN:HD22	1.84	0.42
2:I:64:VAL:O	2:I:65:LYS:C	2.61	0.42
2:K:64:VAL:HA	2:K:67:ARG:HH11	1.83	0.42
1:F:68:LEU:HD11	1:F:149:SER:HA	2.01	0.42
1:C:201:ASP:HB2	1:C:202:PRO:HD2	1.99	0.42
2:J:102:VAL:O	2:J:104:GLY:N	2.52	0.42
2:J:121:GLN:HG3	2:J:122:VAL:N	2.33	0.42
2:H:121:GLN:HG3	2:H:122:VAL:N	2.34	0.42
1:D:234:ARG:HD2	1:D:238:SER:OG	2.18	0.42
2:J:16:GLY:O	2:J:86:LEU:HD13	2.20	0.42
1:F:181:PHE:HB2	1:F:184:ILE:HG13	2.01	0.42
2:L:20:LEU:HD23	2:L:20:LEU:HA	1.56	0.42
1:B:183:TYR:HB2	1:B:251:ILE:HG23	2.02	0.42
2:H:4:LEU:O	2:H:5:VAL:HG23	2.19	0.42
2:H:64:VAL:O	2:H:65:LYS:C	2.61	0.42
1:D:42:ILE:HA	1:D:43:PRO:HD3	1.88	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:142:GLY:N	1:E:143:PRO:CD	2.82	0.42
1:F:190:THR:HG22	1:F:193:ARG:HH11	1.84	0.42
1:B:48:ARG:HA	1:B:77:THR:HG21	2.02	0.42
1:E:226:PHE:HE1	1:E:245:VAL:HG22	1.83	0.42
1:F:171:CYS:O	1:F:172:ILE:C	2.61	0.42
1:F:207:LEU:HD23	1:F:207:LEU:HA	1.93	0.42
1:A:131:GLY:C	1:A:132:ASN:OD1	2.63	0.42
2:G:37:PHE:CD2	2:G:47:PHE:HA	2.54	0.42
2:G:82:GLN:OE1	2:G:82:GLN:HA	2.18	0.42
1:B:64:ASN:HB3	1:B:66:ALA:N	2.34	0.42
2:H:73:ASP:O	2:H:74:ASN:O	2.37	0.42
1:D:91:TYR:OH	1:D:155:SER:HA	2.19	0.42
1:D:151:LEU:HD23	1:D:164:LEU:CD1	2.49	0.42
2:J:74:ASN:OD1	2:J:77:ASN:OD1	2.38	0.42
2:K:14:ALA:H	2:K:125:SER:HB3	1.85	0.42
1:F:199:ALA:HB1	1:F:200:PRO:HD2	2.02	0.42
1:C:123:TYR:O	1:C:124:ASP:C	2.61	0.42
2:I:82:GLN:OE1	2:I:82:GLN:HA	2.20	0.42
1:D:13:THR:HG22	1:D:64:ASN:HA	2.01	0.42
1:D:138:GLU:HG3	2:J:103:ARG:HA	2.00	0.42
1:D:181:PHE:CB	1:D:184:ILE:HG13	2.49	0.42
2:J:102:VAL:CG1	2:J:107:ALA:HB2	2.50	0.42
1:E:64:ASN:HB2	1:E:68:LEU:H	1.84	0.42
1:E:152:TYR:O	1:E:153:TYR:C	2.63	0.42
1:E:205:ILE:O	1:E:208:GLU:N	2.53	0.42
1:E:245:VAL:HG12	1:E:245:VAL:O	2.18	0.42
1:E:189:ARG:HE	1:E:193[A]:ARG:NH2	2.17	0.42
2:K:124:VAL:O	2:K:125:SER:C	2.63	0.42
1:A:132:ASN:OD1	1:A:132:ASN:N	2.53	0.42
1:B:123:TYR:O	1:B:124:ASP:C	2.62	0.42
2:H:60:TYR:CE2	2:H:70:VAL:HG23	2.55	0.42
2:I:109:ARG:O	2:I:110:ALA:C	2.63	0.42
1:D:68:LEU:HD11	1:D:149:SER:HA	2.01	0.42
1:D:181:PHE:CZ	1:D:211:TRP:CD1	3.07	0.42
1:D:199:ALA:HB1	1:D:200:PRO:HD2	2.02	0.42
1:E:144:LEU:O	1:E:144:LEU:HG	2.18	0.42
1:E:261:PRO:HA	1:E:262:PRO:HD3	1.74	0.42
1:F:183:TYR:HB2	1:F:251:ILE:HG23	2.01	0.42
1:F:188:MET:HE1	1:F:191:ARG:CZ	2.50	0.42
1:F:189:ARG:NH2	1:F:193:ARG:HH22	2.18	0.42
1:A:39:ARG:NH2	1:A:261:PRO:HD3	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:197:ARG:O	1:A:197:ARG:HG3	2.19	0.41
1:A:214:LEU:HD23	1:A:214:LEU:HA	1.87	0.41
1:B:13:THR:HG22	1:B:64:ASN:HA	2.02	0.41
1:B:60:VAL:O	1:B:60:VAL:HG12	2.19	0.41
2:H:86:LEU:N	2:H:86:LEU:CD1	2.82	0.41
2:J:82:GLN:OE1	2:J:82:GLN:HA	2.19	0.41
1:F:42:ILE:HA	1:F:43:PRO:HD3	1.88	0.41
1:F:239:LYS:HE3	1:F:239:LYS:HB3	1.46	0.41
2:G:64:VAL:O	2:G:65:LYS:C	2.63	0.41
2:G:67:ARG:HH22	2:G:90:ASP:CG	2.23	0.41
2:G:68:PHE:N	2:G:68:PHE:CD1	2.88	0.41
1:B:107:LEU:HA	1:B:107:LEU:HD23	1.58	0.41
2:H:47:PHE:CG	2:H:108:VAL:CG1	3.02	0.41
2:H:72[A]:ARG:NH1	2:H:72[A]:ARG:CG	2.75	0.41
1:E:94:HIS:HA	1:E:95:PRO:HD2	1.74	0.41
2:K:20:LEU:HD23	2:K:20:LEU:HA	1.59	0.41
1:F:73:ALA:C	1:F:74:LEU:HD12	2.44	0.41
1:F:94:HIS:HB2	1:F:117:PHE:O	2.20	0.41
1:D:25:ILE:O	1:D:26:ARG:C	2.63	0.41
2:J:12:VAL:HG23	2:J:124:VAL:HG12	2.02	0.41
2:K:88:PRO:CA	2:K:124:VAL:HG21	2.48	0.41
2:G:60:TYR:CE2	2:G:70:VAL:HG23	2.55	0.41
2:H:68:PHE:HD1	2:H:68:PHE:N	2.18	0.41
1:C:151:LEU:HD23	1:C:164:LEU:HD12	2.02	0.41
1:E:107:LEU:HD23	1:E:107:LEU:HA	1.58	0.41
1:E:123:TYR:O	1:E:124:ASP:C	2.62	0.41
1:E:239:LYS:HE3	1:E:239:LYS:HB3	1.55	0.41
1:F:78:ASN:O	1:F:79:ALA:CB	2.68	0.41
1:F:169:ILE:O	1:F:173:GLN:HG3	2.20	0.41
2:G:77:ASN:OD1	2:G:78:MET:HG3	2.20	0.41
2:G:99:ASN:HB2	2:G:113:TYR:CD2	2.56	0.41
1:B:189:ARG:HE	1:B:189:ARG:HB3	1.66	0.41
1:C:104:ILE:C	1:C:106:HIS:N	2.76	0.41
1:C:166:ARG:NH2	2:I:112:ASP:O	2.52	0.41
1:C:199:ALA:HB1	1:C:200:PRO:HD2	2.03	0.41
1:E:13:THR:HG22	1:E:64:ASN:HA	2.01	0.41
1:E:88:ASN:OD1	1:E:112:GLN:HG3	2.20	0.41
1:E:247:ILE:HG13	1:E:248:LEU:HD23	2.03	0.41
1:A:151:LEU:HD23	1:A:164:LEU:CD1	2.51	0.41
2:G:73:ASP:O	2:G:74:ASN:O	2.38	0.41
2:H:102:VAL:HG11	2:H:107:ALA:HB2	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:48:ARG:HA	1:C:77:THR:HG21	2.01	0.41
1:E:134:ARG:NH2	1:E:209:ASN:OD1	2.53	0.41
2:K:11:LEU:HA	2:K:123:THR:O	2.19	0.41
1:F:153:TYR:HB3	1:F:159:THR:HG23	2.01	0.41
2:L:31:ARG:HD3	2:L:34:MET:SD	2.61	0.41
1:A:142:GLY:N	1:A:143:PRO:CD	2.83	0.41
1:A:154:TYR:HA	1:A:159:THR:OG1	2.20	0.41
1:A:226:PHE:HE1	1:A:245:VAL:HG22	1.85	0.41
2:I:16:GLY:O	2:I:86:LEU:HD13	2.20	0.41
2:I:18:LEU:HA	2:I:18:LEU:HD23	1.76	0.41
1:D:146:GLU:HA	1:D:146:GLU:OE1	2.21	0.41
1:D:189:ARG:HE	1:D:189:ARG:HB3	1.63	0.41
1:A:122:ASN:O	1:A:123:TYR:C	2.63	0.41
2:H:68:PHE:N	2:H:68:PHE:CD1	2.89	0.41
2:I:68:PHE:N	2:I:68:PHE:CD1	2.88	0.41
1:A:164:LEU:HG	1:A:168:PHE:HE2	1.85	0.41
1:A:216:THR:HG23	1:A:258:ARG:NE	2.36	0.41
2:G:68:PHE:N	2:G:68:PHE:HD1	2.19	0.41
1:B:25:ILE:O	1:B:26:ARG:C	2.62	0.41
2:H:5:VAL:HG12	2:H:6:GLU:N	2.35	0.41
2:H:18:LEU:HA	2:H:18:LEU:HD23	1.73	0.41
2:H:28:THR:HG23	2:H:28:THR:O	2.21	0.41
2:I:68:PHE:N	2:I:68:PHE:HD1	2.19	0.41
2:I:86:LEU:HB3	2:I:124:VAL:HG11	2.03	0.41
1:D:184:ILE:HD13	1:D:204:VAL:HG13	2.03	0.41
2:J:4:LEU:HD11	2:J:98:ASP:HB2	2.03	0.41
2:J:33:SER:HB3	2:J:99:ASN:HD22	1.86	0.41
1:E:17:THR:OG1	1:E:20:SER:HB3	2.20	0.41
1:E:25:ILE:C	1:E:27:ALA:N	2.75	0.41
1:E:39:ARG:O	1:E:41:GLU:N	2.54	0.41
1:E:205:ILE:O	1:E:208:GLU:HB2	2.21	0.41
1:E:247:ILE:CD1	1:F:223:GLN:HE22	2.33	0.41
2:K:2:VAL:O	2:K:3:GLN:HB2	2.21	0.41
2:K:2:VAL:O	2:K:2:VAL:CG1	2.69	0.41
2:K:47:PHE:CZ	2:K:50:SER:HB3	2.56	0.41
2:L:38:ARG:HB2	2:L:92:ALA:HB1	2.02	0.41
2:L:67:ARG:NE	2:L:87:LYS:HE3	2.36	0.41
1:A:13:THR:HG22	1:A:64:ASN:HA	2.02	0.41
1:B:133:LEU:HA	1:B:133:LEU:HD23	1.77	0.41
1:B:146:GLU:HA	1:B:146:GLU:OE1	2.21	0.41
1:B:255:MET:HE3	1:B:255:MET:HB2	1.96	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:77:ASN:OD1	2:H:78:MET:HG3	2.21	0.41
2:H:91:THR:CG2	2:H:123:THR:HG22	2.46	0.41
1:C:125:ARG:NH1	3:C:301:SO4:S	2.93	0.41
1:C:133:LEU:HD23	1:C:133:LEU:HA	1.85	0.41
1:A:74:LEU:CD1	1:A:81:VAL:HG22	2.50	0.40
1:B:17:THR:OG1	1:B:20:SER:HB3	2.21	0.40
1:B:222:ASN:O	1:B:223:GLN:C	2.64	0.40
1:B:232:LEU:HD23	1:B:232:LEU:HA	1.69	0.40
1:C:166:ARG:NH1	2:I:111:ILE:O	2.53	0.40
2:K:16:GLY:O	2:K:86:LEU:HD12	2.22	0.40
2:K:103[B]:ARG:O	2:K:106:VAL:HG23	2.21	0.40
1:F:189:ARG:NH2	5:F:401:HOH:O	2.54	0.40
2:G:102:VAL:O	2:G:103[B]:ARG:C	2.64	0.40
1:B:248:LEU:N	1:B:248:LEU:HD23	2.36	0.40
1:C:92:PHE:HB3	1:C:104:ILE:HD13	2.03	0.40
1:C:232:LEU:HD23	1:C:232:LEU:HA	1.68	0.40
1:D:249:ILE:N	1:D:250:PRO:CD	2.83	0.40
1:E:126:LEU:O	1:E:127:GLU:C	2.63	0.40
2:G:79:VAL:C	2:G:80:TYR:CD1	2.99	0.40
1:B:46:PRO:HG2	1:B:76:VAL:CG1	2.52	0.40
1:B:85:ARG:HD2	1:B:87:GLY:O	2.22	0.40
1:B:236:ASN:H	1:B:236:ASN:ND2	2.20	0.40
1:C:72:LEU:N	1:C:72:LEU:CD1	2.83	0.40
1:D:25:ILE:C	1:D:27:ALA:N	2.78	0.40
1:E:51:LEU:HD12	1:E:51:LEU:HA	1.90	0.40
1:E:223:GLN:HG3	1:F:244:ASP:HB3	2.03	0.40
1:A:68:LEU:C	1:A:68:LEU:HD12	2.47	0.40
2:G:106:VAL:O	2:G:106:VAL:HG12	2.21	0.40
1:B:234:ARG:HD2	1:B:238:SER:OG	2.22	0.40
1:C:171:CYS:O	1:C:172:ILE:C	2.63	0.40

All (4) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:24:ALA:O	2:G:27:ARG:NH2[8_544]	1.85	0.35
2:H:3:GLN:NE2	2:H:3:GLN:NE2[8_544]	1.96	0.24
2:J:85:ASN:ND2	1:F:239:LYS:NZ[15_545]	2.17	0.03
1:A:244:ASP:OD1	1:D:244:ASP:OD1[13_455]	2.18	0.02

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	257/261 (98%)	244 (95%)	13 (5%)	0	100	100
1	B	258/261 (99%)	244 (95%)	14 (5%)	0	100	100
1	C	257/261 (98%)	243 (95%)	14 (5%)	0	100	100
1	D	257/261 (98%)	244 (95%)	13 (5%)	0	100	100
1	E	259/261 (99%)	248 (96%)	11 (4%)	0	100	100
1	F	258/261 (99%)	244 (95%)	14 (5%)	0	100	100
2	G	118/127 (93%)	105 (89%)	13 (11%)	0	100	100
2	H	122/127 (96%)	108 (88%)	14 (12%)	0	100	100
2	I	112/127 (88%)	100 (89%)	12 (11%)	0	100	100
2	J	113/127 (89%)	99 (88%)	14 (12%)	0	100	100
2	K	122/127 (96%)	112 (92%)	10 (8%)	0	100	100
2	L	118/127 (93%)	106 (90%)	12 (10%)	0	100	100
All	All	2251/2328 (97%)	2097 (93%)	154 (7%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	218/220 (99%)	193 (88%)	25 (12%)	5	23
1	B	219/220 (100%)	192 (88%)	27 (12%)	4	20

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	218/220 (99%)	194 (89%)	24 (11%)	6	24
1	D	218/220 (99%)	193 (88%)	25 (12%)	5	23
1	E	220/220 (100%)	198 (90%)	22 (10%)	7	29
1	F	219/220 (100%)	197 (90%)	22 (10%)	7	29
2	G	100/103 (97%)	86 (86%)	14 (14%)	3	15
2	H	101/103 (98%)	85 (84%)	16 (16%)	2	12
2	I	95/103 (92%)	81 (85%)	14 (15%)	3	14
2	J	96/103 (93%)	81 (84%)	15 (16%)	2	12
2	K	101/103 (98%)	80 (79%)	21 (21%)	1	5
2	L	100/103 (97%)	82 (82%)	18 (18%)	2	8
All	All	1905/1938 (98%)	1662 (87%)	243 (13%)	4	18

All (243) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	GLN
1	A	8	ILE
1	A	17	THR
1	A	28	VAL
1	A	34	THR
1	A	38	VAL
1	A	39	ARG
1	A	41	GLU
1	A	64	ASN
1	A	74	LEU
1	A	76	VAL
1	A	82	VAL
1	A	96	ASP
1	A	102	GLU
1	A	114	ARG
1	A	116	THR
1	A	122	ASN
1	A	125	ARG
1	A	132	ASN
1	A	135	GLU
1	A	145	GLU
1	A	156	THR
1	A	166	ARG

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Mol	Chain	Res	Type
1	A	187	GLU
1	A	239	LYS
2	G	2	VAL
2	G	7	SER
2	G	18	LEU
2	G	32	SER
2	G	33	SER
2	G	53	TRP
2	G	55	ASP
2	G	67	ARG
2	G	69	THR
2	G	70	VAL
2	G	72	ARG
2	G	105	LEU
2	G	123	THR
2	G	124	VAL
1	B	5	GLN
1	B	8	ILE
1	B	13	THR
1	B	17	THR
1	B	20	SER
1	B	28	VAL
1	B	34	THR
1	B	38	VAL
1	B	39	ARG
1	B	41	GLU
1	B	64	ASN
1	B	74	LEU
1	B	76	VAL
1	B	82	VAL
1	B	96	ASP
1	B	102	GLU
1	B	114	ARG
1	B	116	THR
1	B	122	ASN
1	B	125	ARG
1	B	132	ASN
1	B	135	GLU
1	B	145	GLU
1	B	156	THR
1	B	166	ARG
1	B	187	GLU

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Mol	Chain	Res	Type
1	B	239	LYS
2	H	7	SER
2	H	18	LEU
2	H	27	ARG
2	H	31	ARG
2	H	32	SER
2	H	33	SER
2	H	55	ASP
2	H	67	ARG
2	H	69	THR
2	H	70	VAL
2	H	72[A]	ARG
2	H	72[B]	ARG
2	H	103	ARG
2	H	105	LEU
2	H	123	THR
2	H	124	VAL
1	C	5	GLN
1	C	8	ILE
1	C	17	THR
1	C	28	VAL
1	C	34	THR
1	C	38	VAL
1	C	39	ARG
1	C	41	GLU
1	C	74	LEU
1	C	76	VAL
1	C	82	VAL
1	C	96	ASP
1	C	102	GLU
1	C	104	ILE
1	C	114	ARG
1	C	116	THR
1	C	122	ASN
1	C	125	ARG
1	C	135	GLU
1	C	145	GLU
1	C	156	THR
1	C	166	ARG
1	C	184	ILE
1	C	239	LYS
2	I	7	SER

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Mol	Chain	Res	Type
2	I	18	LEU
2	I	31	ARG
2	I	32	SER
2	I	33	SER
2	I	53	TRP
2	I	55	ASP
2	I	67	ARG
2	I	69	THR
2	I	70	VAL
2	I	72	ARG
2	I	105	LEU
2	I	123	THR
2	I	124	VAL
1	D	5	GLN
1	D	8	ILE
1	D	17	THR
1	D	28	VAL
1	D	34	THR
1	D	38	VAL
1	D	39	ARG
1	D	41	GLU
1	D	64	ASN
1	D	74	LEU
1	D	76	VAL
1	D	82	VAL
1	D	96	ASP
1	D	102	GLU
1	D	114	ARG
1	D	116	THR
1	D	122	ASN
1	D	125	ARG
1	D	132	ASN
1	D	135	GLU
1	D	145	GLU
1	D	156	THR
1	D	166	ARG
1	D	184	ILE
1	D	187	GLU
2	J	7	SER
2	J	18	LEU
2	J	31	ARG
2	J	32	SER

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Mol	Chain	Res	Type
2	J	33	SER
2	J	53	TRP
2	J	55	ASP
2	J	67	ARG
2	J	69	THR
2	J	70	VAL
2	J	72	ARG
2	J	103	ARG
2	J	105	LEU
2	J	123	THR
2	J	124	VAL
1	E	5	GLN
1	E	8	ILE
1	E	13	THR
1	E	17	THR
1	E	28	VAL
1	E	34	THR
1	E	38	VAL
1	E	39	ARG
1	E	41	GLU
1	E	74	LEU
1	E	76	VAL
1	E	82	VAL
1	E	96	ASP
1	E	102	GLU
1	E	116	THR
1	E	122	ASN
1	E	125	ARG
1	E	145	GLU
1	E	156	THR
1	E	166	ARG
1	E	184	ILE
1	E	239	LYS
2	K	1	GLN
2	K	7	SER
2	K	28	THR
2	K	29	PHE
2	K	30	SER
2	K	33	SER
2	K	59	LEU
2	K	63	SER
2	K	65	LYS

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Mol	Chain	Res	Type
2	K	67	ARG
2	K	69	THR
2	K	71	SER
2	K	78	MET
2	K	79	VAL
2	K	87	LYS
2	K	96	CYS
2	K	105	LEU
2	K	106	VAL
2	K	118	GLN
2	K	120	THR
2	K	124	VAL
1	F	5	GLN
1	F	8	ILE
1	F	17	THR
1	F	28	VAL
1	F	34	THR
1	F	38	VAL
1	F	39	ARG
1	F	41	GLU
1	F	64	ASN
1	F	76	VAL
1	F	96	ASP
1	F	102	GLU
1	F	104	ILE
1	F	114	ARG
1	F	116	THR
1	F	122	ASN
1	F	125	ARG
1	F	135	GLU
1	F	145	GLU
1	F	156	THR
1	F	166	ARG
1	F	197	ARG
2	L	1	GLN
2	L	28	THR
2	L	29	PHE
2	L	30	SER
2	L	33	SER
2	L	63	SER
2	L	65	LYS
2	L	69	THR

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Mol	Chain	Res	Type
2	L	71	SER
2	L	78	MET
2	L	79	VAL
2	L	87	LYS
2	L	96	CYS
2	L	105	LEU
2	L	106	VAL
2	L	118	GLN
2	L	120	THR
2	L	124	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	10	ASN
1	A	141	ASN
2	G	39	GLN
1	B	10	ASN
1	B	65	HIS
2	H	39	GLN
1	C	10	ASN
1	C	64	ASN
1	C	141	ASN
1	C	223	GLN
2	I	39	GLN
1	D	10	ASN
1	D	141	ASN
2	J	39	GLN
1	E	10	ASN
1	E	64	ASN
1	E	65	HIS
1	E	160	GLN
2	K	121	GLN
1	F	10	ASN
1	F	113	ASN
1	F	141	ASN
1	F	160	GLN
1	F	223	GLN
2	L	121	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 23 ligands modelled in this entry, 3 are monoatomic - leaving 20 for Mogul analysis.

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	SO4	B	304	-	4,4,4	0.24	0	6,6,6	0.16	0
3	SO4	F	302	-	4,4,4	0.33	0	6,6,6	0.35	0
3	SO4	C	303	-	4,4,4	0.17	0	6,6,6	0.39	0
3	SO4	J	201	-	4,4,4	0.30	0	6,6,6	0.24	0
3	SO4	G	201	-	4,4,4	0.25	0	6,6,6	0.37	0
3	SO4	E	303	-	4,4,4	0.34	0	6,6,6	0.66	0
3	SO4	C	302	-	4,4,4	0.29	0	6,6,6	0.26	0
3	SO4	F	301	-	4,4,4	0.44	0	6,6,6	0.42	0
3	SO4	A	302	-	4,4,4	0.29	0	6,6,6	0.27	0
3	SO4	C	301	-	4,4,4	0.39	0	6,6,6	0.92	0
3	SO4	B	302	-	4,4,4	0.31	0	6,6,6	0.34	0
3	SO4	B	301	-	4,4,4	0.33	0	6,6,6	1.03	0
3	SO4	B	303	-	4,4,4	0.33	0	6,6,6	0.30	0
3	SO4	L	201	-	4,4,4	0.28	0	6,6,6	0.24	0
3	SO4	D	301	-	4,4,4	0.20	0	6,6,6	0.27	0
3	SO4	E	301	-	4,4,4	0.36	0	6,6,6	0.73	0
3	SO4	A	301	-	4,4,4	0.37	0	6,6,6	0.34	0
3	SO4	E	302	-	4,4,4	0.29	0	6,6,6	0.34	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	SO4	B	305	-	4,4,4	0.18	0	6,6,6	0.32	0
3	SO4	I	201	-	4,4,4	0.28	0	6,6,6	0.32	0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

9 monomers are involved in 18 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	304	SO4	4	0
3	F	302	SO4	1	0
3	C	303	SO4	1	0
3	E	303	SO4	1	0
3	F	301	SO4	3	0
3	C	301	SO4	2	0
3	B	301	SO4	2	0
3	A	301	SO4	3	0
3	B	305	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	A	259/261 (99%)	0.22	3 (1%) 76 58	62, 93, 122, 145	0
1	B	260/261 (99%)	0.12	6 (2%) 61 39	48, 80, 111, 147	0
1	C	259/261 (99%)	0.13	7 (2%) 56 35	60, 90, 119, 140	0
1	D	259/261 (99%)	0.28	7 (2%) 56 35	74, 101, 128, 154	0
1	E	259/261 (99%)	0.14	3 (1%) 76 58	19, 66, 102, 134	2 (0%)
1	F	260/261 (99%)	0.09	4 (1%) 72 52	45, 77, 116, 130	0
2	G	123/127 (96%)	1.30	23 (18%) 3 1	47, 108, 137, 179	1 (0%)
2	H	125/127 (98%)	1.15	18 (14%) 6 3	30, 93, 120, 171	1 (0%)
2	I	118/127 (92%)	1.05	11 (9%) 14 8	77, 104, 135, 156	0
2	J	119/127 (93%)	1.06	14 (11%) 9 5	96, 121, 144, 171	0
2	K	125/127 (98%)	0.29	3 (2%) 59 38	26, 58, 98, 111	1 (0%)
2	L	123/127 (96%)	0.41	9 (7%) 21 11	33, 84, 120, 139	1 (0%)
All	All	2289/2328 (98%)	0.39	108 (4%) 36 19	19, 89, 128, 179	6 (0%)

All (108) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	I	29	PHE	5.6
2	H	3	GLN	5.0
1	D	40	HIS	4.9
2	H	26	GLY	4.8
2	H	25	SER	4.8
2	H	28	THR	4.7
2	H	1	GLN	4.3
2	L	28	THR	4.2
2	J	25	SER	4.2
1	C	40	HIS	4.2
2	G	25	SER	4.2

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Mol	Chain	Res	Type	RSRZ
2	H	-1	ASN	4.1
2	G	2	VAL	3.8
2	G	28	THR	3.7
2	G	1	GLN	3.6
2	L	118	GLN	3.6
2	G	3	GLN	3.5
1	B	40	HIS	3.5
2	L	25	SER	3.4
2	G	24	ALA	3.3
1	C	263	PRO	3.3
2	G	33	SER	3.3
1	F	40	HIS	3.3
2	H	54	ALA	3.2
2	G	111	ILE	3.1
2	L	0	MET	3.1
2	G	60	TYR	3.1
2	J	28	THR	3.1
1	B	264	SER	3.1
1	E	40	HIS	3.0
2	L	1	GLN	3.0
1	F	264	SER	3.0
2	J	105	LEU	3.0
2	I	32	SER	3.0
1	B	262	PRO	3.0
2	H	118	GLN	3.0
2	J	118	GLN	3.0
2	H	71	SER	3.0
2	L	125	SER	3.0
2	J	65	LYS	2.9
2	J	29	PHE	2.9
2	I	85	ASN	2.9
1	D	262	PRO	2.9
1	A	40	HIS	2.8
1	D	263	PRO	2.8
2	I	118	GLN	2.8
2	K	-1	ASN	2.8
2	J	43	LYS	2.8
2	I	72	ARG	2.8
2	L	27	ARG	2.8
2	I	71	SER	2.8
2	H	73	ASP	2.8
2	G	118	GLN	2.8

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Mol	Chain	Res	Type	RSRZ
2	G	104	GLY	2.7
1	A	263	PRO	2.7
2	G	29	PHE	2.6
1	E	17	THR	2.6
1	C	160	GLN	2.6
2	J	104	GLY	2.6
2	G	32	SER	2.6
2	H	104	GLY	2.6
2	G	105	LEU	2.6
1	A	160	GLN	2.5
1	C	65	HIS	2.5
2	L	105	LEU	2.5
2	H	33	SER	2.5
2	I	25	SER	2.5
2	G	11	LEU	2.5
2	G	27	ARG	2.5
2	H	77	ASN	2.4
2	H	106	VAL	2.4
2	J	103	ARG	2.4
1	C	194	TYR	2.4
2	H	111	ILE	2.4
2	I	103	ARG	2.3
2	H	74	ASN	2.3
1	C	136	ASN	2.3
2	I	16	GLY	2.3
1	F	194	TYR	2.3
2	G	54	ALA	2.2
2	H	78	MET	2.2
1	B	17	THR	2.2
2	G	13	GLN	2.2
2	K	118	GLN	2.2
1	C	262	PRO	2.2
1	D	120	GLY	2.2
2	K	125	SER	2.2
1	E	263	PRO	2.2
2	I	63	SER	2.2
2	L	74	ASN	2.2
2	H	29	PHE	2.2
1	D	34	THR	2.1
1	D	194	TYR	2.1
1	F	10	ASN	2.1
2	G	72	ARG	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	195	ASN	2.1
2	I	70	VAL	2.1
1	B	263	PRO	2.1
2	G	30	SER	2.1
2	J	21	SER	2.0
2	J	125	SER	2.0
2	G	4	LEU	2.0
2	G	10	GLY	2.0
2	G	66	GLY	2.0
1	D	88	ASN	2.0
2	J	74	ASN	2.0
2	J	35	GLY	2.0
2	J	56	GLY	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	SO4	C	303	5/5	0.46	0.13	109,132,166,186	0
3	SO4	D	301	5/5	0.47	0.13	89,122,180,197	0
3	SO4	B	304	5/5	0.48	0.14	149,162,186,206	0
4	CL	D	302	1/1	0.62	0.12	46,46,46,46	0
3	SO4	B	302	5/5	0.67	0.17	54,130,184,193	0
3	SO4	F	302	5/5	0.81	0.13	54,97,156,163	0
3	SO4	A	302	5/5	0.82	0.17	58,95,185,235	0
3	SO4	C	302	5/5	0.82	0.15	98,104,154,156	0
3	SO4	I	201	5/5	0.85	0.13	48,90,150,162	0
3	SO4	G	201	5/5	0.86	0.20	57,87,160,182	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	SO4	B	305	5/5	0.89	0.15	84,119,120,156	0
3	SO4	E	302	5/5	0.89	0.17	28,70,183,217	0
3	SO4	J	201	5/5	0.90	0.10	60,119,163,174	0
3	SO4	B	301	5/5	0.91	0.13	40,44,58,115	0
3	SO4	B	303	5/5	0.92	0.13	30,74,172,189	0
3	SO4	E	301	5/5	0.93	0.12	16,52,139,160	0
4	CL	K	201	1/1	0.93	0.17	42,42,42,42	0
3	SO4	A	301	5/5	0.94	0.13	40,47,104,133	0
3	SO4	L	201	5/5	0.94	0.09	87,97,114,115	0
3	SO4	C	301	5/5	0.95	0.10	12,42,80,124	0
3	SO4	E	303	5/5	0.95	0.12	38,66,138,203	0
4	CL	E	304	1/1	0.97	0.20	30,30,30,30	0
3	SO4	F	301	5/5	0.98	0.11	11,25,74,146	0

6.5 Other polymers [i](#)

There are no such residues in this entry.