



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 14, 2020 – 05:34 pm BST

PDB ID : 2V4D
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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

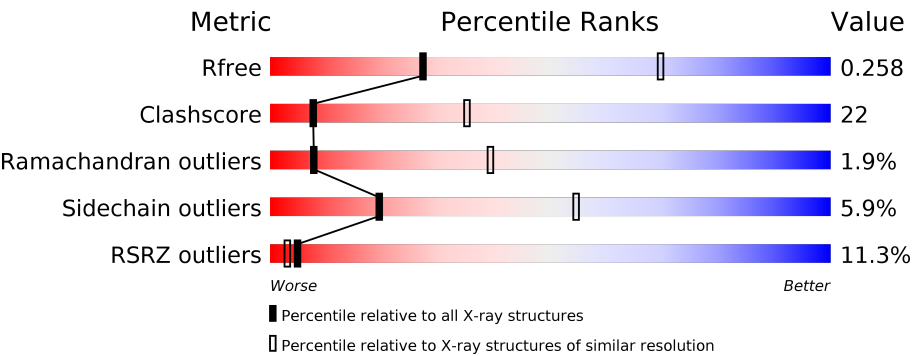
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	130704	1133 (3.20-3.20)
Clashscore	141614	1253 (3.20-3.20)
Ramachandran outliers	138981	1234 (3.20-3.20)
Sidechain outliers	138945	1233 (3.20-3.20)
RSRZ outliers	127900	1095 (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 on 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	<div><div>3%</div><div>31%31%•36%</div></div>
1	B	360	<div><div>6%</div><div>57%32%•9%</div></div>
1	C	360	<div><div>3%</div><div>56%33%•9%</div></div>
1	D	360	<div><div>%</div><div>30%32%•36%</div></div>
1	E	360	<div><div>8%</div><div>57%30%•9%</div></div>
1	F	360	<div><div>2%</div><div>55%34%•9%</div></div>

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Mol	Chain	Length	Quality of chain
1	G	360	
1	H	360	
1	I	360	
1	J	360	
1	K	360	
1	L	360	
1	M	360	

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:

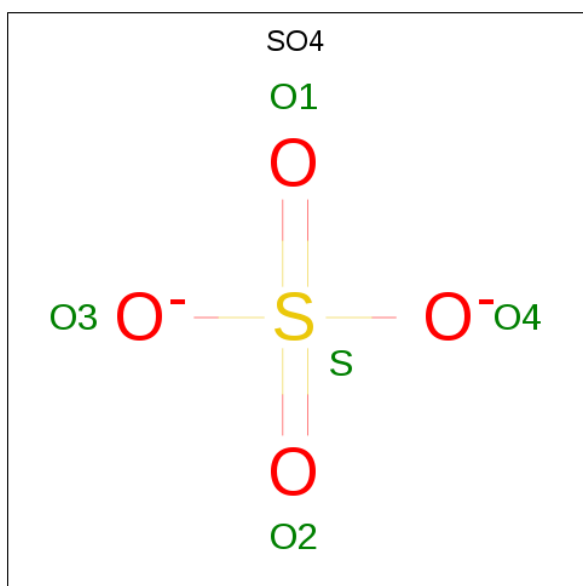
Chain	Residue	Modelled	Actual	Comment	Reference
A	1	SER	CYS	engineered mutation	UNP P52477
B	1	SER	CYS	engineered mutation	UNP P52477
C	1	SER	CYS	engineered mutation	UNP P52477

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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 (three-letter code: SO4) (formula: O₄S).



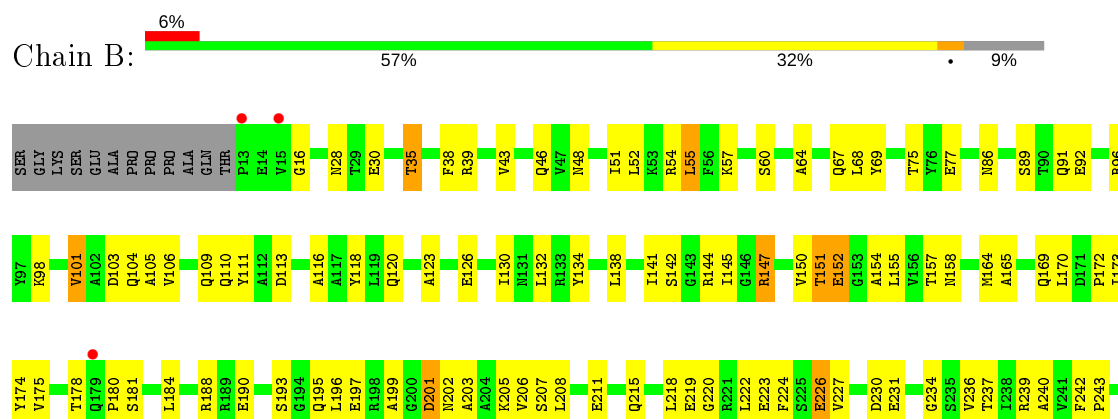
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total O S 5 4 1	0	0
2	A	1	Total O S 5 4 1	0	0
2	B	1	Total O S 5 4 1	0	0
2	B	1	Total O S 5 4 1	0	0
2	C	1	Total O S 5 4 1	0	0
2	E	1	Total O S 5 4 1	0	0

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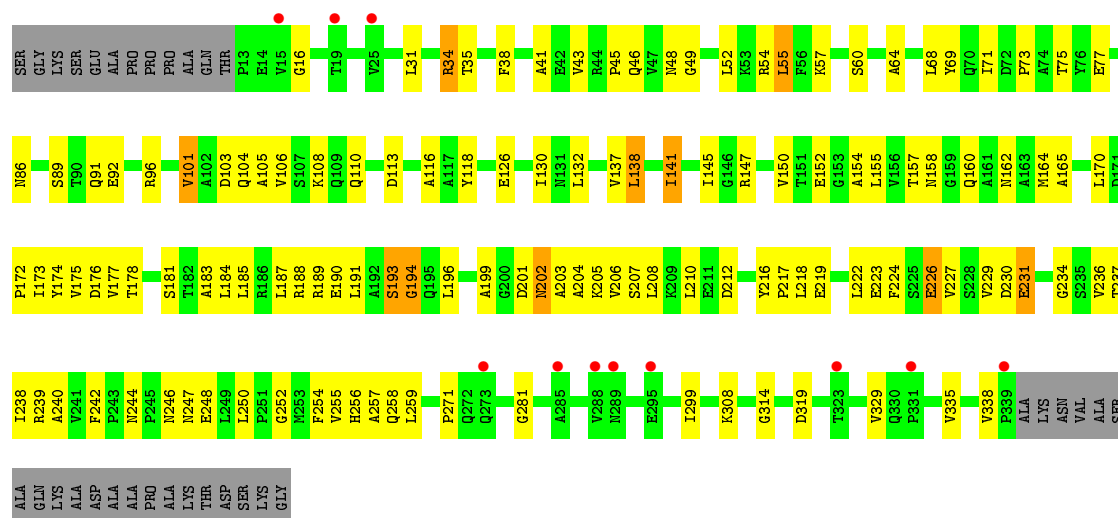
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	E	1	Total	O	S	0	0
			5	4	1		
2	F	1	Total	O	S	0	0
			5	4	1		
2	F	1	Total	O	S	0	0
			5	4	1		
2	G	1	Total	O	S	0	0
			5	4	1		
2	H	1	Total	O	S	0	0
			5	4	1		
2	I	1	Total	O	S	0	0
			5	4	1		
2	J	1	Total	O	S	0	0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

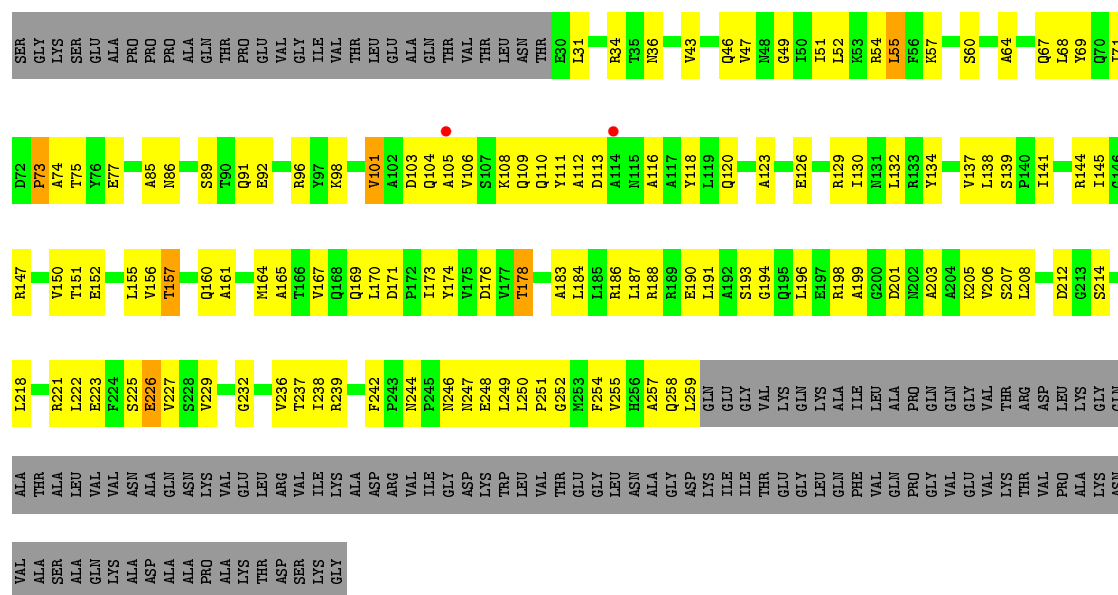
- Molecule 1: MULTIDRUG RESISTANCE PROTEIN MEXA



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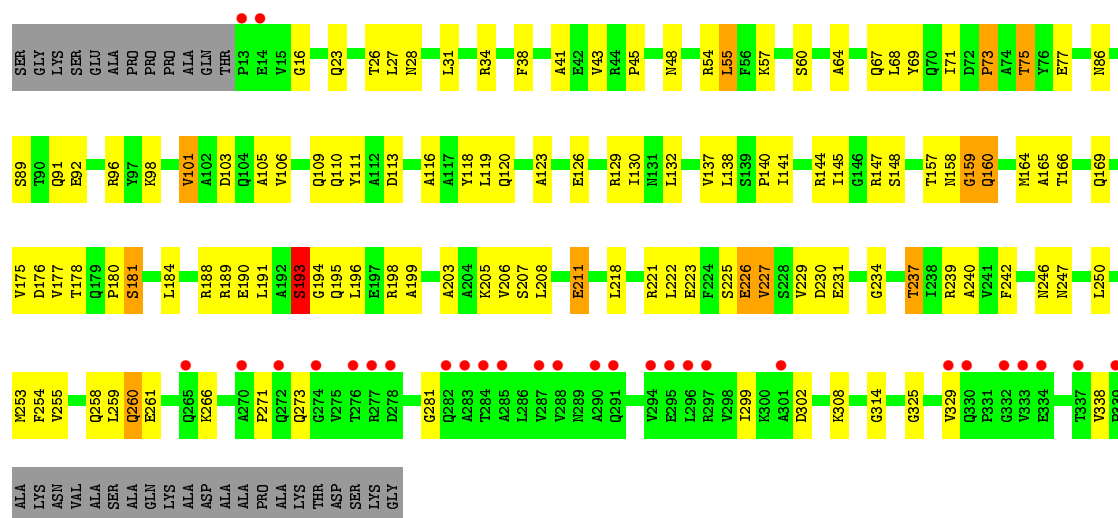


- Molecule 1: MULTIDRUG RESISTANCE PROTEIN MEXA

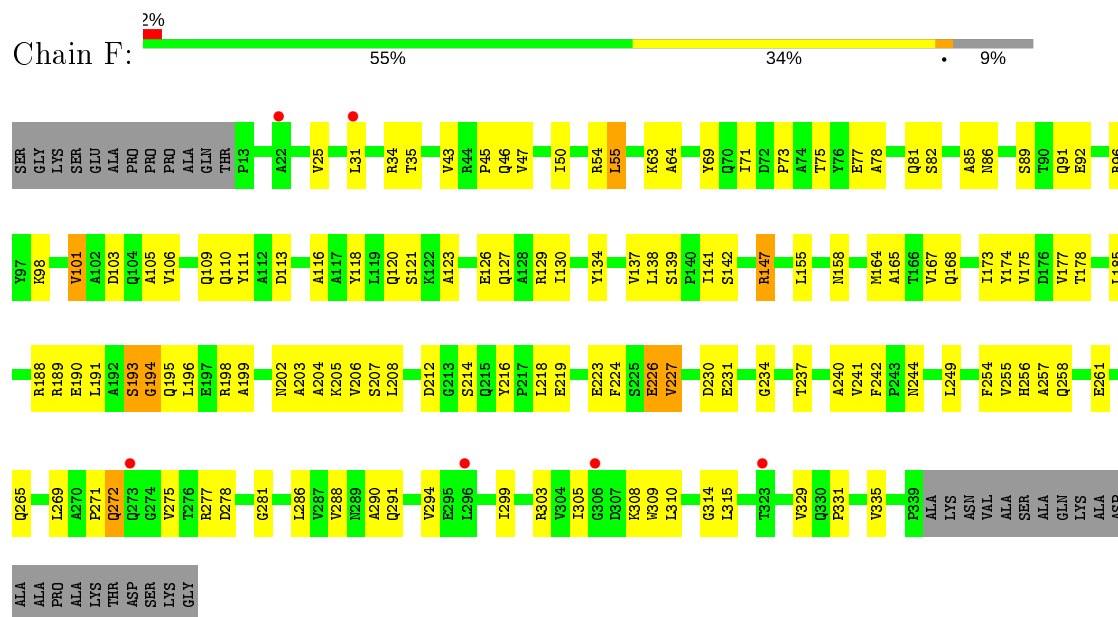


- Molecule 1: MULTIDRUG RESISTANCE PROTEIN MEXA

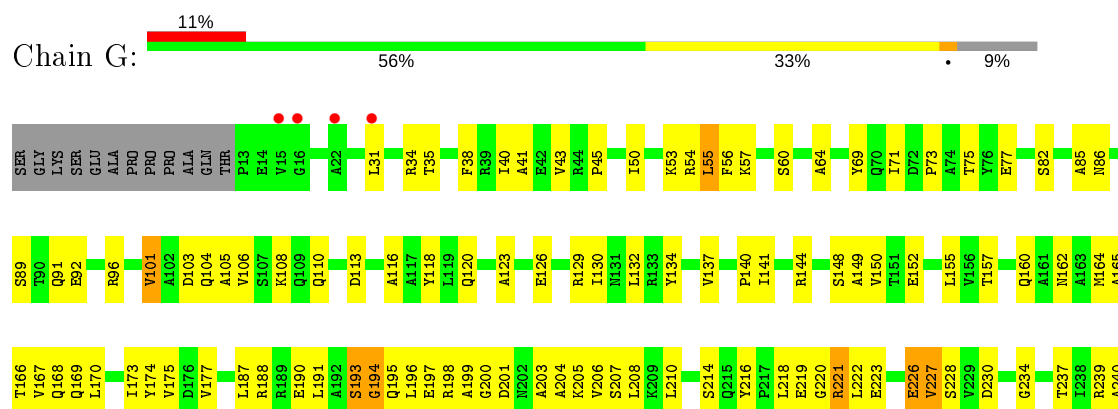


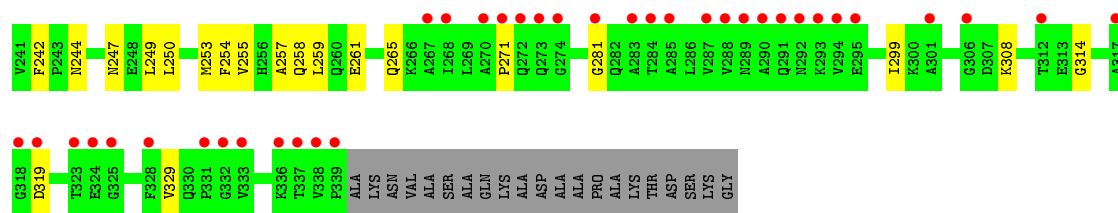


• Molecule 1: MULTIDRUG RESISTANCE PROTEIN MEXA

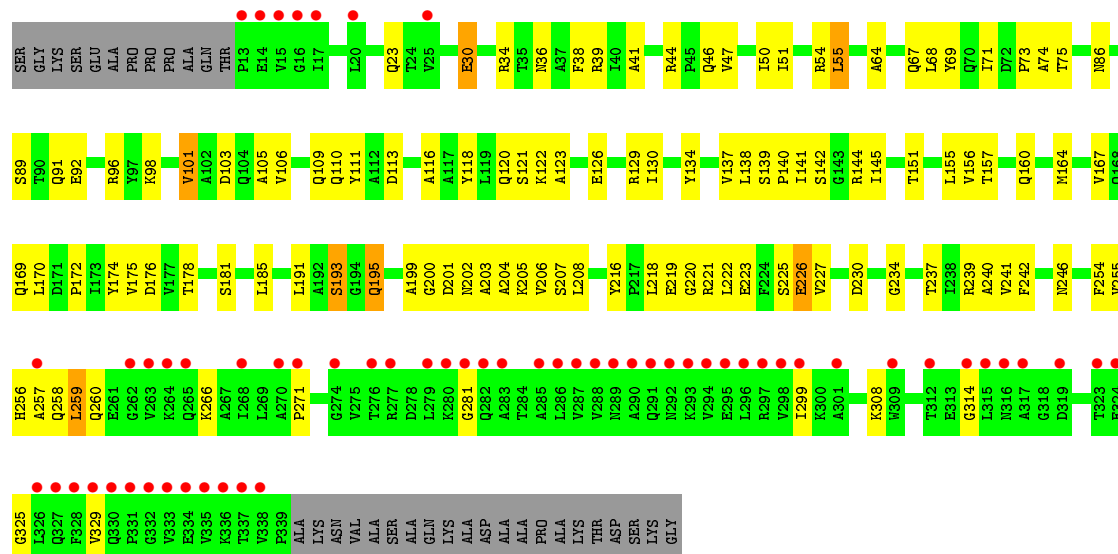


• Molecule 1: MULTIDRUG RESISTANCE PROTEIN MEXA

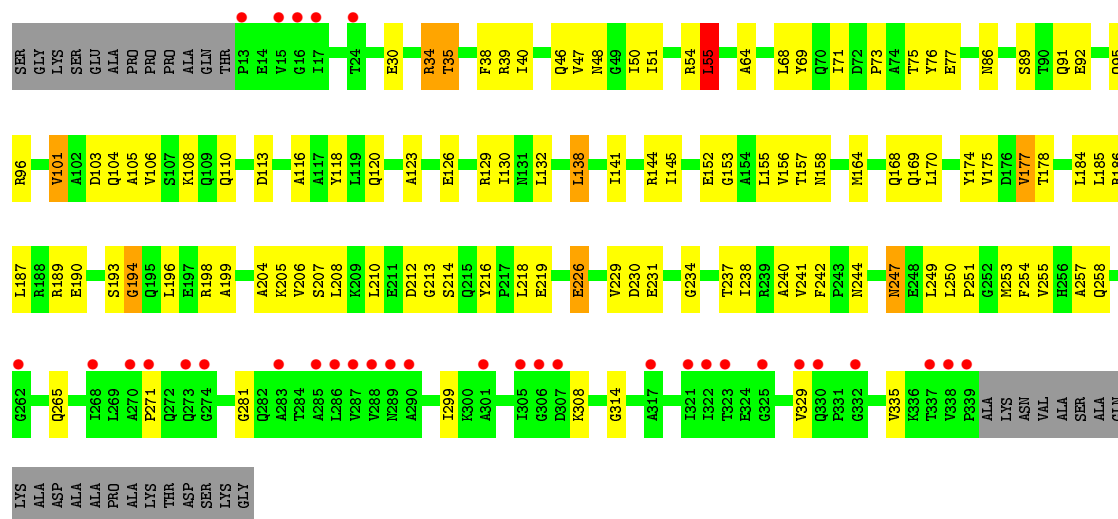




• Molecule 1: MULTIDRUG RESISTANCE PROTEIN MEXA

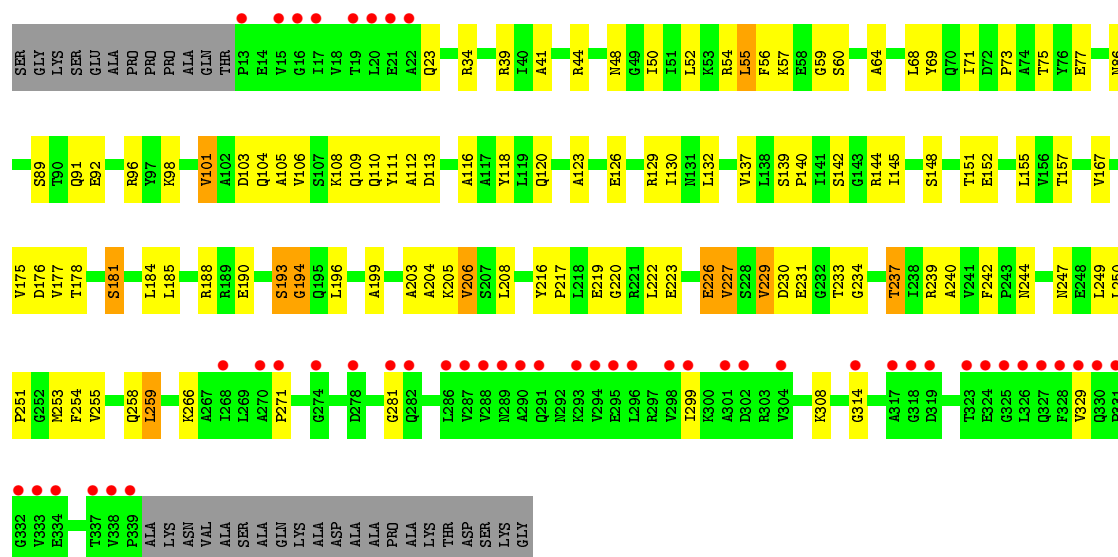


• Molecule 1: MULTIDRUG RESISTANCE PROTEIN MEXA



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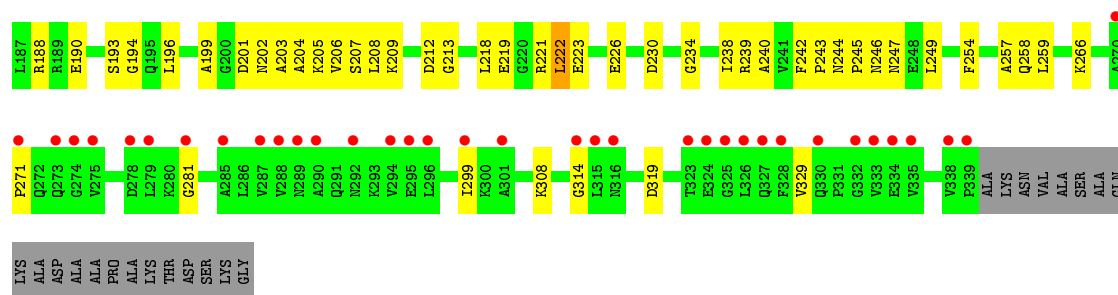


• Molecule 1: MULTIDRUG RESISTANCE PROTEIN MEXA

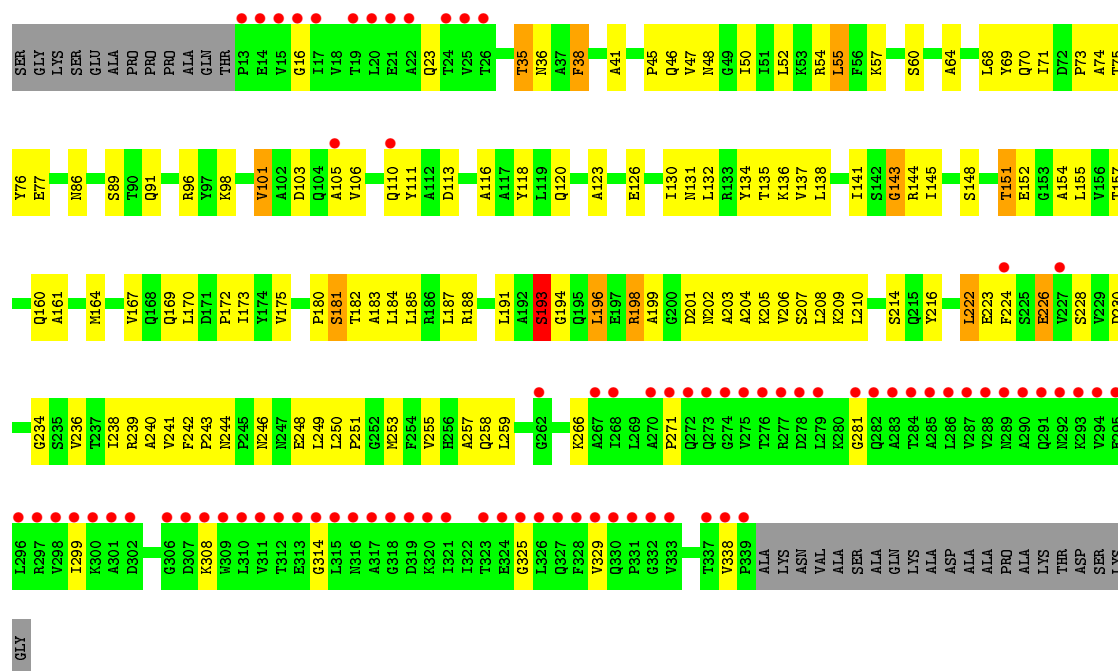


• Molecule 1: MULTIDRUG RESISTANCE PROTEIN MEXA





Molecule 1: MULTIDRUG RESISTANCE PROTEIN MEXA



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 0.233 , 0.258	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 , 77.9	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 [i](#)

5.1 Standard geometry [i](#)

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	0.33	0/1800	0.57	0/2441
1	B	0.35	0/2287	0.59	0/3118
1	C	0.36	0/2278	0.58	0/3107
1	D	0.42	0/1788	0.61	0/2424
1	E	0.43	0/2292	0.61	0/3125
1	F	0.35	0/2445	0.57	0/3325
1	G	0.34	0/2278	0.56	0/3107
1	H	0.42	0/2292	0.62	0/3125
1	I	0.45	0/2278	0.64	0/3107
1	J	0.52	0/2276	0.64	0/3103
1	K	0.47	0/2292	0.65	0/3125
1	L	0.44	0/2278	0.62	0/3107
1	M	0.36	0/2296	0.59	0/3131
All	All	0.41	0/28880	0.60	0/39345

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1776	0	1777	106	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	2259	0	2040	101	0
1	C	2250	0	2021	106	0
1	D	1764	0	1768	105	0
1	E	2264	0	2044	103	0
1	F	2415	0	2358	99	0
1	G	2250	0	2021	108	0
1	H	2264	0	2044	107	0
1	I	2250	0	2021	113	0
1	J	2249	0	2014	79	0
1	K	2264	0	2044	90	0
1	L	2250	0	2021	82	0
1	M	2268	0	2056	106	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	1199	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 22.

All (1199) 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:HB2	1:I:198:ARG:HH11	1.22	1.03
1:D:96:ARG:NH2	1:E:109:GLN:OE1	1.91	1.03
1:G:190:GLU:HB3	1:G:196:LEU:HD13	1.43	1.01
1:J:44:ARG:CD	1:J:44:ARG:CZ	2.41	0.99
1:C:174:TYR:HD1	1:C:239:ARG:HD2	1.27	0.98
1:C:34:ARG:HH11	1:C:34:ARG:HB3	1.29	0.97

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:I:178:THR:HG22	1:I:237:THR:OG1	1.68	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:H	1:C:138:LEU:HD12	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:NH1	1:L:221:ARG:HB2	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: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
1:E:144:ARG:HH11	1:F:226:GLU:HG3	1.44	0.79
1:E:55:LEU:HD12	1:E:55:LEU:H	1.47	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:H	1:J:55:LEU:HD12	1.45	0.78
1:E:193:SER:OG	1:E:195:GLN:HG3	1.83	0.78
1:H:226:GLU:OE2	1:I:144:ARG:HD3	1.83	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:H	1:B:55:LEU:HD12	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:M:35:THR:C	1:M:36:ASN:HD22	1.89	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: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:H	1:L:55:LEU:HD12	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:D:156:VAL:HG11	1:D:164:MET:HE3	1.69	0.73
1:K:199:ALA:HB2	1:K:205:LYS:N	2.03	0.73
1:M:134:TYR:C	1:M:136:LYS:H	1.92	0.73
1:A:184:LEU:HD13	1:A:238:ILE:HD11	1.69	0.73
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:109:GLN:CD	1:I:96:ARG:CZ	2.58	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:F:265:GLN:CD	1:F:265:GLN:H	1.93	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:D:96:ARG:HH21	1:E:109:GLN:CD	1.92	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:HD12	1:I:55:LEU:H	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:D:104:GLN:HG3	1:J:108:LYS:HE3	1.75	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:B:215:GLN:HE22	1:B:258:GLN:NE2	1.89	0.69
1:D:208:LEU:HD11	1:D:255:VAL:HG21	1.73	0.69
1:C:38:PHE:CD1	1:C:174:TYR:HE2	2.11	0.69
1:I:156:VAL:HG11	1:I:164:MET:HE1	1.74	0.69
1:I:30:GLU:OE2	1:I:258:GLN:HG2	1.94	0.69
1:J:206:VAL:HG21	1:J:222:LEU:HB2	1.74	0.68
1:H:169:GLN:C	1:H:170:LEU:HD23	2.13	0.68
1:B:184:LEU:O	1:B:188:ARG:HG3	1.94	0.68
1:B:144:ARG:HH21	1:C:226:GLU:HG3	1.59	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:216:TYR:CE2	1:I:218:LEU:HB2	2.30	0.67
1:I:51:ILE:HD11	1:I:164:MET:CE	2.23	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:H	1:G:55:LEU:HD12	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: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:HD12	1:D:55:LEU:H	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: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:D:156:VAL:HG11	1:D:164:MET:HE2	1.78	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:N	1:J:55:LEU:HD12	2.13	0.64
1:B:195:GLN:HG3	1:B:262:GLY:O	1.98	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:I:51:ILE:HD11	1:I:164:MET:HE1	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:E:227:VAL:HG12	1:E:237:THR:HG22	1.80	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:A:108:LYS:CE	1:G:104:GLN:HG3	2.26	0.62
1:L:34:ARG:HE	1:L:254:PHE:HE1	1.47	0.62
1:M:134:TYR:C	1:M:136:LYS:N	2.52	0.62
1:B:203:ALA:HB2	1:B:223:GLU:HA	1.81	0.62
1:D:170:LEU:HD22	1:D:170:LEU:N	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: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:H:208:LEU:HD11	1:H:255:VAL:CG2	2.30	0.62
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:I:156:VAL:HG11	1:I:164:MET:CE	2.29	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:L:222:LEU:C	1:L:222:LEU:HD12	2.18	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:108:LYS:HE3	1:G:104:GLN:CG	2.25	0.61
1:A:34:ARG:HD2	1:A:252:GLY:O	2.00	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:206:VAL:O	1:F:219:GLU:HG3	2.00	0.61
1:K:222:LEU:HD12	1:K:222:LEU:C	2.21	0.61
1:E:260:GLN:OE1	1:E:260:GLN:HA	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:E:45:PRO:HB3	1:E:164:MET:HE1	1.82	0.60
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: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:199:ALA:HB2	1:F:205:LYS:N	2.17	0.60
1:F:55:LEU:HD12	1:F:55:LEU:N	2.16	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:216:TYR:CE2	1:F:218:LEU:HB2	2.37	0.59
1:F:78:ALA:HA	1:G:85:ALA:HB1	1.84	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:253:MET:HE3	1:C:181:SER:HB3	1.84	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: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:206:VAL:HG12	1:A:207:SER:N	2.18	0.59
1:A:47:VAL:HB	1:A:76:TYR:OH	2.03	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:N	1:I:55:LEU:HD12	2.17	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: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:M:184:LEU:HD22	1:M:236:VAL:HG11	1.86	0.58
1:L:39:ARG:NH1	1:M:54:ARG:NH2	2.47	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:G:50:ILE:CD1	1:G:155:LEU:HB2	2.34	0.58
1:C:104:GLN:HE22	1:I:104:GLN:HE22	1.50	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: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:F:101:VAL:HG13	1:F:106:VAL:HG13	1.85	0.57
1:G:148:SER:C	1:G:150:VAL:H	2.07	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:134:TYR:C	1:A:136:LYS:H	2.08	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:A:227:VAL:O	1:A:227:VAL:HG12	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:101:VAL:HG13	1:E:106:VAL:HG13	1.86	0.57
1:E:38:PHE:HD2	1:E:169:GLN:NE2	2.03	0.57
1:E:75:THR:HG23	1:F:127:GLN:HE22	1.68	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:G:221:ARG:NH1	1:G:221:ARG:HB3	2.20	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:96:ARG:HH21	1:D:109:GLN:CD	2.06	0.56
1:B:101:VAL:HG13	1:B:106:VAL:HG13	1.86	0.56
1:H:41:ALA:HB1	1:H:140:PRO:HG3	1.87	0.56
1:L:39:ARG:HH12	1:M:54:ARG:HH22	1.49	0.56
1:B:215:GLN:NE2	1:B:258:GLN:OE1	2.37	0.56
1:I:206:VAL:HG11	1:I:257:ALA:HB1	1.88	0.56
1:B:55:LEU:N	1:B:55:LEU:HD12	2.19	0.56
1:F:147:ARG:HH11	1:F:147:ARG:HB3	1.71	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:156:VAL:HG11	1:H:164:MET:CE	2.36	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:F:265:GLN:CD	1:F:265:GLN:N	2.59	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: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: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: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: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:CD1	1:C:55:LEU:H	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:D:227:VAL:HG21	1:D:239:ARG:HG2	1.88	0.55
1:J:206:VAL:HG23	1:J:220:GLY:O	2.07	0.55
1:J:55:LEU:H	1:J:55:LEU:CD1	2.09	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:M:64:ALA:HB2	1:M:141:ILE:C	2.28	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:I:64:ALA:HB2	1:I:141:ILE:C	2.28	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
1:G:106:VAL:HG22	1:G:110:GLN:HB2	1.90	0.54
1:G:53:LYS:HA	1:G:152:GLU:OE1	2.08	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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:55:LEU:N	1:G:55:LEU:HD12	2.23	0.53
1:H:144:ARG:HG3	1:H:144:ARG:HH11	1.74	0.53
1:K:106:VAL:HG23	1:K:110:GLN:OE1	2.09	0.53
1:K:34:ARG:NE	1:K:254:PHE:CE1	2.77	0.53
1:M:35:THR:HB	1:M:173:ILE:HD11	1.90	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: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:M:23:GLN:O	1:M:266:LYS:HA	2.08	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: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: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:106:VAL:HG22	1:C:110:GLN:HB2	1.91	0.53
1:C:49:GLY:O	1:C:155:LEU:HD12	2.08	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: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:HD23	1:I:138:LEU:N	2.23	0.53
1:B:240:ALA:HB1	1:B:242:PHE:HE2	1.75	0.52
1:B:64:ALA:HB2	1:B:141:ILE:HA	1.91	0.52
1:D:244:ASN:HD21	1:D:249:LEU:H	1.57	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:158:ASN:C	1:E:160:GLN:H	2.13	0.52
1:E:246:ASN:O	1:F:188:ARG:NH2	2.42	0.52
1:G:221:ARG:HH11	1:G:221:ARG:HB3	1.74	0.52
1:B:253:MET:CE	1:C:181:SER:HB3	2.39	0.52
1:E:189:ARG:HG3	1:E:189:ARG:HH11	1.73	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:169:GLN:C	1:D:170:LEU:HD22	2.30	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:I:193:SER:OG	1:I:194:GLY:N	2.41	0.52
1:H:39:ARG:NH1	1:I:54:ARG:NH2	2.52	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:D:208:LEU:HD22	1:D:242:PHE:CD2	2.45	0.52
1:J:44:ARG:NH1	1:J:44:ARG:CD	2.73	0.52
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:64:ALA:HB2	1:D:141:ILE:C	2.30	0.51
1:D:55:LEU:HD12	1:D:55:LEU:N	2.24	0.51
1:E:106:VAL:HG22	1:E:110:GLN:HB2	1.92	0.51
1:E:54:ARG:HG3	1:E:69:TYR:CE1	2.45	0.51
1:H:156:VAL:HG11	1:H:164:MET:HE3	1.91	0.51
1:K:23:GLN:O	1:K:266:LYS:HA	2.09	0.51
1:A:134:TYR:C	1:A:136:LYS:N	2.62	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:D:251:PRO:HB2	1:E:231:GLU:HG2	1.92	0.51
1:K:206:VAL:HG13	1:K:258:GLN:O	2.09	0.51
1:J:185:LEU:HD11	1:K:248:GLU:HB3	1.92	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:M:206:VAL:HG11	1:M:257:ALA:HB1	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:E:159:GLY:O	1:E:160:GLN:C	2.50	0.51
1:H:51:ILE:HD11	1:H:164:MET:HE1	1.90	0.51
1:H:220:GLY:HA3	1:H:242:PHE:HD1	1.75	0.51
1:H:206:VAL:HG21	1:H:222:LEU:HB2	1.91	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:HH11	1:G:144:ARG:HG3	1.74	0.51
1:B:169:GLN:O	1:B:170:LEU:HD23	2.11	0.51
1:K:39:ARG:HH12	1:L:54:ARG:NH2	2.09	0.51
1:A:208:LEU:HD11	1:A:255:VAL:CG2	2.40	0.51
1:G:155:LEU:C	1:G:155:LEU:HD23	2.31	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:M:222:LEU:HD12	1:M:222:LEU:C	2.31	0.51
1:A:64:ALA:HB2	1:A:141:ILE:C	2.30	0.50
1:F:64:ALA:HB2	1:F:141:ILE:HA	1.93	0.50
1:I:48:ASN:O	1:I:76:TYR:OH	2.22	0.50
1:L:212:ASP:OD1	1:L:213:GLY:N	2.45	0.50
1:B:219:GLU:HG2	1:B:220:GLY:N	2.25	0.50
1:A:54:ARG:NH2	1:B:39:ARG:HH12	2.09	0.50
1:C:162:ASN:N	1:C:162:ASN:HD22	2.09	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:D:67:GLN:HA	1:D:138:LEU:HD23	1.93	0.50
1:D:54:ARG:HG3	1:D:69:TYR:CE1	2.47	0.50
1:H:54:ARG:HG3	1:H:69:TYR:CE1	2.46	0.50
1:J:244:ASN:ND2	1:J:249:LEU:HB2	2.27	0.50
1:J:54:ARG:HG3	1:J:69:TYR:CE1	2.46	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:M:202:ASN:CG	1:M:202:ASN:O	2.49	0.50
1:J:178:THR:CG2	1:J:237:THR:OG1	2.59	0.50
1:L:230:ASP:O	1:L:234:GLY:N	2.41	0.50
1:L:71:ILE:O	1:L:73:PRO:HD3	2.11	0.50
1:M:55:LEU:HD12	1:M:68:LEU:O	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:G:38:PHE:HA	1:G:174:TYR:CD2	2.47	0.50
1:G:206:VAL:HG11	1:G:257:ALA:HB1	1.94	0.50
1:G:50:ILE:HD13	1:G:155:LEU:CA	2.41	0.50
1:I:208:LEU:HD11	1:I:255:VAL:CB	2.41	0.50
1:I:34:ARG:NE	1:I:254:PHE:HE1	2.09	0.50
1:L:55:LEU:H	1:L:55:LEU:CD1	2.15	0.50
1:B:147:ARG:HB3	1:B:147:ARG:HH11	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:I:46:GLN:C	1:I:158:ASN:HB2	2.33	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:195:GLN:HG2	1:G:261:GLU:O	2.12	0.49
1:G:50:ILE:HD11	1:G:155:LEU:HB2	1.95	0.49
1:L:46:GLN:NE2	1:L:134:TYR:HE1	2.10	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:244:ASN:ND2	1:D:249:LEU:H	2.09	0.49
1:D:206:VAL:CG1	1:D:259:LEU:HD13	2.43	0.49
1:G:69:TYR:CD2	1:G:164:MET:HE1	2.47	0.49
1:H:185:LEU:CD2	1:I:210:LEU:HD13	2.42	0.49
1:J:199:ALA:HB2	1:J:204:ALA:C	2.33	0.49
1:K:103:ASP:C	1:K:105:ALA:H	2.16	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:H:113:ASP:O	1:H:116:ALA:HB3	2.13	0.49
1:A:200:GLY:O	1:A:201:ASP:C	2.52	0.48
1:C:138:LEU:N	1:C:138:LEU:HD12	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:CD1	1:I:55:LEU:H	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: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:231:GLU:H	1:I:231:GLU:CD	2.17	0.48
1:I:68:LEU:HD13	1:I:145:ILE:HD12	1.95	0.48
1:I:54:ARG:HG3	1:I:69:TYR:CE1	2.47	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:CD1	1:M:55:LEU:H	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:D:155:LEU:HD12	1:D:156:VAL:N	2.28	0.48
1:I:208:LEU:HD11	1:I:255:VAL:HG21	1.94	0.48
1:I:30:GLU:CD	1:I:258:GLN:HG2	2.34	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:120:GLN:O	1:M:123:ALA:HB3	2.13	0.48
1:M:48:ASN:OD1	1:M:157:THR:HA	2.14	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
1:D:157:THR:O	1:D:160:GLN:HG2	2.13	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: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:B:103:ASP:C	1:B:105:ALA:H	2.16	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:F:193:SER:OG	1:F:194:GLY:N	2.46	0.47
1:F:199:ALA:HB2	1:F:204:ALA:C	2.34	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:H:46:GLN:CD	1:H:134:TYR:CE1	2.88	0.47
1:I:206:VAL:HG12	1:I:207:SER:N	2.29	0.47
1:L:199:ALA:HB2	1:L:204:ALA:C	2.33	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:252:GLY:HA3	1:E:234:GLY:HA2	1.96	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:A:113:ASP:O	1:A:116:ALA:HB3	2.14	0.47
1:A:71:ILE:O	1:A:73:PRO:HD3	2.14	0.47
1:B:69:TYR:CD2	1:B:164:MET:HE1	2.49	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:K:244:ASN:CG	1:K:249:LEU:HB2	2.35	0.47
1:M:38:PHE:HB2	1:M:172:PRO:O	2.14	0.47
1:A:126:GLU:O	1:A:130:ILE:HG13	2.15	0.47
1:A:34:ARG:HD3	1:A:254:PHE:CZ	2.49	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: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:J:175:VAL:HB	1:J:240:ALA:HB3	1.97	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:199:ALA:HB2	1:C:204:ALA:C	2.35	0.47
1:D:73:PRO:O	1:D:74:ALA:C	2.52	0.47
1:G:41:ALA:HB1	1:G:140:PRO:HG3	1.97	0.47
1:K:174:TYR:CD1	1:K:241:VAL:HG22	2.51	0.47
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:91:GLN:HA	1:A:118:TYR:CD1	2.50	0.46
1:A:48:ASN:OD1	1:A:157:THR:HA	2.15	0.46
1:B:68:LEU:HD13	1:B:145:ILE:CD1	2.46	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:C:64:ALA:HB2	1:C:141:ILE:HA	1.97	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:CD2	1:B:242:PHE:N	2.84	0.46
1:C:31:LEU:HB3	1:C:177:VAL:CG1	2.41	0.46
1:E:190:GLU:HG2	1:E:195:GLN:NE2	2.31	0.46
1:E:69:TYR:HB2	1:E:137:VAL:HB	1.98	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: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:206:VAL:HG11	1:H:257:ALA:HB1	1.98	0.46
1:H:30:GLU:HG3	1:H:256:HIS:HB3	1.97	0.46
1:J:190:GLU:HB3	1:J:196:LEU:HD13	1.97	0.46
1:A:178:THR:HG22	1:A:235:SER:HB3	1.96	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:208:LEU:HD11	1:C:255:VAL:CG2	2.45	0.46
1:D:129:ARG:HH11	1:D:129:ARG:HG2	1.81	0.46
1:D:69:TYR:HB2	1:D:137:VAL:HB	1.97	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:222:LEU:O	1:D:222:LEU:HG	2.15	0.46
1:D:96:ARG:NH2	1:E:109:GLN:CD	2.59	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:F:167:VAL:HG12	1:F:168:GLN:N	2.31	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:I:210:LEU:HD22	1:I:253:MET:HE1	1.97	0.46
1:B:52:LEU:HA	1:B:52:LEU:HD23	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:HH11	1:F:129:ARG:HG2	1.80	0.46
1:H:103:ASP:C	1:H:105:ALA:H	2.18	0.46
1:I:103:ASP:C	1:I:105:ALA:H	2.20	0.46
1:J:56:PHE:CZ	1:J:148:SER:HB2	2.51	0.46
1:K:113:ASP:O	1:K:116:ALA:HB3	2.16	0.46
1:K:55:LEU:HD12	1:K:68:LEU:O	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:I:199:ALA:HB2	1:I:204:ALA:C	2.36	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:A:180:PRO:O	1:A:181:SER:C	2.54	0.45
1:D:103:ASP:C	1:D:105:ALA:H	2.19	0.45
1:E:48:ASN:OD1	1:E:157:THR:HA	2.15	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
1:E:27:LEU:O	1:E:260:GLN:OE1	2.33	0.45
1:F:103:ASP:C	1:F:105:ALA:H	2.20	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:K:202:ASN:O	1:K:224:PHE:HD2	1.99	0.45
1:K:64:ALA:HB2	1:K:141:ILE:HA	1.97	0.45
1:L:151:THR:O	1:L:152:GLU:C	2.51	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: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:HA	1:D:52:LEU:HD23	1.82	0.45
1:A:104:GLN:HE22	1:G:104:GLN:HE22	1.64	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:A:103:ASP:C	1:A:105:ALA:H	2.20	0.45
1:D:43:VAL:HG23	1:D:165:ALA:O	2.17	0.45
1:F:147:ARG:HG3	1:F:147:ARG:O	2.16	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:103:ASP:C	1:M:105:ALA:H	2.19	0.45
1:M:57:LYS:HB3	1:M:60:SER:HB3	1.98	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:103:ASP:C	1:L:105:ALA:H	2.20	0.45
1:L:55:LEU:HD12	1:L:68:LEU:O	2.16	0.45
1:M:182:THR:O	1:M:185:LEU:HB2	2.16	0.45
1:M:46:GLN:NE2	1:M:134:TYR:CE1	2.84	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:216:TYR:HA	1:K:217:PRO:HD2	1.85	0.45
1:K:28:ASN:OD1	1:K:260:GLN:HB2	2.16	0.45
1:K:299:ILE:HA	1:K:314:GLY:HA3	1.99	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
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:J:103:ASP:C	1:J:105:ALA:H	2.19	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: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:106:VAL:HG23	1:E:110:GLN:OE1	2.17	0.45
1:E:91:GLN:HA	1:E:118:TYR:CD1	2.52	0.45
1:E:206:VAL:HG21	1:E:222:LEU:CB	2.39	0.45
1:E:86:ASN:O	1:E:89:SER:HB3	2.17	0.45
1:G:106:VAL:HG23	1:G:110:GLN:OE1	2.17	0.45
1:C:108:LYS:HG3	1:I:104:GLN:HB3	1.99	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:CD1	1:A:55:LEU:H	2.16	0.45
1:B:230:ASP:O	1:B:234:GLY:N	2.50	0.45
1:C:103:ASP:C	1:C:105:ALA:H	2.21	0.45
1:C:106:VAL:HG23	1:C:110:GLN:OE1	2.17	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:E:55:LEU:CD1	1:E:55:LEU:H	2.12	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:J:41:ALA:HB1	1:J:140:PRO:CG	2.47	0.45
1:M:38:PHE:CE1	1:M:172:PRO:HD2	2.52	0.45
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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:H:55:LEU:CD1	1:H:55:LEU:H	2.11	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: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:126:GLU:O	1:E:130:ILE:HG13	2.17	0.44
1:E:45:PRO:HD3	1:E:164:MET:HG3	1.99	0.44
1:G:120:GLN:O	1:G:123:ALA:HB3	2.17	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: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:E:207:SER:OG	1:E:258:GLN:HB2	2.17	0.44
1:F:137:VAL:O	1:F:138:LEU:HD23	2.18	0.44
1:F:86:ASN:O	1:F:89:SER:HB3	2.17	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:199:ALA:HB2	1:G:204:ALA:C	2.38	0.44
1:G:250:LEU:H	1:G:253:MET:CE	2.31	0.44
1:G:208:LEU:HD11	1:G:255:VAL:CG2	2.48	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:CB	1:I:198:ARG:HH11	2.11	0.44
1:J:259:LEU:HD23	1:J:259:LEU:HA	1.85	0.44
1:K:199:ALA:HB2	1:K:204:ALA:C	2.37	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:H:299:ILE:HA	1:H:314:GLY:HA3	1.99	0.44
1:A:175:VAL:HG21	1:A:242:PHE:CD2	2.49	0.43
1:D:218:LEU:H	1:D:218:LEU:HD12	1.83	0.43
1:D:57:LYS:HB3	1:D:60:SER:HB3	2.00	0.43
1:E:31:LEU:HB3	1:E:177:VAL:HG11	2.00	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:207:SER:O	1:A:257:ALA:HA	2.17	0.43
1:B:64:ALA:HB2	1:B:141:ILE:C	2.39	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:C:55:LEU:HD12	1:C:68:LEU:O	2.18	0.43
1:D:188:ARG:O	1:D:191:LEU:HB3	2.17	0.43
1:D:49:GLY:O	1:D:155:LEU:HD12	2.17	0.43
1:E:180:PRO:O	1:E:181:SER:C	2.56	0.43
1:J:64:ALA:HB2	1:J:142:SER:N	2.33	0.43
1:L:98:LYS:HG3	1:L:111:TYR:CZ	2.54	0.43
1:L:38:PHE:HB2	1:L:172:PRO:O	2.18	0.43
1:M:77:GLU:HA	1:M:132:LEU:HD22	2.01	0.43
1:M:41:ALA:HB2	1:M:141:ILE:HG23	2.00	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:F:261:GLU:CD	1:F:303:ARG:HH22	2.21	0.43
1:F:288:VAL:HG13	1:F:288:VAL:O	2.17	0.43
1:F:92:GLU:OE2	1:F:96:ARG:NH1	2.52	0.43
1:H:109:GLN:CD	1:I:96:ARG:NE	2.71	0.43
1:H:91:GLN:HA	1:H:118:TYR:CD1	2.53	0.43
1:K:129:ARG:HH11	1:K:129:ARG:HG2	1.84	0.43
1:L:206:VAL:HG21	1:L:222:LEU:HB2	1.99	0.43
1:B:46:GLN:NE2	1:B:134:TYR:CE1	2.86	0.43
1:B:202:ASN:O	1:B:224:PHE:HD2	2.02	0.43
1:B:184:LEU:HD22	1:B:236:VAL:HG11	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:193:SER:OG	1:C:194:GLY:N	2.50	0.43
1:E:45:PRO:CB	1:E:164:MET:HE1	2.47	0.43
1:E:299:ILE:HA	1:E:314:GLY:HA3	2.00	0.43
1:E:92:GLU:OE2	1:E:96:ARG:NH1	2.52	0.43
1:F:208:LEU:HD12	1:F:256:HIS:O	2.18	0.43
1:F:63:LYS:HA	1:F:142:SER:OG	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:195:GLN:O	1:K:196:LEU:HD12	2.18	0.43
1:K:54:ARG:HD2	1:K:148:SER:HB2	2.00	0.43
1:M:244:ASN:CG	1:M:249:LEU:HB2	2.38	0.43
1:A:202:ASN:C	1:A:202:ASN:HD22	2.21	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:M:226:GLU:OE1	1:M:228:SER:N	2.52	0.43
1:M:241:VAL:HG12	1:M:241:VAL:O	2.19	0.43
1:D:55:LEU:CD1	1:D:55:LEU:H	2.20	0.43
1:F:272:GLN:HB2	1:F:309:TRP:CD1	2.53	0.43
1:I:210:LEU:HD21	1:I:249:LEU:HD21	2.01	0.43
1:I:38:PHE:CD2	1:I:169:GLN:NE2	2.87	0.43
1:J:231:GLU:HG3	1:K:251:PRO:CB	2.49	0.43
1:I:229:VAL:HG11	1:J:251:PRO:O	2.19	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:254:PHE:CD2	1:E:254:PHE:N	2.85	0.43
1:E:98:LYS:HG3	1:E:111:TYR:CZ	2.54	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: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
1:G:250:LEU:H	1:G:253:MET:HE3	1.83	0.43
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:D:246:ASN:O	1:D:247:ASN:C	2.56	0.43
1:F:98:LYS:HG3	1:F:111:TYR:CZ	2.54	0.43
1:G:103:ASP:C	1:G:105:ALA:H	2.22	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:218:LEU:HD22	1:H:218:LEU:H	1.84	0.43
1:H:206:VAL:O	1:H:219:GLU:HG3	2.19	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: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:230:ASP:O	1:G:234:GLY:N	2.41	0.42
1:G:86:ASN:O	1:G:89:SER:HB3	2.19	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: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:C:52:LEU:HA	1:C:52:LEU:HD23	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: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: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:HD2	1:M:38:PHE:O	2.01	0.42
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:103:ASP:C	1:E:105:ALA:H	2.21	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:M:180:PRO:O	1:M:181:SER:C	2.57	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: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:G:134:TYR:OH	1:H:74:ALA:CB	2.68	0.42
1:A:173:ILE:HG22	1:A:242:PHE:O	2.20	0.42
1:E:126:GLU:OE2	1:E:129:ARG:NH2	2.52	0.42
1:F:69:TYR:CD2	1:F:164:MET:HE3	2.55	0.42
1:F:174:TYR:CD1	1:F:241:VAL:HG22	2.55	0.42
1:G:191:LEU:N	1:G:196:LEU:HD22	2.35	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:120:GLN:O	1:J:123:ALA:HB3	2.19	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:K:77:GLU:HA	1:K:132:LEU:HD22	2.00	0.42
1:B:250:LEU:HD12	1:C:236:VAL:HG21	2.01	0.42
1:J:109:GLN:O	1:J:112:ALA:HB3	2.19	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: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:K:132:LEU:O	1:K:135:THR:HG23	2.19	0.42
1:L:91:GLN:HA	1:L:118:TYR:CD1	2.55	0.42
1:A:250:LEU:N	1:A:253:MET:SD	2.88	0.42
1:B:180:PRO:O	1:B:181:SER:C	2.58	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:145:ILE:HG23	1:H:145:ILE:O	2.19	0.42
1:H:67:GLN:HA	1:H:138:LEU:HD23	2.01	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:A:158:ASN:C	1:A:158:ASN:OD1	2.58	0.42
1:B:126:GLU:O	1:B:130:ILE:HG13	2.19	0.42
1:D:47:VAL:HG13	1:D:134:TYR:CB	2.50	0.42
1:C:250:LEU:HD12	1:D:236:VAL:HG21	2.01	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:L:92:GLU:OE2	1:L:96:ARG:NH1	2.53	0.42
1:D:101:VAL:HG12	1:D:106:VAL:O	2.20	0.41
1:D:51:ILE:HD11	1:D:164:MET:CE	2.50	0.41
1:E:260:GLN:OE1	1:E:260:GLN:CA	2.67	0.41
1:E:68:LEU:HD13	1:E:145:ILE:CD1	2.50	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:218:LEU:HD23	1:K:218:LEU:N	2.34	0.41
1:K:63:LYS:O	1:K:66:GLN:HB2	2.20	0.41
1:M:182:THR:OG1	1:M:183:ALA:N	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:246:ASN:HB2	1:M:248:GLU:HG3	2.03	0.41
1:M:170:LEU:HD13	1:M:251:PRO:HD3	2.01	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: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:D:129:ARG:HG2	1:D:129:ARG:NH1	2.34	0.41
1:G:38:PHE:CD1	1:G:174:TYR:CE2	3.08	0.41
1:H:121:SER:O	1:H:122:LYS:C	2.59	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: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:H:156:VAL:HG11	1:H:164:MET:HE1	2.02	0.41
1:I:40:ILE:HD13	1:I:168:GLN:HE21	1.85	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: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:77:GLU:HA	1:I:132:LEU:HD22	2.02	0.41
1:I:64:ALA:HA	1:I:141:ILE:O	2.20	0.41
1:J:203:ALA:HB2	1:J:223:GLU:OE1	2.20	0.41
1:J:56:PHE:HZ	1:J:148:SER:HB2	1.85	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: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:D:144:ARG:HE	1:E:226:GLU:CD	2.24	0.41
1:E:34:ARG:NH1	1:E:254:PHE:CD2	2.89	0.41
1:E:64:ALA:HB2	1:E:141:ILE:C	2.40	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:219:GLU:HG3	1:A:220:GLY:H	1.84	0.41
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:I:184:LEU:HD12	1:I:184:LEU:O	2.20	0.41
1:I:187:LEU:N	1:I:187:LEU:HD23	2.35	0.41
1:K:216:TYR:CZ	1:K:249:LEU:HD11	2.56	0.41
1:M:199:ALA:HB2	1:M:204:ALA:C	2.40	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: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:183:ALA:O	1:K:186:ARG:HB3	2.20	0.41
1:K:57:LYS:HB3	1:K:60:SER:HB3	2.02	0.41
1:B:144:ARG:HH11	1:B:144:ARG:HG3	1.86	0.41
1:D:244:ASN:HD21	1:D:249:LEU:N	2.18	0.41
1:D:51:ILE:HD11	1:D:164:MET:HE1	2.02	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: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:F:299:ILE:CG2	1:F:315:LEU:HG	2.51	0.41
1:J:86:ASN:O	1:J:89:SER:HB3	2.21	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:206:VAL:HG21	1:M:222:LEU:HB2	2.02	0.41
1:E:16:GLY:HA2	1:E:338:VAL:O	2.21	0.41
1:F:203:ALA:HB2	1:F:223:GLU:HA	2.03	0.41
1:F:81:GLN:HB3	1:G:82:SER:HA	2.03	0.41
1:J:34:ARG:NE	1:J:254:PHE:CE1	2.89	0.41
1:M:38:PHE:CD2	1:M:38:PHE:C	2.95	0.41
1:M:54:ARG:HD2	1:M:148:SER:HB2	2.03	0.41
1:C:91:GLN:HA	1:C:118:TYR:CD1	2.55	0.41
1:G:38:PHE:HD2	1:G:169:GLN:NE2	2.18	0.41
1:J:52:LEU:HA	1:J:52:LEU:HD23	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:B:215:GLN:NE2	1:B:258:GLN:CD	2.74	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:L:141:ILE:O	1:L:141:ILE:CG1	2.69	0.40
1:C:244:ASN:ND2	1:C:247:ASN:HA	2.37	0.40
1:C:96:ARG:CZ	1:D:109:GLN:OE1	2.69	0.40
1:D:183:ALA:O	1:D:187:LEU:HG	2.22	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:144:ARG:HG3	1:G:144:ARG:NH1	2.36	0.40
1:G:50:ILE:HD13	1:G:155:LEU:HB2	2.02	0.40
1:G:162:ASN:HA	1:G:162:ASN:HD22	1.64	0.40
1:G:166:THR:HG22	1:G:167:VAL:N	2.36	0.40
1:H:170:LEU:HD23	1:H:170:LEU:N	2.35	0.40
1:K:55:LEU:CD1	1:K:55:LEU:H	2.21	0.40
1:M:202:ASN:O	1:M:224:PHE:CD2	2.71	0.40
1:I:91:GLN:HG2	1:I:95:GLN:OE1	2.22	0.40
1:L:46:GLN:CD	1:L:134:TYR:CE1	2.95	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: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:K:200:GLY:O	1:K:202:ASN:N	2.54	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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%)	5	31
1	B	325/360 (90%)	284 (87%)	32 (10%)	9 (3%)	5	29
1	C	325/360 (90%)	279 (86%)	40 (12%)	6 (2%)	8	41
1	D	228/360 (63%)	195 (86%)	31 (14%)	2 (1%)	17	56
1	E	325/360 (90%)	280 (86%)	38 (12%)	7 (2%)	6	35
1	F	325/360 (90%)	277 (85%)	43 (13%)	5 (2%)	10	44
1	G	325/360 (90%)	277 (85%)	41 (13%)	7 (2%)	6	35
1	H	325/360 (90%)	288 (89%)	32 (10%)	5 (2%)	10	44
1	I	325/360 (90%)	281 (86%)	38 (12%)	6 (2%)	8	41
1	J	325/360 (90%)	277 (85%)	43 (13%)	5 (2%)	10	44
1	K	325/360 (90%)	285 (88%)	34 (10%)	6 (2%)	8	41
1	L	325/360 (90%)	279 (86%)	41 (13%)	5 (2%)	10	44
1	M	325/360 (90%)	285 (88%)	32 (10%)	8 (2%)	5	32
All	All	4033/4680 (86%)	3478 (86%)	478 (12%)	77 (2%)	8	39

All (77) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	201	ASP
1	E	160	GLN

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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%)	178 (96%)	8 (4%)	29	64
1	B	193/287 (67%)	182 (94%)	11 (6%)	20	56
1	C	190/287 (66%)	177 (93%)	13 (7%)	16	49
1	D	185/287 (64%)	175 (95%)	10 (5%)	22	58
1	E	194/287 (68%)	177 (91%)	17 (9%)	10	36
1	F	240/287 (84%)	231 (96%)	9 (4%)	33	67
1	G	190/287 (66%)	183 (96%)	7 (4%)	34	68
1	H	194/287 (68%)	181 (93%)	13 (7%)	16	50
1	I	190/287 (66%)	180 (95%)	10 (5%)	22	58
1	J	189/287 (66%)	175 (93%)	14 (7%)	13	46
1	K	194/287 (68%)	183 (94%)	11 (6%)	20	56
1	L	190/287 (66%)	179 (94%)	11 (6%)	20	55
1	M	196/287 (68%)	181 (92%)	15 (8%)	13	44
All	All	2531/3731 (68%)	2382 (94%)	149 (6%)	19	54

All (149) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	55	LEU
1	A	75	THR
1	A	101	VAL
1	A	144	ARG
1	A	151	THR
1	A	186	ARG
1	A	202	ASN
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	152	GLU
1	B	155	LEU
1	B	201	ASP
1	B	226	GLU
1	B	260	GLN
1	C	34	ARG

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Mol	Chain	Res	Type
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	202	ASN
1	C	226	GLU
1	C	227	VAL
1	C	231	GLU
1	C	259	LEU
1	D	36	ASN
1	D	55	LEU
1	D	73	PRO
1	D	75	THR
1	D	101	VAL
1	D	152	GLU
1	D	157	THR
1	D	178	THR
1	D	201	ASP
1	D	226	GLU
1	E	28	ASN
1	E	55	LEU
1	E	73	PRO
1	E	75	THR
1	E	101	VAL
1	E	147	ARG
1	E	166	THR
1	E	193	SER
1	E	196	LEU
1	E	211	GLU
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	55	LEU
1	F	75	THR
1	F	101	VAL

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Mol	Chain	Res	Type
1	F	147	ARG
1	F	226	GLU
1	F	227	VAL
1	F	231	GLU
1	F	272	GLN
1	F	277	ARG
1	G	55	LEU
1	G	75	THR
1	G	101	VAL
1	G	201	ASP
1	G	221	ARG
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	172	PRO
1	H	195	GLN
1	H	201	ASP
1	H	202	ASN
1	H	225	SER
1	H	226	GLU
1	H	227	VAL
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	177	VAL
1	I	226	GLU
1	I	247	ASN
1	J	55	LEU
1	J	75	THR
1	J	101	VAL
1	J	152	GLU
1	J	177	VAL
1	J	181	SER

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Mol	Chain	Res	Type
1	J	206	VAL
1	J	226	GLU
1	J	227	VAL
1	J	229	VAL
1	J	233	THR
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
1	K	197	GLU
1	K	201	ASP
1	K	222	LEU
1	K	226	GLU
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	201	ASP
1	L	202	ASN
1	L	222	LEU
1	L	247	ASN
1	L	259	LEU
1	M	35	THR
1	M	38	PHE
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	193	SER
1	M	196	LEU
1	M	198	ARG
1	M	222	LEU

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Mol	Chain	Res	Type
1	M	226	GLU
1	M	239	ARG
1	M	259	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (85) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	36	ASN
1	A	84	GLN
1	A	86	ASN
1	A	93	GLN
1	A	104	GLN
1	A	109	GLN
1	A	162	ASN
1	A	195	GLN
1	A	202	ASN
1	B	46	GLN
1	B	86	ASN
1	B	93	GLN
1	B	162	ASN
1	B	215	GLN
1	B	258	GLN
1	B	260	GLN
1	C	84	GLN
1	C	86	ASN
1	C	127	GLN
1	C	162	ASN
1	C	202	ASN
1	C	258	GLN
1	D	86	ASN
1	D	127	GLN
1	D	162	ASN
1	D	215	GLN
1	E	46	GLN
1	E	86	ASN
1	E	127	GLN
1	E	168	GLN
1	E	169	GLN
1	E	195	GLN
1	F	84	GLN
1	F	86	ASN
1	F	93	GLN

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Mol	Chain	Res	Type
1	F	127	GLN
1	F	162	ASN
1	F	169	GLN
1	F	195	GLN
1	F	272	GLN
1	F	291	GLN
1	G	46	GLN
1	G	84	GLN
1	G	86	ASN
1	G	93	GLN
1	G	104	GLN
1	G	127	GLN
1	G	162	ASN
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	H	258	GLN
1	I	86	ASN
1	I	104	GLN
1	I	162	ASN
1	I	168	GLN
1	J	46	GLN
1	J	86	ASN
1	J	93	GLN
1	J	127	GLN
1	J	162	ASN
1	J	258	GLN
1	K	46	GLN
1	K	86	ASN
1	K	93	GLN
1	K	127	GLN
1	K	162	ASN
1	K	195	GLN
1	K	256	HIS
1	L	46	GLN
1	L	86	ASN
1	L	93	GLN
1	L	162	ASN

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Mol	Chain	Res	Type
1	L	169	GLN
1	M	36	ASN
1	M	46	GLN
1	M	84	GLN
1	M	86	ASN
1	M	93	GLN
1	M	109	GLN
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 carbohydrates 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	B	1340	-	4,4,4	0.36	0	6,6,6	0.15	0
2	SO4	F	1340	-	4,4,4	0.31	0	6,6,6	0.19	0
2	SO4	F	1341	-	4,4,4	0.35	0	6,6,6	0.09	0
2	SO4	K	1340	-	4,4,4	0.40	0	6,6,6	0.13	0
2	SO4	I	1340	-	4,4,4	0.39	0	6,6,6	0.07	0
2	SO4	E	1341	-	4,4,4	0.30	0	6,6,6	0.13	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	SO4	A	1261	-	4,4,4	0.38	0	6,6,6	0.13	0
2	SO4	M	1340	-	4,4,4	0.35	0	6,6,6	0.10	0
2	SO4	G	1340	-	4,4,4	0.34	0	6,6,6	0.10	0
2	SO4	J	1340	-	4,4,4	0.34	0	6,6,6	0.09	0
2	SO4	B	1341	-	4,4,4	0.31	0	6,6,6	0.13	0
2	SO4	E	1340	-	4,4,4	0.38	0	6,6,6	0.14	0
2	SO4	H	1340	-	4,4,4	0.36	0	6,6,6	0.12	0
2	SO4	A	1260	-	4,4,4	0.38	0	6,6,6	0.09	0
2	SO4	L	1340	-	4,4,4	0.34	0	6,6,6	0.11	0
2	SO4	C	1340	-	4,4,4	0.31	0	6,6,6	0.12	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%)	0.28	9 (3%) 39 25	34, 77, 127, 155	0
1	B	327/360 (90%)	0.18	20 (6%) 21 12	22, 71, 145, 153	0
1	C	327/360 (90%)	0.11	11 (3%) 45 29	20, 73, 141, 158	0
1	D	230/360 (63%)	0.01	2 (0%) 84 75	16, 59, 87, 110	0
1	E	327/360 (90%)	0.37	29 (8%) 9 5	9, 53, 148, 157	0
1	F	327/360 (90%)	0.16	6 (1%) 68 55	28, 66, 131, 148	0
1	G	327/360 (90%)	0.46	41 (12%) 3 2	34, 82, 147, 163	0
1	H	327/360 (90%)	0.79	61 (18%) 1 1	13, 56, 154, 165	0
1	I	327/360 (90%)	0.46	33 (10%) 7 4	9, 52, 147, 163	0
1	J	327/360 (90%)	0.53	49 (14%) 2 1	5, 37, 150, 165	0
1	K	327/360 (90%)	0.81	71 (21%) 0 0	6, 50, 157, 170	0
1	L	327/360 (90%)	0.57	44 (13%) 3 2	8, 56, 154, 173	0
1	M	327/360 (90%)	1.09	81 (24%) 0 0	18, 83, 158, 172	0
All	All	4059/4680 (86%)	0.46	457 (11%) 5 3	5, 65, 151, 173	0

All (457) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	M	339	PRO	9.5
1	M	331	PRO	8.4
1	I	274	GLY	8.3
1	K	317	ALA	7.7
1	K	15	VAL	7.6
1	H	295	GLU	6.9
1	M	315	LEU	6.9
1	K	338	VAL	6.8
1	L	325	GLY	6.7

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Mol	Chain	Res	Type	RSRZ
1	J	339	PRO	6.7
1	K	296	LEU	6.5
1	M	14	GLU	6.5
1	M	288	VAL	6.3
1	M	317	ALA	6.2
1	H	263	VAL	6.2
1	L	327	GLN	5.9
1	M	309	TRP	5.7
1	M	289	ASN	5.7
1	M	13	PRO	5.7
1	M	270	ALA	5.6
1	L	314	GLY	5.6
1	E	332	GLY	5.6
1	H	296	LEU	5.5
1	C	15	VAL	5.5
1	M	316	ASN	5.5
1	G	15	VAL	5.5
1	M	332	GLY	5.4
1	L	15	VAL	5.4
1	K	298	VAL	5.4
1	K	325	GLY	5.4
1	L	332	GLY	5.4
1	M	287	VAL	5.4
1	M	15	VAL	5.4
1	K	324	GLU	5.3
1	K	290	ALA	5.3
1	H	290	ALA	5.3
1	L	339	PRO	5.2
1	L	288	VAL	5.2
1	L	274	GLY	5.2
1	M	337	THR	5.2
1	K	281	GLY	5.2
1	K	16	GLY	5.2
1	M	271	PRO	5.2
1	M	301	ALA	5.2
1	M	338	VAL	5.1
1	L	328	PHE	5.1
1	E	296	LEU	5.1
1	K	316	ASN	5.1
1	L	333	VAL	5.1
1	K	267	ALA	5.1
1	L	334	GLU	5.0

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Mol	Chain	Res	Type	RSRZ
1	M	302	ASP	5.0
1	K	282	GLN	4.9
1	M	25	VAL	4.9
1	G	284	THR	4.9
1	L	289	ASN	4.8
1	H	337	THR	4.8
1	L	19	THR	4.8
1	K	337	THR	4.8
1	M	329	VAL	4.8
1	H	13	PRO	4.7
1	K	328	PHE	4.7
1	I	332	GLY	4.7
1	K	339	PRO	4.7
1	J	270	ALA	4.7
1	J	289	ASN	4.7
1	L	324	GLU	4.7
1	M	313	GLU	4.6
1	M	291	GLN	4.6
1	M	307	ASP	4.6
1	I	339	PRO	4.6
1	H	291	GLN	4.6
1	J	287	VAL	4.6
1	H	314	GLY	4.5
1	M	333	VAL	4.5
1	M	325	GLY	4.4
1	E	14	GLU	4.4
1	M	298	VAL	4.4
1	M	328	PHE	4.4
1	H	327	GLN	4.3
1	K	19	THR	4.3
1	H	287	VAL	4.3
1	M	19	THR	4.3
1	K	278	ASP	4.3
1	K	329	VAL	4.3
1	L	323	THR	4.3
1	H	15	VAL	4.3
1	E	337	THR	4.3
1	M	16	GLY	4.2
1	M	290	ALA	4.2
1	B	296	LEU	4.2
1	B	294	VAL	4.2
1	G	317	ALA	4.2

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Mol	Chain	Res	Type	RSRZ
1	H	332	GLY	4.2
1	M	292	ASN	4.1
1	H	331	PRO	4.1
1	M	21	GLU	4.1
1	M	321	ILE	4.1
1	H	264	LYS	4.1
1	M	296	LEU	4.1
1	K	309	TRP	4.1
1	M	285	ALA	4.1
1	M	314	GLY	4.1
1	B	332	GLY	4.1
1	G	324	GLU	4.1
1	J	295	GLU	4.1
1	L	13	PRO	4.1
1	E	265	GLN	4.0
1	H	294	VAL	4.0
1	K	13	PRO	4.0
1	M	275	VAL	4.0
1	K	295	GLU	4.0
1	H	319	ASP	4.0
1	M	276	THR	4.0
1	M	318	GLY	4.0
1	I	337	THR	4.0
1	M	320	LYS	4.0
1	L	278	ASP	4.0
1	M	330	GLN	4.0
1	F	296	LEU	4.0
1	K	285	ALA	4.0
1	H	289	ASN	3.9
1	M	274	GLY	3.9
1	K	17	ILE	3.9
1	J	288	VAL	3.9
1	K	276	THR	3.9
1	L	21	GLU	3.9
1	H	330	GLN	3.9
1	K	331	PRO	3.9
1	M	278	ASP	3.9
1	M	22	ALA	3.9
1	J	332	GLY	3.8
1	I	338	VAL	3.8
1	K	294	VAL	3.8
1	H	297	ARG	3.8

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Mol	Chain	Res	Type	RSRZ
1	M	319	ASP	3.8
1	J	22	ALA	3.8
1	G	16	GLY	3.8
1	H	281	GLY	3.8
1	H	288	VAL	3.8
1	K	333	VAL	3.8
1	M	294	VAL	3.8
1	M	311	VAL	3.8
1	J	16	GLY	3.8
1	M	299	ILE	3.8
1	G	285	ALA	3.8
1	M	306	GLY	3.7
1	G	337	THR	3.7
1	L	301	ALA	3.7
1	M	268	ILE	3.7
1	H	280	LYS	3.7
1	H	323	THR	3.7
1	I	15	VAL	3.7
1	J	326	LEU	3.7
1	G	294	VAL	3.7
1	H	265	GLN	3.7
1	B	333	VAL	3.7
1	M	295	GLU	3.7
1	K	271	PRO	3.6
1	J	325	GLY	3.6
1	H	334	GLU	3.6
1	H	25	VAL	3.6
1	L	270	ALA	3.6
1	I	271	PRO	3.6
1	G	283	ALA	3.6
1	H	270	ALA	3.6
1	M	277	ARG	3.6
1	G	339	PRO	3.6
1	M	286	LEU	3.6
1	H	333	VAL	3.6
1	J	324	GLU	3.5
1	B	13	PRO	3.5
1	H	292	ASN	3.5
1	K	283	ALA	3.5
1	K	270	ALA	3.5
1	K	334	GLU	3.5
1	J	21	GLU	3.5

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Mol	Chain	Res	Type	RSRZ
1	E	288	VAL	3.5
1	B	288	VAL	3.5
1	A	242	PHE	3.5
1	K	306	GLY	3.5
1	G	270	ALA	3.5
1	L	14	GLU	3.5
1	L	285	ALA	3.5
1	I	317	ALA	3.5
1	M	283	ALA	3.5
1	K	263	VAL	3.4
1	K	314	GLY	3.4
1	E	291	GLN	3.4
1	G	290	ALA	3.4
1	I	307	ASP	3.4
1	H	20	LEU	3.4
1	E	283	ALA	3.4
1	G	338	VAL	3.4
1	J	17	ILE	3.4
1	K	297	ARG	3.4
1	C	339	PRO	3.4
1	G	271	PRO	3.4
1	J	15	VAL	3.3
1	J	294	VAL	3.3
1	H	326	LEU	3.3
1	M	272	GLN	3.3
1	H	285	ALA	3.3
1	G	323	THR	3.3
1	M	297	ARG	3.3
1	J	338	VAL	3.3
1	F	22	ALA	3.2
1	H	16	GLY	3.2
1	M	273	GLN	3.2
1	M	323	THR	3.2
1	E	295	GLU	3.2
1	H	271	PRO	3.2
1	H	282	GLN	3.2
1	C	25	VAL	3.2
1	A	258	GLN	3.2
1	J	337	THR	3.2
1	H	279	LEU	3.2
1	K	293	LYS	3.2
1	M	312	THR	3.1

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Mol	Chain	Res	Type	RSRZ
1	H	262	GLY	3.1
1	L	16	GLY	3.1
1	J	333	VAL	3.1
1	K	330	GLN	3.1
1	M	308	LYS	3.1
1	K	323	THR	3.1
1	L	296	LEU	3.1
1	L	326	LEU	3.1
1	K	299	ILE	3.1
1	K	277	ARG	3.1
1	M	282	GLN	3.1
1	G	22	ALA	3.1
1	L	338	VAL	3.1
1	I	287	VAL	3.1
1	L	294	VAL	3.1
1	K	266	LYS	3.1
1	J	271	PRO	3.1
1	K	284	THR	3.1
1	E	284	THR	3.1
1	H	329	VAL	3.1
1	H	338	VAL	3.0
1	K	14	GLU	3.0
1	L	275	VAL	3.0
1	B	15	VAL	3.0
1	K	300	LYS	3.0
1	L	271	PRO	3.0
1	C	289	ASN	3.0
1	H	335	VAL	3.0
1	E	13	PRO	3.0
1	G	31	LEU	3.0
1	E	290	ALA	3.0
1	B	270	ALA	3.0
1	H	299	ILE	3.0
1	H	14	GLU	3.0
1	J	278	ASP	2.9
1	J	281	GLY	2.9
1	I	283	ALA	2.9
1	K	326	LEU	2.9
1	E	294	VAL	2.9
1	M	20	LEU	2.9
1	H	328	PHE	2.9
1	H	293	LYS	2.9

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Mol	Chain	Res	Type	RSRZ
1	J	13	PRO	2.9
1	G	289	ASN	2.9
1	I	306	GLY	2.9
1	H	257	ALA	2.9
1	L	17	ILE	2.9
1	G	328	PHE	2.9
1	L	290	ALA	2.9
1	K	302	ASP	2.9
1	G	332	GLY	2.9
1	G	312	THR	2.8
1	M	24	THR	2.8
1	I	270	ALA	2.8
1	G	319	ASP	2.8
1	E	272	GLN	2.8
1	K	301	ALA	2.8
1	I	330	GLN	2.8
1	I	288	VAL	2.8
1	C	323	THR	2.8
1	I	24	THR	2.8
1	E	334	GLU	2.8
1	M	284	THR	2.8
1	H	17	ILE	2.8
1	K	22	ALA	2.8
1	H	309	TRP	2.8
1	G	292	ASN	2.8
1	G	274	GLY	2.8
1	I	285	ALA	2.8
1	E	333	VAL	2.8
1	I	17	ILE	2.8
1	J	330	GLN	2.8
1	G	293	LYS	2.8
1	J	331	PRO	2.8
1	H	286	LEU	2.7
1	B	325	GLY	2.7
1	H	336	LYS	2.7
1	M	281	GLY	2.7
1	I	301	ALA	2.7
1	K	274	GLY	2.7
1	G	281	GLY	2.7
1	L	292	ASN	2.7
1	J	328	PHE	2.7
1	J	282	GLN	2.7

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Mol	Chain	Res	Type	RSRZ
1	K	289	ASN	2.7
1	F	323	THR	2.7
1	M	262	GLY	2.7
1	G	273	GLN	2.7
1	B	287	VAL	2.7
1	C	288	VAL	2.6
1	L	281	GLY	2.6
1	G	287	VAL	2.6
1	J	299	ILE	2.6
1	I	305	ILE	2.6
1	B	331	PRO	2.6
1	E	278	ASP	2.6
1	J	327	GLN	2.6
1	C	331	PRO	2.6
1	A	232	GLY	2.6
1	A	233	THR	2.6
1	H	276	THR	2.6
1	E	282	GLN	2.6
1	J	304	VAL	2.6
1	G	268	ILE	2.6
1	I	13	PRO	2.6
1	L	335	VAL	2.6
1	C	295	GLU	2.6
1	J	274	GLY	2.6
1	M	327	GLN	2.5
1	H	298	VAL	2.5
1	J	318	GLY	2.5
1	I	329	VAL	2.5
1	K	291	GLN	2.5
1	I	16	GLY	2.5
1	A	196	LEU	2.5
1	C	19	THR	2.5
1	M	267	ALA	2.5
1	E	339	PRO	2.5
1	G	325	GLY	2.5
1	J	286	LEU	2.5
1	G	295	GLU	2.5
1	E	277	ARG	2.5
1	G	301	ALA	2.5
1	I	322	ILE	2.5
1	L	299	ILE	2.5
1	M	324	GLU	2.5

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Mol	Chain	Res	Type	RSRZ
1	G	306	GLY	2.4
1	I	286	LEU	2.4
1	K	20	LEU	2.4
1	J	293	LYS	2.4
1	M	300	LYS	2.4
1	M	105	ALA	2.4
1	J	323	THR	2.4
1	M	110	GLN	2.4
1	H	312	THR	2.4
1	J	298	VAL	2.4
1	L	279	LEU	2.4
1	J	290	ALA	2.4
1	K	273	GLN	2.4
1	J	319	ASP	2.4
1	K	315	LEU	2.4
1	M	26	THR	2.4
1	I	273	GLN	2.4
1	E	301	ALA	2.4
1	E	274	GLY	2.4
1	H	283	ALA	2.4
1	H	301	ALA	2.4
1	G	318	GLY	2.4
1	E	276	THR	2.4
1	G	288	VAL	2.3
1	L	287	VAL	2.3
1	M	227	VAL	2.3
1	J	302	ASP	2.3
1	I	268	ILE	2.3
1	A	191	LEU	2.3
1	K	262	GLY	2.3
1	E	297	ARG	2.3
1	M	310	LEU	2.3
1	E	287	VAL	2.3
1	K	332	GLY	2.3
1	L	330	GLN	2.3
1	K	292	ASN	2.3
1	J	314	GLY	2.3
1	M	279	LEU	2.3
1	F	306	GLY	2.3
1	G	331	PRO	2.2
1	H	268	ILE	2.2
1	D	114	ALA	2.2

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Mol	Chain	Res	Type	RSRZ
1	I	290	ALA	2.2
1	J	334	GLU	2.2
1	H	315	LEU	2.2
1	K	275	VAL	2.2
1	A	41	ALA	2.2
1	M	293	LYS	2.2
1	B	263	VAL	2.2
1	J	19	THR	2.2
1	G	333	VAL	2.2
1	J	268	ILE	2.2
1	M	17	ILE	2.2
1	G	272	GLN	2.2
1	K	310	LEU	2.2
1	D	105	ALA	2.2
1	M	326	LEU	2.2
1	H	324	GLU	2.2
1	K	335	VAL	2.2
1	E	285	ALA	2.2
1	L	316	ASN	2.2
1	J	291	GLN	2.2
1	K	21	GLU	2.2
1	I	262	GLY	2.2
1	I	325	GLY	2.2
1	K	336	LYS	2.2
1	L	273	GLN	2.1
1	B	278	ASP	2.1
1	K	318	GLY	2.1
1	C	285	ALA	2.1
1	E	330	GLN	2.1
1	B	277	ARG	2.1
1	B	317	ALA	2.1
1	H	316	ASN	2.1
1	I	321	ILE	2.1
1	L	295	GLU	2.1
1	I	289	ASN	2.1
1	I	323	THR	2.1
1	E	270	ALA	2.1
1	A	29	THR	2.1
1	C	273	GLN	2.1
1	E	329	VAL	2.1
1	A	31	LEU	2.1
1	B	257	ALA	2.1

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Mol	Chain	Res	Type	RSRZ
1	L	18	VAL	2.1
1	K	18	VAL	2.1
1	K	279	LEU	2.1
1	K	303	ARG	2.1
1	H	317	ALA	2.1
1	J	301	ALA	2.1
1	K	305	ILE	2.1
1	M	224	PHE	2.1
1	H	274	GLY	2.1
1	K	280	LYS	2.1
1	B	339	PRO	2.0
1	J	329	VAL	2.0
1	K	288	VAL	2.0
1	F	31	LEU	2.0
1	L	315	LEU	2.0
1	B	179	GLN	2.0
1	B	290	ALA	2.0
1	J	20	LEU	2.0
1	F	273	GLN	2.0
1	G	267	ALA	2.0
1	G	336	LYS	2.0
1	J	296	LEU	2.0
1	J	317	ALA	2.0
1	B	295	GLU	2.0
1	K	272	GLN	2.0
1	H	277	ARG	2.0
1	G	291	GLN	2.0
1	L	110	GLN	2.0

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. 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	B	1341	5/5	0.86	0.17	70,75,95,101	0
2	SO4	M	1340	5/5	0.87	0.20	65,69,92,99	0
2	SO4	B	1340	5/5	0.87	0.20	65,78,84,95	0
2	SO4	E	1340	5/5	0.90	0.21	50,60,69,87	0
2	SO4	A	1260	5/5	0.91	0.14	70,77,101,103	0
2	SO4	A	1261	5/5	0.92	0.20	62,66,94,95	0
2	SO4	I	1340	5/5	0.94	0.13	55,56,72,87	0
2	SO4	F	1340	5/5	0.94	0.14	62,76,97,97	0
2	SO4	F	1341	5/5	0.94	0.12	67,75,92,100	0
2	SO4	K	1340	5/5	0.96	0.17	34,34,58,60	0
2	SO4	G	1340	5/5	0.96	0.08	87,89,108,112	0
2	SO4	H	1340	5/5	0.96	0.15	54,57,74,79	0
2	SO4	J	1340	5/5	0.96	0.17	44,50,70,76	0
2	SO4	E	1341	5/5	0.97	0.14	43,52,59,68	0
2	SO4	L	1340	5/5	0.97	0.17	42,44,72,73	0
2	SO4	C	1340	5/5	0.97	0.12	71,71,77,85	0

6.5 Other polymers [i](#)

There are no such residues in this entry.