



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 05:54 AM GMT

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
<http://wwpdb.org/validation/2016/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 : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

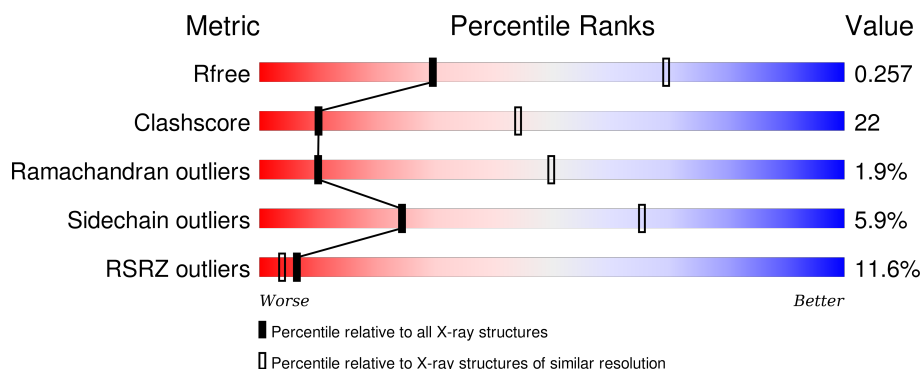
1 Overall quality at a glance ⓘ

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}	91344	1124 (3.24-3.16)
Clashscore	102246	1024 (3.22-3.18)
Ramachandran outliers	100387	1004 (3.22-3.18)
Sidechain outliers	100360	1003 (3.22-3.18)
RSRZ outliers	91569	1129 (3.24-3.16)

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. 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>

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Mol	Chain	Length	Quality of chain
1	F	360	
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:

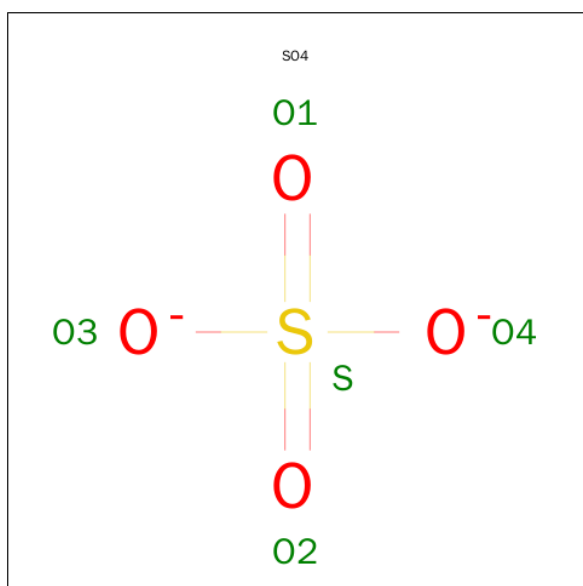
Chain	Residue	Modelled	Actual	Comment	Reference
A	1	SER	CYS	ENGINEERED MUTATION	UNP P52477
B	1	SER	CYS	ENGINEERED MUTATION	UNP P52477
C	1	SER	CYS	ENGINEERED MUTATION	UNP P52477

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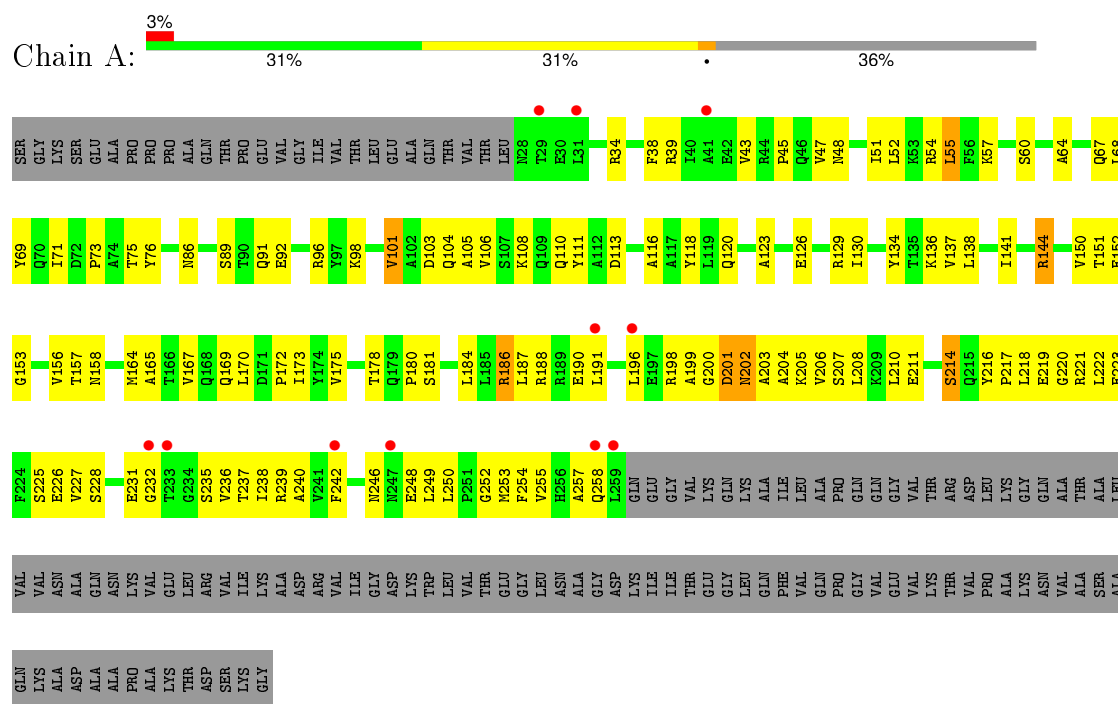
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	E	1	Total	O	S	0	0
			5	4	1		
2	F	1	Total	O	S	0	0
			5	4	1		
2	F	1	Total	O	S	0	0
			5	4	1		
2	G	1	Total	O	S	0	0
			5	4	1		
2	H	1	Total	O	S	0	0
			5	4	1		
2	I	1	Total	O	S	0	0
			5	4	1		
2	J	1	Total	O	S	0	0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

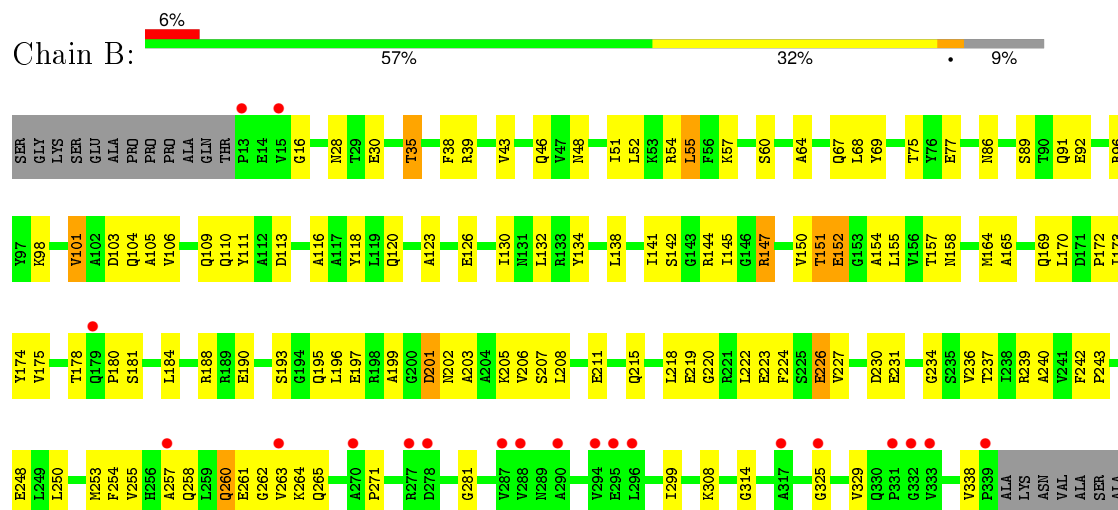
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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



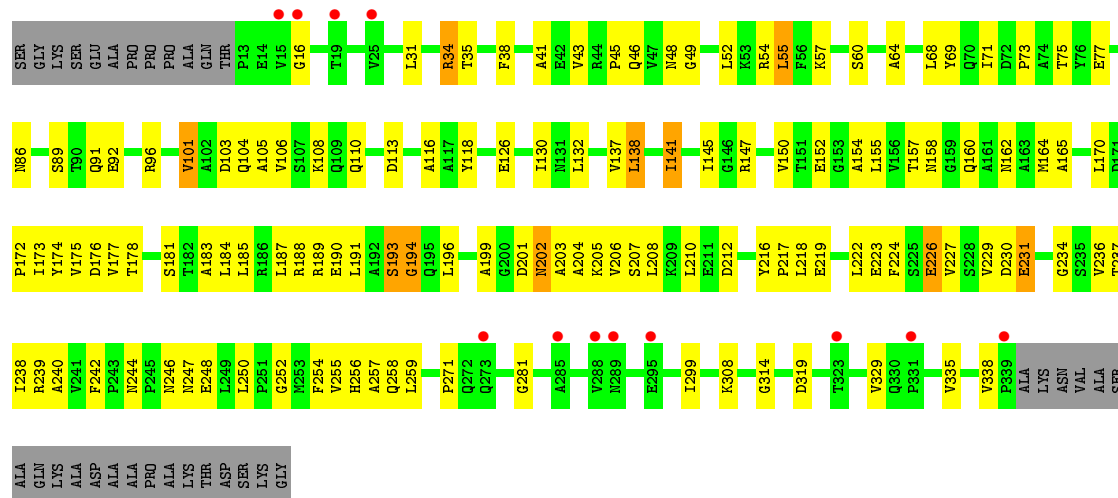
- Molecule 1: MULTIDRUG RESISTANCE PROTEIN MEXA

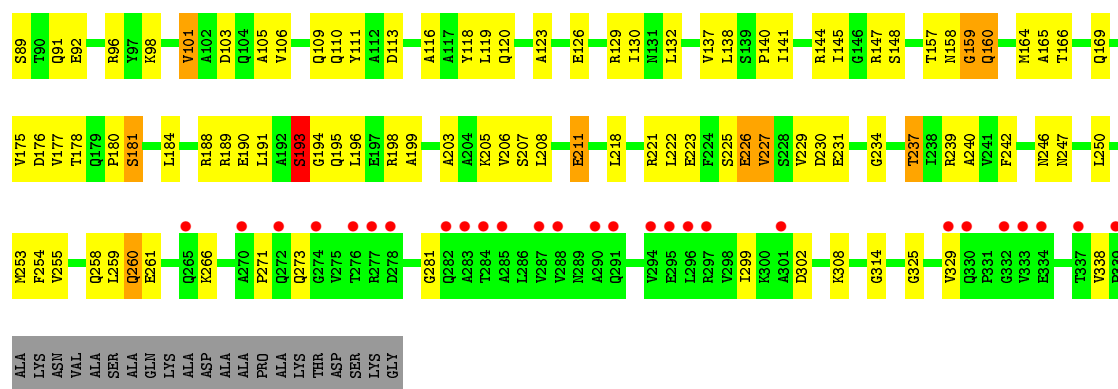


GLN
LYS
ALA
ASP
ALA
ALA
PRO
ALA
LYS
THR
ASP
SER
LYS
GLY

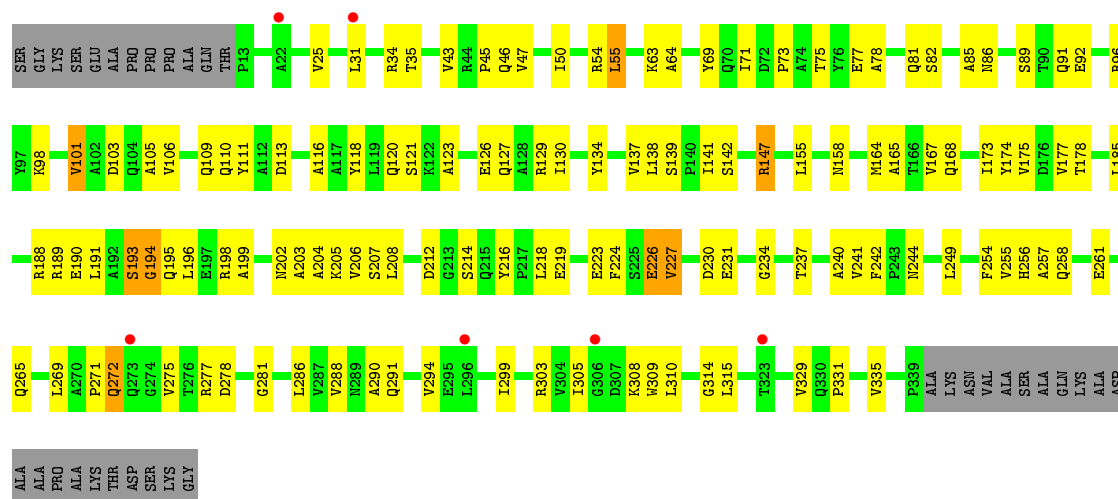
• Molecule 1: MULTIDRUG RESISTANCE PROTEIN MEXA

Chain C: 3% 56% 33% 9%

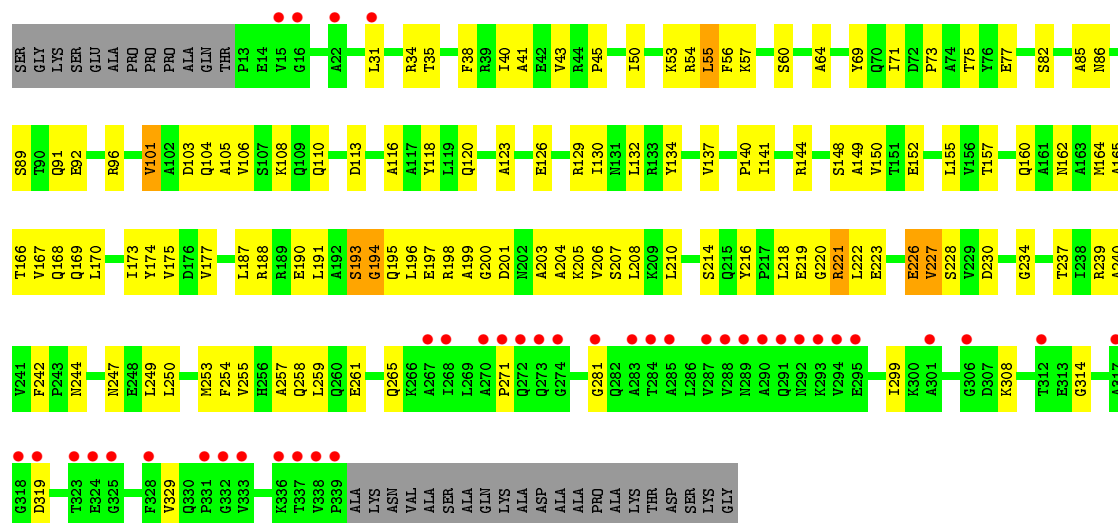




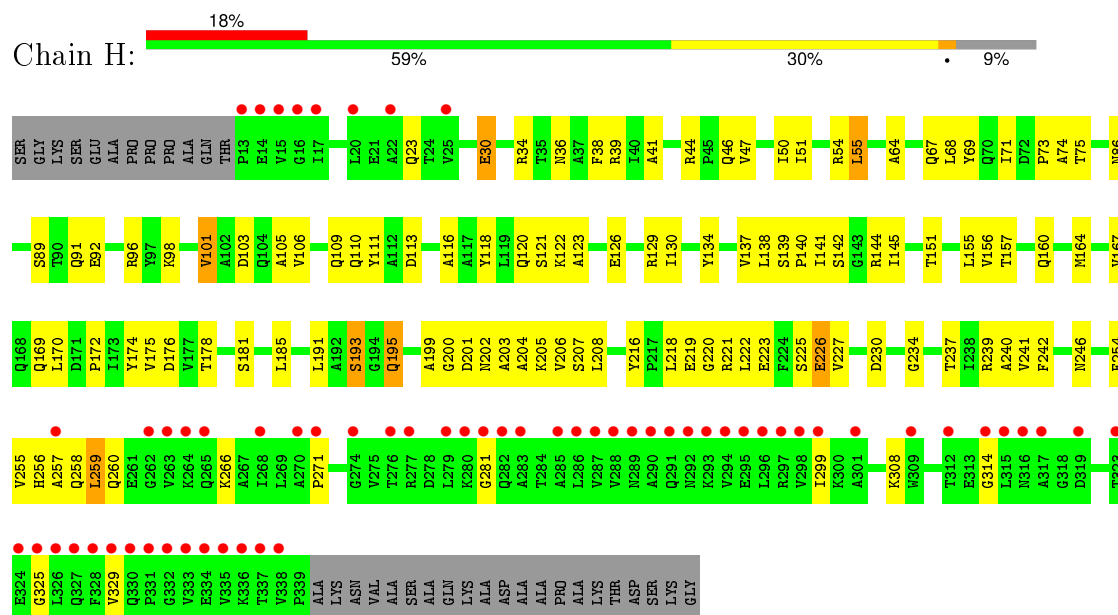
• Molecule 1: MULTIDRUG RESISTANCE PROTEIN MEXA



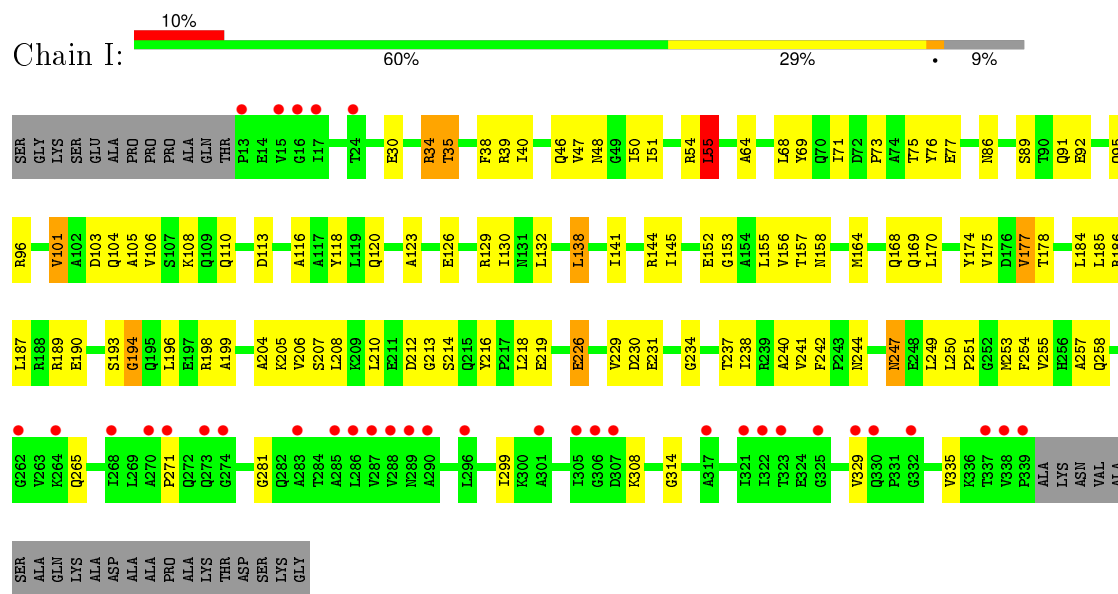
• Molecule 1: MULTIDRUG RESISTANCE PROTEIN MEXA



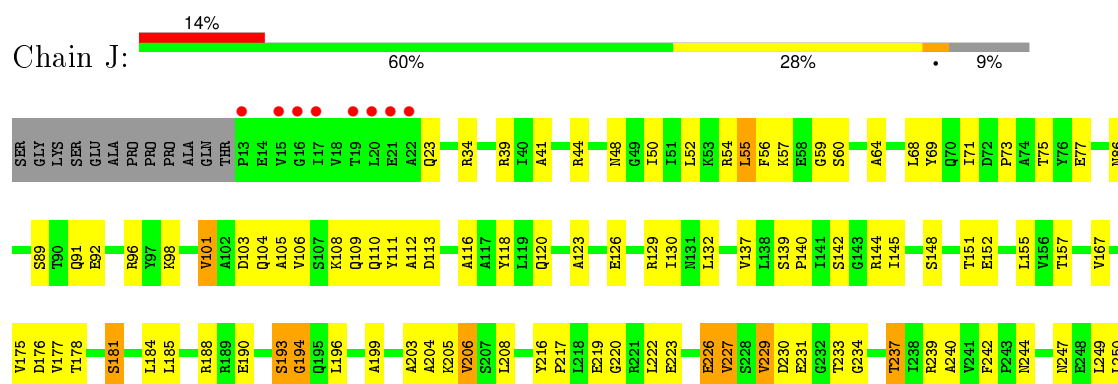
- Molecule 1: MULTIDRUG RESISTANCE PROTEIN MEXA

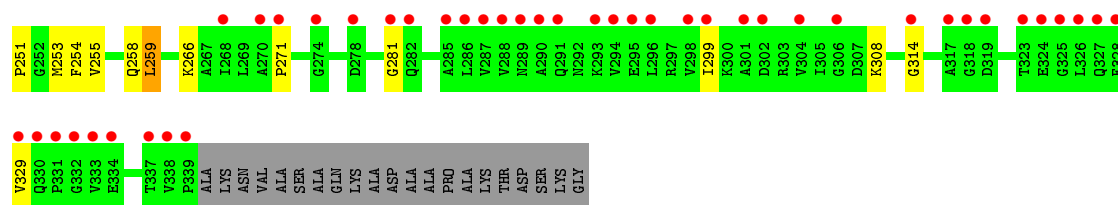


- Molecule 1: MULTIDRUG RESISTANCE PROTEIN MEXA

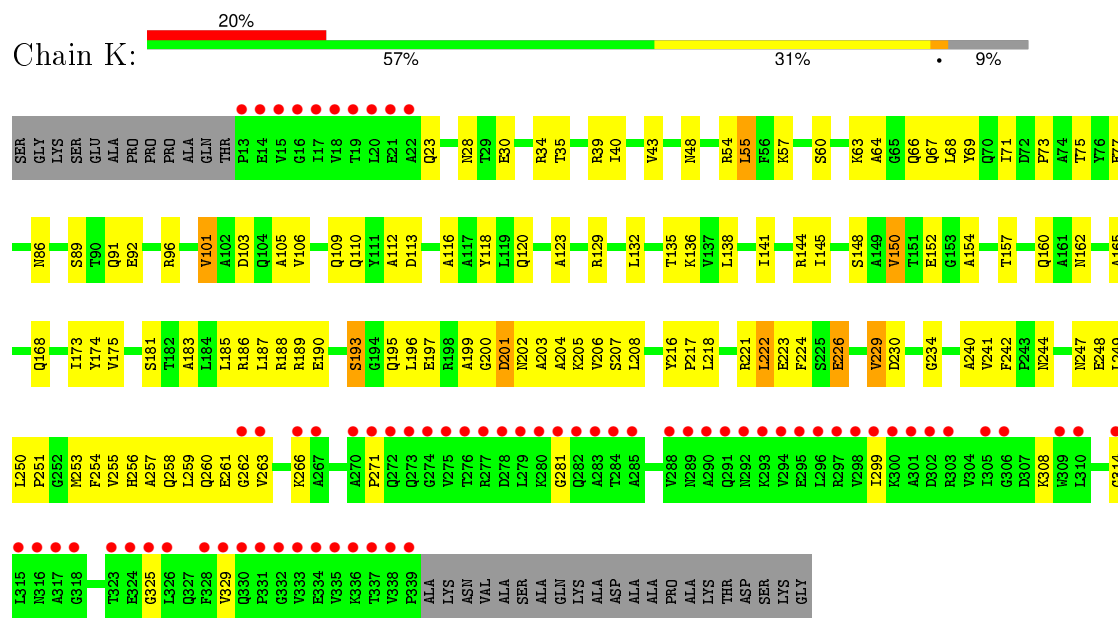


- Molecule 1: MULTIDRUG RESISTANCE PROTEIN MEXA

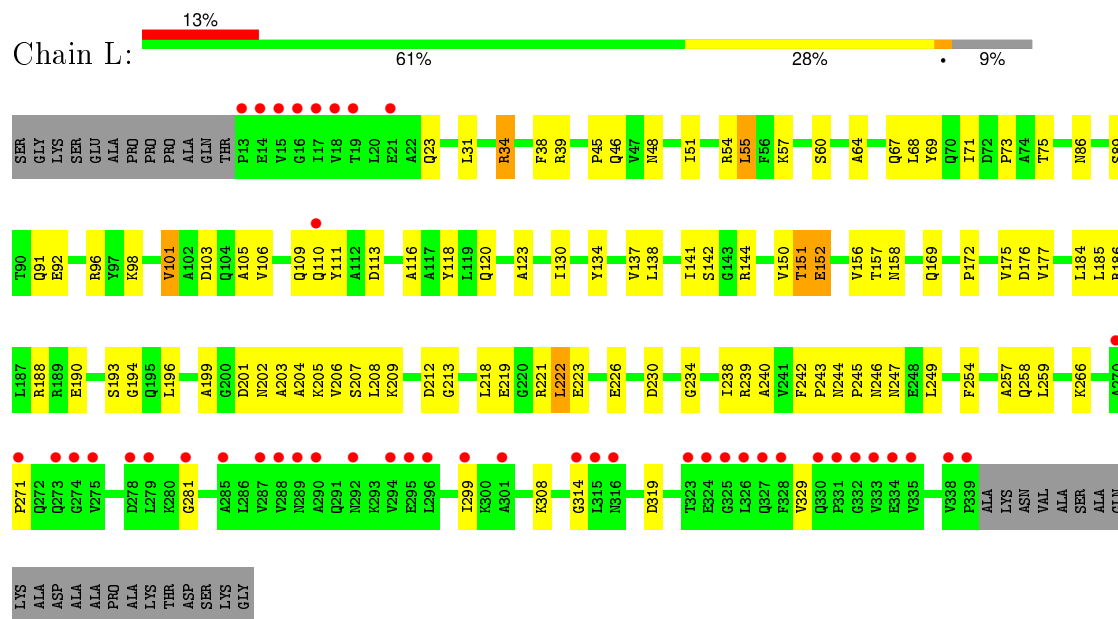




• Molecule 1: MULTIDRUG RESISTANCE PROTEIN MEXA



• Molecule 1: MULTIDRUG RESISTANCE PROTEIN MEXA



• Molecule 1: MULTIDRUG RESISTANCE PROTEIN MEXA





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 , 0.257	Depositor DCC
R_{free} test set	7661 reflections (4.90%)	DCC
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 , 77.4	EDS
Estimated twinning fraction	0.005 for h,-k,-h-l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 156399 reflections	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, 0.375 respectively for untwinned datasets, and 0.333, 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:NH1	1:I:198:ARG:HB2	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: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

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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:M:35:THR:C	1:M:36:ASN:HD22	1.89	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:F:55:LEU:H	1:F:55:LEU:HD12	1.51	0.75
1:C:104:GLN:HG3	1:I:108:LYS:CE	2.15	0.75
1:B:227:VAL:HG22	1:B:237:THR:O	1.87	0.75
1:B:208:LEU:HB2	1:B:242:PHE:CE1	2.20	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:I:216:TYR:HE2	1:I:218:LEU:HB2	1.53	0.74
1:H:157:THR:O	1:H:160:GLN:HG2	1.87	0.74
1:C:174:TYR:CD1	1:C:239:ARG:HD2	2.18	0.74
1:A:43:VAL:HG23	1:A:165:ALA:O	1.86	0.74
1:J:139:SER:OG	1:J:167:VAL:HG21	1.87	0.74
1:H:109:GLN:OE1	1:I:96:ARG:CD	2.35	0.74
1:G:216:TYR:CE2	1:G:218:LEU:HB2	2.23	0.74
1:A:199:ALA:H	1:A:204:ALA:HA	1.52	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:211:GLU:OE2	1:A:254:PHE:HB2	1.89	0.73
1:A:184:LEU:HD13	1:A:238:ILE:HD11	1.69	0.73
1:M:199:ALA:HB2	1:M:205:LYS:N	2.03	0.73
1:F:85:ALA:HB2	1:G:82:SER:HB2	1.69	0.73
1:H:109:GLN:CD	1:I:96:ARG:CZ	2.58	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:35:THR:HB	1:C:173:ILE:HD11	1.72	0.72
1:M:244:ASN:ND2	1:M:249:LEU:HB2	2.03	0.72
1:D:199:ALA:HB2	1:D:205:LYS:N	2.04	0.72
1:A:55:LEU:HD12	1:A:55:LEU:H	1.52	0.72
1:F:265:GLN:CD	1:F:265:GLN:H	1.93	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:G:157:THR:O	1:G:160:GLN:HB2	1.91	0.71
1:B:199:ALA:HB2	1:B:205:LYS:N	2.05	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: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: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: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:144:ARG:HH21	1:C:226:GLU:HG3	1.59	0.68
1:E:221:ARG:HD3	1:E:223:GLU:OE2	1.94	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:184:LEU:O	1:B:188:ARG:HG3	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:H:46:GLN:HB2	1:H:134:TYR:CD1	2.30	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:G:191:LEU:HG	1:G:198:ARG:NH2	2.10	0.67
1:D:246:ASN:HB2	1:D:248:GLU:HG3	1.75	0.67
1:F:82:SER:HA	1:G:82:SER:OG	1.94	0.67
1:F:272:GLN:HB2	1:F:309:TRP:NE1	2.11	0.66
1:E:218:LEU:N	1:E:218:LEU:HD23	2.09	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:M:271:PRO:HA	1:M:308:LYS:HA	1.77	0.66
1:H:271:PRO:HA	1:H: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:J:208:LEU:HD11	1:J:255:VAL:CG2	2.25	0.66
1:H:203:ALA:HB2	1:H:223:GLU:HA	1.77	0.66
1:D:207:SER:OG	1:D:258:GLN:HB2	1.94	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:C:34:ARG:HB3	1:C:34:ARG:NH1	2.06	0.66
1:A:175:VAL:HG21	1:A:242:PHE:HD2	1.61	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:D:208:LEU:HD11	1:D:255:VAL:CG2	2.27	0.65
1:C:208:LEU:HB2	1:C:242:PHE:CZ	2.31	0.65
1:D:156:VAL:HG11	1:D:164:MET:HE2	1.78	0.65
1:L:31:LEU:HB3	1:L:177:VAL:HG11	1.77	0.65
1:J:184:LEU:O	1:J:188:ARG:HG3	1.95	0.65
1:B:43:VAL:HG23	1:B:165:ALA:O	1.97	0.65
1:K:55:LEU:HD12	1:K:55:LEU:H	1.62	0.65
1:B:271:PRO:HA	1:B:308:LYS:HA	1.77	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:J:55:LEU:N	1:J:55:LEU:HD12	2.13	0.64
1:B:175:VAL:HB	1:B:240:ALA:HB3	1.79	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:I:51:ILE:HD11	1:I:164:MET:HE1	1.80	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:B:147:ARG:NH1	1:C:239:ARG:HH21	1.90	0.63
1:A:249:LEU:HD23	1:A:253:MET:SD	2.37	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:M:55:LEU:HD12	1:M:55:LEU:N	2.14	0.63
1:J:199:ALA:HB2	1:J:205:LYS:N	2.13	0.63
1:C:178:THR:HG22	1:C:237:THR:OG1	1.99	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:L:34:ARG:HE	1:L:254:PHE:HE1	1.47	0.62
1:F:271:PRO:HG3	1:F:308:LYS:HE2	1.81	0.62
1:D:184:LEU:O	1:D:188:ARG:HG3	1.99	0.62
1:M:134:TYR:C	1:M:136:LYS:N	2.52	0.62
1:M:222:LEU:HD11	1:M:238:ILE:HD12	1.79	0.62
1:B:203:ALA:HB2	1:B:223:GLU:HA	1.81	0.62
1:E:157:THR:O	1:E:160:GLN:HB2	2.00	0.62
1:D:170:LEU:HD22	1:D:170:LEU:N	2.15	0.62
1:I:206:VAL:O	1:I:219:GLU:HG3	1.98	0.62
1:I:190:GLU:HB3	1:I:196:LEU:HD13	1.82	0.62
1:F:54:ARG:HG3	1:F:69:TYR:CE1	2.34	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: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:G:206:VAL:O	1:G:219:GLU:HG3	1.99	0.62
1:C:55:LEU:HD12	1:C:55:LEU:N	2.15	0.61
1:I:156:VAL:HG11	1:I:164:MET:CE	2.29	0.61
1:C:206:VAL:HG13	1:C:258:GLN:O	2.00	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:L:222:LEU:C	1:L:222:LEU:HD12	2.18	0.61
1:C:54:ARG:HG3	1:C:69:TYR:CE1	2.35	0.61
1:M:54:ARG:HG3	1:M:69:TYR:CE1	2.36	0.61
1:L:299:ILE:HA	1:L:314:GLY:HA3	1.82	0.61
1:F:299:ILE:HA	1:F:314:GLY:HA3	1.82	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:K:222:LEU:HD12	1:K:222:LEU:C	2.21	0.61
1:F:206:VAL:O	1:F:219:GLU:HG3	2.00	0.61
1:L:206:VAL:HG13	1:L:258:GLN:O	2.00	0.61
1:E:260:GLN:OE1	1:E:260:GLN:HA	2.00	0.61
1:M:203:ALA:HB2	1:M:223:GLU:HA	1.81	0.61
1:I:299:ILE:HA	1:I:314:GLY:HA3	1.83	0.61
1:K:195:GLN:O	1:K:262:GLY:N	2.22	0.60
1:E:45:PRO:HB3	1:E:164:MET:HE1	1.82	0.60
1:M:141:ILE:HD11	1:M:167:VAL:O	2.00	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:I:68:LEU:HD13	1:I:145:ILE:CD1	2.31	0.60
1:C:271:PRO:HA	1:C:308:LYS:HA	1.84	0.60
1:G:244:ASN:OD1	1:G:249:LEU:HB2	2.01	0.60
1:F:212:ASP:OD1	1:F:214:SER:N	2.29	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:G:250:LEU:O	1:G:253:MET:HG3	2.02	0.60
1:F:199:ALA:HB2	1:F:205:LYS:N	2.17	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
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

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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: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:E:203:ALA:HB2	1:E:223:GLU:HA	1.84	0.59
1:B:253:MET:HE3	1:C:181:SER:HB3	1.84	0.59
1:C:170:LEU:HD12	1:C:247:ASN:HD21	1.68	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:D:208:LEU:HB2	1:D:242:PHE:CE2	2.38	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:M:101:VAL:HG13	1:M:106:VAL:HG13	1.84	0.59
1:H:101:VAL:HG13	1:H:106:VAL:HG13	1.85	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:F:35:THR:HB	1:F:173:ILE:HD11	1.85	0.58
1:C:199:ALA:HB2	1:C:205:LYS:N	2.18	0.58
1:L:55:LEU:HD12	1:L:55:LEU:N	2.18	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:I:55:LEU:N	1:I:55:LEU:HD12	2.17	0.58
1:E:38:PHE:CD2	1:E:169:GLN:NE2	2.71	0.58
1:B:151:THR:HG23	1:B:154:ALA:HB2	1.84	0.58
1:M:141:ILE:HG13	1:M:143:GLY:H	1.69	0.58
1:H:51:ILE:HD11	1:H:164:MET:CE	2.33	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
1:M:184:LEU:HD22	1:M:236:VAL:HG11	1.86	0.58
1:H:34:ARG:NE	1:H:254:PHE:CE1	2.71	0.58
1:H:55:LEU:HD12	1:H:55:LEU:N	2.14	0.58
1:F:271:PRO:HA	1:F:308:LYS:HA	1.84	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: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:K:207:SER:OG	1:K:258:GLN:HB2	2.03	0.57
1:I:230:ASP:O	1:I:234:GLY:N	2.35	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: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: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: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:L:64:ALA:HB2	1:L:142:SER:N	2.18	0.57
1:L:38:PHE:HD2	1:L:169:GLN:NE2	2.02	0.57
1:J:271:PRO:HA	1:J:308:LYS:HA	1.85	0.57
1:H:139:SER:OG	1:H:167:VAL:HG21	2.04	0.57
1:B:178:THR:HG22	1:B:237:THR:OG1	2.04	0.57
1:A:101:VAL:HG13	1:A:106:VAL:HG13	1.85	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: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: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:A:227:VAL:HG12	1:A:227:VAL:O	2.04	0.57
1:E:38:PHE:HD2	1:E:169:GLN:NE2	2.03	0.57
1:F:25:VAL:HG21	1:F:305:ILE:HD13	1.86	0.57
1:E:101:VAL:HG13	1:E:106:VAL:HG13	1.86	0.57
1:E:75:THR:HG23	1:F:127:GLN:HE22	1.68	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:H:226:GLU:O	1:I:144:ARG:NH1	2.38	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:205:LYS:HE2	1:I:219:GLU:OE2	2.04	0.56
1:G:221:ARG:NH1	1:G:221:ARG:HB3	2.20	0.56
1:C:96:ARG:HH21	1:D:109:GLN:CD	2.06	0.56
1:C:184:LEU:O	1:C:188:ARG:HG3	2.05	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: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: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:M:169:GLN:O	1:M:170:LEU:HD23	2.06	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:G:210:LEU:HD12	1:G:214:SER:OG	2.05	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:K:185:LEU:O	1:K:189:ARG:HG3	2.06	0.55
1:J:176:ASP:OD2	1:J:239:ARG:HG2	2.06	0.55
1:F:271:PRO:HG3	1:F:308:LYS:HG2	1.88	0.55
1:E:23:GLN:O	1:E:266:LYS:HA	2.06	0.55
1:B:35:THR:HB	1:B:173:ILE:HD11	1.88	0.55
1:H:39:ARG:HH12	1:I:54:ARG:HH22	1.50	0.55
1:B:206:VAL:HG13	1:B:258:GLN:O	2.06	0.55
1:A:54:ARG:HG3	1:A:69:TYR:CE1	2.41	0.55
1:C:34:ARG:HH11	1:C:34:ARG:CB	2.10	0.55
1:B:206:VAL:HG21	1:B:222:LEU:HB2	1.88	0.55
1:K:175:VAL:HB	1:K:240:ALA:HB3	1.87	0.55
1:M:207:SER:OG	1:M:258:GLN:HB2	2.07	0.55
1:F:71:ILE:O	1:F:73:PRO:HD3	2.06	0.55
1:E:175:VAL:HB	1:E:240:ALA:HB3	1.87	0.55
1:C:55:LEU:CD1	1:C:55:LEU:H	2.12	0.55
1:J:208:LEU:HB2	1:J:242:PHE:CZ	2.41	0.55
1:B:218:LEU:CD2	1:B:243:PRO:HB2	2.36	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: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:D:227:VAL:HG21	1:D:239:ARG:HG2	1.88	0.55
1:F:206:VAL:HG13	1:F:258:GLN:O	2.06	0.55
1:M:64:ALA:HB2	1:M:141:ILE:C	2.28	0.54
1:I:212:ASP:OD1	1:I:213:GLY:N	2.39	0.54
1:H:144:ARG:HG3	1:H:144:ARG:NH1	2.22	0.54
1:M:191:LEU:HG	1:M:198:ARG:HH12	1.71	0.54
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:A:205:LYS:HB3	1:A:219:GLU:OE2	2.07	0.54
1:A:137:VAL:O	1:A:138:LEU:HD23	2.06	0.54
1:E:34:ARG:HG2	1:E:34:ARG:HH11	1.72	0.54
1:M:35:THR:O	1:M:36:ASN:ND2	2.40	0.54
1:I:64:ALA:HB2	1:I:141:ILE:C	2.28	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:K:68:LEU:HD13	1:K:145:ILE:CD1	2.37	0.54
1:I:208:LEU:HD11	1:I:255:VAL:CG2	2.38	0.54
1:C:183:ALA:O	1:C:187:LEU:HG	2.07	0.54
1:F:50:ILE:HD13	1:F:155:LEU:HA	1.89	0.54
1:H:36:ASN:ND2	1:H:176:ASP:OD2	2.41	0.54
1:G:220:GLY:N	1:G:242:PHE:CE1	2.76	0.54
1:G:244:ASN:ND2	1:G:247:ASN:HA	2.22	0.54
1:G:106:VAL:HG22	1:G:110:GLN:HB2	1.90	0.54
1:I:106:VAL:HG22	1:I:110:GLN:HB2	1.89	0.54
1:A:51:ILE:O	1:A:153:GLY:HA2	2.06	0.54
1:G:53:LYS:HA	1:G:152:GLU:OE1	2.08	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:M:35:THR:HB	1:M:173:ILE:HD11	1.90	0.53
1:A:184:LEU:O	1:A:188:ARG:HG3	2.08	0.53
1:G:55:LEU:N	1:G:55:LEU:HD12	2.23	0.53
1:D:247:ASN:OD1	1:D:250:LEU:HD21	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:106:VAL:HG23	1:K:110:GLN:OE1	2.09	0.53
1:B:106:VAL:HG22	1:B:110:GLN:HB2	1.91	0.53
1:K:34:ARG:NE	1:K:254:PHE:CE1	2.77	0.53
1:H:144:ARG:HG3	1:H:144:ARG:HH11	1.74	0.53
1:F:230:ASP:O	1:F:234:GLY:N	2.39	0.53
1:M:143:GLY:HA2	1:M:169:GLN:HA	1.90	0.53
1:F:206:VAL:HG11	1:F:257:ALA:HB1	1.90	0.53
1:M:23:GLN:O	1:M:266:LYS:HA	2.08	0.53
1:M:187:LEU:HD22	1:M:196:LEU:HD21	1.91	0.53
1:I:185:LEU:O	1:I:189:ARG:HG3	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:K:54:ARG:HG3	1:K:69:TYR:CE1	2.44	0.53
1:H:175:VAL:HB	1:H:240:ALA:HB3	1.89	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:H:106:VAL:HG22	1:H:110:GLN:HB2	1.91	0.53
1:D:108:LYS:HE3	1:J:104:GLN:HG3	1.90	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:H:47:VAL:CG1	1:H:134:TYR:HB2	2.39	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:C:49:GLY:O	1:C:155:LEU:HD12	2.08	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:L:48:ASN:OD1	1:L:158:ASN:N	2.40	0.53
1:I:50:ILE:HD11	1:I:155:LEU:HD13	1.91	0.53
1:G:69:TYR:HB2	1:G:137:VAL:HB	1.91	0.53
1:B:218:LEU:HD23	1:B:243:PRO:HB2	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:L:106:VAL:HG23	1:L:110:GLN:OE1	2.08	0.52
1:D:244:ASN:HD21	1:D:249:LEU:H	1.57	0.52
1:E:158:ASN:C	1:E:160:GLN:H	2.13	0.52
1:A:203:ALA:HB3	1:A:221:ARG:HE	1.75	0.52
1:G:221:ARG:HH11	1:G:221:ARG:HB3	1.74	0.52
1:E:246:ASN:O	1:F:188:ARG:NH2	2.42	0.52
1:B:253:MET:CE	1:C:181:SER:HB3	2.39	0.52
1:G:206:VAL:HG13	1:G:258:GLN:O	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:86:ASN:O	1:L:89:SER:HB3	2.10	0.52
1:E:189:ARG:HG3	1:E:189:ARG:HH11	1.73	0.52
1:C:92:GLU:OE2	1:C:96:ARG:NH1	2.43	0.52
1:H:39:ARG:NH1	1:I:54:ARG:NH2	2.52	0.52
1:E:190:GLU:OE1	1:E:261:GLU:HB3	2.09	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: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: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:A:38:PHE:HB2	1:A:172:PRO:O	2.09	0.52
1:J:44:ARG:NH1	1:J:44:ARG:CD	2.73	0.52
1:D:208:LEU:HD22	1:D:242:PHE:CD2	2.45	0.52
1:M:106:VAL:HG22	1:M:110:GLN:HB2	1.92	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:F:175:VAL:HB	1:F:240:ALA:HB3	1.92	0.52
1:E:208:LEU:HD11	1:E:255:VAL:CG2	2.40	0.52
1:D:55:LEU:HD12	1:D:55:LEU:N	2.24	0.51
1:H:156:VAL:HG11	1:H:164:MET:HE3	1.91	0.51
1:E:106:VAL:HG22	1:E:110:GLN:HB2	1.92	0.51
1:K:23:GLN:O	1:K:266:LYS:HA	2.09	0.51
1:E:54:ARG:HG3	1:E:69:TYR:CE1	2.45	0.51
1:D:64:ALA:HB2	1:D:141:ILE:C	2.30	0.51
1:M:206:VAL:HG12	1:M:207:SER:N	2.26	0.51
1:F:269:LEU:O	1:F:308:LYS:HD3	2.10	0.51
1:F:106:VAL:HG22	1:F:110:GLN:HB2	1.92	0.51
1:A:134:TYR:C	1:A:136:LYS:N	2.62	0.51
1:G:41:ALA:HB1	1:G:140:PRO:CG	2.40	0.51
1:K:206:VAL:HG13	1:K:258:GLN:O	2.09	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:L:31:LEU:HB3	1:L:177:VAL:CG1	2.41	0.51
1:K:55:LEU:HD12	1:K:55:LEU:N	2.25	0.51
1:L:184:LEU:O	1:L:188:ARG:HG3	2.10	0.51
1:C:191:LEU:HD22	1:C:224:PHE:CE2	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
1:A:216:TYR:CE2	1:A:218:LEU:HB2	2.46	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:H:220:GLY:HA3	1:H:242:PHE:HD1	1.75	0.51
1:E:159:GLY:O	1:E:160:GLN:C	2.50	0.51
1:K:221:ARG:HD3	1:K:223:GLU:OE2	2.11	0.51
1:H:51:ILE:HD11	1:H:164:MET:HE1	1.90	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: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:K:39:ARG:HH12	1:L:54:ARG:NH2	2.09	0.51
1:B:169:GLN:O	1:B:170:LEU:HD23	2.11	0.51
1:A:208:LEU:HD11	1:A:255:VAL:CG2	2.40	0.51
1:M:222:LEU:HD12	1:M:222:LEU:C	2.31	0.51
1:G:155:LEU:C	1:G:155:LEU:HD23	2.31	0.51
1:K:186:ARG:NH1	1:K:261:GLU:OE1	2.43	0.51
1:J:231:GLU:HG3	1:K:251:PRO:HB2	1.92	0.51
1:A:64:ALA:HB2	1:A:141:ILE:C	2.30	0.50
1:I:48:ASN:O	1:I:76:TYR:OH	2.22	0.50
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:L:113:ASP:O	1:L:116:ALA:HB3	2.11	0.50
1:C:162:ASN:N	1:C:162:ASN:HD22	2.09	0.50
1:H:68:LEU:HD13	1:H:145:ILE:CD1	2.40	0.50
1:D:106:VAL:HG22	1:D:110:GLN:HB2	1.92	0.50
1:M:68:LEU:HD13	1:M:145:ILE:CD1	2.41	0.50
1:H:54:ARG:HG3	1:H:69:TYR:CE1	2.46	0.50
1:L:106:VAL:HG22	1:L:110:GLN:HB2	1.93	0.50
1:J:54:ARG:HG3	1:J:69:TYR:CE1	2.46	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:J:244:ASN:ND2	1:J:249:LEU:HB2	2.27	0.50
1:M:202:ASN:CG	1:M:202:ASN:O	2.49	0.50
1:M:55:LEU:HD12	1:M:68:LEU:O	2.12	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

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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:E:206:VAL:HG13	1:E:258:GLN:O	2.12	0.50
1:L:38:PHE:CD2	1:L:169:GLN:NE2	2.79	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:K:92:GLU:OE2	1:K:96:ARG:NH1	2.45	0.50
1:L:55:LEU:H	1:L:55:LEU:CD1	2.15	0.50
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:G:38:PHE:HA	1:G:174:TYR:CD2	2.47	0.50
1:B:147:ARG:HB3	1:B:147:ARG:HH11	1.76	0.49
1:L:209:LYS:HD3	1:L:258:GLN:NE2	2.27	0.49
1:D:113:ASP:O	1:D:116:ALA:HB3	2.12	0.49
1:E:184:LEU:O	1:E:188:ARG:HG3	2.12	0.49
1:B:46:GLN:HA	1:B:158:ASN:OD1	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:B:38:PHE:CD1	1:B:172:PRO:HG2	2.47	0.49
1:G:50:ILE:HD11	1:G:155:LEU:HB2	1.95	0.49
1:C:206:VAL:HG12	1:C:207:SER:N	2.27	0.49
1:L:46:GLN:NE2	1:L:134:TYR:HE1	2.10	0.49
1:G:195:GLN:HG2	1:G:261:GLU:O	2.12	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:A:178:THR:HA	1:A:236:VAL:O	2.13	0.49
1:D:206:VAL:CG1	1:D:259:LEU:HD13	2.43	0.49
1:H:185:LEU:CD2	1:I:210:LEU:HD13	2.42	0.49
1:G:69:TYR:CD2	1:G:164:MET:HE1	2.47	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: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:K:67:GLN:HA	1:K:138:LEU:HD23	1.94	0.49
1:I:186:ARG:HG2	1:I:190:GLU:OE2	2.12	0.49
1:E:67:GLN:HA	1:E:138:LEU:HD23	1.95	0.49
1:D:178:THR:OG1	1:D:237:THR:HG22	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:113:ASP:O	1:G:116:ALA:HB3	2.13	0.49
1:B:48:ASN:OD1	1:B:157:THR:HA	2.12	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:D:120:GLN:O	1:D:123:ALA:HB3	2.13	0.49
1:G:197:GLU:O	1:G:205:LYS:HG3	2.13	0.49
1:F:45:PRO:HD3	1:F:164:MET:SD	2.53	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:E:250:LEU:O	1:E:253:MET:HG3	2.13	0.49
1:B:113:ASP:O	1:B:116:ALA:HB3	2.13	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:C:138:LEU:N	1:C:138:LEU:HD12	2.17	0.48
1:M:208:LEU:HB2	1:M:242:PHE:CE2	2.48	0.48
1:I:39:ARG:HH12	1:J:54:ARG:NH2	2.11	0.48
1:E:71:ILE:O	1:E:73:PRO:HD3	2.13	0.48
1:A:200:GLY:O	1:A:201:ASP:C	2.52	0.48
1:M:69:TYR:HB2	1:M:137:VAL:HB	1.94	0.48
1:I:55:LEU:CD1	1:I:55:LEU:H	2.15	0.48
1:K:106:VAL:HG22	1:K:110:GLN:HB2	1.94	0.48
1:H:174:TYR:CE1	1:H:241:VAL:HG22	2.49	0.48
1:K:255:VAL:O	1:K:256:HIS:HD2	1.95	0.48
1:J:129:ARG:HG2	1:J:129:ARG:HH11	1.77	0.48
1:I:54:ARG:HG3	1:I:69:TYR:CE1	2.47	0.48
1:M:55:LEU:CD1	1:M:55:LEU:H	2.09	0.48
1:K:195:GLN:NE2	1:K:263:VAL:CB	2.76	0.48
1:I:68:LEU:HD13	1:I:145:ILE:HD12	1.95	0.48
1:I:48:ASN:OD1	1:I:157:THR:HA	2.14	0.48
1:J:230:ASP:O	1:J:234:GLY:N	2.40	0.48
1:E:230:ASP:O	1:E:234:GLY:N	2.46	0.48
1:I:231:GLU:H	1:I:231:GLU:CD	2.17	0.48
1:C:108:LYS:HG3	1:I:104:GLN:CB	2.44	0.48
1:J:106:VAL:HG22	1:J:110:GLN:HB2	1.93	0.48
1:G:228:SER:OG	1:G:237:THR:HB	2.13	0.48
1:B:64:ALA:HB2	1:B:141:ILE:CA	2.43	0.48
1:M:48:ASN:OD1	1:M:157:THR:HA	2.14	0.48
1:D:155:LEU:HD12	1:D:156:VAL:N	2.28	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:I:208:LEU:HD11	1:I:255:VAL:HG21	1.94	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:J:34:ARG:CZ	1:J:254:PHE:CE1	2.97	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:M:157:THR:O	1:M:160:GLN:HB3	2.13	0.48
1:B:30:GLU:OE1	1:B:258:GLN:HG2	2.14	0.48
1:A:238:ILE:HG22	1:A:239:ARG:N	2.29	0.48
1:J:106:VAL:HG23	1:J:110:GLN:OE1	2.13	0.48
1:G:208:LEU:HB2	1:G:242:PHE:CZ	2.49	0.48
1:M:91:GLN:HA	1:M:118:TYR:CD1	2.49	0.48
1:D:68:LEU:HD11	1:D:139:SER:HB2	1.94	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:A:141:ILE:HD11	1:A:167:VAL:O	2.12	0.48
1:G:222:LEU:HD13	1:G:240:ALA:HB2	1.96	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: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:M:86:ASN:O	1:M:89:SER:HB3	2.13	0.48
1:J:57:LYS:HB3	1:J:60:SER:HB3	1.96	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:M:206:VAL:HG13	1:M:258:GLN:O	2.14	0.47
1:F:199:ALA:HB2	1:F:204:ALA:C	2.34	0.47
1:F:193:SER:OG	1:F:194:GLY:N	2.46	0.47
1:I:206:VAL:HG12	1:I:207:SER:N	2.29	0.47
1:H:46:GLN:CD	1:H:134:TYR:CE1	2.88	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: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:A:92:GLU:OE2	1:A:96:ARG:NH1	2.47	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:126:GLU:O	1:D:130:ILE:HG13	2.13	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:H:208:LEU:HD13	1:H:242:PHE:HE2	1.79	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:B:248:GLU:HG2	1:C:185:LEU:HD11	1.95	0.47
1:L:203:ALA:HB2	1:L:223:GLU:HA	1.96	0.47
1:H:68:LEU:HD11	1:H:139:SER:HB2	1.97	0.47
1:B:51:ILE:HG13	1:B:150:VAL:HG11	1.94	0.47
1:E:34:ARG:NH1	1:E:254:PHE:CG	2.82	0.47
1:D:85:ALA:HB1	1:E:119:LEU:HB3	1.95	0.47
1:I:129:ARG:HG2	1:I:129:ARG:HH11	1.78	0.47
1:D:96:ARG:CZ	1:E:109:GLN:OE1	2.60	0.47
1:K:244:ASN:CG	1:K:249:LEU:HB2	2.35	0.47
1:J:59:GLY:O	1:J:144:ARG:NH1	2.48	0.47
1:B:69:TYR:CD2	1:B:164:MET:HE1	2.49	0.47
1:E:159:GLY:O	1:E:160:GLN:O	2.32	0.47
1:A:71:ILE:O	1:A:73:PRO:HD3	2.14	0.47
1:M:38:PHE:HB2	1:M:172:PRO:O	2.14	0.47
1:A:113:ASP:O	1:A:116:ALA:HB3	2.14	0.47
1:H:226:GLU:HG2	1:I:250:LEU:HD11	1.96	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:J:185:LEU:HD12	1:J:185:LEU:HA	1.77	0.47
1:K:160:GLN:NE2	1:K:162:ASN:O	2.41	0.47
1:A:126:GLU:O	1:A:130:ILE:HG13	2.15	0.47
1:J:193:SER:OG	1:J:194:GLY:N	2.44	0.47
1:H:92:GLU:OE2	1:H:96:ARG:NH1	2.48	0.47
1:K:71:ILE:O	1:K:73:PRO:HD3	2.14	0.47
1:J:175:VAL:HB	1:J:240:ALA:HB3	1.97	0.47
1:K:174:TYR:CE1	1:K:241:VAL:HG22	2.49	0.47
1:F:81:GLN:HG3	1:G:85:ALA:HB2	1.97	0.47
1:A:39:ARG:H	1:A:169:GLN:HB3	1.79	0.47
1:M:106:VAL:HG23	1:M:110:GLN:OE1	2.14	0.47
1:H:64:ALA:HB2	1:H:141:ILE:HA	1.96	0.47
1:C:150:VAL:HG13	1:C:154:ALA:HB3	1.95	0.47
1:K:206:VAL:HG21	1:K:222:LEU:HB2	1.97	0.47
1:G:34:ARG:HE	1:G:254:PHE:HE1	1.63	0.47
1:F:208:LEU:HB2	1:F:242:PHE:CZ	2.50	0.47
1:F:208:LEU:HD11	1:F:255:VAL:HB	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:48:ASN:OD1	1:C:157:THR:HA	2.15	0.47
1:C:199:ALA:HB2	1:C:204:ALA:C	2.35	0.47
1:G:41:ALA:HB1	1:G:140:PRO:HG3	1.97	0.47
1:A:45:PRO:HD3	1:A:164:MET:HG3	1.96	0.47
1:D:73:PRO:O	1:D:74:ALA:C	2.52	0.47
1:K:174:TYR:CD1	1:K:241:VAL:HG22	2.51	0.47
1:J:68:LEU:HD13	1:J:145:ILE:CD1	2.45	0.46
1:D:106:VAL:HG23	1:D:110:GLN:OE1	2.15	0.46
1:M:230:ASP:O	1:M:234:GLY:N	2.45	0.46
1:C:68:LEU:HD13	1:C:145:ILE:CD1	2.45	0.46
1:B:68:LEU:HD13	1:B:145:ILE:CD1	2.46	0.46
1:M:170:LEU:O	1:M:244:ASN:HB3	2.15	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: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: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:C:175:VAL:HB	1:C:240:ALA:HB3	1.96	0.46
1:A:170:LEU:O	1:A:173:ILE:HB	2.15	0.46
1:E:190:GLU:HG2	1:E:195:GLN:NE2	2.31	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: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: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:206:VAL:HG12	1:K:207:SER:N	2.30	0.46
1:G:71:ILE:O	1:G:73:PRO:HD3	2.16	0.46
1:G:206:VAL:CG1	1:G:207:SER:N	2.78	0.46
1:B:190:GLU:HB3	1:B:196:LEU:HG	1.98	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:C:210:LEU:HB2	1:C:212:ASP:OD1	2.15	0.46
1:H:30:GLU:HG3	1:H:256:HIS:HB3	1.97	0.46
1:F:202:ASN:O	1:F:224:PHE:HD2	1.97	0.46
1:A:34:ARG:HD3	1:A:254:PHE:CE2	2.50	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:25:VAL:HG21	1:F:305:ILE:CD1	2.45	0.46
1:D:69:TYR:HB2	1:D:137:VAL:HB	1.97	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:D:129:ARG:HH11	1:D:129:ARG:HG2	1.81	0.46
1:A:86:ASN:O	1:A:89:SER:HB3	2.16	0.46
1:D:96:ARG:NH2	1:E:109:GLN:CD	2.59	0.46
1:M:41:ALA:HB2	1:M:141:ILE:CG2	2.46	0.46
1:D:104:GLN:HG3	1:J:108:LYS:CE	2.44	0.46
1:B:250:LEU:O	1:B:253:MET:HG3	2.16	0.46
1:K:186:ARG:O	1:K:190:GLU:HG3	2.16	0.46
1:D:222:LEU:O	1:D:222:LEU:HG	2.15	0.46
1:G:174:TYR:CD1	1:G:239:ARG:HD3	2.50	0.46
1:E:77:GLU:HA	1:E:132:LEU:HD22	1.98	0.46
1:D:109:GLN:O	1:D:112:ALA:HB3	2.16	0.46
1:B:208:LEU:HD11	1:B:255:VAL:CG2	2.46	0.46
1:I:210:LEU:HD22	1:I:253:MET:HE1	1.97	0.46
1:F:167:VAL:HG12	1:F:168:GLN:N	2.31	0.46
1:I:113:ASP:O	1:I:116: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: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:K:55:LEU:HD12	1:K:68:LEU:O	2.16	0.46
1:I:103:ASP:C	1:I:105:ALA:H	2.20	0.46
1:K:113:ASP:O	1:K:116:ALA:HB3	2.16	0.46
1:J:56:PHE:CZ	1:J:148:SER:HB2	2.51	0.46
1:H:103:ASP:C	1:H:105:ALA:H	2.18	0.46
1:F:129:ARG:HH11	1:F:129:ARG:HG2	1.80	0.46
1:B:52:LEU:HA	1:B:52:LEU:HD23	1.81	0.46
1:I:199:ALA:HB2	1:I:204:ALA:C	2.36	0.46
1:H:46:GLN:NE2	1:H:134:TYR:CE1	2.84	0.46
1:F:106:VAL:HG23	1:F:110:GLN:OE1	2.16	0.46
1:J:185:LEU:HD11	1:K:248:GLU:CB	2.46	0.46
1:L:176:ASP:OD1	1:L:239:ARG:HG2	2.16	0.46
1:K:43:VAL:HG23	1:K:165:ALA:O	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:J:226:GLU:HG3	1:K:144:ARG:HE	1.81	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:D:103:ASP:C	1:D:105:ALA:H	2.19	0.45
1:B:147:ARG:HD2	2:B:1340:SO4:O2	2.16	0.45
1:A:186:ARG:HD3	1:A:190:GLU:OE2	2.16	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:D:98:LYS:HG3	1:D:111:TYR:CZ	2.51	0.45
1:A:120:GLN:O	1:A:123:ALA:HB3	2.16	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:M:216:TYR:OH	1:M:243:PRO:O	2.27	0.45
1:L:175:VAL:HB	1:L:240:ALA:HB3	1.98	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:A:104:GLN:HE22	1:G:104:GLN:HE22	1.64	0.45
1:C:190:GLU:CB	1:C:196:LEU:HD13	2.39	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:C:222:LEU:HD11	1:C:238:ILE:HD12	1.97	0.45
1:C:126:GLU:O	1:C:130:ILE:HG13	2.16	0.45
1:D:52:LEU:HA	1:D:52:LEU:HD23	1.82	0.45
1:F:147:ARG:HG3	1:F:147:ARG:O	2.16	0.45
1:I:106:VAL:HG23	1:I:110:GLN:OE1	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:D:43:VAL:HG23	1:D:165:ALA:O	2.17	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:A:103:ASP:C	1:A:105:ALA:H	2.20	0.45
1:M:57:LYS:HB3	1:M:60:SER:HB3	1.98	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: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:M:182:THR:O	1:M:185:LEU:HB2	2.16	0.45
1:L:103:ASP:C	1:L:105:ALA:H	2.20	0.45
1:H:98:LYS:HG3	1:H:111:TYR:CZ	2.52	0.45
1:E:222:LEU:HD13	1:E:240:ALA:HB2	1.98	0.45
1:K:216:TYR:HA	1:K:217:PRO:HD2	1.85	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:205:LYS:O	1:D:259:LEU:HD13	2.17	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:L:150:VAL:CG1	1:L:151:THR:N	2.80	0.45
1:K:28:ASN:OD1	1:K:260:GLN:HB2	2.16	0.45
1:F:244:ASN:ND2	1:F:249:LEU:O	2.48	0.45
1:H:67:GLN:HA	1:H:138:LEU:CD2	2.47	0.45
1:K:299:ILE:HA	1:K:314:GLY:HA3	1.99	0.45
1:A:206:VAL:HG12	1:A:207:SER:H	1.81	0.45
1:D:203:ALA:HB2	1:D:223:GLU:OE1	2.17	0.45
1:K:187:LEU:H	1:K:187:LEU:HD12	1.81	0.45
1:G:226:GLU:HG3	1:H:144:ARG:HE	1.82	0.45
1:C:113:ASP:O	1:C:116:ALA:HB3	2.16	0.45
1:J:103:ASP:C	1:J:105:ALA:H	2.19	0.45
1:C:108:LYS:HG3	1:I:104:GLN:HB3	1.99	0.45
1:C:38:PHE:CD1	1:C:174:TYR:CE2	2.99	0.45
1:E:206:VAL:HG21	1:E:222:LEU:CB	2.39	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:D:207:SER:OG	1:D:258:GLN:OE1	2.33	0.45
1:B:196:LEU:HD23	1:B:261:GLU:HA	1.99	0.45
1:G:106:VAL:HG23	1:G:110:GLN:OE1	2.17	0.45
1:E:106:VAL:HG23	1:E:110:GLN:OE1	2.17	0.45
1:C:147:ARG:NH2	1:D:176:ASP:OD1	2.49	0.45
1:E:91:GLN:HA	1:E:118:TYR:CD1	2.52	0.45
1:E:86:ASN:O	1:E:89:SER:HB3	2.17	0.45
1:B:299:ILE:HA	1:B:314:GLY:HA3	1.99	0.45
1:E:55:LEU:CD1	1:E:55:LEU:H	2.12	0.45
1:A:55:LEU:CD1	1:A:55:LEU:H	2.16	0.45
1:C:106:VAL:HG23	1:C:110:GLN:OE1	2.17	0.45
1:M:38:PHE:CE1	1:M:172:PRO:HD2	2.52	0.45
1:J:41:ALA:HB1	1:J:140:PRO:CG	2.47	0.45
1:C:103:ASP:C	1:C:105:ALA:H	2.21	0.45
1:B:230:ASP:O	1:B:234:GLY:N	2.50	0.45
1:E:120:GLN:O	1:E:123:ALA:HB3	2.17	0.45
1:F:47:VAL:HG13	1:F:134:TYR:HB2	1.99	0.45
1:E:178:THR:HG23	1:E:178:THR:O	2.17	0.45
1:G:203:ALA:HB2	1:G:223:GLU:HA	1.98	0.45
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:188:ARG:NH2	1:H:246:ASN:O	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:113:ASP:O	1:E:116:ALA:HB3	2.16	0.44
1:M:134:TYR:O	1:M:136:LYS:N	2.49	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:H:208:LEU:HB2	1:H:242:PHE:CZ	2.52	0.44
1:H:55:LEU:CD1	1:H:55:LEU:H	2.11	0.44
1:A:184:LEU:HG	1:A:188:ARG:HD2	1.99	0.44
1:F:206:VAL:HG12	1:F:207:SER:N	2.32	0.44
1:H:216:TYR:CE2	1:H:218:LEU:HB2	2.52	0.44
1:G:64:ALA:HB2	1:G:141:ILE:HA	1.99	0.44
1:D:145:ILE:HB	1:D:167:VAL:HG22	1.98	0.44
1:B:68:LEU:HD13	1:B:145:ILE:HD12	1.98	0.44
1:A:225:SER:O	1:A:227:VAL:HG23	2.18	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:M:244:ASN:ND2	1:M:249:LEU:O	2.48	0.44
1:E:45:PRO:HD3	1:E:164:MET:HG3	1.99	0.44
1:L:64:ALA:HB2	1:L:142:SER:H	1.81	0.44
1:C:202:ASN:O	1:C:224:PHE:HD2	2.00	0.44
1:C:185:LEU:O	1:C:189:ARG:HG3	2.18	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:B:152:GLU:O	1:C:41:ALA:HA	2.17	0.44
1:K:91:GLN:HA	1:K:118:TYR:CD1	2.53	0.44
1:E:126:GLU:O	1:E:130:ILE:HG13	2.17	0.44
1:K:188:ARG:NH1	1:L:246:ASN:O	2.46	0.44
1:E:207:SER:OG	1:E:258:GLN:HB2	2.17	0.44
1:J:203:ALA:HB2	1:J:223:GLU:HA	1.98	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:G:199:ALA:HB2	1:G:204:ALA:C	2.38	0.44
1:K:247:ASN:OD1	1:K:250:LEU:HD21	2.18	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:M:208:LEU:HD11	1:M:255:VAL:HG21	2.00	0.44
1:F:139:SER:OG	1:F:167:VAL:HG21	2.18	0.44
1:H:86:ASN:O	1:H:89:SER:HB3	2.17	0.44
1:G:129:ARG:HG2	1:G:129:ARG:HH11	1.82	0.44
1:I:198:ARG:CB	1:I:198:ARG:HH11	2.11	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:206:VAL:HG11	1:L:257:ALA:HB1	2.00	0.44
1:K:199:ALA:HB2	1:K:204:ALA:C	2.37	0.44
1:E:158:ASN:O	1:E:160:GLN:N	2.49	0.44
1:M:38:PHE:CD1	1:M:172:PRO:HD2	2.52	0.44
1:J:259:LEU:HD23	1:J:259:LEU:HA	1.85	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:B:57:LYS:HB3	1:B:60:SER:HB3	2.00	0.44
1:A:175:VAL:HG21	1:A:242:PHE:CD2	2.49	0.43
1:K:183:ALA:O	1:K:187:LEU:HD12	2.17	0.43
1:H:101:VAL:HG12	1:H:106:VAL:O	2.18	0.43
1:E:31:LEU:HB3	1:E:177:VAL:HG11	2.00	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:D:49:GLY:O	1:D:155:LEU:HD12	2.17	0.43
1:C:55:LEU:HD12	1:C:68:LEU:O	2.18	0.43
1:A:207:SER:O	1:A:257:ALA:HA	2.17	0.43
1:M:41:ALA:HB2	1:M:141:ILE:HG23	2.00	0.43
1:D:188:ARG:O	1:D:191:LEU:HB3	2.17	0.43
1:C:247:ASN:OD1	1:C:250:LEU:HD21	2.18	0.43
1:L:38:PHE:HB2	1:L:172:PRO:O	2.18	0.43
1:B:64:ALA:HB2	1:B:141:ILE:C	2.39	0.43
1:E:180:PRO:O	1:E:181:SER:C	2.56	0.43
1:C:246:ASN:HB3	1:C:248:GLU:OE2	2.18	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:M:77:GLU:HA	1:M:132:LEU:HD22	2.01	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:C:157:THR:O	1:C:160:GLN:HB3	2.19	0.43
1:B:77:GLU:HA	1:B:132:LEU:HD22	2.00	0.43
1:D:91:GLN:HA	1:D:118:TYR:CD1	2.53	0.43
1:H:109:GLN:CD	1:I:96:ARG:NE	2.71	0.43
1:L:206:VAL:HG21	1:L:222:LEU:HB2	1.99	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:K:129:ARG:HH11	1:K:129:ARG:HG2	1.84	0.43
1:H:91:GLN:HA	1:H:118:TYR:CD1	2.53	0.43
1:M:244:ASN:CG	1:M:249:LEU:HB2	2.38	0.43
1:I:244:ASN:ND2	1:I:247:ASN:HA	2.33	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:E:92:GLU:OE2	1:E:96:ARG:NH1	2.52	0.43
1:K:195:GLN:O	1:K:196:LEU:HD12	2.18	0.43
1:E:45:PRO:CB	1:E:164:MET:HE1	2.47	0.43
1:K:54:ARG:HD2	1:K:148:SER:HB2	2.00	0.43
1:B:46:GLN:NE2	1:B:134:TYR:CE1	2.86	0.43
1:F:208:LEU:HD12	1:F:256:HIS:O	2.18	0.43
1:E:299:ILE:HA	1:E:314:GLY:HA3	2.00	0.43
1:C:193:SER:OG	1:C:194:GLY:N	2.50	0.43
1:J:92:GLU:OE2	1:J:96:ARG:NH1	2.51	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:B:202:ASN:O	1:B:224:PHE:HD2	2.02	0.43
1:I:170:LEU:HD22	1:I:251:PRO:HD3	2.01	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:B:92:GLU:OE2	1:B:96:ARG:NH1	2.52	0.43
1:M:241:VAL:HG12	1:M:241:VAL:O	2.19	0.43
1:A:202:ASN:C	1:A:202:ASN:HD22	2.21	0.43
1:M:226:GLU:OE1	1:M:228:SER:N	2.52	0.43
1:I:210:LEU:HD21	1:I:249:LEU:HD21	2.01	0.43
1:F:272:GLN:HB2	1:F:309:TRP:CD1	2.53	0.43
1:D:55:LEU:CD1	1:D:55:LEU:H	2.20	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:I:38:PHE:CD2	1:I:169:GLN:NE2	2.87	0.43
1:C:34:ARG:HH12	1:C:252:GLY:CA	2.30	0.43
1:I:144:ARG:HD2	1:I:170:LEU:HD12	2.00	0.43
1:E:254:PHE:CD2	1:E:254:PHE:N	2.85	0.43
1:A:98:LYS:HG3	1:A:111:TYR:CZ	2.53	0.43
1:J:48:ASN:OD1	1:J:157:THR:HA	2.19	0.43
1:E:98:LYS:HG3	1:E:111:TYR:CZ	2.54	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:B:208:LEU:HD11	1:B:255:VAL:HG21	2.01	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:M:137:VAL:O	1:M:137:VAL:HG12	2.19	0.43
1:D:246:ASN:O	1:D:247:ASN:C	2.56	0.43
1:C:208:LEU:HD12	1:C:256:HIS:O	2.19	0.43
1:H:206:VAL:O	1:H:219:GLU:HG3	2.19	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: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
1:C:38:PHE:HB2	1:C:172:PRO:O	2.18	0.42
1:J:129:ARG:HG2	1:J:129:ARG:NH1	2.34	0.42
1:A:45:PRO:HG3	1:A:156:VAL:HB	2.00	0.42
1:G:230:ASP:O	1:G:234:GLY:N	2.41	0.42
1:L:45:PRO:HG3	1:L:156:VAL:HB	2.01	0.42
1:J:91:GLN:HA	1:J:118:TYR:CD1	2.54	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:B:147:ARG:HH11	1:B:147:ARG:CB	2.32	0.42
1:E:34:ARG:HH11	1:E:34:ARG:CG	2.32	0.42
1:H:204:ALA:O	1:H:206:VAL:HG23	2.19	0.42
1:B:98:LYS:HG3	1:B:111:TYR:CZ	2.54	0.42
1:D:86:ASN:O	1:D:89:SER:HB3	2.18	0.42
1:C:52:LEU:HA	1:C:52:LEU:HD23	1.86	0.42
1:H:191:LEU:O	1:H:191:LEU:HD12	2.19	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:G:193:SER:OG	1:G:194:GLY:N	2.51	0.42
1:C:231:GLU:H	1:C:231:GLU:HG3	1.57	0.42
1:B:91:GLN:HA	1:B:118:TYR:CD1	2.54	0.42
1:F:299:ILE:HG22	1:F:314:GLY:HA3	2.01	0.42
1:B:64:ALA:HB2	1:B:142:SER:N	2.34	0.42
1:I:129:ARG:HG2	1:I:129:ARG:NH1	2.33	0.42
1:E:103:ASP:C	1:E:105:ALA:H	2.21	0.42
1:M:180:PRO:O	1:M:181:SER:C	2.57	0.42
1:F:126:GLU:O	1:F:130:ILE:HG13	2.20	0.42
1:A:129:ARG:HH11	1:A:129:ARG:HG2	1.85	0.42
1:C:185:LEU:HA	1:C:185:LEU:HD12	1.83	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:D:31:LEU:HB2	1:D:257:ALA:HB3	2.01	0.42
1:G:191:LEU:N	1:G:196:LEU:HD22	2.35	0.42
1:A:173:ILE:HG22	1:A:242:PHE:O	2.20	0.42
1:F:69:TYR:CD2	1:F:164:MET:HE3	2.55	0.42
1:K:196:LEU:HD12	1:K:261:GLU:HA	2.01	0.42
1:E:126:GLU:OE2	1:E:129:ARG:NH2	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:174:TYR:CD1	1:F:241:VAL:HG22	2.55	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:B:250:LEU:HD12	1:C:236:VAL:HG21	2.01	0.42
1:M:16:GLY:HA2	1:M:338:VAL:O	2.20	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:B:103:ASP:O	1:B:105:ALA:N	2.53	0.42
1:K:132:LEU:O	1:K:135:THR:HG23	2.19	0.42
1:D:46:GLN:HB2	1:D:134:TYR:CD1	2.55	0.42
1:B:263:VAL:O	1:B:265:GLN:N	2.53	0.42
1:L:91:GLN:HA	1:L:118:TYR:CD1	2.55	0.42
1:L:206:VAL:HG12	1:L:207:SER:N	2.35	0.42
1:A:250:LEU:N	1:A:253:MET:SD	2.88	0.42
1:H:145:ILE:HG23	1:H:145:ILE:O	2.19	0.42
1:L:190:GLU:HB3	1:L:196:LEU:HD13	2.02	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:K:109:GLN:O	1:K:112:ALA:HB3	2.19	0.42
1:J:216:TYR:HA	1:J:217:PRO:HD2	1.86	0.42
1:D:77:GLU:HA	1:D:132:LEU:HD22	2.01	0.42
1:B:180:PRO:O	1:B:181:SER:C	2.58	0.42
1:I:35:THR:OG1	1:I:253:MET:HB2	2.20	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:D:47:VAL:HG13	1:D:134:TYR:CB	2.50	0.42
1:B:126:GLU:O	1:B:130:ILE:HG13	2.19	0.42
1:L:92:GLU:OE2	1:L:96:ARG:NH1	2.53	0.42
1:J:50:ILE:HD13	1:J:155:LEU:HA	2.02	0.42
1:I:86:ASN:O	1:I:89:SER:HB3	2.20	0.42
1:A:158:ASN:C	1:A:158:ASN:OD1	2.58	0.42
1:D:51:ILE:HD11	1:D:164:MET:CE	2.50	0.41
1:K:218:LEU:HD23	1:K:218:LEU:N	2.34	0.41
1:E:68:LEU:HD13	1:E:145:ILE:CD1	2.50	0.41
1:M:170:LEU:HD13	1:M:251:PRO:HD3	2.01	0.41
1:G:56:PHE:CZ	1:G:148:SER:HB2	2.55	0.41
1:E:260:GLN:CA	1:E:260:GLN:OE1	2.67	0.41
1:D:101:VAL:HG12	1:D:106:VAL:O	2.20	0.41
1:M:182:THR:OG1	1:M:183:ALA:N	2.53	0.41
1:M:98:LYS:HG3	1:M:111:TYR:CZ	2.55	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: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:M:52:LEU:HD23	1:M:52:LEU:HA	1.88	0.41
1:J:227:VAL:HG23	1:J:237:THR:O	2.19	0.41
1:G:38:PHE:CD1	1:G:174:TYR:CE2	3.08	0.41
1:B:48:ASN:OD1	1:B:158:ASN:N	2.53	0.41
1:D:129:ARG:HG2	1:D:129:ARG:NH1	2.34	0.41
1:I:116:ALA:O	1:I:120:GLN:HG3	2.19	0.41
1:H:121:SER:O	1:H:122:LYS:C	2.59	0.41
1:C:86:ASN:O	1:C:89:SER:HB3	2.20	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:H:156:VAL:HG11	1:H:164:MET:HE1	2.02	0.41
1:E:41:ALA:CB	1:E:140:PRO:HG2	2.50	0.41
1:I:40:ILE:HD13	1:I:168:GLN:HE21	1.85	0.41
1:C:57:LYS:HB3	1:C:60:SER:HB3	2.02	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:G:77:GLU:HA	1:G:132:LEU:HD22	2.02	0.41
1:L:208:LEU:HB2	1:L:242:PHE:CE1	2.54	0.41
1:I:64:ALA:HA	1:I:141:ILE:O	2.20	0.41
1:D:171:ASP:OD1	1:D:244:ASN:N	2.50	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:G:92:GLU:OE2	1:G:96:ARG:NH1	2.53	0.41
1:E:176:ASP:OD2	1:E:239:ARG:HG2	2.20	0.41
1:I:77:GLU:HA	1:I:132:LEU:HD22	2.02	0.41
1:C:203:ALA:HB2	1:C:223:GLU:HA	2.02	0.41
1:G:91:GLN:HA	1:G:118:TYR:CD1	2.55	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: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:E:34:ARG:NH1	1:E:254:PHE:CD2	2.89	0.41
1:D:144:ARG:HE	1:E:226:GLU:CD	2.24	0.41
1:L:244:ASN:N	1:L:245:PRO:CD	2.83	0.41
1:C:216:TYR:HA	1:C:217:PRO:HD2	1.87	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: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: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:B:240:ALA:CB	1:B:242:PHE:HE2	2.34	0.41
1:A:219:GLU:HG3	1:A:220:GLY:H	1.84	0.41
1:M:199:ALA:HB2	1:M:204:ALA:C	2.40	0.41
1:A:228:SER:HB3	1:A:237:THR:HB	2.02	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:F:206:VAL:CG1	1:F:207:SER:N	2.84	0.41
1:K:183:ALA:O	1:K:186:ARG:HB3	2.20	0.41
1:H:41:ALA:CB	1:H:140:PRO:HG2	2.51	0.41
1:A:54:ARG:N	1:A:152:GLU:OE2	2.54	0.41
1:K:57:LYS:HB3	1:K:60:SER:HB3	2.02	0.41
1:B:16:GLY:HA2	1:B:338:VAL:O	2.20	0.41
1:J:23:GLN:O	1:J:266:LYS:HA	2.21	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: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: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:L:130:ILE:HG21	1:M:74:ALA:HB1	2.01	0.41
1:M:54:ARG:HD2	1:M:148:SER:HB2	2.03	0.41
1:F:81:GLN:HB3	1:G:82:SER:HA	2.03	0.41
1:M:206:VAL:HG21	1:M:222:LEU:HB2	2.02	0.41
1:F:299:ILE:CG2	1:F:315:LEU:HG	2.51	0.41
1:L:208:LEU:HD22	1:L:242:PHE:CD2	2.56	0.41
1:D:64:ALA:HB2	1:D:141:ILE:HA	2.02	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:C:216:TYR:CE2	1:C:218:LEU:HB2	2.56	0.41
1:B:120:GLN:O	1:B:123:ALA:HB3	2.21	0.41
1:J:86:ASN:O	1:J:89:SER:HB3	2.21	0.41
1:F:203:ALA:HB2	1:F:223:GLU:HA	2.03	0.41
1:E:16:GLY:HA2	1:E:338:VAL:O	2.21	0.41
1:J:55:LEU:HD12	1:J:68:LEU:O	2.21	0.41
1:G:38:PHE:HD2	1:G:169:GLN:NE2	2.18	0.41
1:L:150:VAL:HG12	1:L:151:THR:N	2.36	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:K:40:ILE:HG12	1:K:168:GLN:HG2	2.02	0.41
1:J:52:LEU:HA	1:J:52:LEU:HD23	1.85	0.41
1:G:190:GLU:OE1	1:G:196:LEU:HD11	2.20	0.40
1:I:208:LEU:HB2	1:I:242:PHE:CZ	2.55	0.40
1:G:200:GLY:HA3	1:G:221:ARG:NH2	2.36	0.40
1:D:64:ALA:HB2	1:D:141:ILE:CA	2.52	0.40
1:J:69:TYR:HB2	1:J:137:VAL:HB	2.02	0.40
1:D:173:ILE:HG12	1:D:174:TYR:H	1.86	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:16:GLY:HA2	1:C:338:VAL:O	2.22	0.40
1:A:57:LYS:HB3	1:A:60:SER:HB3	2.02	0.40
1:A:52:LEU:HD23	1:A:52:LEU:HA	1.87	0.40
1:C:190:GLU:HB3	1:C:196:LEU:CD1	2.40	0.40
1:B:215:GLN:NE2	1:B:258:GLN:CD	2.74	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:96:ARG:CZ	1:D:109:GLN:OE1	2.69	0.40
1:E:222:LEU:HA	1:E:240:ALA:HA	2.02	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:G:50:ILE:HD13	1:G:155:LEU:HB2	2.02	0.40
1:C:244:ASN:ND2	1:C:247:ASN:HA	2.37	0.40
1:M:202:ASN:O	1:M:224:PHE:CD2	2.71	0.40
1:G:144:ARG:HG3	1:G:144:ARG:NH1	2.36	0.40
1:E:129:ARG:HG2	1:E:129:ARG:HH11	1.85	0.40
1:G:166:THR:HG22	1:G:167:VAL:N	2.36	0.40
1:G:162:ASN:HA	1:G:162:ASN:HD22	1.64	0.40
1:D:183:ALA:O	1:D:187:LEU:HG	2.22	0.40
1:L:46:GLN:CD	1:L:134:TYR:CE1	2.95	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:H:176:ASP:OD1	1:H:239:ARG:HG2	2.22	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
1:F:86:ASN:ND2	1:F:121:SER:OG	2.54	0.40
1:I:38:PHE:HD2	1:I:169:GLN:NE2	2.18	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:91:GLN:HA	1:F:118:TYR:CD1	2.55	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%)	7	40
1	B	325/360 (90%)	284 (87%)	32 (10%)	9 (3%)	6	37
1	C	325/360 (90%)	279 (86%)	40 (12%)	6 (2%)	11	51
1	D	228/360 (63%)	195 (86%)	31 (14%)	2 (1%)	21	67
1	E	325/360 (90%)	280 (86%)	38 (12%)	7 (2%)	8	45
1	F	325/360 (90%)	277 (85%)	43 (13%)	5 (2%)	13	55
1	G	325/360 (90%)	277 (85%)	41 (13%)	7 (2%)	8	45
1	H	325/360 (90%)	288 (89%)	32 (10%)	5 (2%)	13	55
1	I	325/360 (90%)	281 (86%)	38 (12%)	6 (2%)	11	51
1	J	325/360 (90%)	277 (85%)	43 (13%)	5 (2%)	13	55
1	K	325/360 (90%)	285 (88%)	34 (10%)	6 (2%)	11	51
1	L	325/360 (90%)	279 (86%)	41 (13%)	5 (2%)	13	55
1	M	325/360 (90%)	285 (88%)	32 (10%)	8 (2%)	7	41
All	All	4033/4680 (86%)	3478 (86%)	478 (12%)	77 (2%)	10	50

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%)	35	75
1	B	193/287 (67%)	182 (94%)	11 (6%)	25	67
1	C	190/287 (66%)	177 (93%)	13 (7%)	20	59
1	D	185/287 (64%)	175 (95%)	10 (5%)	27	68
1	E	194/287 (68%)	177 (91%)	17 (9%)	12	45
1	F	240/287 (84%)	231 (96%)	9 (4%)	40	78
1	G	190/287 (66%)	183 (96%)	7 (4%)	41	79
1	H	194/287 (68%)	181 (93%)	13 (7%)	20	60
1	I	190/287 (66%)	180 (95%)	10 (5%)	28	69
1	J	189/287 (66%)	175 (93%)	14 (7%)	17	56
1	K	194/287 (68%)	183 (94%)	11 (6%)	25	67
1	L	190/287 (66%)	179 (94%)	11 (6%)	25	66
1	M	196/287 (68%)	181 (92%)	15 (8%)	16	54
All	All	2531/3731 (68%)	2382 (94%)	149 (6%)	24	65

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	A	1260	-	4,4,4	0.40	0	6,6,6	0.19	0
2	SO4	A	1261	-	4,4,4	0.42	0	6,6,6	0.08	0
2	SO4	B	1340	-	4,4,4	0.38	0	6,6,6	0.21	0
2	SO4	B	1341	-	4,4,4	0.40	0	6,6,6	0.21	0
2	SO4	C	1340	-	4,4,4	0.32	0	6,6,6	0.11	0
2	SO4	E	1340	-	4,4,4	0.49	0	6,6,6	0.17	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	SO4	E	1341	-	4,4,4	0.27	0	6,6,6	0.10	0
2	SO4	F	1340	-	4,4,4	0.37	0	6,6,6	0.21	0
2	SO4	F	1341	-	4,4,4	0.36	0	6,6,6	0.10	0
2	SO4	G	1340	-	4,4,4	0.37	0	6,6,6	0.09	0
2	SO4	H	1340	-	4,4,4	0.41	0	6,6,6	0.09	0
2	SO4	I	1340	-	4,4,4	0.45	0	6,6,6	0.10	0
2	SO4	J	1340	-	4,4,4	0.37	0	6,6,6	0.08	0
2	SO4	K	1340	-	4,4,4	0.47	0	6,6,6	0.18	0
2	SO4	L	1340	-	4,4,4	0.44	0	6,6,6	0.14	0
2	SO4	M	1340	-	4,4,4	0.40	0	6,6,6	0.13	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	SO4	A	1260	-	-	0/0/0/0	0/0/0/0
2	SO4	A	1261	-	-	0/0/0/0	0/0/0/0
2	SO4	B	1340	-	-	0/0/0/0	0/0/0/0
2	SO4	B	1341	-	-	0/0/0/0	0/0/0/0
2	SO4	C	1340	-	-	0/0/0/0	0/0/0/0
2	SO4	E	1340	-	-	0/0/0/0	0/0/0/0
2	SO4	E	1341	-	-	0/0/0/0	0/0/0/0
2	SO4	F	1340	-	-	0/0/0/0	0/0/0/0
2	SO4	F	1341	-	-	0/0/0/0	0/0/0/0
2	SO4	G	1340	-	-	0/0/0/0	0/0/0/0
2	SO4	H	1340	-	-	0/0/0/0	0/0/0/0
2	SO4	I	1340	-	-	0/0/0/0	0/0/0/0
2	SO4	J	1340	-	-	0/0/0/0	0/0/0/0
2	SO4	K	1340	-	-	0/0/0/0	0/0/0/0
2	SO4	L	1340	-	-	0/0/0/0	0/0/0/0
2	SO4	M	1340	-	-	0/0/0/0	0/0/0/0

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%)	0.31	11 (4%) 35 22	34, 77, 127, 155	0
1	B	327/360 (90%)	0.21	20 (6%) 25 13	22, 71, 145, 153	0
1	C	327/360 (90%)	0.14	12 (3%) 45 30	20, 73, 141, 158	0
1	D	230/360 (63%)	0.04	3 (1%) 79 67	16, 59, 87, 110	0
1	E	327/360 (90%)	0.40	29 (8%) 12 6	9, 53, 148, 157	0
1	F	327/360 (90%)	0.19	6 (1%) 71 58	28, 66, 131, 148	0
1	G	327/360 (90%)	0.50	41 (12%) 5 3	34, 82, 147, 163	0
1	H	327/360 (90%)	0.84	63 (19%) 2 1	13, 56, 154, 165	0
1	I	327/360 (90%)	0.50	35 (10%) 8 4	9, 52, 147, 163	0
1	J	327/360 (90%)	0.57	51 (15%) 3 2	5, 37, 150, 165	0
1	K	327/360 (90%)	0.85	71 (21%) 1 1	6, 50, 157, 170	0
1	L	327/360 (90%)	0.61	45 (13%) 4 2	8, 56, 154, 173	0
1	M	327/360 (90%)	1.14	82 (25%) 1 1	18, 83, 158, 172	0
All	All	4059/4680 (86%)	0.50	469 (11%) 6 4	5, 65, 151, 173	0

All (469) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	M	339	PRO	9.8
1	M	331	PRO	8.6
1	I	274	GLY	8.5
1	K	317	ALA	7.9
1	K	15	VAL	7.9
1	H	295	GLU	7.1
1	M	315	LEU	7.1
1	K	338	VAL	7.0
1	L	325	GLY	6.9

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Mol	Chain	Res	Type	RSRZ
1	J	339	PRO	6.9
1	K	296	LEU	6.6
1	M	14	GLU	6.6
1	M	288	VAL	6.5
1	H	263	VAL	6.4
1	M	317	ALA	6.4
1	L	327	GLN	6.0
1	M	309	TRP	5.9
1	M	13	PRO	5.8
1	M	289	ASN	5.8
1	L	314	GLY	5.7
1	M	270	ALA	5.7
1	H	296	LEU	5.7
1	E	332	GLY	5.7
1	G	15	VAL	5.7
1	C	15	VAL	5.7
1	M	316	ASN	5.6
1	K	325	GLY	5.6
1	M	332	GLY	5.6
1	K	298	VAL	5.6
1	L	332	GLY	5.5
1	L	15	VAL	5.5
1	M	287	VAL	5.5
1	K	324	GLU	5.5
1	K	290	ALA	5.5
1	M	15	VAL	5.5
1	H	290	ALA	5.4
1	L	339	PRO	5.4
1	K	16	GLY	5.3
1	K	281	GLY	5.3
1	L	274	GLY	5.3
1	L	288	VAL	5.3
1	M	271	PRO	5.3
1	M	337	THR	5.3
1	M	301	ALA	5.3
1	L	328	PHE	5.3
1	M	338	VAL	5.3
1	E	296	LEU	5.2
1	K	267	ALA	5.2
1	L	333	VAL	5.2
1	K	316	ASN	5.2
1	L	334	GLU	5.2

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Mol	Chain	Res	Type	RSRZ
1	M	302	ASP	5.1
1	K	282	GLN	5.0
1	M	25	VAL	5.0
1	G	284	THR	5.0
1	L	19	THR	4.9
1	K	337	THR	4.9
1	H	337	THR	4.9
1	L	289	ASN	4.9
1	H	13	PRO	4.9
1	M	329	VAL	4.9
1	K	328	PHE	4.9
1	K	339	PRO	4.8
1	I	332	GLY	4.8
1	J	270	ALA	4.8
1	J	289	ASN	4.8
1	L	324	GLU	4.8
1	I	339	PRO	4.7
1	M	313	GLU	4.7
1	M	307	ASP	4.7
1	J	287	VAL	4.7
1	H	291	GLN	4.7
1	M	291	GLN	4.7
1	H	314	GLY	4.7
1	M	333	VAL	4.6
1	M	325	GLY	4.5
1	M	298	VAL	4.5
1	M	328	PHE	4.5
1	E	14	GLU	4.5
1	K	19	THR	4.5
1	H	287	VAL	4.4
1	K	329	VAL	4.4
1	K	278	ASP	4.4
1	M	19	THR	4.4
1	H	327	GLN	4.4
1	E	337	THR	4.4
1	L	323	THR	4.4
1	H	15	VAL	4.4
1	M	16	GLY	4.4
1	M	290	ALA	4.4
1	B	296	LEU	4.4
1	H	331	PRO	4.3
1	B	294	VAL	4.3

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Mol	Chain	Res	Type	RSRZ
1	H	332	GLY	4.3
1	G	317	ALA	4.3
1	K	309	TRP	4.2
1	M	21	GLU	4.2
1	H	264	LYS	4.2
1	M	292	ASN	4.2
1	M	296	LEU	4.2
1	L	13	PRO	4.2
1	M	321	ILE	4.2
1	B	332	GLY	4.2
1	M	285	ALA	4.2
1	M	314	GLY	4.2
1	J	295	GLU	4.2
1	E	265	GLN	4.2
1	G	324	GLU	4.2
1	M	318	GLY	4.2
1	K	13	PRO	4.2
1	H	294	VAL	4.1
1	M	275	VAL	4.1
1	M	276	THR	4.1
1	M	320	LYS	4.1
1	I	337	THR	4.1
1	K	295	GLU	4.1
1	H	319	ASP	4.1
1	F	296	LEU	4.1
1	L	278	ASP	4.1
1	K	285	ALA	4.1
1	M	330	GLN	4.1
1	K	276	THR	4.0
1	M	274	GLY	4.0
1	K	17	ILE	4.0
1	L	21	GLU	4.0
1	H	289	ASN	4.0
1	J	288	VAL	4.0
1	H	330	GLN	4.0
1	J	332	GLY	4.0
1	K	331	PRO	4.0
1	M	278	ASP	4.0
1	I	338	VAL	4.0
1	K	294	VAL	4.0
1	H	297	ARG	4.0
1	M	319	ASP	4.0

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Mol	Chain	Res	Type	RSRZ
1	M	22	ALA	3.9
1	H	281	GLY	3.9
1	J	22	ALA	3.9
1	G	16	GLY	3.9
1	H	288	VAL	3.9
1	M	294	VAL	3.9
1	J	16	GLY	3.9
1	M	311	VAL	3.9
1	K	333	VAL	3.9
1	G	337	THR	3.9
1	M	306	GLY	3.9
1	G	285	ALA	3.8
1	M	299	ILE	3.8
1	H	280	LYS	3.8
1	L	301	ALA	3.8
1	H	323	THR	3.8
1	J	326	LEU	3.8
1	G	294	VAL	3.8
1	M	268	ILE	3.8
1	K	271	PRO	3.8
1	M	295	GLU	3.8
1	B	333	VAL	3.8
1	H	265	GLN	3.8
1	I	15	VAL	3.8
1	J	325	GLY	3.8
1	M	277	ARG	3.7
1	G	339	PRO	3.7
1	H	25	VAL	3.7
1	H	270	ALA	3.7
1	I	271	PRO	3.7
1	H	334	GLU	3.7
1	G	283	ALA	3.7
1	L	270	ALA	3.7
1	B	13	PRO	3.7
1	M	286	LEU	3.7
1	J	324	GLU	3.6
1	H	333	VAL	3.6
1	E	288	VAL	3.6
1	K	270	ALA	3.6
1	K	283	ALA	3.6
1	B	288	VAL	3.6
1	A	242	PHE	3.6

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Mol	Chain	Res	Type	RSRZ
1	J	21	GLU	3.6
1	H	292	ASN	3.6
1	K	334	GLU	3.6
1	K	306	GLY	3.6
1	G	270	ALA	3.6
1	K	263	VAL	3.6
1	K	314	GLY	3.6
1	L	285	ALA	3.6
1	L	14	GLU	3.5
1	M	283	ALA	3.5
1	I	307	ASP	3.5
1	K	297	ARG	3.5
1	I	317	ALA	3.5
1	G	290	ALA	3.5
1	E	291	GLN	3.5
1	G	338	VAL	3.5
1	H	20	LEU	3.5
1	C	339	PRO	3.5
1	E	283	ALA	3.5
1	G	271	PRO	3.5
1	J	17	ILE	3.5
1	H	285	ALA	3.5
1	J	294	VAL	3.5
1	H	326	LEU	3.5
1	M	297	ARG	3.4
1	J	15	VAL	3.4
1	M	272	GLN	3.4
1	G	323	THR	3.4
1	H	16	GLY	3.4
1	J	338	VAL	3.3
1	M	323	THR	3.3
1	E	295	GLU	3.3
1	H	271	PRO	3.3
1	C	25	VAL	3.3
1	M	273	GLN	3.3
1	F	22	ALA	3.3
1	H	282	GLN	3.3
1	H	279	LEU	3.3
1	A	258	GLN	3.3
1	J	337	THR	3.3
1	K	277	ARG	3.3
1	K	293	LYS	3.2

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Mol	Chain	Res	Type	RSRZ
1	L	16	GLY	3.2
1	M	312	THR	3.2
1	H	262	GLY	3.2
1	K	323	THR	3.2
1	L	326	LEU	3.2
1	K	330	GLN	3.2
1	J	333	VAL	3.2
1	L	296	LEU	3.2
1	M	282	GLN	3.2
1	G	22	ALA	3.2
1	M	308	LYS	3.2
1	L	338	VAL	3.2
1	K	266	LYS	3.2
1	J	271	PRO	3.2
1	E	284	THR	3.2
1	K	284	THR	3.2
1	K	299	ILE	3.2
1	H	329	VAL	3.2
1	I	287	VAL	3.2
1	L	294	VAL	3.2
1	H	338	VAL	3.2
1	L	275	VAL	3.1
1	L	271	PRO	3.1
1	K	300	LYS	3.1
1	K	14	GLU	3.1
1	E	13	PRO	3.1
1	B	15	VAL	3.1
1	G	31	LEU	3.1
1	H	335	VAL	3.1
1	E	290	ALA	3.1
1	C	289	ASN	3.1
1	B	270	ALA	3.0
1	H	299	ILE	3.0
1	J	278	ASP	3.0
1	H	14	GLU	3.0
1	K	326	LEU	3.0
1	H	328	PHE	3.0
1	M	20	LEU	3.0
1	J	281	GLY	3.0
1	I	283	ALA	3.0
1	E	294	VAL	3.0
1	I	306	GLY	3.0

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Mol	Chain	Res	Type	RSRZ
1	H	293	LYS	3.0
1	J	13	PRO	3.0
1	H	257	ALA	3.0
1	G	328	PHE	2.9
1	K	302	ASP	2.9
1	G	289	ASN	2.9
1	G	312	THR	2.9
1	L	17	ILE	2.9
1	G	332	GLY	2.9
1	M	24	THR	2.9
1	L	290	ALA	2.9
1	I	270	ALA	2.9
1	I	24	THR	2.9
1	G	319	ASP	2.9
1	C	323	THR	2.9
1	E	334	GLU	2.9
1	I	330	GLN	2.9
1	M	284	THR	2.9
1	K	301	ALA	2.9
1	E	272	GLN	2.9
1	I	288	VAL	2.9
1	M	281	GLY	2.9
1	G	293	LYS	2.9
1	H	309	TRP	2.9
1	I	285	ALA	2.9
1	K	22	ALA	2.9
1	B	325	GLY	2.9
1	H	17	ILE	2.8
1	H	286	LEU	2.8
1	J	331	PRO	2.8
1	E	333	VAL	2.8
1	G	274	GLY	2.8
1	G	292	ASN	2.8
1	H	336	LYS	2.8
1	J	330	GLN	2.8
1	I	17	ILE	2.8
1	K	274	GLY	2.8
1	I	301	ALA	2.8
1	J	328	PHE	2.8
1	F	323	THR	2.8
1	J	282	GLN	2.8
1	G	281	GLY	2.8

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Mol	Chain	Res	Type	RSRZ
1	M	262	GLY	2.8
1	L	292	ASN	2.8
1	K	289	ASN	2.7
1	B	287	VAL	2.7
1	C	288	VAL	2.7
1	G	287	VAL	2.7
1	G	273	GLN	2.7
1	B	331	PRO	2.7
1	L	281	GLY	2.7
1	E	278	ASP	2.7
1	C	331	PRO	2.7
1	H	276	THR	2.7
1	I	305	ILE	2.7
1	A	232	GLY	2.7
1	A	233	THR	2.7
1	J	304	VAL	2.7
1	J	299	ILE	2.7
1	J	327	GLN	2.7
1	G	268	ILE	2.7
1	J	274	GLY	2.7
1	I	13	PRO	2.7
1	L	335	VAL	2.7
1	E	282	GLN	2.7
1	J	318	GLY	2.6
1	C	295	GLU	2.6
1	H	298	VAL	2.6
1	M	327	GLN	2.6
1	A	196	LEU	2.6
1	C	19	THR	2.6
1	G	325	GLY	2.6
1	J	286	LEU	2.6
1	I	16	GLY	2.6
1	K	291	GLN	2.6
1	E	339	PRO	2.6
1	I	329	VAL	2.6
1	E	277	ARG	2.6
1	G	295	GLU	2.6
1	G	301	ALA	2.5
1	M	267	ALA	2.5
1	G	306	GLY	2.5
1	I	286	LEU	2.5
1	J	323	THR	2.5

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Mol	Chain	Res	Type	RSRZ
1	K	20	LEU	2.5
1	L	299	ILE	2.5
1	J	293	LYS	2.5
1	M	105	ALA	2.5
1	M	300	LYS	2.5
1	M	324	GLU	2.5
1	I	322	ILE	2.5
1	M	26	THR	2.5
1	L	279	LEU	2.5
1	M	110	GLN	2.5
1	H	312	THR	2.5
1	J	319	ASP	2.5
1	J	298	VAL	2.5
1	K	315	LEU	2.5
1	E	301	ALA	2.5
1	J	290	ALA	2.5
1	K	273	GLN	2.5
1	H	301	ALA	2.4
1	E	274	GLY	2.4
1	G	318	GLY	2.4
1	I	273	GLN	2.4
1	E	276	THR	2.4
1	G	288	VAL	2.4
1	L	287	VAL	2.4
1	J	302	ASP	2.4
1	H	283	ALA	2.4
1	A	191	LEU	2.4
1	M	227	VAL	2.4
1	E	297	ARG	2.4
1	K	262	GLY	2.4
1	I	268	ILE	2.4
1	E	287	VAL	2.4
1	J	314	GLY	2.4
1	K	332	GLY	2.4
1	M	279	LEU	2.4
1	M	310	LEU	2.4
1	L	330	GLN	2.4
1	F	306	GLY	2.3
1	K	292	ASN	2.3
1	G	331	PRO	2.3
1	I	290	ALA	2.3
1	D	114	ALA	2.3

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Mol	Chain	Res	Type	RSRZ
1	H	315	LEU	2.3
1	K	275	VAL	2.3
1	J	334	GLU	2.3
1	J	19	THR	2.3
1	M	293	LYS	2.3
1	H	268	ILE	2.3
1	A	41	ALA	2.3
1	K	310	LEU	2.3
1	B	263	VAL	2.3
1	G	333	VAL	2.3
1	J	268	ILE	2.3
1	G	272	GLN	2.3
1	M	326	LEU	2.3
1	K	335	VAL	2.3
1	M	17	ILE	2.3
1	D	105	ALA	2.2
1	H	324	GLU	2.2
1	I	262	GLY	2.2
1	I	325	GLY	2.2
1	K	336	LYS	2.2
1	E	285	ALA	2.2
1	L	316	ASN	2.2
1	J	291	GLN	2.2
1	L	273	GLN	2.2
1	K	21	GLU	2.2
1	I	323	THR	2.2
1	B	277	ARG	2.2
1	K	318	GLY	2.2
1	B	278	ASP	2.2
1	C	285	ALA	2.2
1	E	330	GLN	2.2
1	I	321	ILE	2.2
1	A	29	THR	2.2
1	L	295	GLU	2.2
1	H	316	ASN	2.2
1	I	289	ASN	2.2
1	B	317	ALA	2.2
1	A	31	LEU	2.2
1	E	329	VAL	2.2
1	L	18	VAL	2.2
1	E	270	ALA	2.2
1	K	303	ARG	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	257	ALA	2.2
1	C	273	GLN	2.2
1	K	279	LEU	2.2
1	M	224	PHE	2.2
1	K	18	VAL	2.2
1	H	317	ALA	2.1
1	K	280	LYS	2.1
1	J	20	LEU	2.1
1	H	274	GLY	2.1
1	B	339	PRO	2.1
1	F	31	LEU	2.1
1	J	329	VAL	2.1
1	K	288	VAL	2.1
1	K	305	ILE	2.1
1	J	301	ALA	2.1
1	L	315	LEU	2.1
1	H	277	ARG	2.1
1	G	336	LYS	2.1
1	C	16	GLY	2.1
1	B	179	GLN	2.1
1	J	296	LEU	2.1
1	B	290	ALA	2.1
1	B	295	GLU	2.1
1	G	267	ALA	2.1
1	H	22	ALA	2.1
1	J	317	ALA	2.1
1	K	272	GLN	2.1
1	F	273	GLN	2.1
1	G	291	GLN	2.1
1	D	96	ARG	2.1
1	L	110	GLN	2.1
1	A	247	ASN	2.0
1	J	306	GLY	2.0
1	L	331	PRO	2.0
1	A	259	LEU	2.0
1	I	264	LYS	2.0
1	I	296	LEU	2.0
1	M	334	GLU	2.0
1	H	325	GLY	2.0
1	J	285	ALA	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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(\AA^2)	Q<0.9
2	SO4	E	1340	5/5	0.90	0.21	-0.40	50,60,69,87	0
2	SO4	B	1340	5/5	0.87	0.20	-0.66	65,78,84,95	0
2	SO4	M	1340	5/5	0.87	0.20	-0.69	65,69,92,99	0
2	SO4	A	1260	5/5	0.91	0.14	-1.11	70,77,101,103	0
2	SO4	A	1261	5/5	0.92	0.20	-1.44	62,66,94,95	0
2	SO4	B	1341	5/5	0.86	0.17	-1.57	70,75,95,101	0
2	SO4	C	1340	5/5	0.97	0.12	-2.49	71,71,77,85	0
2	SO4	J	1340	5/5	0.96	0.17	-2.89	44,50,70,76	0
2	SO4	L	1340	5/5	0.97	0.17	-3.24	42,44,72,73	0
2	SO4	E	1341	5/5	0.97	0.14	-3.49	43,52,59,68	0
2	SO4	K	1340	5/5	0.96	0.17	-3.50	34,34,58,60	0
2	SO4	H	1340	5/5	0.96	0.15	-3.52	54,57,74,79	0
2	SO4	I	1340	5/5	0.93	0.13	-4.11	55,56,72,87	0
2	SO4	F	1340	5/5	0.94	0.14	-	62,76,97,97	0
2	SO4	G	1340	5/5	0.96	0.08	-	87,89,108,112	0
2	SO4	F	1341	5/5	0.94	0.12	-	67,75,92,100	0

6.5 Other polymers [i](#)

There are no such residues in this entry.