



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 09:33 AM UTC

PDB ID : 2V4D / pdb_00002v4d
Title : Re-refinement of MexA adaptor protein
Authors : Symmons, M.F.; Bokma, E.; Koronakis, E.; Hughes, C.; Koronakis, V.
Deposited on : 2008-09-18
Resolution : 3.20 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

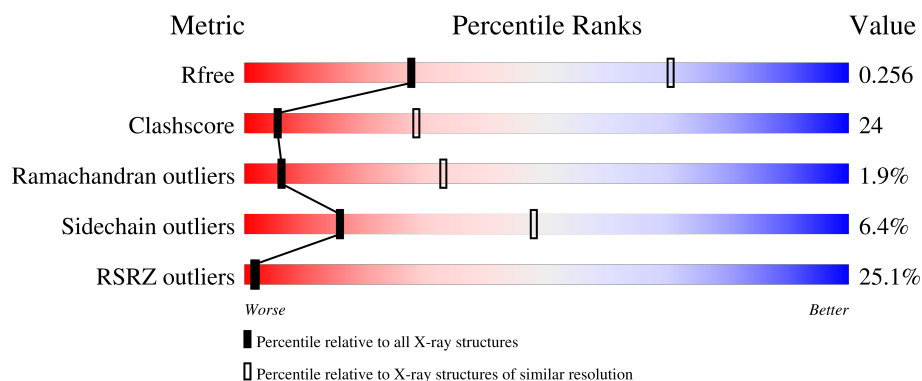
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.20 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	1466 (3.20-3.20)
Clashscore	190562	1573 (3.20-3.20)
Ramachandran outliers	187476	1548 (3.20-3.20)
Sidechain outliers	187428	1547 (3.20-3.20)
RSRZ outliers	180081	1466 (3.20-3.20)

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	360	
1	B	360	
1	C	360	
1	D	360	
1	E	360	

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Mol	Chain	Length	Quality of chain
1	F	360	15% 54% 35% 9%
1	G	360	28% 55% 34% 9%
1	H	360	28% 56% 33% 9%
1	I	360	24% 56% 31% 9%
1	J	360	23% 56% 32% 9%
1	K	360	24% 53% 35% 9%
1	L	360	26% 59% 29% 9%
1	M	360	30% 52% 35% 9%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 28603 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 MULTIDRUG RESISTANCE PROTEIN MEXA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	232	Total	C	N	O	S	0	0	0
			1776	1104	320	350	2			
1	B	327	Total	C	N	O	S	0	0	0
			2259	1394	417	446	2			
1	C	327	Total	C	N	O	S	0	0	0
			2250	1388	415	445	2			
1	D	230	Total	C	N	O	S	0	0	0
			1764	1097	318	347	2			
1	E	327	Total	C	N	O	S	0	0	0
			2264	1396	417	449	2			
1	F	327	Total	C	N	O	S	0	0	0
			2415	1498	438	477	2			
1	G	327	Total	C	N	O	S	0	0	0
			2250	1388	415	445	2			
1	H	327	Total	C	N	O	S	0	0	0
			2264	1396	417	449	2			
1	I	327	Total	C	N	O	S	0	0	0
			2250	1388	415	445	2			
1	J	327	Total	C	N	O	S	0	0	0
			2249	1388	414	445	2			
1	K	327	Total	C	N	O	S	0	0	0
			2264	1396	417	449	2			
1	L	327	Total	C	N	O	S	0	0	0
			2250	1388	415	445	2			
1	M	327	Total	C	N	O	S	0	0	0
			2268	1399	417	450	2			

There are 13 discrepancies between the modelled and reference sequences:

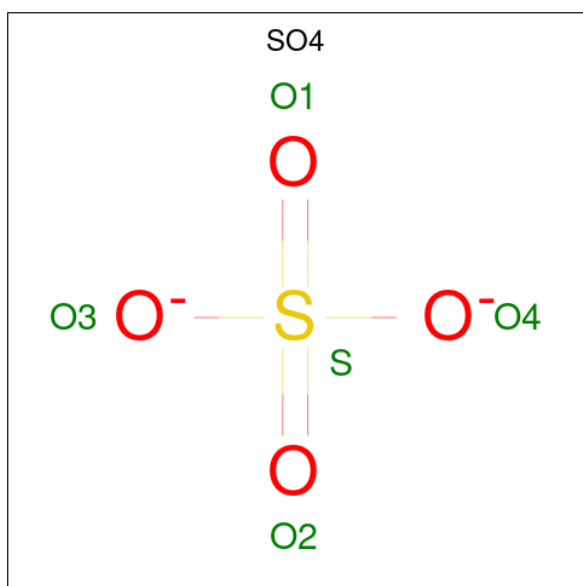
Chain	Residue	Modelled	Actual	Comment	Reference
A	1	SER	CYS	engineered mutation	UNP P52477
B	1	SER	CYS	engineered mutation	UNP P52477
C	1	SER	CYS	engineered mutation	UNP P52477

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Chain	Residue	Modelled	Actual	Comment	Reference
D	1	SER	CYS	engineered mutation	UNP P52477
E	1	SER	CYS	engineered mutation	UNP P52477
F	1	SER	CYS	engineered mutation	UNP P52477
G	1	SER	CYS	engineered mutation	UNP P52477
H	1	SER	CYS	engineered mutation	UNP P52477
I	1	SER	CYS	engineered mutation	UNP P52477
J	1	SER	CYS	engineered mutation	UNP P52477
K	1	SER	CYS	engineered mutation	UNP P52477
L	1	SER	CYS	engineered mutation	UNP P52477
M	1	SER	CYS	engineered mutation	UNP P52477

- Molecule 2 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total O S 5 4 1	0	0
2	A	1	Total O S 5 4 1	0	0
2	B	1	Total O S 5 4 1	0	0
2	B	1	Total O S 5 4 1	0	0
2	C	1	Total O S 5 4 1	0	0
2	E	1	Total O S 5 4 1	0	0

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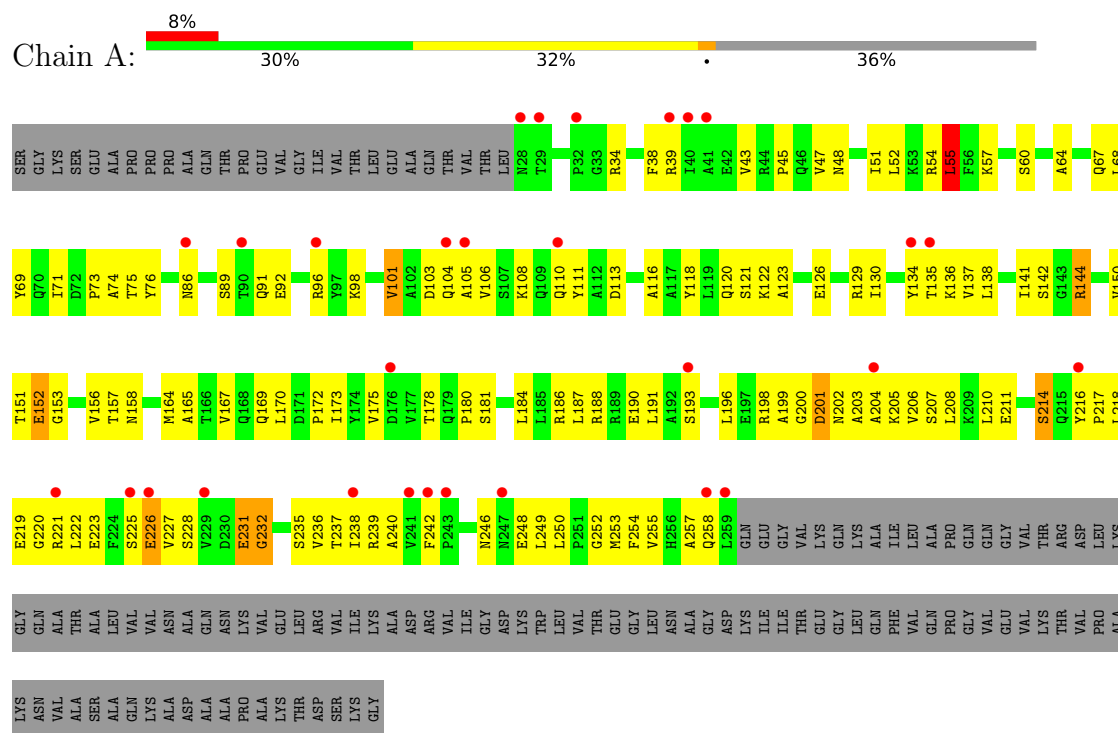
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	E	1	Total	O	S	0	0
			5	4	1		
2	F	1	Total	O	S	0	0
			5	4	1		
2	F	1	Total	O	S	0	0
			5	4	1		
2	G	1	Total	O	S	0	0
			5	4	1		
2	H	1	Total	O	S	0	0
			5	4	1		
2	I	1	Total	O	S	0	0
			5	4	1		
2	J	1	Total	O	S	0	0
			5	4	1		
2	K	1	Total	O	S	0	0
			5	4	1		
2	L	1	Total	O	S	0	0
			5	4	1		
2	M	1	Total	O	S	0	0
			5	4	1		

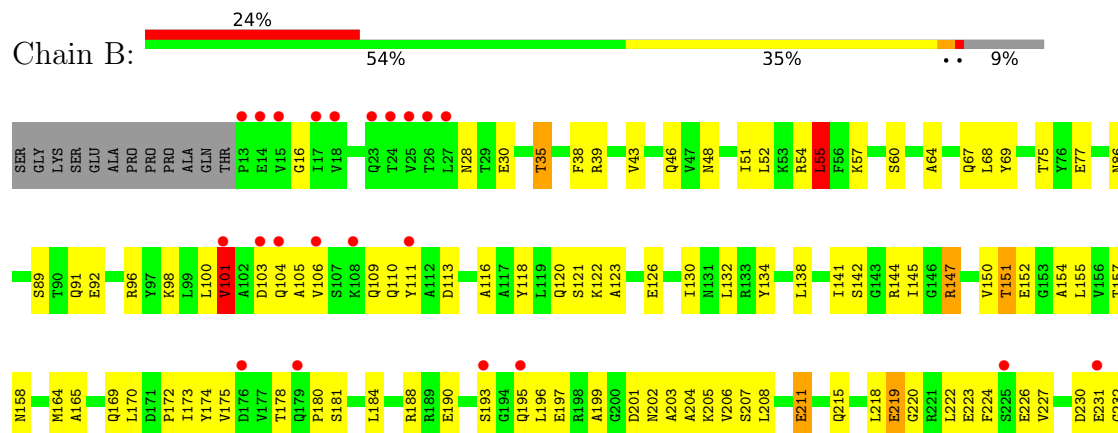
3 Residue-property plots [i](#)

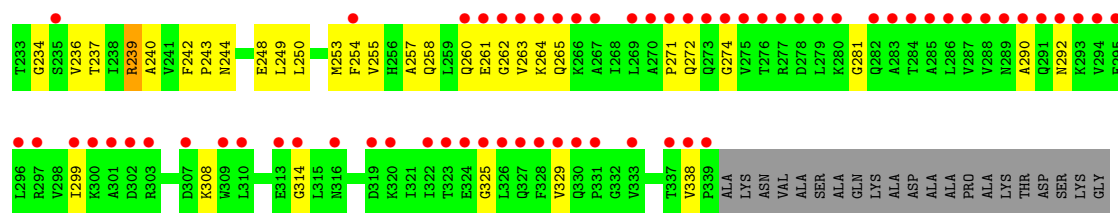
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: MULTIDRUG RESISTANCE PROTEIN MEXA

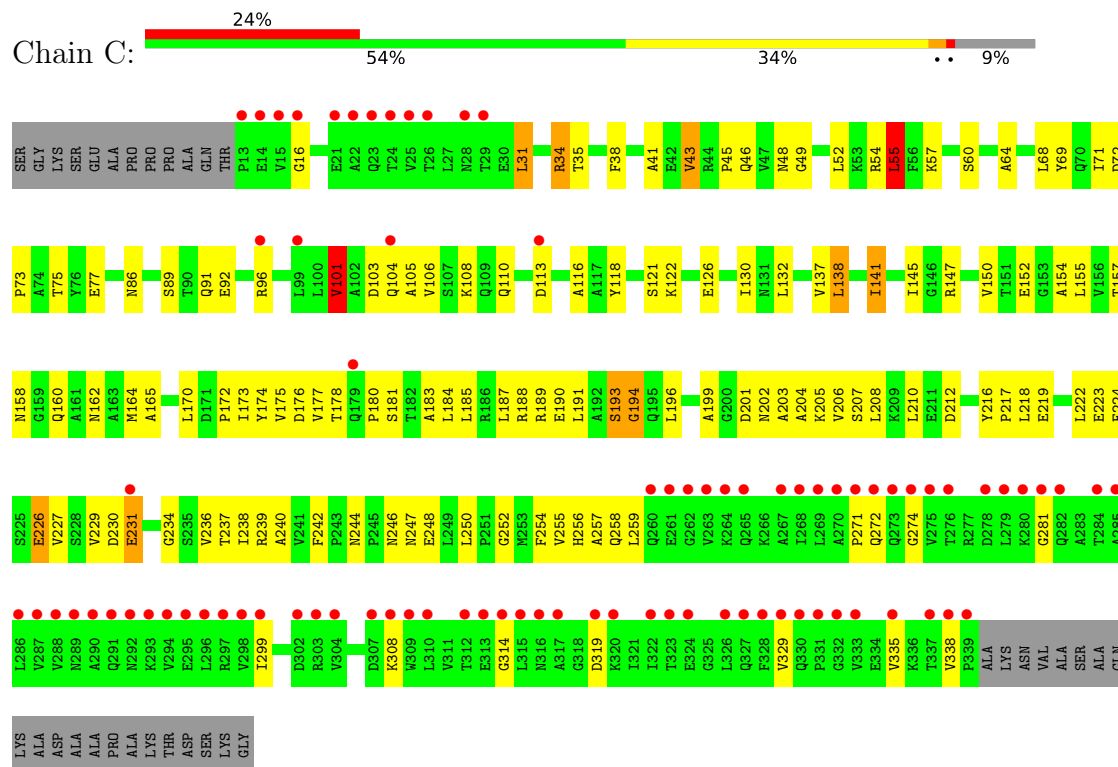


• Molecule 1: MULTIDRUG RESISTANCE PROTEIN MEXA

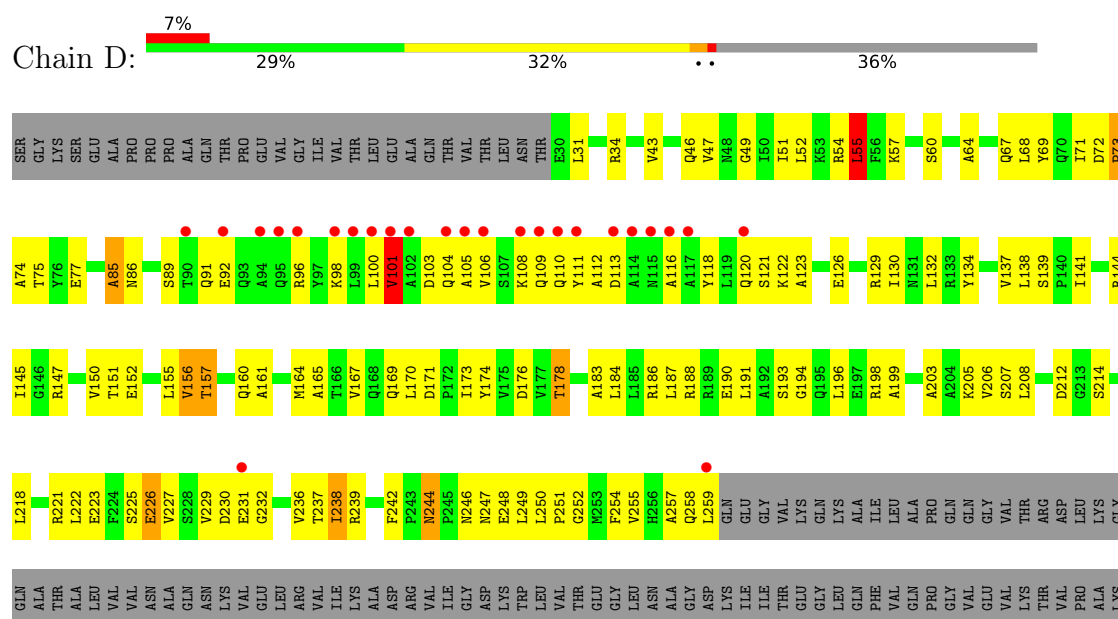


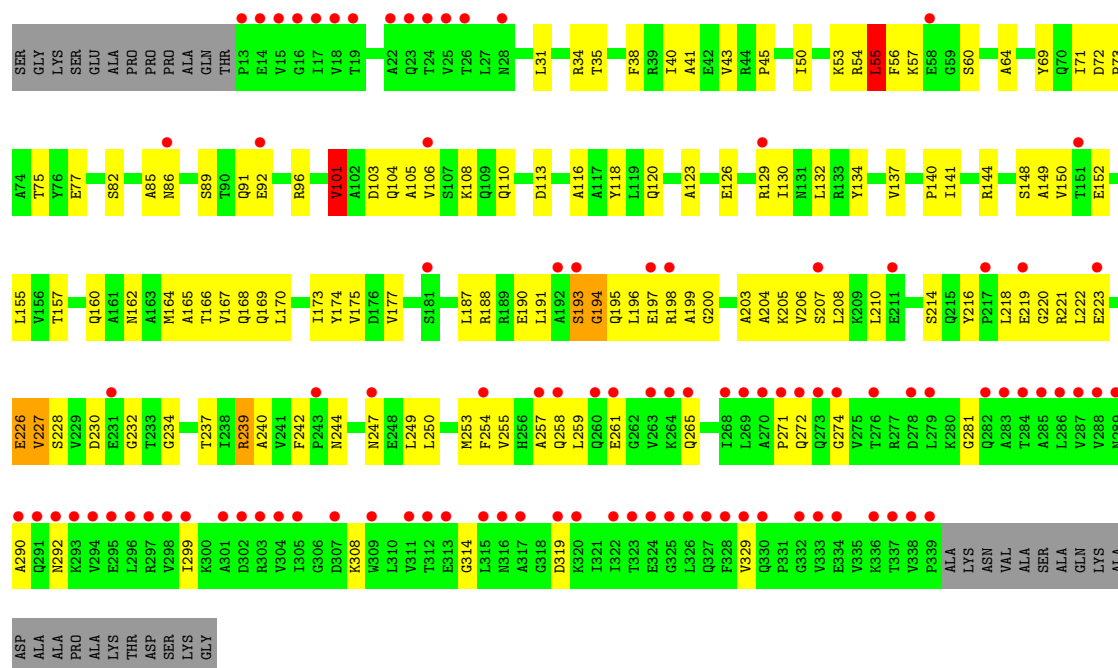


- Molecule 1: MULTIDRUG RESISTANCE PROTEIN MEXA

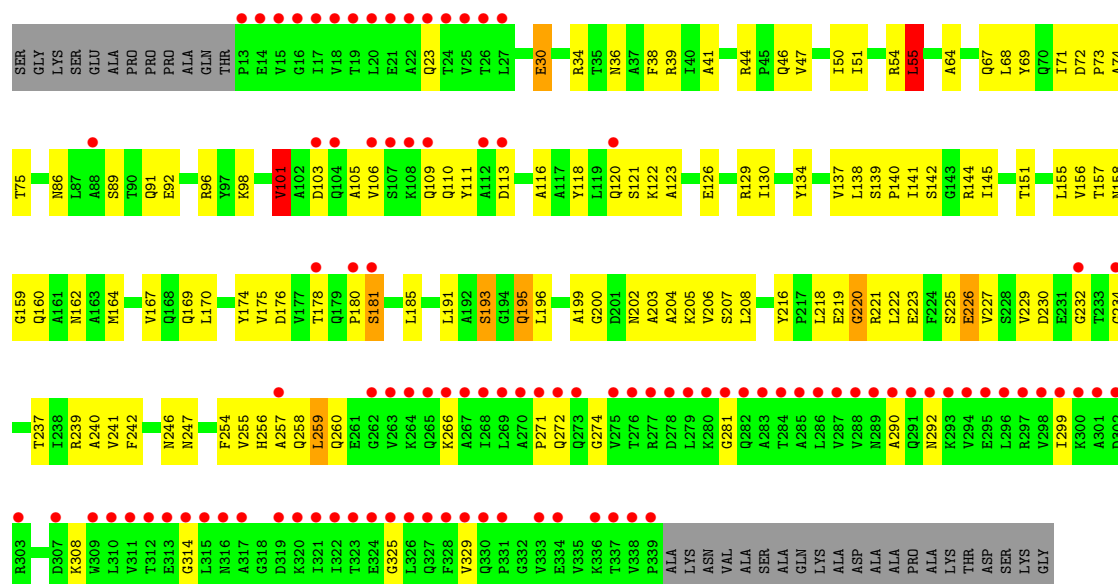


- Molecule 1: MULTIDRUG RESISTANCE PROTEIN MEXA



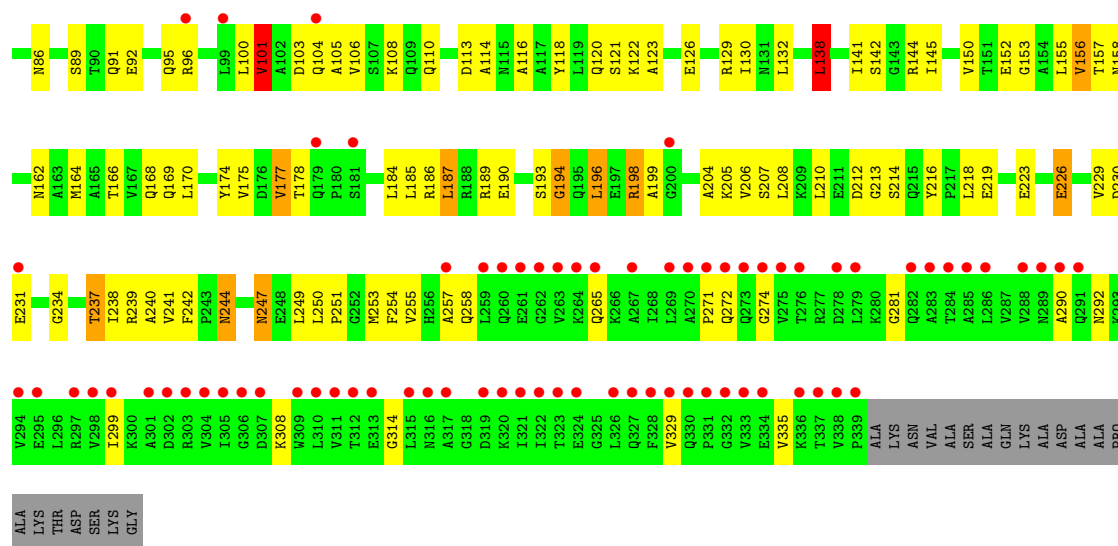


• Molecule 1: MULTIDRUG RESISTANCE PROTEIN MEXA

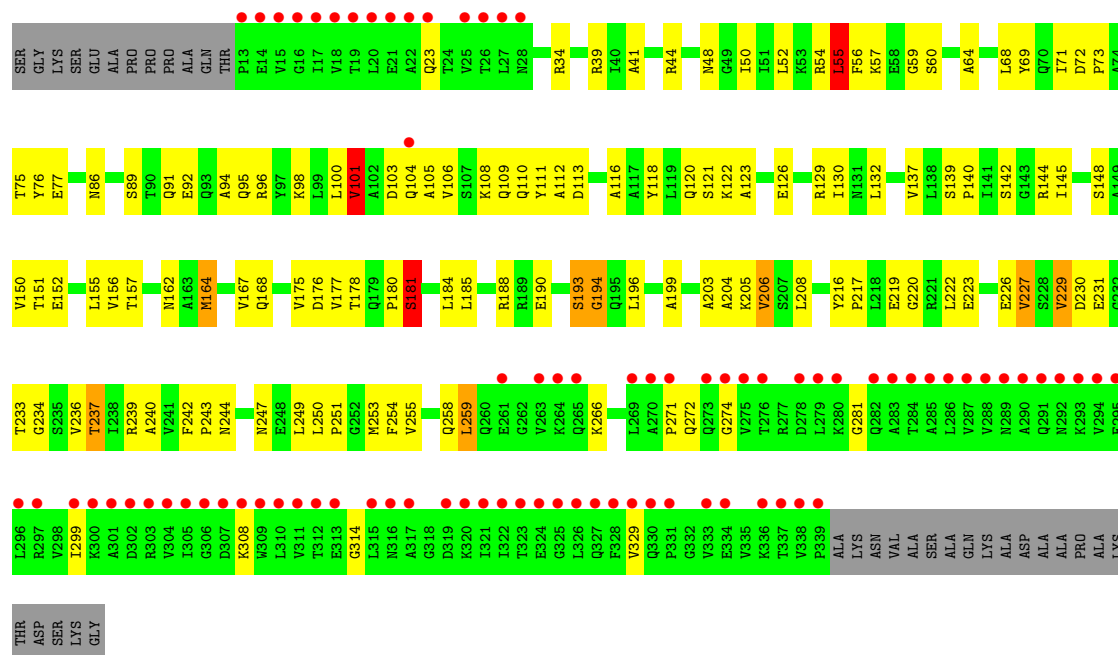


• Molecule 1: MULTIDRUG RESISTANCE PROTEIN MEXA

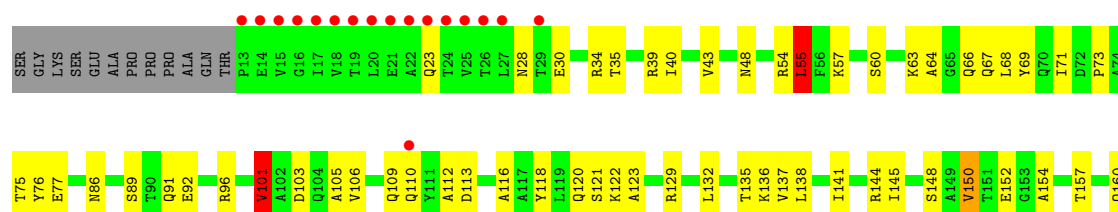




• Molecule 1: MULTIDRUG RESISTANCE PROTEIN MEXA



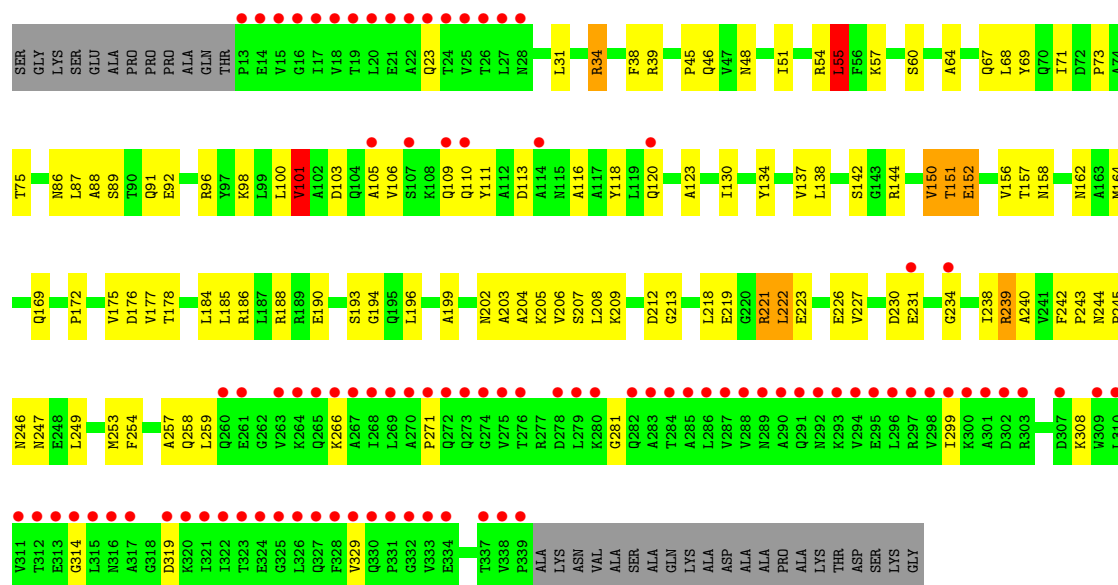
• Molecule 1: MULTIDRUG RESISTANCE PROTEIN MEXA





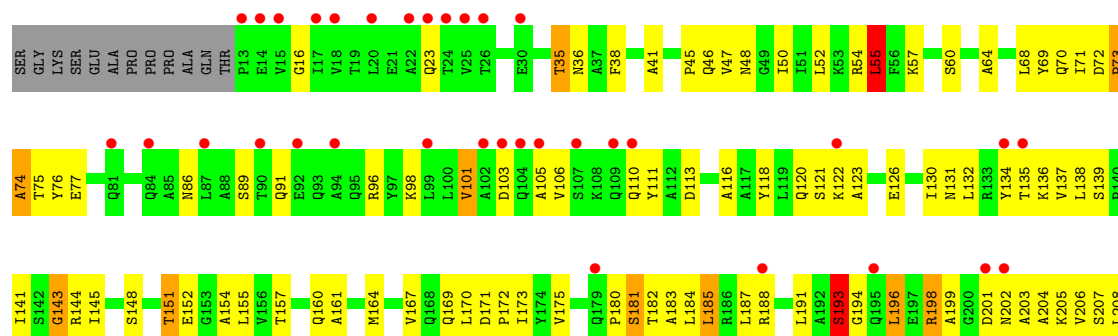
• Molecule 1: MULTIDRUG RESISTANCE PROTEIN MEXA

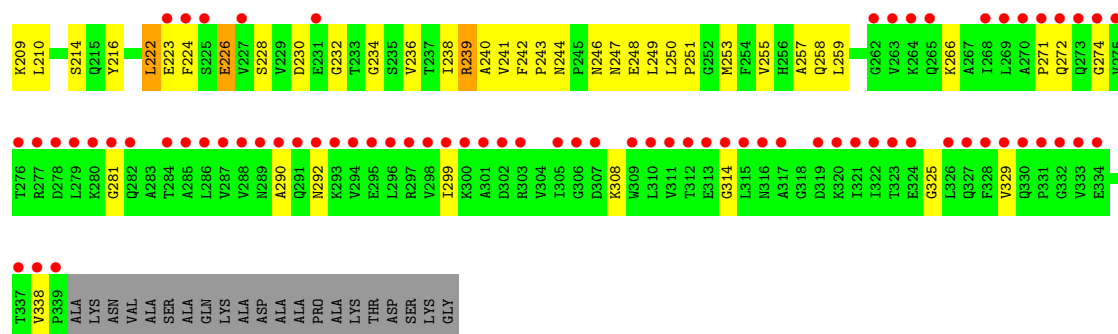
Chain L: 26% 59% 29% 9%



• Molecule 1: MULTIDRUG RESISTANCE PROTEIN MEXA

Chain M: 30% 52% 35% 9%





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	130.55Å 183.59Å 213.31Å 90.00° 107.38° 90.00°	Depositor
Resolution (Å)	65.58 – 3.20 65.58 – 3.20	Depositor EDS
% Data completeness (in resolution range)	99.0 (65.58-3.20) 99.0 (65.58-3.20)	Depositor EDS
R_{merge}	0.45	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.38 (at 3.19Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.239 , 0.264 0.231 , 0.256	Depositor DCC
R_{free} test set	7672 reflections (4.91%)	wwPDB-VP
Wilson B-factor (Å ²)	67.0	Xtriage
Anisotropy	0.022	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 73.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.005 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	28603	wwPDB-VP
Average B, all atoms (Å ²)	68.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.88% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	0.41	0/1800	0.87	4/2441 (0.2%)
1	B	0.44	0/2287	0.91	3/3118 (0.1%)
1	C	0.47	0/2278	0.91	4/3107 (0.1%)
1	D	0.52	0/1788	0.96	7/2424 (0.3%)
1	E	0.55	0/2292	0.93	6/3125 (0.2%)
1	F	0.44	0/2445	0.89	4/3325 (0.1%)
1	G	0.44	0/2278	0.88	5/3107 (0.2%)
1	H	0.56	0/2292	0.94	6/3125 (0.2%)
1	I	0.58	0/2278	0.97	10/3107 (0.3%)
1	J	0.68	1/2276 (0.0%)	0.99	6/3103 (0.2%)
1	K	0.61	0/2292	0.97	7/3125 (0.2%)
1	L	0.58	0/2278	0.95	5/3107 (0.2%)
1	M	0.47	0/2296	0.91	6/3131 (0.2%)
All	All	0.53	1/28880 (0.0%)	0.93	73/39345 (0.2%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	J	164	MET	SD-CE	-6.40	1.63	1.79

All (73) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	J	162	ASN	N-CA-C	8.26	122.50	110.28
1	D	72	ASP	CA-C-N	7.46	128.45	120.47
1	D	72	ASP	C-N-CA	7.46	128.45	120.47
1	E	72	ASP	CA-C-N	7.27	128.25	120.47
1	E	72	ASP	C-N-CA	7.27	128.25	120.47
1	B	55	LEU	N-CA-C	7.18	121.83	110.70
1	I	166	THR	N-CA-C	6.48	119.00	107.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	K	101	VAL	N-CA-C	-6.38	104.28	110.72
1	D	101	VAL	N-CA-C	-6.37	104.28	110.72
1	M	139	SER	CA-C-N	6.32	125.54	118.97
1	M	139	SER	C-N-CA	6.32	125.54	118.97
1	B	101	VAL	N-CA-C	-6.12	104.54	110.72
1	I	101	VAL	N-CA-C	-6.03	104.63	110.72
1	F	72	ASP	CA-C-N	6.03	126.98	120.83
1	F	72	ASP	C-N-CA	6.03	126.98	120.83
1	L	55	LEU	N-CA-C	6.01	123.60	110.80
1	I	244	ASN	CA-C-N	5.98	125.60	119.56
1	I	244	ASN	C-N-CA	5.98	125.60	119.56
1	E	101	VAL	N-CA-C	-5.97	104.69	110.72
1	J	101	VAL	N-CA-C	-5.96	104.71	110.72
1	A	135	THR	N-CA-C	-5.92	106.14	113.19
1	C	101	VAL	N-CA-C	-5.90	104.76	110.72
1	L	101	VAL	N-CA-C	-5.89	104.77	110.72
1	I	55	LEU	N-CA-C	5.85	123.26	110.80
1	A	74	ALA	N-CA-C	5.84	117.34	110.97
1	M	239	ARG	N-CA-C	5.83	118.91	109.40
1	L	150	VAL	N-CA-C	-5.78	103.75	110.05
1	D	55	LEU	N-CA-C	5.67	122.89	110.80
1	G	101	VAL	N-CA-C	-5.65	105.02	110.72
1	K	244	ASN	CA-C-N	5.64	125.73	119.87
1	K	244	ASN	C-N-CA	5.64	125.73	119.87
1	G	72	ASP	CA-C-N	5.61	127.67	120.89
1	G	72	ASP	C-N-CA	5.61	127.67	120.89
1	J	72	ASP	CA-C-N	5.59	127.66	120.89
1	J	72	ASP	C-N-CA	5.59	127.66	120.89
1	H	55	LEU	N-CA-C	5.57	122.66	110.80
1	K	55	LEU	N-CA-C	5.56	122.65	110.80
1	G	55	LEU	N-CA-C	5.53	122.59	110.80
1	F	101	VAL	N-CA-C	-5.51	105.16	110.72
1	E	152	GLU	N-CA-C	-5.50	103.23	110.43
1	H	101	VAL	N-CA-C	-5.47	105.19	110.72
1	F	55	LEU	N-CA-C	5.46	122.44	110.80
1	M	74	ALA	N-CA-C	5.42	117.61	111.11
1	H	162	ASN	N-CA-C	5.39	118.72	110.20
1	A	55	LEU	N-CA-C	5.38	122.26	110.80
1	I	162	ASN	N-CA-C	5.38	118.08	110.50
1	H	72	ASP	CA-C-N	5.34	127.20	121.00
1	H	72	ASP	C-N-CA	5.34	127.20	121.00
1	B	239	ARG	N-CA-C	5.34	118.10	109.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	142	SER	N-CA-C	-5.31	101.05	109.76
1	I	239	ARG	N-CA-C	5.30	118.05	109.40
1	K	162	ASN	N-CA-C	5.30	118.58	110.20
1	C	55	LEU	N-CA-C	5.29	122.07	110.80
1	J	55	LEU	N-CA-C	5.27	122.02	110.80
1	D	244	ASN	CA-C-N	5.25	125.33	119.87
1	D	244	ASN	C-N-CA	5.25	125.33	119.87
1	M	73	PRO	N-CA-C	5.20	122.18	114.80
1	E	239	ARG	N-CA-C	5.20	117.87	109.40
1	I	72	ASP	CA-C-N	5.19	127.17	120.89
1	I	72	ASP	C-N-CA	5.19	127.17	120.89
1	K	220	GLY	N-CA-C	5.19	118.68	111.10
1	L	162	ASN	N-CA-C	5.15	117.90	110.28
1	D	85	ALA	N-CA-C	-5.14	105.57	111.07
1	L	239	ARG	N-CA-C	5.09	117.70	109.40
1	I	138	LEU	N-CA-C	5.08	118.05	110.52
1	J	168	GLN	N-CA-C	5.08	115.84	107.20
1	M	55	LEU	N-CA-C	5.05	121.57	110.80
1	C	72	ASP	CA-C-N	5.05	127.00	120.89
1	C	72	ASP	C-N-CA	5.05	127.00	120.89
1	G	239	ARG	N-CA-C	5.04	117.61	109.40
1	K	239	ARG	N-CA-C	5.02	117.59	109.40
1	E	55	LEU	N-CA-C	5.01	121.48	110.80
1	H	220	GLY	N-CA-C	5.01	118.41	111.10

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1776	0	1777	114	0
1	B	2259	0	2040	110	0
1	C	2250	0	2021	113	0
1	D	1764	0	1768	110	0
1	E	2264	0	2044	112	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	F	2415	0	2358	104	0
1	G	2250	0	2021	113	0
1	H	2264	0	2044	116	0
1	I	2250	0	2021	125	0
1	J	2249	0	2014	88	0
1	K	2264	0	2044	102	0
1	L	2250	0	2021	87	0
1	M	2268	0	2056	116	0
2	A	10	0	0	0	0
2	B	10	0	0	1	0
2	C	5	0	0	0	0
2	E	10	0	0	0	0
2	F	10	0	0	0	0
2	G	5	0	0	0	0
2	H	5	0	0	0	0
2	I	5	0	0	0	0
2	J	5	0	0	0	0
2	K	5	0	0	0	0
2	L	5	0	0	0	0
2	M	5	0	0	0	0
All	All	28603	0	26229	1302	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 24.

All (1302) 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:C:104:GLN:HG3	1:I:108:LYS:HE3	1.36	1.05
1:C:108:LYS:HE3	1:I:104:GLN:HG3	1.32	1.05
1:A:104:GLN:HG3	1:G:108:LYS:HE3	1.38	1.04
1:I:198:ARG:HH11	1:I:198:ARG:HB2	1.22	1.03
1:D:96:ARG:NH2	1:E:109:GLN:OE1	1.91	1.03
1:D:156:VAL:HG11	1:D:164:MET:HE3	1.38	1.03
1:G:190:GLU:HB3	1:G:196:LEU:HD13	1.43	1.01
1:J:44:ARG:CZ	1:J:44:ARG:CD	2.41	0.99
1:C:174:TYR:HD1	1:C:239:ARG:HD2	1.27	0.98
1:C:34:ARG:HB3	1:C:34:ARG:HH11	1.29	0.97
1:A:108:LYS:HE3	1:G:104:GLN:HG3	1.47	0.96
1:F:34:ARG:HE	1:F:254:PHE:HE1	0.99	0.96
1:B:253:MET:HE3	1:C:181:SER:HB3	1.44	0.96

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:96:ARG:NH2	1:B:109:GLN:OE1	1.98	0.96
1:L:226:GLU:OE2	1:M:144:ARG:HD3	1.69	0.93
1:H:156:VAL:HG11	1:H:164:MET:HE3	1.50	0.93
1:I:178:THR:HG22	1:I:237:THR:OG1	1.68	0.93
1:I:156:VAL:HG11	1:I:164:MET:HE3	1.49	0.93
1:L:221:ARG:HB2	1:L:221:ARG:HH11	1.34	0.92
1:B:147:ARG:HH12	1:C:239:ARG:HH21	1.16	0.92
1:L:130:ILE:HD13	1:M:74:ALA:HB1	1.53	0.91
1:H:109:GLN:OE1	1:I:96:ARG:HD3	1.71	0.91
1:H:208:LEU:HB2	1:H:242:PHE:CE2	2.06	0.90
1:L:222:LEU:HD11	1:L:238:ILE:HD12	1.54	0.89
1:I:177:VAL:HG23	1:I:238:ILE:HG13	1.55	0.89
1:H:109:GLN:OE1	1:I:96:ARG:NH1	2.05	0.89
1:A:190:GLU:HB3	1:A:196:LEU:HD13	1.53	0.89
1:C:138:LEU:HD12	1:C:138:LEU:H	1.39	0.88
1:C:96:ARG:NH2	1:D:109:GLN:OE1	2.06	0.88
1:L:39:ARG:HH12	1:M:54:ARG:NH2	1.70	0.87
1:H:39:ARG:HH12	1:I:54:ARG:NH2	1.72	0.87
1:H:200:GLY:HA3	1:H:221:ARG:HH12	1.41	0.86
1:L:221:ARG:HB2	1:L:221:ARG:NH1	1.91	0.85
1:M:48:ASN:O	1:M:76:TYR:OH	1.93	0.85
1:C:190:GLU:HB3	1:C:196:LEU:HD13	1.56	0.85
1:D:156:VAL:HG11	1:D:164:MET:CE	2.08	0.84
1:L:109:GLN:OE1	1:M:96:ARG:CZ	2.26	0.84
1:E:206:VAL:HG21	1:E:222:LEU:HB2	1.60	0.84
1:D:190:GLU:HB3	1:D:196:LEU:HD13	1.59	0.82
1:B:211:GLU:HG2	1:B:254:PHE:O	1.80	0.82
1:K:244:ASN:ND2	1:K:249:LEU:HB2	1.95	0.82
1:M:55:LEU:HD12	1:M:55:LEU:H	1.44	0.82
1:F:31:LEU:HB3	1:F:177:VAL:HG11	1.61	0.82
1:H:109:GLN:OE1	1:I:96:ARG:CZ	2.28	0.81
1:C:108:LYS:CE	1:I:104:GLN:HG3	2.10	0.81
1:I:198:ARG:HB2	1:I:198:ARG:NH1	1.95	0.81
1:F:286:LEU:HD11	1:F:331:PRO:HG3	1.63	0.81
1:M:35:THR:C	1:M:36:ASN:HD22	1.89	0.81
1:K:137:VAL:HG21	1:K:164:MET:HE1	1.62	0.81
1:A:249:LEU:HA	1:A:253:MET:SD	2.20	0.81
1:G:190:GLU:HB3	1:G:196:LEU:CD1	2.10	0.80
1:A:175:VAL:HB	1:A:240:ALA:HB3	1.64	0.80
1:M:210:LEU:HD12	1:M:214:SER:HB2	1.63	0.80
1:H:55:LEU:HD12	1:H:55:LEU:H	1.47	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:55:LEU:HD12	1:E:55:LEU:H	1.47	0.79
1:E:144:ARG:HH11	1:F:226:GLU:HG3	1.44	0.79
1:F:34:ARG:NE	1:F:254:PHE:HE1	1.79	0.79
1:L:109:GLN:OE1	1:M:96:ARG:NH1	2.15	0.79
1:H:178:THR:HG22	1:H:237:THR:OG1	1.81	0.78
1:C:55:LEU:HD12	1:C:55:LEU:H	1.48	0.78
1:J:55:LEU:HD12	1:J:55:LEU:H	1.45	0.78
1:E:193:SER:OG	1:E:195:GLN:HG3	1.83	0.78
1:D:96:ARG:HH21	1:E:109:GLN:CD	1.92	0.77
1:H:226:GLU:OE2	1:I:144:ARG:HD3	1.83	0.77
1:F:265:GLN:CD	1:F:265:GLN:H	1.93	0.77
1:H:109:GLN:CD	1:I:96:ARG:CZ	2.58	0.77
1:L:221:ARG:HH11	1:L:221:ARG:CB	1.96	0.77
1:B:215:GLN:HE22	1:B:258:GLN:HE22	1.33	0.77
1:B:55:LEU:HD12	1:B:55:LEU:H	1.49	0.77
1:A:144:ARG:HD3	1:B:226:GLU:OE2	1.86	0.76
1:G:31:LEU:HB3	1:G:177:VAL:HG11	1.66	0.76
1:F:178:THR:HG22	1:F:237:THR:OG1	1.86	0.76
1:G:216:TYR:HE2	1:G:218:LEU:HB2	1.50	0.76
1:I:226:GLU:OE2	1:J:144:ARG:HD3	1.86	0.75
1:M:134:TYR:C	1:M:136:LYS:H	1.92	0.75
1:F:55:LEU:HD12	1:F:55:LEU:H	1.51	0.75
1:C:104:GLN:HG3	1:I:108:LYS:CE	2.15	0.75
1:B:208:LEU:HB2	1:B:242:PHE:CE1	2.20	0.75
1:B:227:VAL:HG22	1:B:237:THR:O	1.87	0.75
1:G:40:ILE:HG12	1:G:168:GLN:HG2	1.68	0.75
1:E:144:ARG:HD3	1:F:226:GLU:OE2	1.87	0.75
1:B:67:GLN:HA	1:B:138:LEU:HD23	1.69	0.75
1:E:302:ASP:HA	1:F:278:ASP:OD2	1.87	0.74
1:L:55:LEU:HD12	1:L:55:LEU:H	1.52	0.74
1:H:157:THR:O	1:H:160:GLN:HG2	1.87	0.74
1:I:216:TYR:HE2	1:I:218:LEU:HB2	1.53	0.74
1:A:43:VAL:HG23	1:A:165:ALA:O	1.86	0.74
1:C:174:TYR:CD1	1:C:239:ARG:HD2	2.18	0.74
1:J:139:SER:OG	1:J:167:VAL:HG21	1.87	0.74
1:A:199:ALA:H	1:A:204:ALA:HA	1.52	0.74
1:G:216:TYR:CE2	1:G:218:LEU:HB2	2.23	0.74
1:H:109:GLN:OE1	1:I:96:ARG:CD	2.35	0.74
1:K:199:ALA:HB2	1:K:205:LYS:N	2.03	0.73
1:H:169:GLN:C	1:H:170:LEU:HD23	2.13	0.73
1:A:184:LEU:HD13	1:A:238:ILE:HD11	1.69	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:211:GLU:OE2	1:A:254:PHE:HB2	1.89	0.73
1:F:85:ALA:HB2	1:G:82:SER:HB2	1.69	0.73
1:M:199:ALA:HB2	1:M:205:LYS:N	2.03	0.73
1:C:35:THR:HB	1:C:173:ILE:HD11	1.72	0.72
1:A:55:LEU:HD12	1:A:55:LEU:H	1.52	0.72
1:D:199:ALA:HB2	1:D:205:LYS:N	2.04	0.72
1:M:244:ASN:ND2	1:M:249:LEU:HB2	2.03	0.72
1:C:104:GLN:CG	1:I:108:LYS:HE3	2.18	0.72
1:I:244:ASN:OD1	1:I:249:LEU:HB2	1.89	0.72
1:J:208:LEU:HD11	1:J:255:VAL:HG21	1.71	0.72
1:A:104:GLN:HG3	1:G:108:LYS:CE	2.19	0.72
1:F:294:VAL:HG23	1:F:331:PRO:HA	1.72	0.71
1:J:178:THR:HG22	1:J:237:THR:OG1	1.90	0.71
1:G:197:GLU:HB3	1:G:205:LYS:HD3	1.71	0.71
1:B:199:ALA:HB2	1:B:205:LYS:N	2.05	0.71
1:G:157:THR:O	1:G:160:GLN:HB2	1.91	0.71
1:A:210:LEU:HD12	1:A:214:SER:HB2	1.72	0.71
1:H:199:ALA:HB2	1:H:205:LYS:N	2.05	0.71
1:G:43:VAL:HG23	1:G:165:ALA:O	1.90	0.71
1:C:31:LEU:HB3	1:C:177:VAL:HG11	1.72	0.71
1:E:199:ALA:HB2	1:E:205:LYS:N	2.04	0.71
1:I:178:THR:HG22	1:I:237:THR:HG1	1.56	0.70
1:K:35:THR:HB	1:K:173:ILE:HD11	1.72	0.70
1:M:209:LYS:HD2	1:M:258:GLN:NE2	2.07	0.70
1:M:250:LEU:O	1:M:253:MET:HG3	1.91	0.70
1:G:148:SER:O	1:G:150:VAL:N	2.25	0.69
1:I:55:LEU:H	1:I:55:LEU:HD12	1.55	0.69
1:I:206:VAL:HG13	1:I:258:GLN:O	1.93	0.69
1:A:206:VAL:HG11	1:A:257:ALA:HB1	1.73	0.69
1:B:28:ASN:OD1	1:B:260:GLN:HG2	1.93	0.69
1:B:215:GLN:HE22	1:B:258:GLN:NE2	1.89	0.69
1:D:104:GLN:HG3	1:J:108:LYS:HE3	1.75	0.69
1:D:208:LEU:HD11	1:D:255:VAL:HG21	1.73	0.69
1:K:250:LEU:O	1:K:253:MET:HG3	1.93	0.69
1:L:206:VAL:O	1:L:219:GLU:HG3	1.93	0.69
1:C:38:PHE:CD1	1:C:174:TYR:HE2	2.11	0.69
1:I:30:GLU:OE2	1:I:258:GLN:HG2	1.94	0.69
1:I:51:ILE:HD11	1:I:164:MET:HE1	1.74	0.69
1:J:206:VAL:HG21	1:J:222:LEU:HB2	1.74	0.68
1:B:144:ARG:HH21	1:C:226:GLU:HG3	1.59	0.68
1:B:184:LEU:O	1:B:188:ARG:HG3	1.94	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:221:ARG:HD3	1:E:223:GLU:OE2	1.94	0.68
1:A:186:ARG:HH11	1:A:187:LEU:HD23	1.58	0.68
1:K:271:PRO:HA	1:K:308:LYS:HA	1.76	0.68
1:E:96:ARG:NH2	1:F:109:GLN:OE1	2.23	0.68
1:I:51:ILE:HD11	1:I:164:MET:CE	2.23	0.67
1:I:216:TYR:CE2	1:I:218:LEU:HB2	2.30	0.67
1:E:45:PRO:CD	1:E:164:MET:HE2	2.24	0.67
1:E:43:VAL:HG23	1:E:165:ALA:O	1.95	0.67
1:F:216:TYR:HE2	1:F:218:LEU:HB2	1.60	0.67
1:G:55:LEU:HD12	1:G:55:LEU:H	1.60	0.67
1:H:46:GLN:HB2	1:H:134:TYR:CD1	2.30	0.67
1:D:246:ASN:HB2	1:D:248:GLU:HG3	1.75	0.67
1:G:191:LEU:HG	1:G:198:ARG:NH2	2.10	0.67
1:F:82:SER:HA	1:G:82:SER:OG	1.94	0.67
1:E:218:LEU:N	1:E:218:LEU:HD23	2.09	0.66
1:F:272:GLN:HB2	1:F:309:TRP:NE1	2.11	0.66
1:B:150:VAL:HG21	1:B:164:MET:HG2	1.77	0.66
1:L:222:LEU:HD12	1:L:222:LEU:C	2.18	0.66
1:C:46:GLN:HA	1:C:158:ASN:OD1	1.95	0.66
1:H:271:PRO:HA	1:H:308:LYS:HA	1.77	0.66
1:M:271:PRO:HA	1:M:308:LYS:HA	1.77	0.66
1:A:199:ALA:HB2	1:A:205:LYS:N	2.11	0.66
1:C:229:VAL:HG12	1:C:236:VAL:HG22	1.78	0.66
1:D:55:LEU:H	1:D:55:LEU:HD12	1.60	0.66
1:D:207:SER:OG	1:D:258:GLN:HB2	1.94	0.66
1:H:203:ALA:HB2	1:H:223:GLU:HA	1.77	0.66
1:J:208:LEU:HD11	1:J:255:VAL:CG2	2.25	0.66
1:D:206:VAL:HG12	1:D:259:LEU:HD13	1.76	0.66
1:K:67:GLN:OE1	1:K:136:LYS:HD3	1.96	0.66
1:A:175:VAL:HG21	1:A:242:PHE:HD2	1.61	0.66
1:C:34:ARG:HB3	1:C:34:ARG:NH1	2.06	0.66
1:F:303:ARG:HD2	1:F:310:LEU:HD23	1.78	0.66
1:E:144:ARG:NH1	1:F:226:GLU:HG3	2.09	0.65
1:K:222:LEU:C	1:K:222:LEU:HD12	2.21	0.65
1:C:208:LEU:HB2	1:C:242:PHE:CZ	2.31	0.65
1:D:208:LEU:HD11	1:D:255:VAL:CG2	2.27	0.65
1:J:184:LEU:O	1:J:188:ARG:HG3	1.95	0.65
1:L:31:LEU:HB3	1:L:177:VAL:HG11	1.77	0.65
1:B:43:VAL:HG23	1:B:165:ALA:O	1.97	0.65
1:B:271:PRO:HA	1:B:308:LYS:HA	1.77	0.65
1:K:55:LEU:HD12	1:K:55:LEU:H	1.62	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:215:GLN:NE2	1:B:258:GLN:HE22	1.95	0.65
1:J:226:GLU:OE1	1:J:229:VAL:HG22	1.96	0.65
1:M:134:TYR:C	1:M:136:LYS:N	2.52	0.65
1:I:212:ASP:OD1	1:I:214:SER:N	2.23	0.64
1:L:186:ARG:HG2	1:L:190:GLU:OE2	1.97	0.64
1:A:207:SER:OG	1:A:258:GLN:HB2	1.96	0.64
1:B:175:VAL:HB	1:B:240:ALA:HB3	1.79	0.64
1:J:55:LEU:HD12	1:J:55:LEU:N	2.13	0.64
1:B:195:GLN:HG3	1:B:262:GLY:O	1.98	0.64
1:E:45:PRO:HD3	1:E:164:MET:HE2	1.78	0.64
1:I:150:VAL:HG11	1:I:164:MET:HE2	1.78	0.64
1:C:34:ARG:HH12	1:C:252:GLY:HA2	1.63	0.63
1:E:271:PRO:HA	1:E:308:LYS:HA	1.80	0.63
1:L:199:ALA:HB2	1:L:205:LYS:N	2.12	0.63
1:G:50:ILE:HD13	1:G:155:LEU:HA	1.78	0.63
1:A:249:LEU:HD23	1:A:253:MET:SD	2.37	0.63
1:B:147:ARG:NH1	1:C:239:ARG:HH21	1.90	0.63
1:A:181:SER:O	1:A:184:LEU:HB3	1.98	0.63
1:L:67:GLN:HA	1:L:138:LEU:HD23	1.80	0.63
1:B:54:ARG:HG3	1:B:69:TYR:CE1	2.33	0.63
1:M:175:VAL:HB	1:M:240:ALA:HB3	1.81	0.63
1:C:178:THR:HG22	1:C:237:THR:OG1	1.99	0.63
1:J:199:ALA:HB2	1:J:205:LYS:N	2.13	0.63
1:M:55:LEU:HD12	1:M:55:LEU:N	2.14	0.63
1:L:137:VAL:HG21	1:L:164:MET:HE1	1.80	0.63
1:E:227:VAL:HG12	1:E:237:THR:HG22	1.80	0.62
1:A:108:LYS:CE	1:G:104:GLN:HG3	2.26	0.62
1:D:184:LEU:O	1:D:188:ARG:HG3	1.99	0.62
1:F:271:PRO:HG3	1:F:308:LYS:HE2	1.81	0.62
1:L:34:ARG:HE	1:L:254:PHE:HE1	1.47	0.62
1:B:203:ALA:HB2	1:B:223:GLU:HA	1.81	0.62
1:D:170:LEU:N	1:D:170:LEU:HD22	2.15	0.62
1:E:157:THR:O	1:E:160:GLN:HB2	2.00	0.62
1:M:222:LEU:HD11	1:M:238:ILE:HD12	1.79	0.62
1:F:54:ARG:HG3	1:F:69:TYR:CE1	2.34	0.62
1:G:148:SER:C	1:G:150:VAL:H	2.07	0.62
1:I:190:GLU:HB3	1:I:196:LEU:HD13	1.82	0.62
1:I:206:VAL:O	1:I:219:GLU:HG3	1.98	0.62
1:K:203:ALA:HB2	1:K:223:GLU:HA	1.80	0.62
1:A:134:TYR:C	1:A:136:LYS:H	2.08	0.62
1:H:208:LEU:HD11	1:H:255:VAL:CG2	2.30	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:206:VAL:O	1:G:219:GLU:HG3	1.99	0.62
1:H:208:LEU:HD11	1:H:255:VAL:HG21	1.81	0.62
1:M:151:THR:HG23	1:M:154:ALA:HB2	1.81	0.62
1:C:55:LEU:HD12	1:C:55:LEU:N	2.15	0.61
1:C:206:VAL:HG13	1:C:258:GLN:O	2.00	0.61
1:D:221:ARG:HD3	1:D:223:GLU:OE1	2.00	0.61
1:C:54:ARG:HG3	1:C:69:TYR:CE1	2.35	0.61
1:C:96:ARG:HH21	1:D:109:GLN:CD	2.06	0.61
1:F:299:ILE:HA	1:F:314:GLY:HA3	1.82	0.61
1:L:299:ILE:HA	1:L:314:GLY:HA3	1.82	0.61
1:M:54:ARG:HG3	1:M:69:TYR:CE1	2.36	0.61
1:A:34:ARG:HD2	1:A:252:GLY:O	2.00	0.61
1:A:108:LYS:HE3	1:G:104:GLN:CG	2.25	0.61
1:C:206:VAL:O	1:C:219:GLU:HG3	2.00	0.61
1:D:203:ALA:HB2	1:D:223:GLU:HA	1.82	0.61
1:F:265:GLN:CD	1:F:265:GLN:N	2.59	0.61
1:F:206:VAL:O	1:F:219:GLU:HG3	2.00	0.61
1:E:260:GLN:HA	1:E:260:GLN:OE1	2.00	0.61
1:I:299:ILE:HA	1:I:314:GLY:HA3	1.83	0.61
1:L:206:VAL:HG13	1:L:258:GLN:O	2.00	0.61
1:M:203:ALA:HB2	1:M:223:GLU:HA	1.81	0.61
1:K:195:GLN:O	1:K:262:GLY:N	2.22	0.60
1:B:196:LEU:HD21	1:B:261:GLU:HG2	1.84	0.60
1:C:45:PRO:HD3	1:C:164:MET:SD	2.42	0.60
1:M:141:ILE:HD11	1:M:167:VAL:O	2.00	0.60
1:C:271:PRO:HA	1:C:308:LYS:HA	1.84	0.60
1:I:68:LEU:HD13	1:I:145:ILE:CD1	2.31	0.60
1:F:212:ASP:OD1	1:F:214:SER:N	2.29	0.60
1:G:244:ASN:OD1	1:G:249:LEU:HB2	2.01	0.60
1:H:51:ILE:HD11	1:H:164:MET:HE1	1.83	0.60
1:I:210:LEU:HD22	1:I:253:MET:HE1	1.83	0.60
1:C:299:ILE:HA	1:C:314:GLY:HA3	1.82	0.60
1:I:34:ARG:HE	1:I:254:PHE:HE1	1.49	0.60
1:D:186:ARG:HG2	1:D:190:GLU:OE2	2.00	0.60
1:A:208:LEU:HD11	1:A:255:VAL:HG21	1.82	0.60
1:F:55:LEU:HD12	1:F:55:LEU:N	2.16	0.60
1:F:199:ALA:HB2	1:F:205:LYS:N	2.17	0.60
1:G:250:LEU:O	1:G:253:MET:HG3	2.02	0.60
1:J:299:ILE:HA	1:J:314:GLY:HA3	1.83	0.60
1:H:185:LEU:HD21	1:I:210:LEU:HD13	1.84	0.60
1:F:78:ALA:HA	1:G:85:ALA:HB1	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:216:TYR:CE2	1:F:218:LEU:HB2	2.37	0.59
1:L:208:LEU:HB2	1:L:242:PHE:CZ	2.37	0.59
1:A:144:ARG:HH11	1:B:226:GLU:HG3	1.67	0.59
1:D:101:VAL:HG13	1:D:106:VAL:HG13	1.84	0.59
1:D:229:VAL:HG12	1:D:236:VAL:HG22	1.84	0.59
1:A:188:ARG:O	1:A:191:LEU:HB3	2.02	0.59
1:G:271:PRO:HA	1:G:308:LYS:HA	1.82	0.59
1:A:39:ARG:O	1:A:169:GLN:N	2.35	0.59
1:G:299:ILE:HA	1:G:314:GLY:HA3	1.82	0.59
1:C:170:LEU:HD12	1:C:247:ASN:HD21	1.68	0.59
1:E:203:ALA:HB2	1:E:223:GLU:HA	1.84	0.59
1:H:220:GLY:HA3	1:H:242:PHE:CD1	2.37	0.59
1:I:64:ALA:HB2	1:I:141:ILE:C	2.28	0.59
1:M:64:ALA:HA	1:M:141:ILE:O	2.02	0.59
1:F:31:LEU:HB3	1:F:177:VAL:CG1	2.31	0.59
1:M:193:SER:OG	1:M:194:GLY:N	2.34	0.59
1:J:206:VAL:HG12	1:J:258:GLN:O	2.02	0.59
1:A:47:VAL:HB	1:A:76:TYR:OH	2.03	0.59
1:A:206:VAL:HG12	1:A:207:SER:N	2.18	0.59
1:C:43:VAL:HG21	1:C:165:ALA:HB3	1.85	0.59
1:D:208:LEU:HB2	1:D:242:PHE:CE2	2.38	0.59
1:H:101:VAL:HG13	1:H:106:VAL:HG13	1.85	0.59
1:M:101:VAL:HG13	1:M:106:VAL:HG13	1.84	0.59
1:A:96:ARG:CZ	1:B:109:GLN:OE1	2.50	0.59
1:C:71:ILE:O	1:C:73:PRO:HD3	2.03	0.59
1:L:271:PRO:HA	1:L:308:LYS:HA	1.84	0.59
1:C:199:ALA:HB2	1:C:205:LYS:N	2.18	0.58
1:F:35:THR:HB	1:F:173:ILE:HD11	1.85	0.58
1:H:69:TYR:HB2	1:H:137:VAL:HB	1.85	0.58
1:I:271:PRO:HA	1:I:308:LYS:HA	1.84	0.58
1:L:55:LEU:HD12	1:L:55:LEU:N	2.18	0.58
1:B:151:THR:HG23	1:B:154:ALA:HB2	1.84	0.58
1:E:38:PHE:CD2	1:E:169:GLN:NE2	2.71	0.58
1:I:55:LEU:HD12	1:I:55:LEU:N	2.17	0.58
1:M:64:ALA:HB2	1:M:141:ILE:C	2.28	0.58
1:H:51:ILE:HD11	1:H:164:MET:CE	2.33	0.58
1:M:141:ILE:HG13	1:M:143:GLY:H	1.69	0.58
1:E:45:PRO:N	1:E:164:MET:HE2	2.18	0.58
1:H:34:ARG:NE	1:H:254:PHE:CE1	2.71	0.58
1:H:109:GLN:NE2	1:I:96:ARG:CZ	2.67	0.58
1:L:39:ARG:NH1	1:M:54:ARG:NH2	2.47	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:184:LEU:HD22	1:M:236:VAL:HG11	1.86	0.58
1:C:69:TYR:CD2	1:C:164:MET:HE2	2.39	0.58
1:F:271:PRO:HA	1:F:308:LYS:HA	1.84	0.58
1:H:55:LEU:HD12	1:H:55:LEU:N	2.14	0.58
1:I:208:LEU:HD11	1:I:255:VAL:HB	1.85	0.58
1:J:250:LEU:O	1:J:253:MET:HG3	2.04	0.58
1:M:202:ASN:O	1:M:224:PHE:HD2	1.86	0.58
1:A:221:ARG:HG2	1:A:222:LEU:H	1.69	0.58
1:G:199:ALA:HB2	1:G:205:LYS:N	2.18	0.58
1:G:31:LEU:HB3	1:G:177:VAL:CG1	2.32	0.58
1:L:46:GLN:NE2	1:L:134:TYR:CE1	2.72	0.58
1:C:104:GLN:HE22	1:I:104:GLN:HE22	1.50	0.58
1:G:50:ILE:CD1	1:G:155:LEU:HB2	2.34	0.58
1:I:71:ILE:O	1:I:73:PRO:HD3	2.04	0.58
1:L:101:VAL:HG13	1:L:106:VAL:HG13	1.85	0.58
1:I:230:ASP:O	1:I:234:GLY:N	2.35	0.57
1:K:207:SER:OG	1:K:258:GLN:HB2	2.03	0.57
1:F:46:GLN:O	1:F:158:ASN:ND2	2.37	0.57
1:M:70:GLN:NE2	1:M:135:THR:O	2.38	0.57
1:B:51:ILE:HD11	1:B:164:MET:HE3	1.86	0.57
1:B:207:SER:OG	1:B:258:GLN:HB2	2.04	0.57
1:C:101:VAL:HG13	1:C:106:VAL:HG13	1.86	0.57
1:E:158:ASN:C	1:E:160:GLN:H	2.13	0.57
1:F:101:VAL:HG13	1:F:106:VAL:HG13	1.85	0.57
1:G:54:ARG:HG3	1:G:69:TYR:CE1	2.39	0.57
1:H:47:VAL:HG13	1:H:134:TYR:CB	2.33	0.57
1:A:246:ASN:HB2	1:A:248:GLU:HG3	1.86	0.57
1:J:271:PRO:HA	1:J:308:LYS:HA	1.85	0.57
1:L:38:PHE:HD2	1:L:169:GLN:NE2	2.02	0.57
1:L:64:ALA:HB2	1:L:142:SER:N	2.18	0.57
1:A:101:VAL:HG13	1:A:106:VAL:HG13	1.85	0.57
1:B:178:THR:HG22	1:B:237:THR:OG1	2.04	0.57
1:H:139:SER:OG	1:H:167:VAL:HG21	2.04	0.57
1:A:67:GLN:HA	1:A:138:LEU:HD23	1.86	0.57
1:F:191:LEU:HG	1:F:198:ARG:NH2	2.18	0.57
1:G:101:VAL:HG13	1:G:106:VAL:HG13	1.86	0.57
1:H:109:GLN:OE1	1:I:96:ARG:NE	2.37	0.57
1:K:30:GLU:OE2	1:K:258:GLN:HG2	2.04	0.57
1:E:55:LEU:HD12	1:E:55:LEU:N	2.17	0.57
1:H:169:GLN:O	1:H:170:LEU:HD23	2.04	0.57
1:E:38:PHE:HD2	1:E:169:GLN:NE2	2.03	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:75:THR:HG23	1:F:127:GLN:HE22	1.68	0.57
1:E:101:VAL:HG13	1:E:106:VAL:HG13	1.86	0.57
1:F:25:VAL:HG21	1:F:305:ILE:HD13	1.86	0.57
1:A:144:ARG:NH1	1:B:226:GLU:HG3	2.19	0.57
1:I:199:ALA:HB2	1:I:205:LYS:N	2.20	0.57
1:K:101:VAL:HG13	1:K:106:VAL:HG13	1.87	0.57
1:B:215:GLN:NE2	1:B:258:GLN:NE2	2.52	0.57
1:D:169:GLN:C	1:D:170:LEU:HD22	2.30	0.57
1:G:221:ARG:NH1	1:G:221:ARG:HB3	2.20	0.56
1:H:226:GLU:O	1:I:144:ARG:NH1	2.38	0.56
1:I:205:LYS:HE2	1:I:219:GLU:OE2	2.04	0.56
1:C:184:LEU:O	1:C:188:ARG:HG3	2.05	0.56
1:B:101:VAL:HG13	1:B:106:VAL:HG13	1.86	0.56
1:B:215:GLN:NE2	1:B:258:GLN:OE1	2.37	0.56
1:H:41:ALA:HB1	1:H:140:PRO:HG3	1.87	0.56
1:I:206:VAL:HG11	1:I:257:ALA:HB1	1.88	0.56
1:L:39:ARG:HH12	1:M:54:ARG:HH22	1.49	0.56
1:B:55:LEU:HD12	1:B:55:LEU:N	2.19	0.56
1:D:64:ALA:HB2	1:D:141:ILE:C	2.30	0.56
1:F:147:ARG:HH11	1:F:147:ARG:HB3	1.71	0.56
1:J:156:VAL:HG11	1:J:164:MET:HE3	1.86	0.56
1:A:134:TYR:C	1:A:136:LYS:N	2.62	0.56
1:J:101:VAL:HG13	1:J:106:VAL:HG13	1.87	0.56
1:L:54:ARG:HG3	1:L:69:TYR:CE1	2.41	0.56
1:G:210:LEU:HD12	1:G:214:SER:OG	2.05	0.56
1:H:71:ILE:O	1:H:73:PRO:HD3	2.05	0.56
1:M:169:GLN:O	1:M:170:LEU:HD23	2.06	0.56
1:A:55:LEU:HD12	1:A:55:LEU:N	2.20	0.56
1:H:47:VAL:HG13	1:H:134:TYR:HB2	1.87	0.56
1:M:184:LEU:O	1:M:188:ARG:HG3	2.06	0.56
1:A:227:VAL:HG12	1:A:227:VAL:O	2.04	0.56
1:E:159:GLY:O	1:E:160:GLN:C	2.50	0.56
1:F:272:GLN:HE21	1:F:272:GLN:HA	1.70	0.56
1:J:176:ASP:OD2	1:J:239:ARG:HG2	2.06	0.55
1:K:185:LEU:O	1:K:189:ARG:HG3	2.06	0.55
1:M:69:TYR:CD2	1:M:164:MET:HE2	2.40	0.55
1:A:64:ALA:HB2	1:A:141:ILE:C	2.30	0.55
1:B:35:THR:HB	1:B:173:ILE:HD11	1.88	0.55
1:E:23:GLN:O	1:E:266:LYS:HA	2.06	0.55
1:F:271:PRO:HG3	1:F:308:LYS:HG2	1.88	0.55
1:M:222:LEU:HD12	1:M:222:LEU:C	2.31	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:54:ARG:HG3	1:A:69:TYR:CE1	2.41	0.55
1:B:206:VAL:HG13	1:B:258:GLN:O	2.06	0.55
1:H:39:ARG:HH12	1:I:54:ARG:HH22	1.50	0.55
1:B:206:VAL:HG21	1:B:222:LEU:HB2	1.88	0.55
1:C:34:ARG:HH11	1:C:34:ARG:CB	2.10	0.55
1:G:155:LEU:C	1:G:155:LEU:HD23	2.31	0.55
1:K:175:VAL:HB	1:K:240:ALA:HB3	1.87	0.55
1:F:71:ILE:O	1:F:73:PRO:HD3	2.06	0.55
1:M:207:SER:OG	1:M:258:GLN:HB2	2.07	0.55
1:B:218:LEU:CD2	1:B:243:PRO:HB2	2.36	0.55
1:C:55:LEU:H	1:C:55:LEU:CD1	2.12	0.55
1:E:175:VAL:HB	1:E:240:ALA:HB3	1.87	0.55
1:J:208:LEU:HB2	1:J:242:PHE:CZ	2.41	0.55
1:M:64:ALA:CA	1:M:141:ILE:O	2.55	0.55
1:M:71:ILE:O	1:M:73:PRO:HD3	2.06	0.55
1:E:26:THR:O	1:E:27:LEU:HD23	2.06	0.55
1:G:35:THR:HB	1:G:173:ILE:HD11	1.87	0.55
1:K:34:ARG:CZ	1:K:254:PHE:CE1	2.90	0.55
1:M:202:ASN:O	1:M:202:ASN:CG	2.49	0.55
1:D:227:VAL:HG21	1:D:239:ARG:HG2	1.88	0.55
1:J:55:LEU:H	1:J:55:LEU:CD1	2.09	0.55
1:J:206:VAL:HG23	1:J:220:GLY:O	2.07	0.55
1:F:206:VAL:HG13	1:F:258:GLN:O	2.06	0.55
1:D:34:ARG:NE	1:D:254:PHE:HE2	2.04	0.54
1:G:227:VAL:HG12	1:G:237:THR:O	2.06	0.54
1:H:144:ARG:HG3	1:H:144:ARG:NH1	2.22	0.54
1:I:212:ASP:OD1	1:I:213:GLY:N	2.39	0.54
1:M:191:LEU:HG	1:M:198:ARG:HH12	1.71	0.54
1:A:137:VAL:O	1:A:138:LEU:HD23	2.06	0.54
1:A:205:LYS:HB3	1:A:219:GLU:OE2	2.07	0.54
1:E:34:ARG:HG2	1:E:34:ARG:HH11	1.72	0.54
1:D:222:LEU:HD11	1:D:238:ILE:HD13	1.90	0.54
1:H:206:VAL:HG13	1:H:258:GLN:O	2.07	0.54
1:M:35:THR:O	1:M:36:ASN:ND2	2.40	0.54
1:C:183:ALA:O	1:C:187:LEU:HG	2.07	0.54
1:I:208:LEU:HD11	1:I:255:VAL:CG2	2.38	0.54
1:K:68:LEU:HD13	1:K:145:ILE:CD1	2.37	0.54
1:F:50:ILE:HD13	1:F:155:LEU:HA	1.89	0.54
1:G:220:GLY:N	1:G:242:PHE:CE1	2.76	0.54
1:H:36:ASN:ND2	1:H:176:ASP:OD2	2.41	0.54
1:A:51:ILE:O	1:A:153:GLY:HA2	2.06	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:53:LYS:HA	1:G:152:GLU:OE1	2.08	0.54
1:G:106:VAL:HG22	1:G:110:GLN:HB2	1.90	0.54
1:G:244:ASN:ND2	1:G:247:ASN:HA	2.22	0.54
1:I:106:VAL:HG22	1:I:110:GLN:HB2	1.89	0.54
1:J:199:ALA:HB2	1:J:204:ALA:C	2.33	0.54
1:K:103:ASP:C	1:K:105:ALA:H	2.16	0.54
1:H:41:ALA:HB1	1:H:140:PRO:CG	2.37	0.54
1:I:175:VAL:HB	1:I:240:ALA:HB3	1.90	0.54
1:L:199:ALA:HB2	1:L:204:ALA:C	2.33	0.54
1:D:147:ARG:NH2	1:E:237:THR:HG21	2.23	0.54
1:H:106:VAL:HG23	1:H:110:GLN:OE1	2.08	0.54
1:K:226:GLU:OE1	1:K:229:VAL:HG22	2.07	0.54
1:A:104:GLN:HB3	1:G:108:LYS:HG3	1.90	0.53
1:A:184:LEU:O	1:A:188:ARG:HG3	2.08	0.53
1:B:106:VAL:HG22	1:B:110:GLN:HB2	1.91	0.53
1:D:247:ASN:OD1	1:D:250:LEU:HD21	2.08	0.53
1:F:230:ASP:O	1:F:234:GLY:N	2.39	0.53
1:G:55:LEU:HD12	1:G:55:LEU:N	2.23	0.53
1:H:144:ARG:HG3	1:H:144:ARG:HH11	1.74	0.53
1:K:34:ARG:NE	1:K:254:PHE:CE1	2.77	0.53
1:K:106:VAL:HG23	1:K:110:GLN:OE1	2.09	0.53
1:M:35:THR:HB	1:M:173:ILE:HD11	1.90	0.53
1:A:200:GLY:O	1:A:201:ASP:C	2.52	0.53
1:F:206:VAL:HG11	1:F:257:ALA:HB1	1.90	0.53
1:I:185:LEU:O	1:I:189:ARG:HG3	2.08	0.53
1:M:23:GLN:O	1:M:266:LYS:HA	2.08	0.53
1:M:143:GLY:HA2	1:M:169:GLN:HA	1.90	0.53
1:M:187:LEU:HD22	1:M:196:LEU:HD21	1.91	0.53
1:F:137:VAL:HG21	1:F:164:MET:HE1	1.90	0.53
1:A:206:VAL:N	1:A:220:GLY:O	2.41	0.53
1:A:221:ARG:HG2	1:A:222:LEU:N	2.24	0.53
1:H:175:VAL:HB	1:H:240:ALA:HB3	1.89	0.53
1:I:231:GLU:CD	1:I:231:GLU:H	2.17	0.53
1:K:54:ARG:HG3	1:K:69:TYR:CE1	2.44	0.53
1:B:206:VAL:HG12	1:B:207:SER:N	2.23	0.53
1:G:170:LEU:O	1:G:173:ILE:HB	2.09	0.53
1:D:108:LYS:HE3	1:J:104:GLN:HG3	1.90	0.53
1:H:106:VAL:HG22	1:H:110:GLN:HB2	1.91	0.53
1:I:30:GLU:CD	1:I:258:GLN:HG2	2.34	0.53
1:I:46:GLN:C	1:I:158:ASN:HB2	2.33	0.53
1:I:48:ASN:O	1:I:76:TYR:OH	2.22	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:39:ARG:NE	1:K:152:GLU:OE2	2.42	0.53
1:A:180:PRO:HA	1:A:235:SER:HA	1.91	0.53
1:C:49:GLY:O	1:C:155:LEU:HD12	2.08	0.53
1:C:106:VAL:HG22	1:C:110:GLN:HB2	1.91	0.53
1:H:23:GLN:O	1:H:266:LYS:HA	2.09	0.53
1:H:47:VAL:CG1	1:H:134:TYR:HB2	2.39	0.53
1:D:92:GLU:OE2	1:D:96:ARG:NH1	2.42	0.53
1:E:41:ALA:HB1	1:E:140:PRO:CG	2.38	0.53
1:I:50:ILE:HD11	1:I:155:LEU:HD13	1.91	0.53
1:L:48:ASN:OD1	1:L:158:ASN:N	2.40	0.53
1:B:103:ASP:C	1:B:105:ALA:H	2.16	0.53
1:B:218:LEU:HD23	1:B:243:PRO:HB2	1.91	0.53
1:G:69:TYR:HB2	1:G:137:VAL:HB	1.91	0.53
1:I:138:LEU:N	1:I:138:LEU:HD23	2.23	0.53
1:B:64:ALA:HB2	1:B:141:ILE:HA	1.91	0.52
1:B:240:ALA:HB1	1:B:242:PHE:HE2	1.75	0.52
1:B:253:MET:HE3	1:C:181:SER:CB	2.28	0.52
1:D:244:ASN:HD21	1:D:249:LEU:H	1.57	0.52
1:I:156:VAL:HG11	1:I:164:MET:CE	2.29	0.52
1:L:106:VAL:HG23	1:L:110:GLN:OE1	2.08	0.52
1:A:203:ALA:HB3	1:A:221:ARG:HE	1.75	0.52
1:E:246:ASN:O	1:F:188:ARG:NH2	2.42	0.52
1:F:199:ALA:HB2	1:F:204:ALA:C	2.34	0.52
1:G:221:ARG:HB3	1:G:221:ARG:HH11	1.74	0.52
1:H:46:GLN:CD	1:H:134:TYR:CE1	2.88	0.52
1:E:189:ARG:HG3	1:E:189:ARG:HH11	1.73	0.52
1:G:206:VAL:HG13	1:G:258:GLN:O	2.09	0.52
1:L:86:ASN:O	1:L:89:SER:HB3	2.10	0.52
1:C:92:GLU:OE2	1:C:96:ARG:NH1	2.43	0.52
1:D:34:ARG:NE	1:D:254:PHE:CE2	2.78	0.52
1:E:190:GLU:OE1	1:E:261:GLU:HB3	2.09	0.52
1:H:39:ARG:NH1	1:I:54:ARG:NH2	2.52	0.52
1:I:193:SER:OG	1:I:194:GLY:N	2.41	0.52
1:M:208:LEU:HB2	1:M:242:PHE:CZ	2.44	0.52
1:B:174:TYR:CD1	1:B:239:ARG:HD3	2.45	0.52
1:A:38:PHE:HB2	1:A:172:PRO:O	2.09	0.52
1:B:55:LEU:HD12	1:B:68:LEU:O	2.10	0.52
1:E:41:ALA:HB1	1:E:140:PRO:HG3	1.90	0.52
1:K:244:ASN:CG	1:K:249:LEU:HB2	2.35	0.52
1:D:208:LEU:HD22	1:D:242:PHE:CD2	2.45	0.52
1:J:44:ARG:CD	1:J:44:ARG:NH1	2.73	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:203:ALA:HB2	1:A:223:GLU:HA	1.92	0.52
1:B:106:VAL:HG23	1:B:110:GLN:OE1	2.10	0.52
1:E:208:LEU:HD11	1:E:255:VAL:CG2	2.40	0.52
1:F:175:VAL:HB	1:F:240:ALA:HB3	1.92	0.52
1:M:106:VAL:HG22	1:M:110:GLN:HB2	1.92	0.52
1:D:55:LEU:HD12	1:D:55:LEU:N	2.24	0.51
1:E:54:ARG:HG3	1:E:69:TYR:CE1	2.45	0.51
1:E:106:VAL:HG22	1:E:110:GLN:HB2	1.92	0.51
1:I:64:ALA:H	1:I:142:SER:HG	1.59	0.51
1:K:23:GLN:O	1:K:266:LYS:HA	2.09	0.51
1:F:106:VAL:HG22	1:F:110:GLN:HB2	1.92	0.51
1:F:269:LEU:O	1:F:308:LYS:HD3	2.10	0.51
1:G:41:ALA:HB1	1:G:140:PRO:CG	2.40	0.51
1:M:206:VAL:HG12	1:M:207:SER:N	2.26	0.51
1:C:199:ALA:HB2	1:C:204:ALA:C	2.35	0.51
1:D:73:PRO:O	1:D:74:ALA:C	2.52	0.51
1:D:251:PRO:HB2	1:E:231:GLU:HG2	1.92	0.51
1:J:185:LEU:HD11	1:K:248:GLU:HB3	1.92	0.51
1:K:206:VAL:HG13	1:K:258:GLN:O	2.09	0.51
1:C:191:LEU:HD22	1:C:224:PHE:CE2	2.46	0.51
1:K:55:LEU:HD12	1:K:55:LEU:N	2.25	0.51
1:L:31:LEU:HB3	1:L:177:VAL:CG1	2.41	0.51
1:L:184:LEU:O	1:L:188:ARG:HG3	2.10	0.51
1:A:216:TYR:CE2	1:A:218:LEU:HB2	2.46	0.51
1:F:227:VAL:HG23	1:F:237:THR:O	2.10	0.51
1:I:51:ILE:CD1	1:I:164:MET:HE1	2.40	0.51
1:I:156:VAL:CG1	1:I:164:MET:HE3	2.31	0.51
1:M:206:VAL:HG11	1:M:257:ALA:HB1	1.92	0.51
1:F:195:GLN:HE21	1:F:261:GLU:HB3	1.76	0.51
1:H:193:SER:OG	1:H:195:GLN:HG3	2.10	0.51
1:I:210:LEU:HD22	1:I:253:MET:CE	2.40	0.51
1:J:206:VAL:O	1:J:219:GLU:HG3	2.09	0.51
1:D:225:SER:O	1:D:238:ILE:HG22	2.10	0.51
1:H:206:VAL:HG21	1:H:222:LEU:HB2	1.91	0.51
1:H:220:GLY:HA3	1:H:242:PHE:HD1	1.75	0.51
1:K:221:ARG:HD3	1:K:223:GLU:OE2	2.11	0.51
1:M:50:ILE:HD11	1:M:155:LEU:HD13	1.91	0.51
1:G:144:ARG:HG3	1:G:144:ARG:HH11	1.74	0.51
1:B:169:GLN:O	1:B:170:LEU:HD23	2.11	0.51
1:D:51:ILE:HD11	1:D:164:MET:HE2	1.91	0.51
1:K:39:ARG:HH12	1:L:54:ARG:NH2	2.09	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:208:LEU:HD11	1:A:255:VAL:CG2	2.40	0.51
1:D:96:ARG:NH2	1:E:109:GLN:CD	2.59	0.51
1:J:231:GLU:HG3	1:K:251:PRO:HB2	1.92	0.51
1:K:186:ARG:NH1	1:K:261:GLU:OE1	2.43	0.51
1:F:64:ALA:HB2	1:F:141:ILE:HA	1.93	0.50
1:L:212:ASP:OD1	1:L:213:GLY:N	2.45	0.50
1:A:54:ARG:NH2	1:B:39:ARG:HH12	2.09	0.50
1:B:219:GLU:HG2	1:B:220:GLY:N	2.25	0.50
1:C:162:ASN:N	1:C:162:ASN:HD22	2.09	0.50
1:G:69:TYR:CD2	1:G:164:MET:HE2	2.45	0.50
1:L:113:ASP:O	1:L:116:ALA:HB3	2.11	0.50
1:D:106:VAL:HG22	1:D:110:GLN:HB2	1.92	0.50
1:H:68:LEU:HD13	1:H:145:ILE:CD1	2.40	0.50
1:I:199:ALA:HB2	1:I:204:ALA:C	2.36	0.50
1:A:180:PRO:O	1:A:181:SER:C	2.54	0.50
1:D:54:ARG:HG3	1:D:69:TYR:CE1	2.47	0.50
1:D:67:GLN:HA	1:D:138:LEU:HD23	1.93	0.50
1:H:54:ARG:HG3	1:H:69:TYR:CE1	2.46	0.50
1:H:103:ASP:C	1:H:105:ALA:H	2.18	0.50
1:J:54:ARG:HG3	1:J:69:TYR:CE1	2.46	0.50
1:J:244:ASN:ND2	1:J:249:LEU:HB2	2.27	0.50
1:L:106:VAL:HG22	1:L:110:GLN:HB2	1.93	0.50
1:M:68:LEU:HD13	1:M:145:ILE:CD1	2.41	0.50
1:D:103:ASP:C	1:D:105:ALA:H	2.19	0.50
1:F:103:ASP:C	1:F:105:ALA:H	2.20	0.50
1:J:178:THR:CG2	1:J:237:THR:OG1	2.59	0.50
1:L:71:ILE:O	1:L:73:PRO:HD3	2.11	0.50
1:L:151:THR:O	1:L:152:GLU:C	2.51	0.50
1:L:230:ASP:O	1:L:234:GLY:N	2.41	0.50
1:M:55:LEU:HD12	1:M:68:LEU:O	2.12	0.50
1:E:208:LEU:HB2	1:E:242:PHE:CZ	2.47	0.50
1:F:185:LEU:O	1:F:189:ARG:HG3	2.11	0.50
1:I:174:TYR:CE1	1:I:241:VAL:HG22	2.47	0.50
1:A:106:VAL:HG22	1:A:110:GLN:HB2	1.93	0.50
1:E:191:LEU:HD11	1:E:198:ARG:HG3	1.94	0.50
1:E:206:VAL:HG13	1:E:258:GLN:O	2.12	0.50
1:I:103:ASP:C	1:I:105:ALA:H	2.20	0.50
1:K:92:GLU:OE2	1:K:96:ARG:NH1	2.45	0.50
1:L:38:PHE:CD2	1:L:169:GLN:NE2	2.79	0.50
1:M:103:ASP:C	1:M:105:ALA:H	2.19	0.50
1:G:38:PHE:HA	1:G:174:TYR:CD2	2.47	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:50:ILE:HD13	1:G:155:LEU:CA	2.41	0.50
1:G:206:VAL:HG11	1:G:257:ALA:HB1	1.94	0.50
1:I:34:ARG:NE	1:I:254:PHE:HE1	2.09	0.50
1:I:208:LEU:HD11	1:I:255:VAL:CB	2.41	0.50
1:L:55:LEU:H	1:L:55:LEU:CD1	2.15	0.50
1:B:147:ARG:HH11	1:B:147:ARG:HB3	1.76	0.49
1:D:113:ASP:O	1:D:116:ALA:HB3	2.12	0.49
1:L:209:LYS:HD3	1:L:258:GLN:NE2	2.27	0.49
1:B:38:PHE:CD1	1:B:172:PRO:HG2	2.47	0.49
1:B:46:GLN:HA	1:B:158:ASN:OD1	2.12	0.49
1:E:184:LEU:O	1:E:188:ARG:HG3	2.12	0.49
1:H:64:ALA:HB2	1:H:142:SER:N	2.27	0.49
1:L:103:ASP:C	1:L:105:ALA:H	2.20	0.49
1:J:48:ASN:O	1:J:76:TYR:OH	2.27	0.49
1:C:103:ASP:C	1:C:105:ALA:H	2.21	0.49
1:C:206:VAL:HG12	1:C:207:SER:N	2.27	0.49
1:D:212:ASP:OD2	1:D:214:SER:N	2.46	0.49
1:F:290:ALA:HB3	1:F:291:GLN:NE2	2.27	0.49
1:G:50:ILE:HD11	1:G:155:LEU:HB2	1.95	0.49
1:G:195:GLN:HG2	1:G:261:GLU:O	2.12	0.49
1:L:46:GLN:NE2	1:L:134:TYR:HE1	2.10	0.49
1:A:103:ASP:C	1:A:105:ALA:H	2.20	0.49
1:A:178:THR:HA	1:A:236:VAL:O	2.13	0.49
1:C:206:VAL:HG11	1:C:257:ALA:HB1	1.94	0.49
1:D:206:VAL:CG1	1:D:259:LEU:HD13	2.43	0.49
1:D:244:ASN:ND2	1:D:249:LEU:H	2.09	0.49
1:H:185:LEU:CD2	1:I:210:LEU:HD13	2.42	0.49
1:C:176:ASP:OD1	1:C:239:ARG:HD3	2.13	0.49
1:D:178:THR:OG1	1:D:237:THR:HG22	2.12	0.49
1:E:67:GLN:HA	1:E:138:LEU:HD23	1.95	0.49
1:G:69:TYR:CE2	1:G:164:MET:HE2	2.48	0.49
1:G:113:ASP:O	1:G:116:ALA:HB3	2.13	0.49
1:I:186:ARG:HG2	1:I:190:GLU:OE2	2.12	0.49
1:J:103:ASP:C	1:J:105:ALA:H	2.19	0.49
1:K:67:GLN:HA	1:K:138:LEU:HD23	1.94	0.49
1:B:48:ASN:OD1	1:B:157:THR:HA	2.12	0.49
1:D:120:GLN:O	1:D:123:ALA:HB3	2.13	0.49
1:D:193:SER:OG	1:D:194:GLY:N	2.46	0.49
1:J:113:ASP:O	1:J:116:ALA:HB3	2.13	0.49
1:B:113:ASP:O	1:B:116:ALA:HB3	2.13	0.49
1:E:250:LEU:O	1:E:253:MET:HG3	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:45:PRO:HD3	1:F:164:MET:SD	2.53	0.49
1:G:197:GLU:O	1:G:205:LYS:HG3	2.13	0.49
1:I:101:VAL:HG13	1:I:106:VAL:HG13	1.94	0.49
1:K:157:THR:O	1:K:160:GLN:HG2	2.12	0.49
1:K:230:ASP:O	1:K:234:GLY:N	2.44	0.49
1:B:206:VAL:HG11	1:B:257:ALA:HB1	1.95	0.49
1:E:208:LEU:HD11	1:E:255:VAL:HG21	1.94	0.49
1:G:199:ALA:HB2	1:G:204:ALA:C	2.38	0.49
1:H:113:ASP:O	1:H:116:ALA:HB3	2.13	0.49
1:C:138:LEU:HD12	1:C:138:LEU:N	2.17	0.48
1:E:71:ILE:O	1:E:73:PRO:HD3	2.13	0.48
1:I:39:ARG:HH12	1:J:54:ARG:NH2	2.11	0.48
1:M:208:LEU:HB2	1:M:242:PHE:CE2	2.48	0.48
1:H:174:TYR:CE1	1:H:241:VAL:HG22	2.49	0.48
1:I:55:LEU:H	1:I:55:LEU:CD1	2.15	0.48
1:J:129:ARG:HG2	1:J:129:ARG:HH11	1.77	0.48
1:K:106:VAL:HG22	1:K:110:GLN:HB2	1.94	0.48
1:K:199:ALA:HB2	1:K:204:ALA:C	2.37	0.48
1:K:255:VAL:O	1:K:256:HIS:HD2	1.95	0.48
1:M:69:TYR:HB2	1:M:137:VAL:HB	1.94	0.48
1:E:230:ASP:O	1:E:234:GLY:N	2.46	0.48
1:I:48:ASN:OD1	1:I:157:THR:HA	2.14	0.48
1:I:54:ARG:HG3	1:I:69:TYR:CE1	2.47	0.48
1:I:68:LEU:HD13	1:I:145:ILE:HD12	1.95	0.48
1:J:230:ASP:O	1:J:234:GLY:N	2.40	0.48
1:K:195:GLN:NE2	1:K:263:VAL:CB	2.76	0.48
1:M:55:LEU:H	1:M:55:LEU:CD1	2.09	0.48
1:B:64:ALA:HB2	1:B:141:ILE:CA	2.43	0.48
1:C:108:LYS:HG3	1:I:104:GLN:CB	2.44	0.48
1:G:228:SER:OG	1:G:237:THR:HB	2.13	0.48
1:J:106:VAL:HG22	1:J:110:GLN:HB2	1.93	0.48
1:B:64:ALA:HB2	1:B:141:ILE:C	2.39	0.48
1:D:155:LEU:HD12	1:D:156:VAL:N	2.28	0.48
1:E:180:PRO:O	1:E:181:SER:C	2.56	0.48
1:I:208:LEU:HD11	1:I:255:VAL:HG21	1.94	0.48
1:J:34:ARG:CZ	1:J:254:PHE:CE1	2.97	0.48
1:K:226:GLU:HG3	1:L:144:ARG:NH1	2.29	0.48
1:M:48:ASN:OD1	1:M:157:THR:HA	2.14	0.48
1:M:120:GLN:O	1:M:123:ALA:HB3	2.13	0.48
1:A:104:GLN:CB	1:G:108:LYS:HG3	2.43	0.48
1:B:144:ARG:NH2	1:C:226:GLU:HG3	2.27	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:157:THR:O	1:D:160:GLN:HG2	2.13	0.48
1:F:261:GLU:CD	1:F:303:ARG:HH22	2.21	0.48
1:A:238:ILE:HG22	1:A:239:ARG:N	2.29	0.48
1:B:30:GLU:OE1	1:B:258:GLN:HG2	2.14	0.48
1:D:68:LEU:HD11	1:D:139:SER:HB2	1.94	0.48
1:G:208:LEU:HB2	1:G:242:PHE:CZ	2.49	0.48
1:J:106:VAL:HG23	1:J:110:GLN:OE1	2.13	0.48
1:M:91:GLN:HA	1:M:118:TYR:CD1	2.49	0.48
1:M:157:THR:O	1:M:160:GLN:HB3	2.13	0.48
1:M:244:ASN:CG	1:M:249:LEU:HB2	2.38	0.48
1:A:141:ILE:HD11	1:A:167:VAL:O	2.12	0.48
1:A:208:LEU:HB2	1:A:242:PHE:CZ	2.49	0.48
1:D:170:LEU:N	1:D:170:LEU:CD2	2.77	0.48
1:G:222:LEU:HD13	1:G:240:ALA:HB2	1.96	0.48
1:A:106:VAL:HG23	1:A:110:GLN:OE1	2.13	0.48
1:F:43:VAL:HG23	1:F:165:ALA:O	2.13	0.48
1:H:178:THR:CG2	1:H:237:THR:OG1	2.59	0.48
1:K:206:VAL:HG11	1:K:257:ALA:HB1	1.94	0.48
1:M:86:ASN:O	1:M:89:SER:HB3	2.13	0.48
1:A:150:VAL:HG23	1:A:164:MET:HA	1.95	0.48
1:D:71:ILE:O	1:D:73:PRO:HD3	2.14	0.48
1:J:57:LYS:HB3	1:J:60:SER:HB3	1.96	0.48
1:A:202:ASN:C	1:A:202:ASN:HD22	2.21	0.47
1:M:206:VAL:HG13	1:M:258:GLN:O	2.14	0.47
1:E:54:ARG:HD2	1:E:148:SER:HB2	1.95	0.47
1:G:175:VAL:HB	1:G:240:ALA:HB3	1.95	0.47
1:I:206:VAL:HG12	1:I:207:SER:N	2.29	0.47
1:M:202:ASN:OD1	1:M:224:PHE:HB2	2.14	0.47
1:A:92:GLU:OE2	1:A:96:ARG:NH1	2.47	0.47
1:D:126:GLU:O	1:D:130:ILE:HG13	2.13	0.47
1:D:246:ASN:O	1:D:247:ASN:C	2.56	0.47
1:D:252:GLY:HA3	1:E:234:GLY:HA2	1.96	0.47
1:G:103:ASP:C	1:G:105:ALA:H	2.22	0.47
1:H:109:GLN:CD	1:I:96:ARG:NE	2.71	0.47
1:I:40:ILE:O	1:J:151:THR:HB	2.14	0.47
1:K:216:TYR:HE2	1:K:218:LEU:HB2	1.79	0.47
1:K:226:GLU:OE2	1:L:144:ARG:HD3	2.14	0.47
1:M:47:VAL:HG12	1:M:131:ASN:OD1	2.13	0.47
1:B:147:ARG:H	1:B:147:ARG:HG3	1.51	0.47
1:B:248:GLU:HG2	1:C:185:LEU:HD11	1.95	0.47
1:C:69:TYR:HB2	1:C:137:VAL:HB	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:211:GLU:HG2	1:E:254:PHE:O	2.14	0.47
1:H:208:LEU:HD13	1:H:242:PHE:HE2	1.79	0.47
1:L:203:ALA:HB2	1:L:223:GLU:HA	1.96	0.47
1:B:51:ILE:HG13	1:B:150:VAL:HG11	1.94	0.47
1:D:85:ALA:HB1	1:E:119:LEU:HB3	1.95	0.47
1:E:34:ARG:NH1	1:E:254:PHE:CG	2.82	0.47
1:H:68:LEU:HD11	1:H:139:SER:HB2	1.97	0.47
1:I:129:ARG:HG2	1:I:129:ARG:HH11	1.78	0.47
1:L:134:TYR:OH	1:M:72:ASP:OD2	2.32	0.47
1:A:71:ILE:O	1:A:73:PRO:HD3	2.14	0.47
1:A:113:ASP:O	1:A:116:ALA:HB3	2.14	0.47
1:D:96:ARG:CZ	1:E:109:GLN:OE1	2.60	0.47
1:E:159:GLY:O	1:E:160:GLN:O	2.32	0.47
1:J:59:GLY:O	1:J:144:ARG:NH1	2.48	0.47
1:M:38:PHE:HB2	1:M:172:PRO:O	2.14	0.47
1:A:34:ARG:HD3	1:A:254:PHE:CZ	2.49	0.47
1:A:126:GLU:O	1:A:130:ILE:HG13	2.15	0.47
1:E:103:ASP:C	1:E:105:ALA:H	2.21	0.47
1:F:272:GLN:HB2	1:F:309:TRP:HE1	1.78	0.47
1:H:92:GLU:OE2	1:H:96:ARG:NH1	2.48	0.47
1:H:226:GLU:HG2	1:I:250:LEU:HD11	1.96	0.47
1:J:175:VAL:HB	1:J:240:ALA:HB3	1.97	0.47
1:J:185:LEU:HD12	1:J:185:LEU:HA	1.77	0.47
1:J:193:SER:OG	1:J:194:GLY:N	2.44	0.47
1:K:71:ILE:O	1:K:73:PRO:HD3	2.14	0.47
1:K:160:GLN:NE2	1:K:162:ASN:O	2.41	0.47
1:K:174:TYR:CE1	1:K:241:VAL:HG22	2.49	0.47
1:M:180:PRO:O	1:M:181:SER:C	2.57	0.47
1:M:226:GLU:C	1:M:226:GLU:CD	2.82	0.47
1:A:39:ARG:H	1:A:169:GLN:HB3	1.79	0.47
1:C:150:VAL:HG13	1:C:154:ALA:HB3	1.95	0.47
1:F:81:GLN:HG3	1:G:85:ALA:HB2	1.97	0.47
1:H:64:ALA:HB2	1:H:141:ILE:HA	1.96	0.47
1:M:106:VAL:HG23	1:M:110:GLN:OE1	2.14	0.47
1:C:48:ASN:OD1	1:C:157:THR:HA	2.15	0.47
1:F:208:LEU:HD11	1:F:255:VAL:HB	1.97	0.47
1:F:208:LEU:HB2	1:F:242:PHE:CZ	2.50	0.47
1:G:34:ARG:HE	1:G:254:PHE:HE1	1.63	0.47
1:K:206:VAL:HG21	1:K:222:LEU:HB2	1.97	0.47
1:A:45:PRO:HD3	1:A:164:MET:HG3	1.96	0.47
1:G:41:ALA:HB1	1:G:140:PRO:HG3	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:174:TYR:CD1	1:K:241:VAL:HG22	2.51	0.47
1:B:180:PRO:O	1:B:181:SER:C	2.58	0.46
1:D:106:VAL:HG23	1:D:110:GLN:OE1	2.15	0.46
1:J:68:LEU:HD13	1:J:145:ILE:CD1	2.45	0.46
1:M:230:ASP:O	1:M:234:GLY:N	2.45	0.46
1:A:48:ASN:OD1	1:A:157:THR:HA	2.15	0.46
1:A:91:GLN:HA	1:A:118:TYR:CD1	2.50	0.46
1:A:158:ASN:OD1	1:A:158:ASN:C	2.58	0.46
1:B:68:LEU:HD13	1:B:145:ILE:CD1	2.46	0.46
1:C:64:ALA:HB2	1:C:141:ILE:HA	1.97	0.46
1:C:68:LEU:HD13	1:C:145:ILE:CD1	2.45	0.46
1:C:175:VAL:HB	1:C:240:ALA:HB3	1.96	0.46
1:J:77:GLU:HA	1:J:132:LEU:HD22	1.97	0.46
1:K:196:LEU:HD11	1:K:261:GLU:HG2	1.96	0.46
1:L:69:TYR:HB2	1:L:137:VAL:HB	1.97	0.46
1:M:170:LEU:O	1:M:244:ASN:HB3	2.15	0.46
1:A:170:LEU:O	1:A:173:ILE:HB	2.15	0.46
1:B:242:PHE:N	1:B:242:PHE:CD2	2.84	0.46
1:C:31:LEU:HB3	1:C:177:VAL:CG1	2.41	0.46
1:E:69:TYR:HB2	1:E:137:VAL:HB	1.98	0.46
1:E:190:GLU:HG2	1:E:195:GLN:NE2	2.31	0.46
1:F:120:GLN:O	1:F:123:ALA:HB3	2.15	0.46
1:G:130:ILE:HG21	1:H:74:ALA:HB1	1.96	0.46
1:H:121:SER:O	1:H:122:LYS:C	2.59	0.46
1:K:48:ASN:OD1	1:K:157:THR:HG23	2.15	0.46
1:K:86:ASN:O	1:K:89:SER:HB3	2.16	0.46
1:L:120:GLN:O	1:L:123:ALA:HB3	2.15	0.46
1:G:71:ILE:O	1:G:73:PRO:HD3	2.16	0.46
1:K:206:VAL:HG12	1:K:207:SER:N	2.30	0.46
1:B:190:GLU:HB3	1:B:196:LEU:HG	1.98	0.46
1:C:210:LEU:HB2	1:C:212:ASP:OD1	2.15	0.46
1:F:202:ASN:O	1:F:224:PHE:HD2	1.97	0.46
1:G:206:VAL:CG1	1:G:207:SER:N	2.78	0.46
1:H:30:GLU:HG3	1:H:256:HIS:HB3	1.97	0.46
1:H:206:VAL:HG11	1:H:257:ALA:HB1	1.98	0.46
1:J:190:GLU:HB3	1:J:196:LEU:HD13	1.97	0.46
1:A:34:ARG:HD3	1:A:254:PHE:CE2	2.50	0.46
1:A:86:ASN:O	1:A:89:SER:HB3	2.16	0.46
1:A:178:THR:HG22	1:A:235:SER:HB3	1.96	0.46
1:C:208:LEU:HD11	1:C:255:VAL:CG2	2.45	0.46
1:D:69:TYR:HB2	1:D:137:VAL:HB	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:129:ARG:HG2	1:D:129:ARG:HH11	1.81	0.46
1:F:25:VAL:HG21	1:F:305:ILE:CD1	2.45	0.46
1:H:216:TYR:HE2	1:H:218:LEU:HB2	1.81	0.46
1:H:230:ASP:O	1:H:234:GLY:N	2.48	0.46
1:M:113:ASP:O	1:M:116:ALA:HB3	2.15	0.46
1:B:250:LEU:O	1:B:253:MET:HG3	2.16	0.46
1:D:104:GLN:HG3	1:J:108:LYS:CE	2.44	0.46
1:D:144:ARG:HE	1:E:226:GLU:CD	2.24	0.46
1:D:222:LEU:O	1:D:222:LEU:HG	2.15	0.46
1:E:64:ALA:HB2	1:E:141:ILE:C	2.40	0.46
1:E:77:GLU:HA	1:E:132:LEU:HD22	1.98	0.46
1:G:174:TYR:CD1	1:G:239:ARG:HD3	2.50	0.46
1:K:186:ARG:O	1:K:190:GLU:HG3	2.16	0.46
1:M:41:ALA:HB2	1:M:141:ILE:CG2	2.46	0.46
1:B:208:LEU:HD11	1:B:255:VAL:CG2	2.46	0.46
1:D:109:GLN:O	1:D:112:ALA:HB3	2.16	0.46
1:F:113:ASP:O	1:F:116:ALA:HB3	2.16	0.46
1:H:50:ILE:HD13	1:H:155:LEU:HA	1.98	0.46
1:I:113:ASP:O	1:I:116:ALA:HB3	2.16	0.46
1:M:199:ALA:HB2	1:M:204:ALA:C	2.40	0.46
1:B:52:LEU:HD23	1:B:52:LEU:HA	1.81	0.46
1:C:34:ARG:NE	1:C:254:PHE:CE1	2.84	0.46
1:E:55:LEU:HD12	1:E:68:LEU:O	2.15	0.46
1:F:129:ARG:HG2	1:F:129:ARG:HH11	1.80	0.46
1:J:56:PHE:CZ	1:J:148:SER:HB2	2.51	0.46
1:K:55:LEU:HD12	1:K:68:LEU:O	2.16	0.46
1:K:113:ASP:O	1:K:116:ALA:HB3	2.16	0.46
1:F:106:VAL:HG23	1:F:110:GLN:OE1	2.16	0.46
1:H:46:GLN:NE2	1:H:134:TYR:CE1	2.84	0.46
1:J:185:LEU:HD11	1:K:248:GLU:CB	2.46	0.46
1:K:43:VAL:HG23	1:K:165:ALA:O	2.16	0.46
1:L:176:ASP:OD1	1:L:239:ARG:HG2	2.16	0.46
1:M:299:ILE:HA	1:M:314:GLY:HA3	1.98	0.46
1:E:48:ASN:OD1	1:E:157:THR:HA	2.15	0.45
1:J:226:GLU:HG3	1:K:144:ARG:HE	1.81	0.45
1:A:120:GLN:O	1:A:123:ALA:HB3	2.16	0.45
1:A:186:ARG:HD3	1:A:190:GLU:OE2	2.16	0.45
1:B:147:ARG:HD2	2:B:1340:SO4:O2	2.16	0.45
1:B:215:GLN:NE2	1:B:258:GLN:CD	2.74	0.45
1:D:98:LYS:HG3	1:D:111:TYR:CZ	2.51	0.45
1:D:191:LEU:HD11	1:D:198:ARG:NH1	2.31	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:27:LEU:O	1:E:260:GLN:OE1	2.33	0.45
1:A:210:LEU:HD23	1:A:255:VAL:HG12	1.98	0.45
1:B:86:ASN:O	1:B:89:SER:HB3	2.16	0.45
1:C:230:ASP:O	1:C:234:GLY:N	2.41	0.45
1:F:167:VAL:HG12	1:F:168:GLN:N	2.31	0.45
1:K:64:ALA:HB2	1:K:141:ILE:HA	1.97	0.45
1:K:202:ASN:O	1:K:224:PHE:HD2	1.99	0.45
1:L:175:VAL:HB	1:L:240:ALA:HB3	1.98	0.45
1:M:216:TYR:OH	1:M:243:PRO:O	2.27	0.45
1:A:104:GLN:HE22	1:G:104:GLN:HE22	1.64	0.45
1:C:126:GLU:O	1:C:130:ILE:HG13	2.16	0.45
1:C:190:GLU:CB	1:C:196:LEU:HD13	2.39	0.45
1:C:222:LEU:HD11	1:C:238:ILE:HD12	1.97	0.45
1:D:52:LEU:HD23	1:D:52:LEU:HA	1.82	0.45
1:H:46:GLN:NE2	1:H:134:TYR:HE1	2.14	0.45
1:M:208:LEU:HD11	1:M:255:VAL:CG2	2.46	0.45
1:D:43:VAL:HG23	1:D:165:ALA:O	2.17	0.45
1:G:126:GLU:O	1:G:130:ILE:HG13	2.17	0.45
1:H:120:GLN:O	1:H:123:ALA:HB3	2.16	0.45
1:I:106:VAL:HG23	1:I:110:GLN:OE1	2.16	0.45
1:J:126:GLU:O	1:J:130:ILE:HG13	2.16	0.45
1:M:57:LYS:HB3	1:M:60:SER:HB3	1.98	0.45
1:A:191:LEU:C	1:A:193:SER:H	2.24	0.45
1:C:162:ASN:N	1:C:162:ASN:ND2	2.63	0.45
1:E:57:LYS:HB3	1:E:60:SER:HB3	1.98	0.45
1:H:98:LYS:HG3	1:H:111:TYR:CZ	2.52	0.45
1:L:55:LEU:HD12	1:L:68:LEU:O	2.16	0.45
1:M:46:GLN:NE2	1:M:134:TYR:CE1	2.84	0.45
1:M:182:THR:O	1:M:185:LEU:HB2	2.16	0.45
1:D:205:LYS:O	1:D:259:LEU:HD13	2.17	0.45
1:E:222:LEU:HD13	1:E:240:ALA:HB2	1.98	0.45
1:F:244:ASN:ND2	1:F:249:LEU:O	2.48	0.45
1:G:54:ARG:HD2	1:G:148:SER:CB	2.46	0.45
1:G:55:LEU:H	1:G:55:LEU:CD1	2.20	0.45
1:H:67:GLN:HA	1:H:138:LEU:CD2	2.47	0.45
1:K:28:ASN:OD1	1:K:260:GLN:HB2	2.16	0.45
1:K:216:TYR:HA	1:K:217:PRO:HD2	1.85	0.45
1:K:299:ILE:HA	1:K:314:GLY:HA3	1.99	0.45
1:L:46:GLN:CD	1:L:134:TYR:CE1	2.95	0.45
1:L:150:VAL:CG1	1:L:151:THR:N	2.80	0.45
1:A:206:VAL:HG12	1:A:207:SER:H	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:272:GLN:C	1:B:274:GLY:H	2.25	0.45
1:C:113:ASP:O	1:C:116:ALA:HB3	2.16	0.45
1:D:203:ALA:HB2	1:D:223:GLU:OE1	2.17	0.45
1:G:226:GLU:HG3	1:H:144:ARG:HE	1.82	0.45
1:K:103:ASP:C	1:K:105:ALA:N	2.75	0.45
1:K:187:LEU:H	1:K:187:LEU:HD12	1.81	0.45
1:B:196:LEU:HD23	1:B:261:GLU:HA	1.99	0.45
1:B:299:ILE:HA	1:B:314:GLY:HA3	1.99	0.45
1:C:38:PHE:CD1	1:C:174:TYR:CE2	2.99	0.45
1:C:108:LYS:HG3	1:I:104:GLN:HB3	1.99	0.45
1:C:147:ARG:NH2	1:D:176:ASP:OD1	2.49	0.45
1:D:207:SER:OG	1:D:258:GLN:OE1	2.33	0.45
1:E:86:ASN:O	1:E:89:SER:HB3	2.17	0.45
1:E:91:GLN:HA	1:E:118:TYR:CD1	2.52	0.45
1:E:106:VAL:HG23	1:E:110:GLN:OE1	2.17	0.45
1:E:206:VAL:HG21	1:E:222:LEU:CB	2.39	0.45
1:F:193:SER:OG	1:F:194:GLY:N	2.46	0.45
1:G:106:VAL:HG23	1:G:110:GLN:OE1	2.17	0.45
1:H:180:PRO:O	1:H:181:SER:C	2.59	0.45
1:K:216:TYR:CE2	1:K:218:LEU:HB2	2.51	0.45
1:M:68:LEU:HD13	1:M:145:ILE:HD12	1.99	0.45
1:A:55:LEU:H	1:A:55:LEU:CD1	2.16	0.45
1:B:230:ASP:O	1:B:234:GLY:N	2.50	0.45
1:C:106:VAL:HG23	1:C:110:GLN:OE1	2.17	0.45
1:E:55:LEU:H	1:E:55:LEU:CD1	2.12	0.45
1:E:120:GLN:O	1:E:123:ALA:HB3	2.17	0.45
1:E:178:THR:HG23	1:E:178:THR:O	2.17	0.45
1:F:47:VAL:HG13	1:F:134:TYR:HB2	1.99	0.45
1:G:203:ALA:HB2	1:G:223:GLU:HA	1.98	0.45
1:H:199:ALA:HB2	1:H:204:ALA:C	2.41	0.45
1:J:41:ALA:HB1	1:J:140:PRO:CG	2.47	0.45
1:M:38:PHE:C	1:M:38:PHE:CD2	2.95	0.45
1:M:38:PHE:CE1	1:M:172:PRO:HD2	2.52	0.45
1:D:92:GLU:CD	1:D:96:ARG:HH12	2.25	0.44
1:E:113:ASP:O	1:E:116:ALA:HB3	2.16	0.44
1:G:188:ARG:NH2	1:H:246:ASN:O	2.51	0.44
1:G:206:VAL:HG12	1:G:207:SER:N	2.31	0.44
1:K:190:GLU:HB3	1:K:196:LEU:HD13	1.99	0.44
1:G:45:PRO:HD3	1:G:164:MET:SD	2.56	0.44
1:K:208:LEU:HB2	1:K:242:PHE:CZ	2.52	0.44
1:M:134:TYR:O	1:M:136:LYS:N	2.49	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:184:LEU:HG	1:A:188:ARG:HD2	1.99	0.44
1:D:145:ILE:HB	1:D:167:VAL:HG22	1.98	0.44
1:F:206:VAL:HG12	1:F:207:SER:N	2.32	0.44
1:G:64:ALA:HB2	1:G:141:ILE:HA	1.99	0.44
1:H:55:LEU:H	1:H:55:LEU:CD1	2.11	0.44
1:H:208:LEU:HB2	1:H:242:PHE:CZ	2.52	0.44
1:H:216:TYR:CE2	1:H:218:LEU:HB2	2.52	0.44
1:A:225:SER:O	1:A:227:VAL:HG23	2.18	0.44
1:B:68:LEU:HD13	1:B:145:ILE:HD12	1.98	0.44
1:D:244:ASN:ND2	1:D:249:LEU:O	2.50	0.44
1:I:120:GLN:O	1:I:123:ALA:HB3	2.17	0.44
1:K:120:GLN:O	1:K:123:ALA:HB3	2.18	0.44
1:A:208:LEU:HD13	1:A:242:PHE:CE2	2.53	0.44
1:B:103:ASP:C	1:B:105:ALA:N	2.75	0.44
1:B:152:GLU:O	1:C:41:ALA:HA	2.17	0.44
1:C:185:LEU:O	1:C:189:ARG:HG3	2.18	0.44
1:C:202:ASN:O	1:C:224:PHE:HD2	2.00	0.44
1:E:45:PRO:HD3	1:E:164:MET:HG3	1.99	0.44
1:E:126:GLU:O	1:E:130:ILE:HG13	2.17	0.44
1:G:120:GLN:O	1:G:123:ALA:HB3	2.17	0.44
1:H:158:ASN:C	1:H:158:ASN:OD1	2.58	0.44
1:I:91:GLN:HA	1:I:118:TYR:CD1	2.53	0.44
1:K:91:GLN:HA	1:K:118:TYR:CD1	2.53	0.44
1:K:186:ARG:HH12	1:K:261:GLU:CD	2.26	0.44
1:K:188:ARG:NH1	1:L:246:ASN:O	2.46	0.44
1:L:64:ALA:HB2	1:L:142:SER:H	1.81	0.44
1:M:244:ASN:ND2	1:M:249:LEU:O	2.48	0.44
1:B:169:GLN:C	1:B:170:LEU:HD23	2.42	0.44
1:E:207:SER:OG	1:E:258:GLN:HB2	2.17	0.44
1:F:86:ASN:O	1:F:89:SER:HB3	2.17	0.44
1:F:137:VAL:O	1:F:138:LEU:HD23	2.18	0.44
1:I:103:ASP:C	1:I:105:ALA:N	2.76	0.44
1:J:203:ALA:HB2	1:J:223:GLU:HA	1.98	0.44
1:F:139:SER:OG	1:F:167:VAL:HG21	2.18	0.44
1:G:129:ARG:HG2	1:G:129:ARG:HH11	1.82	0.44
1:G:208:LEU:HD11	1:G:255:VAL:CG2	2.48	0.44
1:G:250:LEU:H	1:G:253:MET:CE	2.31	0.44
1:H:86:ASN:O	1:H:89:SER:HB3	2.17	0.44
1:K:247:ASN:OD1	1:K:250:LEU:HD21	2.18	0.44
1:M:208:LEU:HD11	1:M:255:VAL:HG21	2.00	0.44
1:E:158:ASN:O	1:E:160:GLN:N	2.49	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:198:ARG:HH11	1:I:198:ARG:CB	2.11	0.44
1:J:259:LEU:HD23	1:J:259:LEU:HA	1.85	0.44
1:K:212:ASP:OD2	1:K:212:ASP:C	2.61	0.44
1:L:206:VAL:HG11	1:L:257:ALA:HB1	2.00	0.44
1:M:38:PHE:CD1	1:M:172:PRO:HD2	2.52	0.44
1:B:57:LYS:HB3	1:B:60:SER:HB3	2.00	0.44
1:D:226:GLU:HG2	1:D:227:VAL:N	2.33	0.44
1:F:147:ARG:HG3	1:F:147:ARG:O	2.16	0.44
1:H:299:ILE:HA	1:H:314:GLY:HA3	1.99	0.44
1:I:272:GLN:C	1:I:274:GLY:H	2.26	0.44
1:A:175:VAL:HG21	1:A:242:PHE:CD2	2.49	0.43
1:D:57:LYS:HB3	1:D:60:SER:HB3	2.00	0.43
1:D:218:LEU:HD12	1:D:218:LEU:H	1.83	0.43
1:E:31:LEU:HB3	1:E:177:VAL:HG11	2.00	0.43
1:G:244:ASN:CG	1:G:249:LEU:HB2	2.43	0.43
1:H:101:VAL:HG12	1:H:106:VAL:O	2.18	0.43
1:K:183:ALA:O	1:K:187:LEU:HD12	2.17	0.43
1:A:103:ASP:C	1:A:105:ALA:N	2.76	0.43
1:A:207:SER:O	1:A:257:ALA:HA	2.17	0.43
1:C:55:LEU:HD12	1:C:68:LEU:O	2.18	0.43
1:C:246:ASN:HB3	1:C:248:GLU:OE2	2.18	0.43
1:C:247:ASN:OD1	1:C:250:LEU:HD21	2.18	0.43
1:D:49:GLY:O	1:D:155:LEU:HD12	2.17	0.43
1:D:188:ARG:O	1:D:191:LEU:HB3	2.17	0.43
1:J:64:ALA:HB2	1:J:142:SER:N	2.33	0.43
1:L:38:PHE:HB2	1:L:172:PRO:O	2.18	0.43
1:L:98:LYS:HG3	1:L:111:TYR:CZ	2.54	0.43
1:M:41:ALA:HB2	1:M:141:ILE:HG23	2.00	0.43
1:M:77:GLU:HA	1:M:132:LEU:HD22	2.01	0.43
1:B:77:GLU:HA	1:B:132:LEU:HD22	2.00	0.43
1:C:157:THR:O	1:C:160:GLN:HB3	2.19	0.43
1:D:91:GLN:HA	1:D:118:TYR:CD1	2.53	0.43
1:E:273:GLN:HA	1:F:331:PRO:O	2.18	0.43
1:H:140:PRO:C	1:H:141:ILE:CG2	2.91	0.43
1:M:103:ASP:C	1:M:105:ALA:N	2.77	0.43
1:F:92:GLU:OE2	1:F:96:ARG:NH1	2.52	0.43
1:F:288:VAL:HG13	1:F:288:VAL:O	2.17	0.43
1:H:91:GLN:HA	1:H:118:TYR:CD1	2.53	0.43
1:K:129:ARG:HG2	1:K:129:ARG:HH11	1.84	0.43
1:L:206:VAL:HG21	1:L:222:LEU:HB2	1.99	0.43
1:A:205:LYS:HD3	1:A:219:GLU:CD	2.43	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:46:GLN:NE2	1:B:134:TYR:CE1	2.86	0.43
1:B:184:LEU:HD22	1:B:236:VAL:HG11	1.99	0.43
1:B:202:ASN:O	1:B:224:PHE:HD2	2.02	0.43
1:C:64:ALA:HB2	1:C:141:ILE:C	2.44	0.43
1:C:193:SER:OG	1:C:194:GLY:N	2.50	0.43
1:E:92:GLU:OE2	1:E:96:ARG:NH1	2.52	0.43
1:E:299:ILE:HA	1:E:314:GLY:HA3	2.00	0.43
1:F:63:LYS:HA	1:F:142:SER:OG	2.18	0.43
1:F:208:LEU:HD12	1:F:256:HIS:O	2.18	0.43
1:H:129:ARG:HH11	1:H:129:ARG:HG2	1.83	0.43
1:I:244:ASN:ND2	1:I:247:ASN:HA	2.33	0.43
1:J:92:GLU:OE2	1:J:96:ARG:NH1	2.51	0.43
1:K:54:ARG:HD2	1:K:148:SER:HB2	2.00	0.43
1:K:195:GLN:O	1:K:196:LEU:HD12	2.18	0.43
1:A:231:GLU:O	1:A:232:GLY:C	2.62	0.43
1:B:92:GLU:OE2	1:B:96:ARG:NH1	2.52	0.43
1:F:195:GLN:HG2	1:F:261:GLU:O	2.18	0.43
1:I:47:VAL:N	1:I:158:ASN:HB2	2.34	0.43
1:I:170:LEU:HD22	1:I:251:PRO:HD3	2.01	0.43
1:J:272:GLN:C	1:J:274:GLY:H	2.26	0.43
1:M:226:GLU:OE1	1:M:228:SER:N	2.52	0.43
1:M:241:VAL:O	1:M:241:VAL:HG12	2.19	0.43
1:A:121:SER:O	1:A:122:LYS:C	2.62	0.43
1:D:55:LEU:H	1:D:55:LEU:CD1	2.20	0.43
1:F:272:GLN:HB2	1:F:309:TRP:CD1	2.53	0.43
1:I:38:PHE:CD2	1:I:169:GLN:NE2	2.87	0.43
1:I:210:LEU:HD21	1:I:249:LEU:HD21	2.01	0.43
1:I:229:VAL:HG11	1:J:251:PRO:O	2.19	0.43
1:J:231:GLU:HG3	1:K:251:PRO:CB	2.49	0.43
1:M:272:GLN:C	1:M:274:GLY:H	2.26	0.43
1:A:98:LYS:HG3	1:A:111:TYR:CZ	2.53	0.43
1:C:34:ARG:HH12	1:C:252:GLY:CA	2.30	0.43
1:E:98:LYS:HG3	1:E:111:TYR:CZ	2.54	0.43
1:E:254:PHE:CD2	1:E:254:PHE:N	2.85	0.43
1:I:144:ARG:HD2	1:I:170:LEU:HD12	2.00	0.43
1:J:48:ASN:OD1	1:J:157:THR:HA	2.19	0.43
1:J:100:LEU:C	1:J:106:VAL:HG12	2.44	0.43
1:B:208:LEU:HD11	1:B:255:VAL:HG21	2.01	0.43
1:D:190:GLU:CB	1:D:196:LEU:HD13	2.41	0.43
1:E:193:SER:OG	1:E:194:GLY:N	2.52	0.43
1:F:275:VAL:CG1	1:F:299:ILE:HD11	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:57:LYS:HB3	1:G:60:SER:HB3	2.01	0.43
1:C:208:LEU:HD12	1:C:256:HIS:O	2.19	0.43
1:E:121:SER:O	1:E:122:LYS:C	2.62	0.43
1:E:244:ASN:CG	1:E:249:LEU:HB2	2.43	0.43
1:E:272:GLN:C	1:E:274:GLY:H	2.26	0.43
1:F:98:LYS:HG3	1:F:111:TYR:CZ	2.54	0.43
1:H:206:VAL:O	1:H:219:GLU:HG3	2.19	0.43
1:H:218:LEU:H	1:H:218:LEU:HD22	1.84	0.43
1:K:180:PRO:O	1:K:181:SER:C	2.61	0.43
1:K:290:ALA:C	1:K:292:ASN:H	2.27	0.43
1:M:137:VAL:O	1:M:137:VAL:HG12	2.19	0.43
1:A:45:PRO:HG3	1:A:156:VAL:HB	2.00	0.42
1:A:226:GLU:C	1:A:226:GLU:OE1	2.62	0.42
1:C:38:PHE:HB2	1:C:172:PRO:O	2.18	0.42
1:E:226:GLU:OE1	1:E:229:VAL:HG23	2.19	0.42
1:G:86:ASN:O	1:G:89:SER:HB3	2.19	0.42
1:G:230:ASP:O	1:G:234:GLY:N	2.41	0.42
1:H:103:ASP:C	1:H:105:ALA:N	2.76	0.42
1:H:290:ALA:C	1:H:292:ASN:H	2.27	0.42
1:J:91:GLN:HA	1:J:118:TYR:CD1	2.54	0.42
1:J:129:ARG:HG2	1:J:129:ARG:NH1	2.34	0.42
1:L:45:PRO:HG3	1:L:156:VAL:HB	2.01	0.42
1:L:87:LEU:O	1:L:88:ALA:C	2.62	0.42
1:B:98:LYS:HG3	1:B:111:TYR:CZ	2.54	0.42
1:B:147:ARG:HH11	1:B:147:ARG:CB	2.32	0.42
1:B:230:ASP:C	1:B:232:GLY:N	2.75	0.42
1:B:244:ASN:CG	1:B:249:LEU:HB2	2.43	0.42
1:C:52:LEU:HD23	1:C:52:LEU:HA	1.86	0.42
1:D:86:ASN:O	1:D:89:SER:HB3	2.18	0.42
1:E:34:ARG:HH11	1:E:34:ARG:CG	2.32	0.42
1:H:191:LEU:O	1:H:191:LEU:HD12	2.19	0.42
1:H:204:ALA:O	1:H:206:VAL:HG23	2.19	0.42
1:J:216:TYR:OH	1:J:243:PRO:O	2.33	0.42
1:B:91:GLN:HA	1:B:118:TYR:CD1	2.54	0.42
1:C:231:GLU:H	1:C:231:GLU:HG3	1.57	0.42
1:D:121:SER:O	1:D:122:LYS:C	2.62	0.42
1:G:193:SER:OG	1:G:194:GLY:N	2.51	0.42
1:H:55:LEU:HD12	1:H:68:LEU:O	2.19	0.42
1:L:48:ASN:OD1	1:L:157:THR:HA	2.19	0.42
1:M:38:PHE:C	1:M:38:PHE:HD2	2.28	0.42
1:M:38:PHE:HD2	1:M:38:PHE:O	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:129:ARG:HH11	1:A:129:ARG:HG2	1.85	0.42
1:B:64:ALA:HB2	1:B:142:SER:N	2.34	0.42
1:E:158:ASN:C	1:E:160:GLN:N	2.78	0.42
1:F:126:GLU:O	1:F:130:ILE:HG13	2.20	0.42
1:F:299:ILE:HG22	1:F:314:GLY:HA3	2.01	0.42
1:I:129:ARG:HG2	1:I:129:ARG:NH1	2.33	0.42
1:B:199:ALA:HB2	1:B:204:ALA:C	2.44	0.42
1:C:185:LEU:HD12	1:C:185:LEU:HA	1.83	0.42
1:D:31:LEU:HB2	1:D:257:ALA:HB3	2.01	0.42
1:G:134:TYR:OH	1:H:74:ALA:CB	2.68	0.42
1:H:126:GLU:O	1:H:130:ILE:HG13	2.19	0.42
1:H:259:LEU:HD23	1:H:260:GLN:H	1.84	0.42
1:K:48:ASN:O	1:K:76:TYR:OH	2.34	0.42
1:K:272:GLN:C	1:K:274:GLY:H	2.27	0.42
1:M:230:ASP:C	1:M:232:GLY:N	2.77	0.42
1:A:173:ILE:HG22	1:A:242:PHE:O	2.20	0.42
1:C:103:ASP:C	1:C:105:ALA:N	2.77	0.42
1:D:92:GLU:CD	1:D:96:ARG:NH1	2.77	0.42
1:E:126:GLU:OE2	1:E:129:ARG:NH2	2.52	0.42
1:F:174:TYR:CD1	1:F:241:VAL:HG22	2.55	0.42
1:F:272:GLN:C	1:F:274:GLY:H	2.27	0.42
1:G:191:LEU:N	1:G:196:LEU:HD22	2.35	0.42
1:J:120:GLN:O	1:J:123:ALA:HB3	2.19	0.42
1:K:77:GLU:HA	1:K:132:LEU:HD22	2.00	0.42
1:K:150:VAL:HG23	1:K:154:ALA:HB3	2.01	0.42
1:K:196:LEU:HD12	1:K:261:GLU:HA	2.01	0.42
1:B:250:LEU:HD12	1:C:236:VAL:HG21	2.01	0.42
1:C:121:SER:O	1:C:122:LYS:C	2.62	0.42
1:J:109:GLN:O	1:J:112:ALA:HB3	2.19	0.42
1:J:180:PRO:O	1:J:181:SER:C	2.63	0.42
1:L:218:LEU:HD12	1:L:243:PRO:HB2	2.02	0.42
1:M:16:GLY:HA2	1:M:338:VAL:O	2.20	0.42
1:A:225:SER:O	1:A:226:GLU:C	2.63	0.42
1:B:103:ASP:O	1:B:105:ALA:N	2.53	0.42
1:B:263:VAL:O	1:B:265:GLN:N	2.53	0.42
1:D:46:GLN:HB2	1:D:134:TYR:CD1	2.55	0.42
1:E:212:ASP:OD1	1:E:212:ASP:C	2.62	0.42
1:H:191:LEU:HD12	1:H:191:LEU:C	2.44	0.42
1:K:132:LEU:O	1:K:135:THR:HG23	2.19	0.42
1:K:181:SER:HB3	1:L:253:MET:HE3	2.02	0.42
1:L:91:GLN:HA	1:L:118:TYR:CD1	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:250:LEU:N	1:A:253:MET:SD	2.88	0.42
1:D:77:GLU:HA	1:D:132:LEU:HD22	2.01	0.42
1:G:41:ALA:CB	1:G:140:PRO:HG2	2.50	0.42
1:H:67:GLN:HA	1:H:138:LEU:HD23	2.01	0.42
1:H:145:ILE:HG23	1:H:145:ILE:O	2.19	0.42
1:J:121:SER:O	1:J:122:LYS:C	2.63	0.42
1:J:216:TYR:HA	1:J:217:PRO:HD2	1.86	0.42
1:K:109:GLN:O	1:K:112:ALA:HB3	2.19	0.42
1:L:190:GLU:HB3	1:L:196:LEU:HD13	2.02	0.42
1:L:206:VAL:HG12	1:L:207:SER:N	2.35	0.42
1:B:100:LEU:C	1:B:106:VAL:HG12	2.44	0.42
1:B:126:GLU:O	1:B:130:ILE:HG13	2.19	0.42
1:C:180:PRO:O	1:C:181:SER:C	2.63	0.42
1:C:250:LEU:HD12	1:D:236:VAL:HG21	2.01	0.42
1:D:47:VAL:HG13	1:D:134:TYR:CB	2.50	0.42
1:H:206:VAL:HG12	1:H:207:SER:N	2.35	0.42
1:I:35:THR:OG1	1:I:253:MET:HB2	2.20	0.42
1:I:86:ASN:O	1:I:89:SER:HB3	2.20	0.42
1:J:50:ILE:HD13	1:J:155:LEU:HA	2.02	0.42
1:K:67:GLN:CD	1:K:136:LYS:HD3	2.44	0.42
1:K:121:SER:O	1:K:122:LYS:C	2.62	0.42
1:L:92:GLU:OE2	1:L:96:ARG:NH1	2.53	0.42
1:M:121:SER:O	1:M:122:LYS:C	2.62	0.42
1:M:290:ALA:C	1:M:292:ASN:H	2.28	0.42
1:D:101:VAL:HG12	1:D:106:VAL:O	2.20	0.41
1:E:68:LEU:HD13	1:E:145:ILE:CD1	2.50	0.41
1:E:199:ALA:HB2	1:E:204:ALA:C	2.45	0.41
1:E:260:GLN:OE1	1:E:260:GLN:CA	2.67	0.41
1:G:56:PHE:CZ	1:G:148:SER:HB2	2.55	0.41
1:I:126:GLU:O	1:I:130:ILE:HG13	2.20	0.41
1:K:63:LYS:O	1:K:66:GLN:HB2	2.20	0.41
1:K:218:LEU:N	1:K:218:LEU:HD23	2.34	0.41
1:M:52:LEU:HD23	1:M:52:LEU:HA	1.88	0.41
1:M:98:LYS:HG3	1:M:111:TYR:CZ	2.55	0.41
1:M:170:LEU:HD13	1:M:251:PRO:HD3	2.01	0.41
1:M:182:THR:OG1	1:M:183:ALA:N	2.53	0.41
1:M:246:ASN:HB2	1:M:248:GLU:HG3	2.03	0.41
1:B:48:ASN:OD1	1:B:158:ASN:N	2.53	0.41
1:C:86:ASN:O	1:C:89:SER:HB3	2.20	0.41
1:C:272:GLN:C	1:C:274:GLY:H	2.27	0.41
1:D:129:ARG:HG2	1:D:129:ARG:NH1	2.34	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:38:PHE:CD1	1:G:174:TYR:CE2	3.08	0.41
1:H:272:GLN:C	1:H:274:GLY:H	2.26	0.41
1:I:116:ALA:O	1:I:120:GLN:HG3	2.19	0.41
1:J:227:VAL:HG23	1:J:237:THR:O	2.19	0.41
1:L:103:ASP:C	1:L:105:ALA:N	2.78	0.41
1:M:45:PRO:HD3	1:M:164:MET:SD	2.60	0.41
1:A:55:LEU:HD12	1:A:68:LEU:O	2.20	0.41
1:C:57:LYS:HB3	1:C:60:SER:HB3	2.02	0.41
1:E:41:ALA:CB	1:E:140:PRO:HG2	2.50	0.41
1:G:77:GLU:HA	1:G:132:LEU:HD22	2.02	0.41
1:G:193:SER:HG	1:G:194:GLY:H	1.67	0.41
1:I:40:ILE:HD13	1:I:168:GLN:HE21	1.85	0.41
1:I:114:ALA:C	1:I:116:ALA:N	2.76	0.41
1:J:71:ILE:O	1:J:73:PRO:HD3	2.20	0.41
1:J:98:LYS:HG3	1:J:111:TYR:CZ	2.55	0.41
1:B:290:ALA:C	1:B:292:ASN:H	2.28	0.41
1:C:203:ALA:HB2	1:C:223:GLU:HA	2.02	0.41
1:D:171:ASP:OD1	1:D:244:ASN:N	2.50	0.41
1:E:176:ASP:OD2	1:E:239:ARG:HG2	2.20	0.41
1:G:91:GLN:HA	1:G:118:TYR:CD1	2.55	0.41
1:G:92:GLU:OE2	1:G:96:ARG:NH1	2.53	0.41
1:I:64:ALA:HA	1:I:141:ILE:O	2.20	0.41
1:I:77:GLU:HA	1:I:132:LEU:HD22	2.02	0.41
1:J:56:PHE:HZ	1:J:148:SER:HB2	1.85	0.41
1:J:203:ALA:HB2	1:J:223:GLU:OE1	2.20	0.41
1:L:208:LEU:HB2	1:L:242:PHE:CE1	2.54	0.41
1:L:244:ASN:ND2	1:L:249:LEU:O	2.50	0.41
1:M:171:ASP:OD1	1:M:244:ASN:C	2.64	0.41
1:C:104:GLN:HB3	1:I:108:LYS:HG3	2.01	0.41
1:C:216:TYR:HA	1:C:217:PRO:HD2	1.87	0.41
1:E:34:ARG:NH1	1:E:254:PHE:CD2	2.89	0.41
1:F:103:ASP:C	1:F:105:ALA:N	2.78	0.41
1:G:187:LEU:HD22	1:G:259:LEU:CD2	2.50	0.41
1:I:92:GLU:OE2	1:I:96:ARG:NH1	2.53	0.41
1:I:121:SER:O	1:I:122:LYS:C	2.64	0.41
1:K:230:ASP:C	1:K:232:GLY:N	2.78	0.41
1:L:100:LEU:C	1:L:106:VAL:HG12	2.46	0.41
1:L:101:VAL:HG12	1:L:106:VAL:O	2.20	0.41
1:L:244:ASN:N	1:L:245:PRO:CD	2.83	0.41
1:A:186:ARG:HH11	1:A:187:LEU:CD2	2.29	0.41
1:A:219:GLU:HG3	1:A:220:GLY:H	1.84	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:228:SER:HB3	1:A:237:THR:HB	2.02	0.41
1:B:240:ALA:CB	1:B:242:PHE:HE2	2.34	0.41
1:C:77:GLU:HA	1:C:132:LEU:HD22	2.01	0.41
1:D:150:VAL:HG22	1:D:151:THR:N	2.36	0.41
1:H:205:LYS:C	1:H:206:VAL:HG23	2.46	0.41
1:I:184:LEU:O	1:I:184:LEU:HD12	2.20	0.41
1:I:187:LEU:N	1:I:187:LEU:HD23	2.35	0.41
1:J:94:ALA:O	1:J:95:GLN:C	2.63	0.41
1:K:216:TYR:CZ	1:K:249:LEU:HD11	2.56	0.41
1:L:185:LEU:CD2	1:M:210:LEU:HD13	2.50	0.41
1:A:54:ARG:N	1:A:152:GLU:OE2	2.54	0.41
1:B:16:GLY:HA2	1:B:338:VAL:O	2.20	0.41
1:F:43:VAL:HG23	1:F:165:ALA:C	2.45	0.41
1:F:206:VAL:CG1	1:F:207:SER:N	2.84	0.41
1:H:41:ALA:CB	1:H:140:PRO:HG2	2.51	0.41
1:J:23:GLN:O	1:J:266:LYS:HA	2.21	0.41
1:K:57:LYS:HB3	1:K:60:SER:HB3	2.02	0.41
1:K:183:ALA:O	1:K:186:ARG:HB3	2.20	0.41
1:B:121:SER:O	1:B:122:LYS:C	2.63	0.41
1:B:144:ARG:HG3	1:B:144:ARG:HH11	1.86	0.41
1:D:51:ILE:HD11	1:D:164:MET:CE	2.50	0.41
1:D:244:ASN:HD21	1:D:249:LEU:N	2.18	0.41
1:E:206:VAL:HG12	1:E:207:SER:N	2.36	0.41
1:H:38:PHE:HD2	1:H:169:GLN:NE2	2.18	0.41
1:H:44:ARG:HD2	1:I:153:GLY:O	2.21	0.41
1:M:126:GLU:O	1:M:130:ILE:HG13	2.20	0.41
1:A:202:ASN:C	1:A:202:ASN:ND2	2.79	0.41
1:B:120:GLN:O	1:B:123:ALA:HB3	2.21	0.41
1:C:216:TYR:CE2	1:C:218:LEU:HB2	2.56	0.41
1:D:64:ALA:HB2	1:D:141:ILE:HA	2.02	0.41
1:E:16:GLY:HA2	1:E:338:VAL:O	2.21	0.41
1:F:81:GLN:HB3	1:G:82:SER:HA	2.03	0.41
1:F:203:ALA:HB2	1:F:223:GLU:HA	2.03	0.41
1:F:299:ILE:CG2	1:F:315:LEU:HG	2.51	0.41
1:J:34:ARG:NE	1:J:254:PHE:CE1	2.89	0.41
1:J:86:ASN:O	1:J:89:SER:HB3	2.21	0.41
1:J:103:ASP:C	1:J:105:ALA:N	2.78	0.41
1:L:130:ILE:HG21	1:M:74:ALA:HB1	2.01	0.41
1:L:208:LEU:HD22	1:L:242:PHE:CD2	2.56	0.41
1:M:54:ARG:HD2	1:M:148:SER:HB2	2.03	0.41
1:M:206:VAL:HG21	1:M:222:LEU:HB2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:91:GLN:HA	1:C:118:TYR:CD1	2.55	0.41
1:D:103:ASP:C	1:D:105:ALA:N	2.78	0.41
1:F:46:GLN:C	1:F:158:ASN:ND2	2.79	0.41
1:G:38:PHE:HD2	1:G:169:GLN:NE2	2.18	0.41
1:J:52:LEU:HD23	1:J:52:LEU:HA	1.85	0.41
1:J:55:LEU:HD12	1:J:68:LEU:O	2.21	0.41
1:K:40:ILE:HG12	1:K:168:GLN:HG2	2.02	0.41
1:L:150:VAL:HG12	1:L:151:THR:N	2.36	0.41
1:A:52:LEU:HD23	1:A:52:LEU:HA	1.87	0.40
1:A:57:LYS:HB3	1:A:60:SER:HB3	2.02	0.40
1:C:16:GLY:HA2	1:C:338:VAL:O	2.22	0.40
1:D:64:ALA:HB2	1:D:141:ILE:CA	2.52	0.40
1:D:173:ILE:HG12	1:D:174:TYR:H	1.86	0.40
1:E:290:ALA:C	1:E:292:ASN:H	2.28	0.40
1:G:190:GLU:OE1	1:G:196:LEU:HD11	2.20	0.40
1:G:200:GLY:HA3	1:G:221:ARG:NH2	2.36	0.40
1:I:208:LEU:HB2	1:I:242:PHE:CZ	2.55	0.40
1:J:69:TYR:HB2	1:J:137:VAL:HB	2.02	0.40
1:L:23:GLN:O	1:L:266:LYS:HA	2.21	0.40
1:L:57:LYS:HB3	1:L:60:SER:HB3	2.04	0.40
1:C:92:GLU:CD	1:C:96:ARG:HH12	2.28	0.40
1:C:190:GLU:HB3	1:C:196:LEU:CD1	2.40	0.40
1:E:54:ARG:HD2	1:E:148:SER:CB	2.51	0.40
1:F:129:ARG:HG2	1:F:129:ARG:NH1	2.37	0.40
1:F:190:GLU:HB3	1:F:196:LEU:HD13	2.03	0.40
1:I:100:LEU:C	1:I:106:VAL:HG12	2.46	0.40
1:C:96:ARG:CZ	1:D:109:GLN:OE1	2.69	0.40
1:C:244:ASN:ND2	1:C:247:ASN:HA	2.37	0.40
1:D:183:ALA:O	1:D:187:LEU:HG	2.22	0.40
1:D:230:ASP:O	1:D:231:GLU:C	2.64	0.40
1:E:100:LEU:C	1:E:106:VAL:HG12	2.47	0.40
1:E:129:ARG:HG2	1:E:129:ARG:HH11	1.85	0.40
1:E:222:LEU:HA	1:E:240:ALA:HA	2.02	0.40
1:G:50:ILE:HD13	1:G:155:LEU:HB2	2.02	0.40
1:G:144:ARG:HG3	1:G:144:ARG:NH1	2.36	0.40
1:G:162:ASN:HD22	1:G:162:ASN:HA	1.64	0.40
1:G:166:THR:HG22	1:G:167:VAL:N	2.36	0.40
1:G:272:GLN:C	1:G:274:GLY:H	2.28	0.40
1:G:290:ALA:C	1:G:292:ASN:H	2.29	0.40
1:H:170:LEU:HD23	1:H:170:LEU:N	2.35	0.40
1:I:194:GLY:C	1:I:196:LEU:H	2.29	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:249:LEU:HD23	1:I:253:MET:HE1	2.02	0.40
1:K:55:LEU:H	1:K:55:LEU:CD1	2.21	0.40
1:M:202:ASN:O	1:M:224:PHE:CD2	2.71	0.40
1:D:100:LEU:C	1:D:106:VAL:HG12	2.47	0.40
1:H:230:ASP:C	1:H:232:GLY:N	2.77	0.40
1:I:91:GLN:HG2	1:I:95:GLN:OE1	2.22	0.40
1:A:206:VAL:CG1	1:A:207:SER:N	2.85	0.40
1:F:73:PRO:O	1:F:77:GLU:HB3	2.22	0.40
1:F:86:ASN:ND2	1:F:121:SER:OG	2.54	0.40
1:F:91:GLN:HA	1:F:118:TYR:CD1	2.55	0.40
1:F:203:ALA:HB2	1:F:223:GLU:CD	2.46	0.40
1:G:230:ASP:C	1:G:232:GLY:N	2.79	0.40
1:H:159:GLY:O	1:H:160:GLN:C	2.63	0.40
1:H:176:ASP:OD1	1:H:239:ARG:HG2	2.22	0.40
1:I:38:PHE:HD2	1:I:169:GLN:NE2	2.18	0.40
1:I:290:ALA:C	1:I:292:ASN:H	2.29	0.40
1:K:200:GLY:O	1:K:202:ASN:N	2.54	0.40
1:L:51:ILE:HG13	1:L:150:VAL:CG1	2.51	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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	230/360 (64%)	191 (83%)	33 (14%)	6 (3%)	4	26
1	B	325/360 (90%)	284 (87%)	32 (10%)	9 (3%)	4	25
1	C	325/360 (90%)	279 (86%)	40 (12%)	6 (2%)	6	34
1	D	228/360 (63%)	195 (86%)	31 (14%)	2 (1%)	14	47
1	E	325/360 (90%)	280 (86%)	38 (12%)	7 (2%)	5	29
1	F	325/360 (90%)	277 (85%)	43 (13%)	5 (2%)	8	37

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	G	325/360 (90%)	277 (85%)	41 (13%)	7 (2%)	5	29
1	H	325/360 (90%)	288 (89%)	32 (10%)	5 (2%)	8	37
1	I	325/360 (90%)	281 (86%)	38 (12%)	6 (2%)	6	34
1	J	325/360 (90%)	277 (85%)	43 (13%)	5 (2%)	8	37
1	K	325/360 (90%)	285 (88%)	34 (10%)	6 (2%)	6	34
1	L	325/360 (90%)	279 (86%)	41 (13%)	5 (2%)	8	37
1	M	325/360 (90%)	285 (88%)	32 (10%)	8 (2%)	4	27
All	All	4033/4680 (86%)	3478 (86%)	478 (12%)	77 (2%)	6	33

All (77) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	201	ASP
1	E	160	GLN
1	G	149	ALA
1	C	329	VAL
1	E	329	VAL
1	F	329	VAL
1	G	329	VAL
1	I	329	VAL
1	J	329	VAL
1	L	329	VAL
1	M	143	GLY
1	M	161	ALA
1	A	198	ARG
1	A	231	GLU
1	B	329	VAL
1	H	329	VAL
1	K	193	SER
1	K	201	ASP
1	K	329	VAL
1	M	329	VAL
1	A	214	SER
1	B	193	SER
1	B	201	ASP
1	B	231	GLU
1	C	194	GLY
1	C	319	ASP
1	D	161	ALA
1	D	232	GLY

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Mol	Chain	Res	Type
1	E	181	SER
1	E	193	SER
1	F	194	GLY
1	G	194	GLY
1	G	265	GLN
1	H	181	SER
1	H	193	SER
1	I	194	GLY
1	I	265	GLN
1	J	193	SER
1	J	194	GLY
1	L	193	SER
1	L	194	GLY
1	M	201	ASP
1	B	197	GLU
1	B	264	LYS
1	C	193	SER
1	G	193	SER
1	J	181	SER
1	K	181	SER
1	L	319	ASP
1	M	181	SER
1	B	104	GLN
1	F	193	SER
1	G	319	ASP
1	I	55	LEU
1	M	193	SER
1	A	217	PRO
1	A	232	GLY
1	E	159	GLY
1	B	281	GLY
1	B	325	GLY
1	C	281	GLY
1	E	281	GLY
1	E	325	GLY
1	F	281	GLY
1	G	281	GLY
1	H	281	GLY
1	H	325	GLY
1	I	281	GLY
1	J	281	GLY
1	K	281	GLY

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Mol	Chain	Res	Type
1	K	325	GLY
1	L	281	GLY
1	M	281	GLY
1	M	325	GLY
1	I	335	VAL
1	C	335	VAL
1	F	335	VAL

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	186/287 (65%)	179 (96%)	7 (4%)	29	62
1	B	193/287 (67%)	184 (95%)	9 (5%)	23	57
1	C	190/287 (66%)	176 (93%)	14 (7%)	13	43
1	D	185/287 (64%)	175 (95%)	10 (5%)	20	53
1	E	194/287 (68%)	173 (89%)	21 (11%)	6	27
1	F	240/287 (84%)	229 (95%)	11 (5%)	24	58
1	G	190/287 (66%)	185 (97%)	5 (3%)	40	69
1	H	194/287 (68%)	180 (93%)	14 (7%)	13	44
1	I	190/287 (66%)	174 (92%)	16 (8%)	10	38
1	J	189/287 (66%)	174 (92%)	15 (8%)	11	40
1	K	194/287 (68%)	184 (95%)	10 (5%)	21	54
1	L	190/287 (66%)	176 (93%)	14 (7%)	13	43
1	M	196/287 (68%)	180 (92%)	16 (8%)	10	39
All	All	2531/3731 (68%)	2369 (94%)	162 (6%)	16	48

All (162) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	55	LEU

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Mol	Chain	Res	Type
1	A	75	THR
1	A	101	VAL
1	A	144	ARG
1	A	151	THR
1	A	152	GLU
1	A	226	GLU
1	B	35	THR
1	B	55	LEU
1	B	75	THR
1	B	101	VAL
1	B	147	ARG
1	B	151	THR
1	B	155	LEU
1	B	211	GLU
1	B	219	GLU
1	C	31	LEU
1	C	34	ARG
1	C	43	VAL
1	C	55	LEU
1	C	75	THR
1	C	101	VAL
1	C	138	LEU
1	C	141	ILE
1	C	152	GLU
1	C	201	ASP
1	C	226	GLU
1	C	227	VAL
1	C	231	GLU
1	C	259	LEU
1	D	55	LEU
1	D	73	PRO
1	D	75	THR
1	D	101	VAL
1	D	152	GLU
1	D	156	VAL
1	D	157	THR
1	D	178	THR
1	D	226	GLU
1	D	238	ILE
1	E	28	ASN
1	E	55	LEU
1	E	73	PRO

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Mol	Chain	Res	Type
1	E	75	THR
1	E	101	VAL
1	E	147	ARG
1	E	151	THR
1	E	155	LEU
1	E	166	THR
1	E	177	VAL
1	E	193	SER
1	E	196	LEU
1	E	211	GLU
1	E	218	LEU
1	E	225	SER
1	E	226	GLU
1	E	227	VAL
1	E	237	THR
1	E	247	ASN
1	E	259	LEU
1	E	260	GLN
1	F	43	VAL
1	F	55	LEU
1	F	75	THR
1	F	101	VAL
1	F	147	ARG
1	F	150	VAL
1	F	211	GLU
1	F	226	GLU
1	F	227	VAL
1	F	231	GLU
1	F	277	ARG
1	G	55	LEU
1	G	75	THR
1	G	101	VAL
1	G	226	GLU
1	G	227	VAL
1	H	30	GLU
1	H	55	LEU
1	H	75	THR
1	H	101	VAL
1	H	151	THR
1	H	195	GLN
1	H	196	LEU
1	H	202	ASN

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Mol	Chain	Res	Type
1	H	225	SER
1	H	226	GLU
1	H	227	VAL
1	H	229	VAL
1	H	247	ASN
1	H	259	LEU
1	I	34	ARG
1	I	35	THR
1	I	55	LEU
1	I	75	THR
1	I	101	VAL
1	I	138	LEU
1	I	152	GLU
1	I	156	VAL
1	I	177	VAL
1	I	187	LEU
1	I	196	LEU
1	I	198	ARG
1	I	223	GLU
1	I	226	GLU
1	I	237	THR
1	I	247	ASN
1	J	55	LEU
1	J	75	THR
1	J	101	VAL
1	J	150	VAL
1	J	152	GLU
1	J	177	VAL
1	J	181	SER
1	J	206	VAL
1	J	227	VAL
1	J	229	VAL
1	J	233	THR
1	J	236	VAL
1	J	237	THR
1	J	247	ASN
1	J	259	LEU
1	K	55	LEU
1	K	75	THR
1	K	101	VAL
1	K	150	VAL
1	K	193	SER

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Mol	Chain	Res	Type
1	K	197	GLU
1	K	201	ASP
1	K	222	LEU
1	K	229	VAL
1	K	259	LEU
1	L	34	ARG
1	L	55	LEU
1	L	75	THR
1	L	101	VAL
1	L	151	THR
1	L	152	GLU
1	L	178	THR
1	L	202	ASN
1	L	221	ARG
1	L	222	LEU
1	L	227	VAL
1	L	231	GLU
1	L	247	ASN
1	L	259	LEU
1	M	35	THR
1	M	55	LEU
1	M	75	THR
1	M	101	VAL
1	M	138	LEU
1	M	151	THR
1	M	152	GLU
1	M	185	LEU
1	M	193	SER
1	M	196	LEU
1	M	198	ARG
1	M	222	LEU
1	M	226	GLU
1	M	239	ARG
1	M	247	ASN
1	M	259	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (101) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	36	ASN
1	A	86	ASN
1	A	104	GLN

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Mol	Chain	Res	Type
1	A	109	GLN
1	A	160	GLN
1	A	162	ASN
1	A	202	ASN
1	A	215	GLN
1	B	46	GLN
1	B	86	ASN
1	B	93	GLN
1	B	127	GLN
1	B	162	ASN
1	B	215	GLN
1	B	258	GLN
1	B	260	GLN
1	C	46	GLN
1	C	86	ASN
1	C	109	GLN
1	C	115	ASN
1	C	127	GLN
1	C	162	ASN
1	C	179	GLN
1	C	202	ASN
1	D	46	GLN
1	D	86	ASN
1	D	104	GLN
1	D	127	GLN
1	D	162	ASN
1	D	179	GLN
1	D	215	GLN
1	E	86	ASN
1	E	115	ASN
1	E	127	GLN
1	E	168	GLN
1	E	169	GLN
1	E	179	GLN
1	E	195	GLN
1	F	84	GLN
1	F	86	ASN
1	F	127	GLN
1	F	162	ASN
1	F	169	GLN
1	F	195	GLN
1	F	272	GLN

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Mol	Chain	Res	Type
1	F	291	GLN
1	G	46	GLN
1	G	84	GLN
1	G	109	GLN
1	G	115	ASN
1	G	127	GLN
1	G	162	ASN
1	G	169	GLN
1	G	179	GLN
1	H	36	ASN
1	H	46	GLN
1	H	84	GLN
1	H	86	ASN
1	H	93	GLN
1	H	162	ASN
1	H	169	GLN
1	I	67	GLN
1	I	70	GLN
1	I	86	ASN
1	I	104	GLN
1	I	127	GLN
1	I	162	ASN
1	I	168	GLN
1	J	46	GLN
1	J	86	ASN
1	J	104	GLN
1	J	127	GLN
1	J	162	ASN
1	J	247	ASN
1	K	46	GLN
1	K	86	ASN
1	K	104	GLN
1	K	109	GLN
1	K	127	GLN
1	K	162	ASN
1	K	195	GLN
1	K	256	HIS
1	K	260	GLN
1	L	46	GLN
1	L	86	ASN
1	L	93	GLN
1	L	115	ASN

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Mol	Chain	Res	Type
1	L	162	ASN
1	L	168	GLN
1	L	169	GLN
1	L	247	ASN
1	M	36	ASN
1	M	46	GLN
1	M	84	GLN
1	M	86	ASN
1	M	109	GLN
1	M	115	ASN
1	M	169	GLN
1	M	179	GLN
1	M	247	ASN
1	M	258	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

16 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
2	SO4	C	1340	-	4,4,4	0.42	0	6,6,6	0.13	0
2	SO4	F	1340	-	4,4,4	0.41	0	6,6,6	0.19	0
2	SO4	A	1260	-	4,4,4	0.48	0	6,6,6	0.13	0
2	SO4	B	1341	-	4,4,4	0.41	0	6,6,6	0.12	0
2	SO4	F	1341	-	4,4,4	0.45	0	6,6,6	0.11	0
2	SO4	G	1340	-	4,4,4	0.44	0	6,6,6	0.11	0
2	SO4	J	1340	-	4,4,4	0.44	0	6,6,6	0.10	0
2	SO4	E	1340	-	4,4,4	0.47	0	6,6,6	0.15	0
2	SO4	L	1340	-	4,4,4	0.44	0	6,6,6	0.12	0
2	SO4	H	1340	-	4,4,4	0.46	0	6,6,6	0.12	0
2	SO4	E	1341	-	4,4,4	0.40	0	6,6,6	0.14	0
2	SO4	B	1340	-	4,4,4	0.46	0	6,6,6	0.19	0
2	SO4	A	1261	-	4,4,4	0.47	0	6,6,6	0.12	0
2	SO4	M	1340	-	4,4,4	0.45	0	6,6,6	0.13	0
2	SO4	K	1340	-	4,4,4	0.49	0	6,6,6	0.17	0
2	SO4	I	1340	-	4,4,4	0.48	0	6,6,6	0.10	0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	1340	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	232/360 (64%)	0.88	29 (12%) 8 6	34, 77, 127, 155	0
1	B	327/360 (90%)	1.23	87 (26%) 1 1	22, 71, 145, 153	0
1	C	327/360 (90%)	1.13	85 (25%) 1 2	20, 73, 141, 158	0
1	D	230/360 (63%)	0.48	25 (10%) 10 7	16, 59, 87, 110	0
1	E	327/360 (90%)	0.84	81 (24%) 2 2	9, 53, 148, 157	0
1	F	327/360 (90%)	0.95	54 (16%) 4 3	28, 66, 131, 148	0
1	G	327/360 (90%)	1.42	99 (30%) 1 1	34, 82, 147, 163	0
1	H	327/360 (90%)	1.18	101 (30%) 1 1	13, 56, 154, 165	0
1	I	327/360 (90%)	1.04	88 (26%) 1 1	9, 52, 147, 163	0
1	J	327/360 (90%)	0.92	83 (25%) 1 2	5, 37, 150, 165	0
1	K	327/360 (90%)	1.09	86 (26%) 1 2	6, 50, 157, 170	0
1	L	327/360 (90%)	1.11	94 (28%) 1 1	8, 56, 154, 173	0
1	M	327/360 (90%)	1.63	108 (33%) 1 1	18, 83, 158, 172	0
All	All	4059/4680 (86%)	1.09	1020 (25%) 1 2	5, 65, 151, 173	0

All (1020) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	I	274	GLY	12.5
1	M	315	LEU	8.6
1	M	270	ALA	7.7
1	L	315	LEU	7.7
1	K	317	ALA	7.6
1	M	14	GLU	7.6
1	B	23	GLN	7.5
1	K	15	VAL	7.5
1	H	295	GLU	7.1

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Mol	Chain	Res	Type	RSRZ
1	M	302	ASP	7.1
1	C	295	GLU	7.0
1	J	295	GLU	6.9
1	H	263	VAL	6.9
1	M	289	ASN	6.8
1	M	288	VAL	6.8
1	J	323	THR	6.7
1	I	339	PRO	6.6
1	J	273	GLN	6.6
1	M	316	ASN	6.5
1	B	263	VAL	6.5
1	G	15	VAL	6.5
1	J	302	ASP	6.5
1	M	278	ASP	6.4
1	C	273	GLN	6.2
1	B	270	ALA	6.2
1	J	282	GLN	6.1
1	K	324	GLU	6.1
1	L	289	ASN	6.0
1	L	326	LEU	6.0
1	I	264	LYS	5.9
1	G	324	GLU	5.9
1	K	302	ASP	5.9
1	K	316	ASN	5.9
1	G	317	ALA	5.9
1	J	270	ALA	5.9
1	M	301	ALA	5.8
1	D	99	LEU	5.8
1	G	319	ASP	5.7
1	M	338	VAL	5.7
1	B	273	GLN	5.7
1	M	271	PRO	5.7
1	I	307	ASP	5.7
1	C	289	ASN	5.7
1	K	270	ALA	5.6
1	L	328	PHE	5.6
1	J	322	ILE	5.6
1	M	285	ALA	5.6
1	J	287	VAL	5.6
1	M	299	ILE	5.6
1	L	265	GLN	5.5
1	G	316	ASN	5.5

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Mol	Chain	Res	Type	RSRZ
1	J	278	ASP	5.5
1	J	309	TRP	5.5
1	L	288	VAL	5.5
1	K	315	LEU	5.5
1	L	327	GLN	5.4
1	L	325	GLY	5.4
1	K	338	VAL	5.4
1	H	315	LEU	5.4
1	M	337	THR	5.4
1	B	231	GLU	5.4
1	H	302	ASP	5.4
1	J	289	ASN	5.4
1	J	274	GLY	5.4
1	L	15	VAL	5.3
1	E	323	THR	5.3
1	E	337	THR	5.3
1	I	322	ILE	5.3
1	I	315	LEU	5.2
1	H	339	PRO	5.2
1	G	291	GLN	5.2
1	J	324	GLU	5.2
1	L	295	GLU	5.2
1	E	315	LEU	5.2
1	K	289	ASN	5.2
1	K	267	ALA	5.2
1	J	271	PRO	5.1
1	J	307	ASP	5.1
1	C	265	GLN	5.1
1	J	286	LEU	5.1
1	J	316	ASN	5.1
1	H	322	ILE	5.0
1	B	324	GLU	5.0
1	C	291	GLN	5.0
1	E	278	ASP	5.0
1	K	278	ASP	5.0
1	J	338	VAL	5.0
1	J	279	LEU	5.0
1	I	28	ASN	5.0
1	L	284	THR	5.0
1	J	288	VAL	5.0
1	B	302	ASP	5.0
1	B	307	ASP	5.0

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Mol	Chain	Res	Type	RSRZ
1	M	22	ALA	5.0
1	J	304	VAL	5.0
1	L	274	GLY	5.0
1	L	333	VAL	5.0
1	M	339	PRO	4.9
1	L	301	ALA	4.9
1	J	294	VAL	4.9
1	B	296	LEU	4.9
1	L	286	LEU	4.9
1	M	291	GLN	4.9
1	H	24	THR	4.9
1	L	319	ASP	4.9
1	G	278	ASP	4.9
1	M	311	VAL	4.8
1	A	32	PRO	4.8
1	K	22	ALA	4.8
1	C	286	LEU	4.8
1	H	15	VAL	4.8
1	L	334	GLU	4.8
1	L	273	GLN	4.8
1	G	269	LEU	4.8
1	K	328	PHE	4.7
1	E	265	GLN	4.7
1	E	291	GLN	4.7
1	I	291	GLN	4.7
1	J	327	GLN	4.7
1	F	339	PRO	4.7
1	F	279	LEU	4.7
1	L	285	ALA	4.7
1	E	277	ARG	4.7
1	H	271	PRO	4.7
1	H	316	ASN	4.7
1	M	295	GLU	4.7
1	G	327	GLN	4.7
1	I	23	GLN	4.7
1	C	15	VAL	4.7
1	M	324	GLU	4.7
1	K	13	PRO	4.6
1	M	317	ALA	4.6
1	K	299	ILE	4.6
1	C	284	THR	4.6
1	K	295	GLU	4.6

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Mol	Chain	Res	Type	RSRZ
1	H	291	GLN	4.6
1	L	17	ILE	4.6
1	G	293	LYS	4.6
1	E	322	ILE	4.6
1	H	331	PRO	4.6
1	M	273	GLN	4.6
1	L	276	THR	4.6
1	I	26	THR	4.6
1	J	337	THR	4.6
1	J	15	VAL	4.6
1	G	322	ILE	4.5
1	H	22	ALA	4.5
1	M	286	LEU	4.5
1	K	292	ASN	4.5
1	K	337	THR	4.5
1	M	333	VAL	4.5
1	G	17	ILE	4.5
1	C	315	LEU	4.5
1	H	19	THR	4.5
1	J	339	PRO	4.5
1	G	265	GLN	4.5
1	K	282	GLN	4.5
1	L	314	GLY	4.4
1	E	292	ASN	4.4
1	K	323	THR	4.4
1	E	13	PRO	4.4
1	E	295	GLU	4.4
1	H	309	TRP	4.4
1	J	299	ILE	4.4
1	G	339	PRO	4.4
1	H	287	VAL	4.4
1	F	326	LEU	4.4
1	G	307	ASP	4.4
1	F	337	THR	4.4
1	M	276	THR	4.4
1	B	294	VAL	4.4
1	M	331	PRO	4.4
1	H	324	GLU	4.4
1	E	319	ASP	4.4
1	G	289	ASN	4.4
1	M	275	VAL	4.4
1	E	22	ALA	4.3

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Mol	Chain	Res	Type	RSRZ
1	I	265	GLN	4.3
1	G	311	VAL	4.3
1	M	319	ASP	4.3
1	I	282	GLN	4.3
1	L	330	GLN	4.3
1	J	275	VAL	4.3
1	E	331	PRO	4.3
1	J	326	LEU	4.3
1	F	327	GLN	4.3
1	M	15	VAL	4.3
1	K	291	GLN	4.3
1	L	110	GLN	4.3
1	M	227	VAL	4.3
1	B	337	THR	4.3
1	I	286	LEU	4.3
1	E	332	GLY	4.3
1	H	292	ASN	4.3
1	I	311	VAL	4.3
1	M	309	TRP	4.2
1	K	339	PRO	4.2
1	J	276	THR	4.2
1	J	315	LEU	4.2
1	J	13	PRO	4.2
1	J	331	PRO	4.2
1	I	25	VAL	4.2
1	F	22	ALA	4.2
1	K	262	GLY	4.2
1	B	316	ASN	4.2
1	M	262	GLY	4.2
1	E	313	GLU	4.2
1	D	96	ARG	4.2
1	C	260	GLN	4.2
1	H	272	GLN	4.2
1	L	302	ASP	4.2
1	B	323	THR	4.2
1	J	284	THR	4.2
1	E	288	VAL	4.1
1	B	319	ASP	4.1
1	C	276	THR	4.1
1	K	288	VAL	4.1
1	C	322	ILE	4.1
1	L	282	GLN	4.1

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Mol	Chain	Res	Type	RSRZ
1	K	301	ALA	4.1
1	B	13	PRO	4.1
1	I	309	TRP	4.1
1	B	24	THR	4.1
1	E	316	ASN	4.1
1	C	25	VAL	4.1
1	K	271	PRO	4.1
1	E	324	GLU	4.1
1	I	330	GLN	4.1
1	H	338	VAL	4.0
1	G	312	THR	4.0
1	M	26	THR	4.0
1	E	317	ALA	4.0
1	H	109	GLN	4.0
1	L	339	PRO	4.0
1	M	292	ASN	4.0
1	K	319	ASP	4.0
1	B	26	THR	4.0
1	M	284	THR	4.0
1	M	322	ILE	4.0
1	L	14	GLU	4.0
1	L	260	GLN	4.0
1	G	315	LEU	4.0
1	H	264	LYS	4.0
1	L	307	ASP	4.0
1	J	296	LEU	4.0
1	K	298	VAL	4.0
1	K	309	TRP	4.0
1	C	28	ASN	4.0
1	B	179	GLN	4.0
1	I	18	VAL	4.0
1	C	288	VAL	3.9
1	J	333	VAL	3.9
1	C	282	GLN	3.9
1	J	17	ILE	3.9
1	J	22	ALA	3.9
1	H	326	LEU	3.9
1	H	288	VAL	3.9
1	L	18	VAL	3.9
1	C	13	PRO	3.9
1	M	272	GLN	3.9
1	F	26	THR	3.9

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Mol	Chain	Res	Type	RSRZ
1	G	26	THR	3.9
1	M	313	GLU	3.9
1	K	294	VAL	3.9
1	K	16	GLY	3.9
1	M	264	LYS	3.9
1	H	270	ALA	3.9
1	K	286	LEU	3.9
1	L	296	LEU	3.9
1	B	289	ASN	3.9
1	C	313	GLU	3.9
1	L	303	ARG	3.9
1	H	289	ASN	3.9
1	I	316	ASN	3.9
1	K	293	LYS	3.9
1	M	320	LYS	3.9
1	H	286	LEU	3.9
1	K	311	VAL	3.9
1	K	333	VAL	3.9
1	E	24	THR	3.9
1	L	313	GLU	3.9
1	M	323	THR	3.9
1	M	268	ILE	3.9
1	B	291	GLN	3.9
1	L	23	GLN	3.9
1	B	310	LEU	3.9
1	G	285	ALA	3.9
1	G	271	PRO	3.8
1	J	330	GLN	3.8
1	E	294	VAL	3.8
1	E	14	GLU	3.8
1	G	323	THR	3.8
1	I	271	PRO	3.8
1	L	19	THR	3.8
1	M	224	PHE	3.8
1	G	273	GLN	3.8
1	G	296	LEU	3.8
1	I	338	VAL	3.8
1	L	294	VAL	3.8
1	G	284	THR	3.8
1	I	279	LEU	3.8
1	J	28	ASN	3.8
1	H	296	LEU	3.8

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Mol	Chain	Res	Type	RSRZ
1	M	310	LEU	3.8
1	E	273	GLN	3.8
1	J	291	GLN	3.8
1	K	327	GLN	3.8
1	B	288	VAL	3.8
1	G	288	VAL	3.8
1	K	18	VAL	3.8
1	K	266	LYS	3.8
1	L	300	LYS	3.8
1	M	287	VAL	3.8
1	G	231	GLU	3.8
1	E	296	LEU	3.8
1	B	327	GLN	3.7
1	B	15	VAL	3.7
1	H	319	ASP	3.7
1	K	268	ILE	3.7
1	K	24	THR	3.7
1	G	338	VAL	3.7
1	K	265	GLN	3.7
1	C	278	ASP	3.7
1	I	319	ASP	3.7
1	K	21	GLU	3.7
1	C	26	THR	3.7
1	E	293	LYS	3.7
1	M	312	THR	3.7
1	C	327	GLN	3.7
1	D	95	GLN	3.7
1	B	309	TRP	3.7
1	B	14	GLU	3.7
1	G	22	ALA	3.7
1	J	303	ARG	3.7
1	K	17	ILE	3.7
1	L	299	ILE	3.7
1	M	17	ILE	3.7
1	G	290	ALA	3.7
1	J	23	GLN	3.7
1	A	259	LEU	3.7
1	J	20	LEU	3.7
1	E	289	ASN	3.7
1	B	339	PRO	3.6
1	L	331	PRO	3.6
1	G	295	GLU	3.6

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Mol	Chain	Res	Type	RSRZ
1	J	21	GLU	3.6
1	L	329	VAL	3.6
1	J	297	ARG	3.6
1	F	296	LEU	3.6
1	G	23	GLN	3.6
1	F	280	LYS	3.6
1	C	309	TRP	3.6
1	L	278	ASP	3.6
1	C	24	THR	3.6
1	J	310	LEU	3.6
1	C	330	GLN	3.6
1	A	247	ASN	3.6
1	G	192	ALA	3.6
1	C	21	GLU	3.6
1	I	324	GLU	3.6
1	K	280	LYS	3.6
1	C	23	GLN	3.6
1	E	330	GLN	3.6
1	J	306	GLY	3.6
1	K	325	GLY	3.6
1	L	309	TRP	3.6
1	C	331	PRO	3.6
1	B	285	ALA	3.6
1	G	28	ASN	3.6
1	C	293	LYS	3.6
1	B	282	GLN	3.6
1	J	265	GLN	3.6
1	M	327	GLN	3.6
1	M	13	PRO	3.6
1	A	28	ASN	3.6
1	D	98	LYS	3.6
1	F	324	GLU	3.6
1	J	308	LYS	3.6
1	L	293	LYS	3.6
1	B	254	PHE	3.5
1	C	314	GLY	3.5
1	B	275	VAL	3.5
1	L	298	VAL	3.5
1	M	25	VAL	3.5
1	M	280	LYS	3.5
1	C	297	ARG	3.5
1	I	24	THR	3.5

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Mol	Chain	Res	Type	RSRZ
1	K	297	ARG	3.5
1	L	312	THR	3.5
1	C	302	ASP	3.5
1	E	15	VAL	3.5
1	J	311	VAL	3.5
1	K	23	GLN	3.5
1	C	319	ASP	3.5
1	G	13	PRO	3.5
1	B	295	GLU	3.5
1	J	14	GLU	3.5
1	C	274	GLY	3.5
1	F	304	VAL	3.5
1	F	329	VAL	3.5
1	G	260	GLN	3.5
1	K	25	VAL	3.5
1	G	283	ALA	3.5
1	K	307	ASP	3.5
1	E	339	PRO	3.5
1	H	320	LYS	3.5
1	B	284	THR	3.5
1	C	298	VAL	3.5
1	I	273	GLN	3.5
1	I	306	GLY	3.5
1	H	279	LEU	3.5
1	J	18	VAL	3.4
1	B	279	LEU	3.4
1	C	326	LEU	3.4
1	L	323	THR	3.4
1	H	330	GLN	3.4
1	I	270	ALA	3.4
1	I	299	ILE	3.4
1	K	305	ILE	3.4
1	M	99	LEU	3.4
1	A	29	THR	3.4
1	C	290	ALA	3.4
1	K	272	GLN	3.4
1	H	13	PRO	3.4
1	J	313	GLU	3.4
1	B	287	VAL	3.4
1	H	257	ALA	3.4
1	E	104	GLN	3.4
1	G	282	GLN	3.4

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Mol	Chain	Res	Type	RSRZ
1	I	337	THR	3.4
1	L	324	GLU	3.4
1	M	334	GLU	3.4
1	H	18	VAL	3.4
1	H	280	LYS	3.4
1	M	265	GLN	3.4
1	F	99	LEU	3.4
1	G	294	VAL	3.4
1	J	25	VAL	3.4
1	M	269	LEU	3.4
1	H	290	ALA	3.4
1	K	285	ALA	3.4
1	E	300	LYS	3.4
1	M	321	ILE	3.4
1	C	272	GLN	3.4
1	C	338	VAL	3.3
1	E	287	VAL	3.3
1	G	320	LYS	3.3
1	C	296	LEU	3.3
1	E	333	VAL	3.3
1	L	275	VAL	3.3
1	E	21	GLU	3.3
1	C	281	GLY	3.3
1	E	19	THR	3.3
1	G	24	THR	3.3
1	I	323	THR	3.3
1	K	110	GLN	3.3
1	I	298	VAL	3.3
1	G	270	ALA	3.3
1	L	290	ALA	3.3
1	C	307	ASP	3.3
1	M	277	ARG	3.3
1	D	101	VAL	3.3
1	F	264	LYS	3.3
1	G	292	ASN	3.3
1	H	278	ASP	3.3
1	B	326	LEU	3.3
1	E	336	LYS	3.3
1	I	15	VAL	3.3
1	H	299	ILE	3.3
1	I	14	GLU	3.3
1	J	301	ALA	3.3

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Mol	Chain	Res	Type	RSRZ
1	B	278	ASP	3.2
1	F	104	GLN	3.2
1	K	320	LYS	3.2
1	G	329	VAL	3.2
1	B	280	LYS	3.2
1	L	269	LEU	3.2
1	C	328	PHE	3.2
1	C	231	GLU	3.2
1	I	331	PRO	3.2
1	I	181	SER	3.2
1	I	17	ILE	3.2
1	L	322	ILE	3.2
1	D	105	ALA	3.2
1	J	290	ALA	3.2
1	K	277	ARG	3.2
1	I	261	GLU	3.2
1	I	289	ASN	3.2
1	K	279	LEU	3.2
1	G	217	PRO	3.2
1	I	13	PRO	3.2
1	B	260	GLN	3.2
1	H	181	SER	3.2
1	I	272	GLN	3.2
1	H	317	ALA	3.2
1	H	14	GLU	3.2
1	A	96	ARG	3.2
1	B	330	GLN	3.2
1	H	323	THR	3.2
1	L	26	THR	3.2
1	L	332	GLY	3.1
1	C	261	GLU	3.1
1	C	333	VAL	3.1
1	H	17	ILE	3.1
1	H	293	LYS	3.1
1	J	283	ALA	3.1
1	M	297	ARG	3.1
1	B	322	ILE	3.1
1	H	267	ALA	3.1
1	G	286	LEU	3.1
1	L	24	THR	3.1
1	M	281	GLY	3.1
1	M	307	ASP	3.1

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Mol	Chain	Res	Type	RSRZ
1	E	275	VAL	3.1
1	G	106	VAL	3.1
1	L	338	VAL	3.1
1	L	292	ASN	3.1
1	C	179	GLN	3.1
1	D	104	GLN	3.1
1	E	327	GLN	3.1
1	F	330	GLN	3.1
1	H	327	GLN	3.1
1	I	301	ALA	3.1
1	M	290	ALA	3.1
1	H	26	THR	3.1
1	K	313	GLU	3.1
1	J	300	LYS	3.1
1	H	265	GLN	3.1
1	C	337	THR	3.1
1	I	312	THR	3.1
1	H	25	VAL	3.1
1	H	294	VAL	3.1
1	G	14	GLU	3.1
1	L	280	LYS	3.1
1	E	302	ASP	3.1
1	L	20	LEU	3.0
1	M	202	ASN	3.0
1	D	90	THR	3.0
1	K	312	THR	3.0
1	G	25	VAL	3.0
1	C	264	LYS	3.0
1	B	17	ILE	3.0
1	B	301	ALA	3.0
1	D	114	ALA	3.0
1	G	279	LEU	3.0
1	K	269	LEU	3.0
1	B	104	GLN	3.0
1	F	179	GLN	3.0
1	J	104	GLN	3.0
1	L	272	GLN	3.0
1	G	337	THR	3.0
1	I	276	THR	3.0
1	K	275	VAL	3.0
1	L	21	GLU	3.0
1	I	99	LEU	3.0

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Mol	Chain	Res	Type	RSRZ
1	M	134	TYR	3.0
1	M	303	ARG	3.0
1	F	289	ASN	3.0
1	K	26	THR	3.0
1	G	193	SER	3.0
1	C	270	ALA	3.0
1	E	290	ALA	3.0
1	F	198	ARG	3.0
1	K	283	ALA	3.0
1	B	101	VAL	3.0
1	C	104	GLN	3.0
1	A	242	PHE	3.0
1	J	305	ILE	3.0
1	C	279	LEU	3.0
1	J	319	ASP	3.0
1	B	329	VAL	3.0
1	I	263	VAL	3.0
1	C	269	LEU	2.9
1	I	326	LEU	2.9
1	F	295	GLU	2.9
1	F	309	TRP	2.9
1	K	334	GLU	2.9
1	H	108	LYS	2.9
1	L	22	ALA	2.9
1	M	225	SER	2.9
1	F	25	VAL	2.9
1	G	274	GLY	2.9
1	H	307	ASP	2.9
1	I	321	ILE	2.9
1	C	316	ASN	2.9
1	D	115	ASN	2.9
1	M	296	LEU	2.9
1	E	309	TRP	2.9
1	J	334	GLU	2.9
1	C	267	ALA	2.9
1	M	94	ALA	2.9
1	E	311	VAL	2.9
1	G	258	GLN	2.9
1	G	268	ILE	2.9
1	I	327	GLN	2.9
1	M	282	GLN	2.9
1	K	296	LEU	2.9

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Mol	Chain	Res	Type	RSRZ
1	G	276	THR	2.9
1	J	26	THR	2.9
1	H	21	GLU	2.9
1	L	13	PRO	2.9
1	L	270	ALA	2.9
1	L	25	VAL	2.9
1	L	287	VAL	2.9
1	H	262	GLY	2.9
1	H	20	LEU	2.9
1	M	326	LEU	2.9
1	E	231	GLU	2.9
1	D	111	TYR	2.9
1	H	277	ARG	2.9
1	E	279	LEU	2.9
1	H	88	ALA	2.9
1	J	19	THR	2.9
1	G	18	VAL	2.9
1	A	39	ARG	2.9
1	M	328	PHE	2.9
1	B	108	LYS	2.9
1	F	17	ILE	2.9
1	J	320	LYS	2.9
1	K	300	LYS	2.9
1	E	23	GLN	2.8
1	C	339	PRO	2.8
1	I	290	ALA	2.8
1	K	284	THR	2.8
1	C	324	GLU	2.8
1	B	303	ARG	2.8
1	L	264	LYS	2.8
1	C	99	LEU	2.8
1	H	282	GLN	2.8
1	L	291	GLN	2.8
1	H	113	ASP	2.8
1	H	333	VAL	2.8
1	I	297	ARG	2.8
1	M	263	VAL	2.8
1	C	22	ALA	2.8
1	C	304	VAL	2.8
1	C	14	GLU	2.8
1	E	334	GLU	2.8
1	G	151	THR	2.8

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Mol	Chain	Res	Type	RSRZ
1	I	333	VAL	2.8
1	M	329	VAL	2.8
1	M	201	ASP	2.8
1	C	332	GLY	2.8
1	B	195	GLN	2.8
1	G	287	VAL	2.8
1	J	329	VAL	2.8
1	M	298	VAL	2.8
1	F	92	GLU	2.8
1	H	284	THR	2.8
1	H	334	GLU	2.8
1	I	21	GLU	2.8
1	B	265	GLN	2.8
1	B	272	GLN	2.8
1	H	285	ALA	2.8
1	J	317	ALA	2.8
1	J	280	LYS	2.8
1	K	273	GLN	2.8
1	C	335	VAL	2.8
1	E	335	VAL	2.8
1	I	294	VAL	2.8
1	E	326	LEU	2.8
1	G	313	GLU	2.8
1	K	14	GLU	2.8
1	J	321	ILE	2.8
1	H	314	GLY	2.7
1	C	292	ASN	2.7
1	L	316	ASN	2.7
1	A	216	TYR	2.7
1	B	297	ARG	2.7
1	K	303	ARG	2.7
1	B	264	LYS	2.7
1	M	293	LYS	2.7
1	C	275	VAL	2.7
1	C	329	VAL	2.7
1	F	15	VAL	2.7
1	I	288	VAL	2.7
1	M	87	LEU	2.7
1	C	312	THR	2.7
1	J	312	THR	2.7
1	F	281	GLY	2.7
1	A	221	ARG	2.7

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Mol	Chain	Res	Type	RSRZ
1	H	303	ARG	2.7
1	J	264	LYS	2.7
1	G	301	ALA	2.7
1	L	263	VAL	2.7
1	B	271	PRO	2.7
1	H	269	LEU	2.7
1	H	310	LEU	2.7
1	L	279	LEU	2.7
1	G	261	GLU	2.7
1	J	325	GLY	2.7
1	H	297	ARG	2.7
1	E	113	ASP	2.7
1	B	283	ALA	2.7
1	I	283	ALA	2.7
1	D	100	LEU	2.7
1	K	27	LEU	2.7
1	B	299	ILE	2.7
1	I	328	PHE	2.7
1	H	234	GLY	2.7
1	A	193	SER	2.7
1	F	53	LYS	2.7
1	A	41	ALA	2.7
1	B	290	ALA	2.7
1	D	94	ALA	2.7
1	G	326	LEU	2.7
1	L	28	ASN	2.7
1	C	303	ARG	2.7
1	L	231	GLU	2.7
1	H	337	THR	2.7
1	A	134	TYR	2.7
1	B	292	ASN	2.7
1	G	272	GLN	2.6
1	B	293	LYS	2.6
1	C	16	GLY	2.6
1	B	269	LEU	2.6
1	C	294	VAL	2.6
1	I	269	LEU	2.6
1	I	317	ALA	2.6
1	K	322	ILE	2.6
1	A	86	ASN	2.6
1	J	292	ASN	2.6
1	M	84	GLN	2.6

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Mol	Chain	Res	Type	RSRZ
1	D	231	GLU	2.6
1	F	14	GLU	2.6
1	G	263	VAL	2.6
1	H	275	VAL	2.6
1	I	275	VAL	2.6
1	H	107	SER	2.6
1	G	299	ILE	2.6
1	E	307	ASP	2.6
1	J	261	GLU	2.6
1	G	333	VAL	2.6
1	H	276	THR	2.6
1	L	310	LEU	2.6
1	K	290	ALA	2.6
1	M	305	ILE	2.6
1	I	260	GLN	2.6
1	K	20	LEU	2.6
1	F	263	VAL	2.6
1	I	285	ALA	2.6
1	K	263	VAL	2.6
1	A	135	THR	2.6
1	L	267	ALA	2.6
1	E	320	LYS	2.6
1	J	293	LYS	2.6
1	K	264	LYS	2.6
1	D	110	GLN	2.6
1	E	272	GLN	2.6
1	I	278	ASP	2.6
1	D	92	GLU	2.6
1	M	300	LYS	2.6
1	K	29	THR	2.6
1	F	282	GLN	2.5
1	L	16	GLY	2.5
1	M	110	GLN	2.5
1	B	27	LEU	2.5
1	K	326	LEU	2.5
1	D	106	VAL	2.5
1	G	219	GLU	2.5
1	H	266	LYS	2.5
1	I	295	GLU	2.5
1	M	294	VAL	2.5
1	E	26	THR	2.5
1	L	337	THR	2.5

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Mol	Chain	Res	Type	RSRZ
1	L	271	PRO	2.5
1	G	181	SER	2.5
1	D	120	GLN	2.5
1	G	330	GLN	2.5
1	H	273	GLN	2.5
1	K	330	GLN	2.5
1	H	106	VAL	2.5
1	I	329	VAL	2.5
1	F	334	GLU	2.5
1	J	285	ALA	2.5
1	E	297	ARG	2.5
1	E	303	ARG	2.5
1	J	27	LEU	2.5
1	F	181	SER	2.5
1	F	338	VAL	2.5
1	D	102	ALA	2.5
1	M	105	ALA	2.5
1	F	278	ASP	2.5
1	H	268	ILE	2.5
1	K	331	PRO	2.5
1	E	269	LEU	2.5
1	J	269	LEU	2.5
1	G	16	GLY	2.5
1	M	332	GLY	2.5
1	M	330	GLN	2.5
1	C	268	ILE	2.5
1	G	302	ASP	2.5
1	H	103	ASP	2.5
1	D	259	LEU	2.5
1	G	297	ARG	2.5
1	E	274	GLY	2.5
1	A	241	VAL	2.5
1	B	25	VAL	2.5
1	B	333	VAL	2.5
1	L	105	ALA	2.4
1	E	17	ILE	2.4
1	G	207	SER	2.4
1	I	313	GLU	2.4
1	B	176	ASP	2.4
1	C	96	ARG	2.4
1	G	19	THR	2.4
1	I	302	ASP	2.4

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Mol	Chain	Res	Type	RSRZ
1	H	329	VAL	2.4
1	D	109	GLN	2.4
1	G	264	LYS	2.4
1	M	188	ARG	2.4
1	E	284	THR	2.4
1	F	316	ASN	2.4
1	M	24	THR	2.4
1	M	135	THR	2.4
1	F	301	ALA	2.4
1	F	322	ILE	2.4
1	L	317	ALA	2.4
1	I	104	GLN	2.4
1	I	310	LEU	2.4
1	M	279	LEU	2.4
1	C	29	THR	2.4
1	G	298	VAL	2.4
1	E	314	GLY	2.4
1	F	267	ALA	2.4
1	H	321	ILE	2.4
1	B	266	LYS	2.4
1	M	109	GLN	2.4
1	B	277	ARG	2.4
1	E	20	LEU	2.4
1	F	211	GLU	2.4
1	B	193	SER	2.4
1	K	276	THR	2.4
1	I	262	GLY	2.4
1	M	314	GLY	2.4
1	A	105	ALA	2.4
1	C	317	ALA	2.4
1	L	297	ARG	2.4
1	F	23	GLN	2.4
1	K	310	LEU	2.4
1	B	261	GLU	2.4
1	I	334	GLU	2.4
1	M	223	GLU	2.4
1	E	25	VAL	2.4
1	F	13	PRO	2.4
1	I	96	ARG	2.3
1	L	283	ALA	2.3
1	H	23	GLN	2.3
1	M	179	GLN	2.3

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Mol	Chain	Res	Type	RSRZ
1	G	197	GLU	2.3
1	C	287	VAL	2.3
1	L	321	ILE	2.3
1	B	103	ASP	2.3
1	J	328	PHE	2.3
1	I	30	GLU	2.3
1	C	263	VAL	2.3
1	E	298	VAL	2.3
1	G	304	VAL	2.3
1	I	336	LYS	2.3
1	B	225	SER	2.3
1	B	314	GLY	2.3
1	L	234	GLY	2.3
1	E	285	ALA	2.3
1	H	178	THR	2.3
1	L	114	ALA	2.3
1	I	259	LEU	2.3
1	L	27	LEU	2.3
1	A	110	GLN	2.3
1	G	211	GLU	2.3
1	D	108	LYS	2.3
1	F	288	VAL	2.3
1	H	311	VAL	2.3
1	F	305	ILE	2.3
1	I	332	GLY	2.3
1	K	281	GLY	2.3
1	F	317	ALA	2.3
1	I	284	THR	2.3
1	M	20	LEU	2.3
1	B	328	PHE	2.3
1	A	104	GLN	2.3
1	B	320	LYS	2.3
1	G	336	LYS	2.3
1	A	226	GLU	2.3
1	G	58	GLU	2.3
1	B	331	PRO	2.3
1	I	305	ILE	2.3
1	F	290	ALA	2.3
1	H	325	GLY	2.3
1	A	90	THR	2.3
1	C	323	THR	2.3
1	K	19	THR	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	300	LYS	2.3
1	F	96	ARG	2.3
1	H	104	GLN	2.3
1	L	109	GLN	2.3
1	G	92	GLU	2.2
1	B	325	GLY	2.2
1	E	281	GLY	2.2
1	B	286	LEU	2.2
1	J	336	LYS	2.2
1	G	198	ARG	2.2
1	G	86	ASN	2.2
1	M	23	GLN	2.2
1	M	231	GLU	2.2
1	L	268	ILE	2.2
1	C	271	PRO	2.2
1	C	310	LEU	2.2
1	H	16	GLY	2.2
1	G	328	PHE	2.2
1	E	178	THR	2.2
1	H	300	LYS	2.2
1	I	19	THR	2.2
1	M	107	SER	2.2
1	L	311	VAL	2.2
1	M	18	VAL	2.2
1	C	299	ILE	2.2
1	A	204	ALA	2.2
1	E	270	ALA	2.2
1	F	274	GLY	2.2
1	H	180	PRO	2.2
1	C	280	LYS	2.2
1	L	320	LYS	2.2
1	G	254	PHE	2.2
1	H	298	VAL	2.2
1	A	258	GLN	2.2
1	M	195	GLN	2.2
1	A	238	ILE	2.2
1	H	313	GLU	2.2
1	L	261	GLU	2.2
1	C	262	GLY	2.2
1	M	102	ALA	2.2
1	F	328	PHE	2.2
1	B	276	THR	2.2

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Mol	Chain	Res	Type	RSRZ
1	E	312	THR	2.2
1	F	273	GLN	2.2
1	H	283	ALA	2.2
1	A	243	PRO	2.2
1	G	332	GLY	2.2
1	A	176	ASP	2.2
1	C	113	ASP	2.2
1	I	304	VAL	2.1
1	E	286	LEU	2.1
1	I	179	GLN	2.1
1	L	120	GLN	2.1
1	M	81	GLN	2.1
1	I	22	ALA	2.1
1	L	107	SER	2.1
1	I	303	ARG	2.1
1	M	30	GLU	2.1
1	M	306	GLY	2.1
1	D	113	ASP	2.1
1	B	106	VAL	2.1
1	H	27	LEU	2.1
1	M	122	LYS	2.1
1	H	120	GLN	2.1
1	G	257	ALA	2.1
1	A	225	SER	2.1
1	B	274	GLY	2.1
1	F	33	GLY	2.1
1	F	332	GLY	2.1
1	J	16	GLY	2.1
1	C	308	LYS	2.1
1	E	310	LEU	2.1
1	G	305	ILE	2.1
1	M	90	THR	2.1
1	G	129	ARG	2.1
1	K	198	ARG	2.1
1	B	262	GLY	2.1
1	E	16	GLY	2.1
1	M	92	GLU	2.1
1	B	235	SER	2.1
1	G	309	TRP	2.1
1	H	336	LYS	2.1
1	I	320	LYS	2.1
1	E	276	THR	2.1

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Mol	Chain	Res	Type	RSRZ
1	H	112	ALA	2.1
1	H	301	ALA	2.1
1	I	257	ALA	2.1
1	M	104	GLN	2.1
1	E	325	GLY	2.1
1	B	18	VAL	2.1
1	B	338	VAL	2.1
1	G	247	ASN	2.1
1	L	266	LYS	2.1
1	F	302	ASP	2.1
1	M	103	ASP	2.1
1	E	97	TYR	2.1
1	E	267	ALA	2.1
1	G	325	GLY	2.1
1	K	306	GLY	2.1
1	K	318	GLY	2.1
1	M	274	GLY	2.1
1	G	243	PRO	2.1
1	H	328	PHE	2.1
1	A	229	VAL	2.0
1	C	320	LYS	2.0
1	A	40	ILE	2.0
1	E	321	ILE	2.0
1	B	111	TYR	2.0
1	D	116	ALA	2.0
1	D	117	ALA	2.0
1	H	312	THR	2.0
1	E	328	PHE	2.0
1	I	200	GLY	2.0
1	B	313	GLU	2.0
1	F	231	GLU	2.0
1	G	223	GLU	2.0
1	G	334	GLU	2.0
1	I	231	GLU	2.0
1	E	304	VAL	2.0
1	J	263	VAL	2.0
1	B	267	ALA	2.0
1	C	285	ALA	2.0
1	I	267	ALA	2.0
1	H	232	GLY	2.0
1	H	281	GLY	2.0
1	E	282	GLN	2.0

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Mol	Chain	Res	Type	RSRZ
1	F	298	VAL	2.0
1	G	303	ARG	2.0
1	E	99	LEU	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
2	SO4	G	1340	5/5	0.73	0.16	87,89,108,112	0
2	SO4	B	1340	5/5	0.82	0.15	65,78,84,95	0
2	SO4	A	1260	5/5	0.82	0.15	70,77,101,103	0
2	SO4	M	1340	5/5	0.85	0.16	65,69,92,99	0
2	SO4	A	1261	5/5	0.87	0.18	62,66,94,95	0
2	SO4	F	1340	5/5	0.87	0.13	62,76,97,97	0
2	SO4	B	1341	5/5	0.88	0.16	70,75,95,101	0
2	SO4	F	1341	5/5	0.88	0.11	67,75,92,100	0
2	SO4	H	1340	5/5	0.90	0.12	54,57,74,79	0
2	SO4	C	1340	5/5	0.90	0.10	71,71,77,85	0
2	SO4	L	1340	5/5	0.91	0.14	42,44,72,73	0
2	SO4	E	1340	5/5	0.92	0.09	50,60,69,87	0
2	SO4	I	1340	5/5	0.92	0.13	55,56,72,87	0
2	SO4	J	1340	5/5	0.93	0.14	44,50,70,76	0
2	SO4	E	1341	5/5	0.94	0.10	43,52,59,68	0
2	SO4	K	1340	5/5	0.95	0.10	34,34,58,60	0

6.5 Other polymers [i](#)

There are no such residues in this entry.