



Full wwPDB X-ray Structure Validation Report

Feb 27, 2014 – 11:19 PM 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 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/ValidationPDFNotes.html>

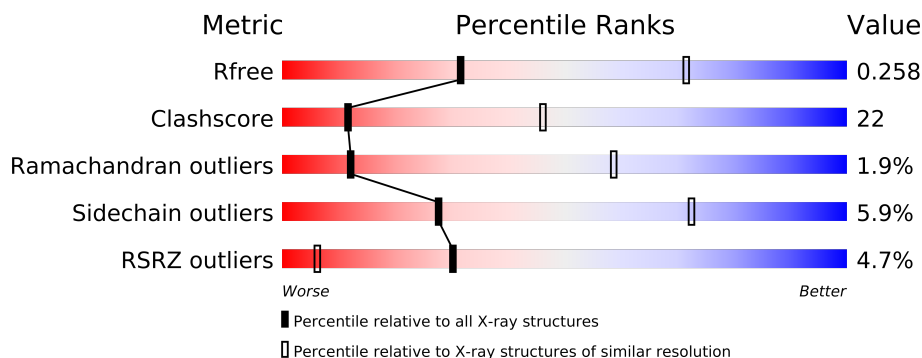
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

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}	66092	1824 (3.30-3.10)
Clashscore	79885	1078 (3.26-3.14)
Ramachandran outliers	78287	1059 (3.26-3.14)
Sidechain outliers	78261	1058 (3.26-3.14)
RSRZ outliers	66119	1825 (3.30-3.10)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	360	
1	B	360	
1	C	360	
1	D	360	
1	E	360	
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 hydrogen and 0 are deuterium.

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:

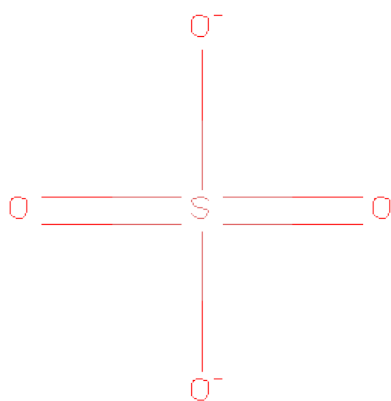
Chain	Residue	Modelled	Actual	Comment	Reference
A	1	SER	CYS	ENGINEERED MUTATION	UNP P52477
B	1	SER	CYS	ENGINEERED MUTATION	UNP P52477
C	1	SER	CYS	ENGINEERED MUTATION	UNP P52477

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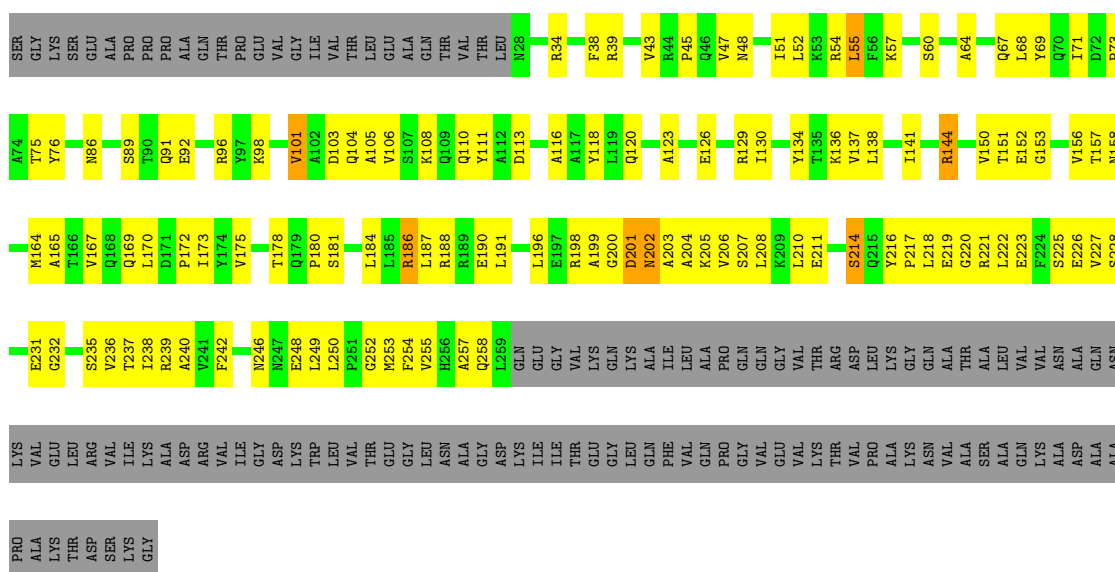
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	E	1	Total	O	S	0	0
			5	4	1		
2	F	1	Total	O	S	0	0
			5	4	1		
2	F	1	Total	O	S	0	0
			5	4	1		
2	G	1	Total	O	S	0	0
			5	4	1		
2	H	1	Total	O	S	0	0
			5	4	1		
2	I	1	Total	O	S	0	0
			5	4	1		
2	J	1	Total	O	S	0	0
			5	4	1		
2	K	1	Total	O	S	0	0
			5	4	1		
2	L	1	Total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

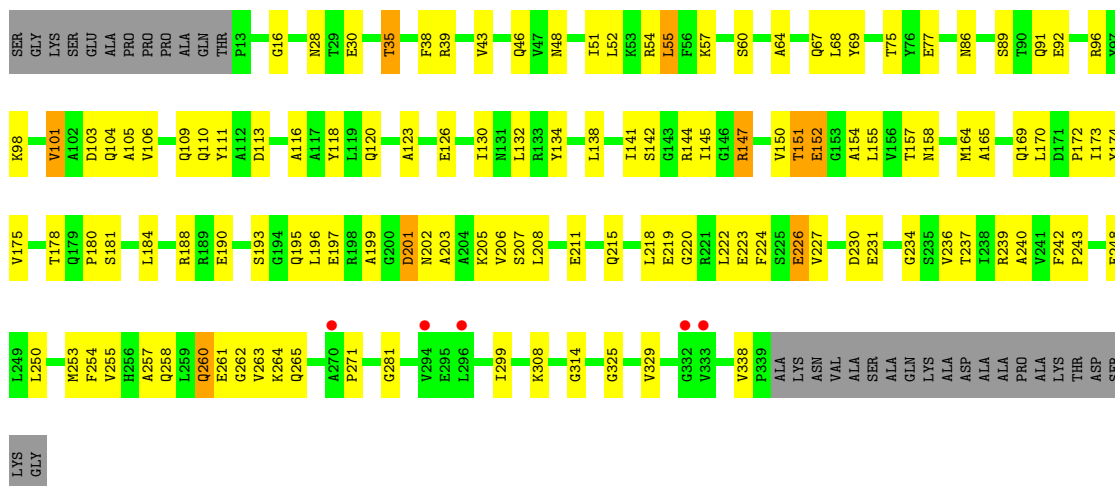
• Molecule 1: MULTIDRUG RESISTANCE PROTEIN MEXA

Chain A:



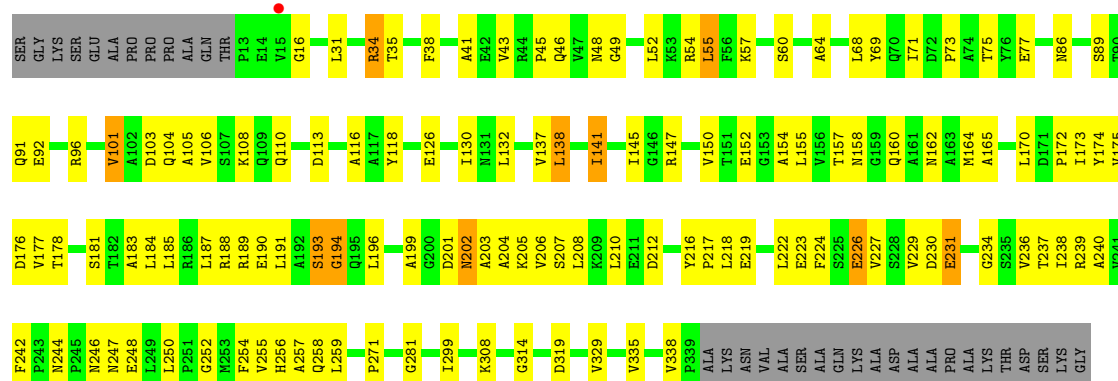
• Molecule 1: MULTIDRUG RESISTANCE PROTEIN MEXA

Chain B:



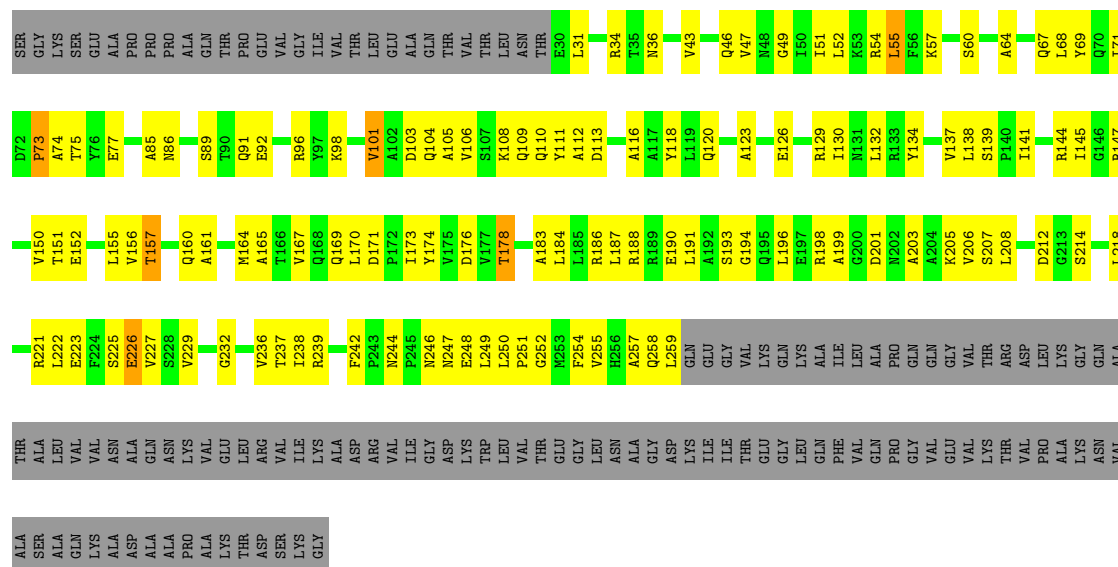
- Molecule 1: MULTIDRUG RESISTANCE PROTEIN MEXA

Chain C:



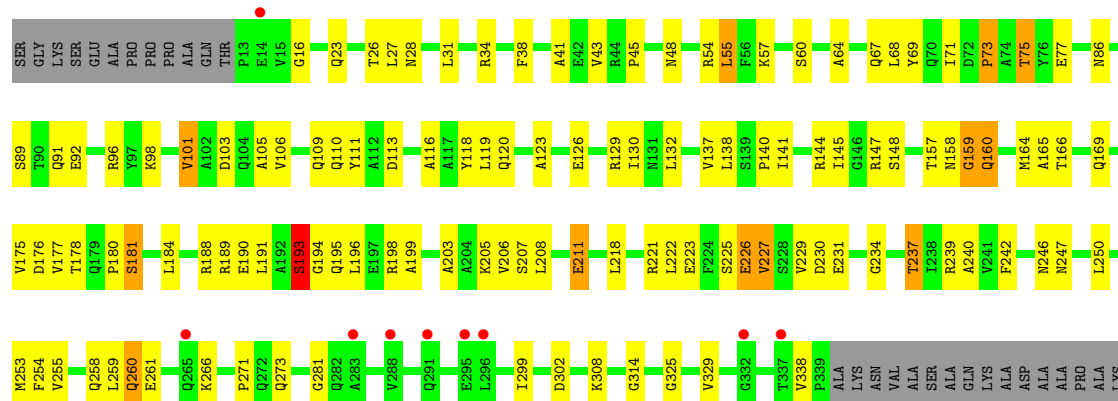
- Molecule 1: MULTIDRUG RESISTANCE PROTEIN MEXA

Chain D:



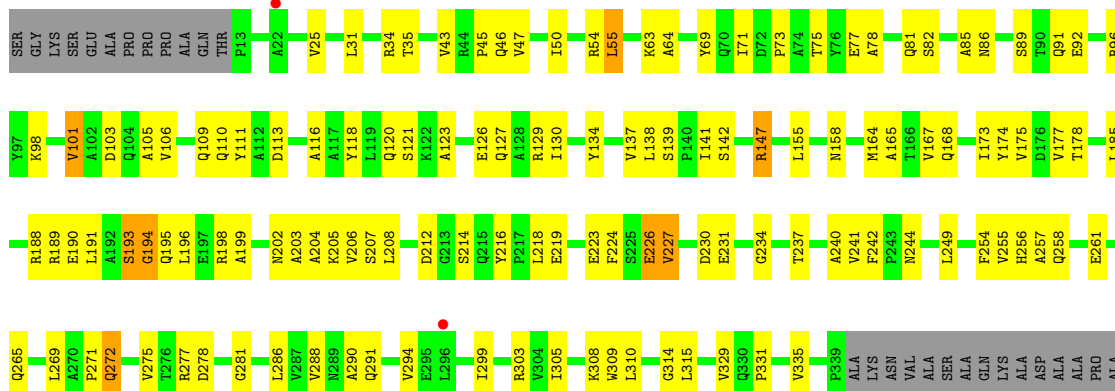
- Molecule 1: MULTIDRUG RESISTANCE PROTEIN MEXA

Chain E:



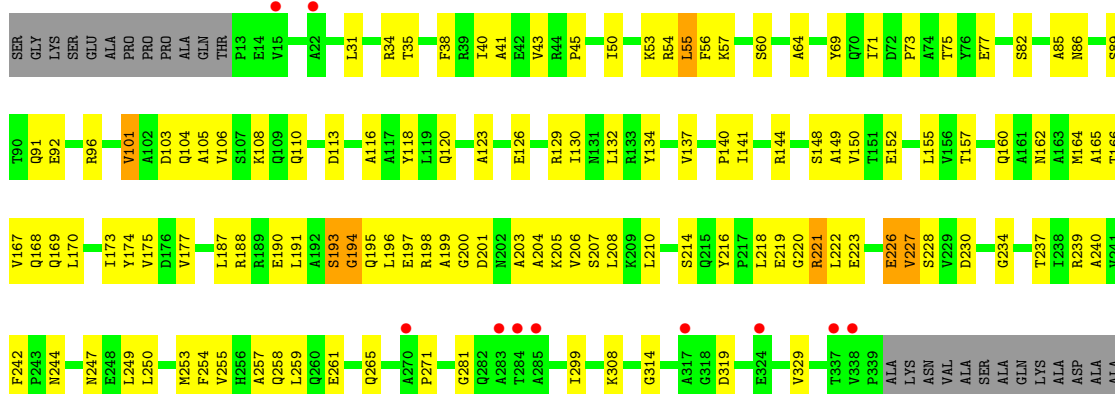
THR
ASP
SER
LYS
GLY

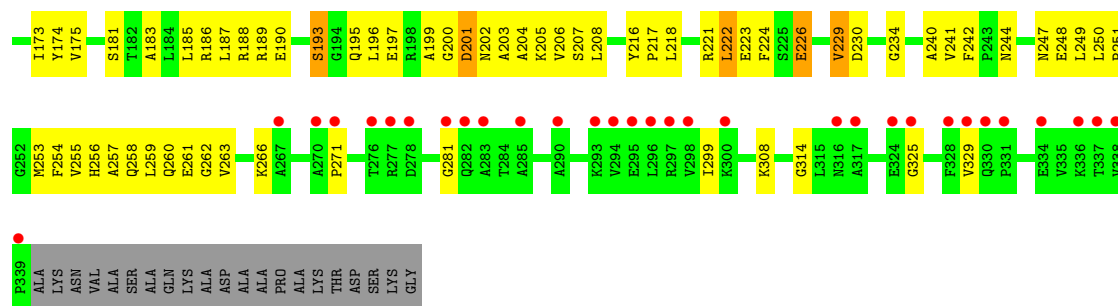
• Molecule 1: MULTIDRUG RESISTANCE PROTEIN MEXA

Chain F: 

LYS
THR
ASP
SER
LYS
GLY

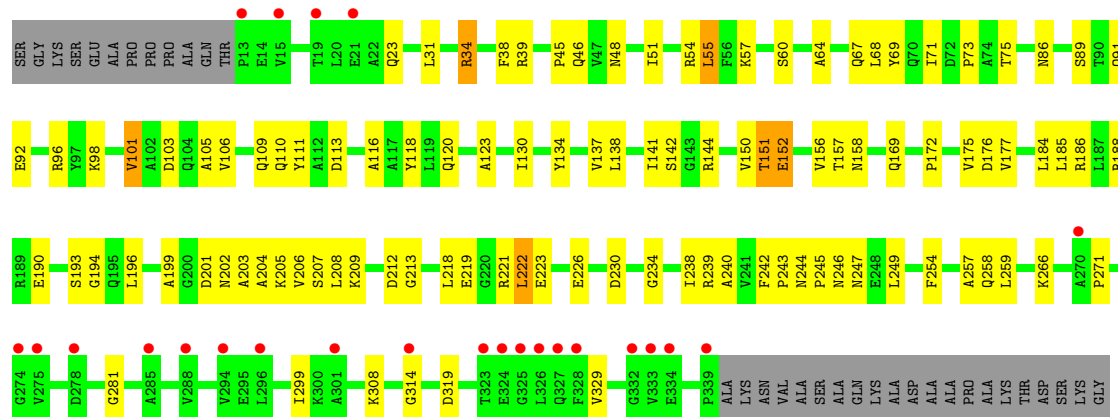
• Molecule 1: MULTIDRUG RESISTANCE PROTEIN MEXA

Chain G: 



• Molecule 1: MULTIDRUG RESISTANCE PROTEIN MEXA

Chain L:



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	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 , 37.5	EDS
Estimated twinning fraction	0.005 for h,-k,-h-l	Xtriage
L-test for twinning	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	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.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.33	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 Close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

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

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 22.

All (1199) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:96:ARG:NH2	1:B:109:GLN:OE1	1.98	0.96
1:L:226:GLU:OE2	1:M:144:ARG:HD3	1.69	0.93
1: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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
1:F:91:GLN:HA	1:F:118:TYR:CD1	2.55	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	230/360 (64%)	191 (83%)	33 (14%)	6 (3%)	8	47
1	B	325/360 (90%)	284 (87%)	32 (10%)	9 (3%)	8	44
1	C	325/360 (90%)	279 (86%)	40 (12%)	6 (2%)	13	60
1	D	228/360 (63%)	195 (86%)	31 (14%)	2 (1%)	25	76
1	E	325/360 (90%)	280 (86%)	38 (12%)	7 (2%)	10	53
1	F	325/360 (90%)	277 (85%)	43 (13%)	5 (2%)	15	64
1	G	325/360 (90%)	277 (85%)	41 (13%)	7 (2%)	10	53
1	H	325/360 (90%)	288 (89%)	32 (10%)	5 (2%)	15	64
1	I	325/360 (90%)	281 (86%)	38 (12%)	6 (2%)	13	60
1	J	325/360 (90%)	277 (85%)	43 (13%)	5 (2%)	15	64
1	K	325/360 (90%)	285 (88%)	34 (10%)	6 (2%)	13	60
1	L	325/360 (90%)	279 (86%)	41 (13%)	5 (2%)	15	64

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	M	325/360 (90%)	285 (88%)	32 (10%)	8 (2%)	9	49
All	All	4033/4680 (86%)	3478 (86%)	478 (12%)	77 (2%)	12	59

All (77) Ramachandran outliers are listed below:

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

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Mol	Chain	Res	Type
1	I	265	GLN
1	J	193	SER
1	J	194	GLY
1	L	193	SER
1	L	194	GLY
1	M	201	ASP
1	B	197	GLU
1	B	264	LYS
1	C	193	SER
1	G	193	SER
1	J	181	SER
1	K	181	SER
1	L	319	ASP
1	M	181	SER
1	B	104	GLN
1	F	193	SER
1	G	319	ASP
1	I	55	LEU
1	M	193	SER
1	A	217	PRO
1	A	232	GLY
1	E	159	GLY
1	B	281	GLY
1	B	325	GLY
1	C	281	GLY
1	E	281	GLY
1	E	325	GLY
1	F	281	GLY
1	G	281	GLY
1	H	281	GLY
1	H	325	GLY
1	I	281	GLY
1	J	281	GLY
1	K	281	GLY
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%)	40	81
1	B	193/287 (67%)	182 (94%)	11 (6%)	29	74
1	C	190/287 (66%)	177 (93%)	13 (7%)	22	65
1	D	185/287 (64%)	175 (95%)	10 (5%)	31	75
1	E	194/287 (68%)	177 (91%)	17 (9%)	14	50
1	F	240/287 (84%)	231 (96%)	9 (4%)	44	84
1	G	190/287 (66%)	183 (96%)	7 (4%)	45	85
1	H	194/287 (68%)	181 (93%)	13 (7%)	23	66
1	I	190/287 (66%)	180 (95%)	10 (5%)	32	75
1	J	189/287 (66%)	175 (93%)	14 (7%)	20	62
1	K	194/287 (68%)	183 (94%)	11 (6%)	29	74
1	L	190/287 (66%)	179 (94%)	11 (6%)	28	73
1	M	196/287 (68%)	181 (92%)	15 (8%)	18	59
All	All	2531/3731 (68%)	2382 (94%)	149 (6%)	28	72

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

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Mol	Chain	Res	Type
1	B	152	GLU
1	B	155	LEU
1	B	201	ASP
1	B	226	GLU
1	B	260	GLN
1	C	34	ARG
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

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Mol	Chain	Res	Type
1	E	247	ASN
1	E	259	LEU
1	E	260	GLN
1	F	55	LEU
1	F	75	THR
1	F	101	VAL
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

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Mol	Chain	Res	Type
1	J	55	LEU
1	J	75	THR
1	J	101	VAL
1	J	152	GLU
1	J	177	VAL
1	J	181	SER
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

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Mol	Chain	Res	Type
1	M	151	THR
1	M	152	GLU
1	M	193	SER
1	M	196	LEU
1	M	198	ARG
1	M	222	LEU
1	M	226	GLU
1	M	239	ARG
1	M	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

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Mol	Chain	Res	Type
1	E	168	GLN
1	E	169	GLN
1	E	195	GLN
1	F	84	GLN
1	F	86	ASN
1	F	93	GLN
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

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Mol	Chain	Res	Type
1	K	195	GLN
1	K	256	HIS
1	L	46	GLN
1	L	86	ASN
1	L	93	GLN
1	L	162	ASN
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 ⓘ

There are no RNA chains in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

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	0.45	0	6,6,6	0.18	0
2	SO4	A	1261	-	4,4,4	0.47	0	6,6,6	0.08	0
2	SO4	B	1340	-	4,4,4	0.43	0	6,6,6	0.19	0
2	SO4	B	1341	-	4,4,4	0.45	0	6,6,6	0.20	0
2	SO4	C	1340	-	4,4,4	0.37	0	6,6,6	0.10	0
2	SO4	E	1340	-	4,4,4	0.55	0	6,6,6	0.16	0
2	SO4	E	1341	-	4,4,4	0.32	0	6,6,6	0.09	0
2	SO4	F	1340	-	4,4,4	0.42	0	6,6,6	0.20	0
2	SO4	F	1341	-	4,4,4	0.41	0	6,6,6	0.09	0
2	SO4	G	1340	-	4,4,4	0.42	0	6,6,6	0.08	0
2	SO4	H	1340	-	4,4,4	0.46	0	6,6,6	0.09	0
2	SO4	I	1340	-	4,4,4	0.51	0	6,6,6	0.09	0
2	SO4	J	1340	-	4,4,4	0.42	0	6,6,6	0.07	0
2	SO4	K	1340	-	4,4,4	0.53	0	6,6,6	0.16	0
2	SO4	L	1340	-	4,4,4	0.50	0	6,6,6	0.13	0
2	SO4	M	1340	-	4,4,4	0.45	0	6,6,6	0.12	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.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

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%)	0.09	0 100 100	34, 77, 127, 155	0
1	B	327/360 (90%)	0.08	5 (1%) 70 21	22, 71, 145, 153	0
1	C	327/360 (90%)	-0.00	1 (0%) 91 58	20, 73, 141, 158	0
1	D	230/360 (63%)	-0.04	0 100 100	16, 59, 87, 110	0
1	E	327/360 (90%)	0.17	9 (2%) 50 11	9, 53, 148, 157	0
1	F	327/360 (90%)	0.05	2 (0%) 86 41	28, 66, 131, 148	0
1	G	327/360 (90%)	0.24	10 (3%) 47 10	34, 82, 147, 163	0
1	H	327/360 (90%)	0.42	27 (8%) 11 3	13, 56, 154, 165	0
1	I	327/360 (90%)	0.22	7 (2%) 60 15	9, 52, 147, 163	0
1	J	327/360 (90%)	0.26	12 (3%) 39 8	5, 37, 150, 165	0
1	K	327/360 (90%)	0.44	37 (11%) 6 2	6, 50, 157, 170	0
1	L	327/360 (90%)	0.30	24 (7%) 15 3	8, 56, 154, 173	0
1	M	327/360 (90%)	0.59	57 (17%) 2 1	18, 83, 158, 172	0
All	All	4059/4680 (86%)	0.23	191 (4%) 30 6	5, 65, 151, 173	0

All (191) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	M	339	PRO	6.5
1	K	317	ALA	5.0
1	H	295	GLU	4.9
1	M	14	GLU	4.7
1	M	331	PRO	4.6
1	K	296	LEU	4.6
1	K	15	VAL	4.4
1	L	327	GLN	4.2
1	M	315	LEU	4.2

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Mol	Chain	Res	Type	RSRZ
1	K	338	VAL	4.1
1	M	317	ALA	4.1
1	I	274	GLY	4.0
1	J	339	PRO	3.9
1	M	270	ALA	3.9
1	K	324	GLU	3.8
1	K	290	ALA	3.8
1	M	288	VAL	3.8
1	H	296	LEU	3.7
1	H	264	LYS	3.6
1	L	325	GLY	3.5
1	K	16	GLY	3.5
1	L	314	GLY	3.5
1	L	334	GLU	3.4
1	M	271	PRO	3.4
1	M	301	ALA	3.3
1	H	263	VAL	3.3
1	E	296	LEU	3.3
1	L	332	GLY	3.3
1	E	332	GLY	3.3
1	M	13	PRO	3.3
1	M	313	GLU	3.2
1	M	320	LYS	3.2
1	K	325	GLY	3.1
1	J	270	ALA	3.1
1	L	274	GLY	3.1
1	L	324	GLU	3.1
1	M	330	GLN	3.1
1	M	338	VAL	3.1
1	M	332	GLY	3.1
1	M	15	VAL	3.0
1	B	296	LEU	3.0
1	I	339	PRO	3.0
1	K	295	GLU	3.0
1	K	17	ILE	3.0
1	K	267	ALA	3.0
1	J	295	GLU	3.0
1	E	14	GLU	2.9
1	K	337	THR	2.9
1	H	280	LYS	2.9
1	M	337	THR	2.9
1	L	328	PHE	2.8

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Mol	Chain	Res	Type	RSRZ
1	K	316	ASN	2.8
1	L	339	PRO	2.8
1	G	324	GLU	2.8
1	G	15	VAL	2.8
1	M	291	GLN	2.8
1	K	282	GLN	2.8
1	K	339	PRO	2.8
1	L	333	VAL	2.8
1	M	287	VAL	2.8
1	M	25	VAL	2.7
1	K	281	GLY	2.7
1	H	291	GLN	2.7
1	L	15	VAL	2.7
1	F	296	LEU	2.7
1	H	290	ALA	2.7
1	H	13	PRO	2.7
1	G	283	ALA	2.7
1	L	19	THR	2.6
1	H	330	GLN	2.6
1	M	285	ALA	2.6
1	K	328	PHE	2.6
1	J	21	GLU	2.6
1	E	295	GLU	2.6
1	M	296	LEU	2.6
1	L	21	GLU	2.6
1	J	287	VAL	2.6
1	M	21	GLU	2.6
1	M	325	GLY	2.6
1	M	321	ILE	2.6
1	M	268	ILE	2.6
1	M	16	GLY	2.6
1	C	15	VAL	2.6
1	M	316	ASN	2.5
1	L	13	PRO	2.5
1	M	289	ASN	2.5
1	L	301	ALA	2.5
1	M	272	GLN	2.5
1	H	297	ARG	2.5
1	H	331	PRO	2.5
1	K	298	VAL	2.5
1	I	332	GLY	2.5
1	G	337	THR	2.5

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Mol	Chain	Res	Type	RSRZ
1	M	302	ASP	2.5
1	H	265	GLN	2.5
1	B	294	VAL	2.5
1	L	326	LEU	2.5
1	J	324	GLU	2.4
1	M	277	ARG	2.4
1	E	337	THR	2.4
1	H	15	VAL	2.4
1	M	297	ARG	2.4
1	B	332	GLY	2.4
1	L	288	VAL	2.4
1	M	307	ASP	2.4
1	H	327	GLN	2.4
1	J	289	ASN	2.4
1	M	318	GLY	2.4
1	K	277	ARG	2.4
1	G	270	ALA	2.3
1	H	332	GLY	2.3
1	K	13	PRO	2.3
1	M	329	VAL	2.3
1	M	275	VAL	2.3
1	L	296	LEU	2.3
1	H	314	GLY	2.3
1	B	270	ALA	2.3
1	K	270	ALA	2.3
1	M	290	ALA	2.3
1	M	306	GLY	2.3
1	E	288	VAL	2.3
1	L	285	ALA	2.3
1	L	323	THR	2.3
1	M	333	VAL	2.3
1	K	300	LYS	2.3
1	G	317	ALA	2.3
1	L	278	ASP	2.3
1	E	265	GLN	2.3
1	M	295	GLU	2.3
1	G	284	THR	2.2
1	K	293	LYS	2.2
1	M	298	VAL	2.2
1	M	282	GLN	2.2
1	I	337	THR	2.2
1	H	20	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
1	K	271	PRO	2.2
1	L	275	VAL	2.2
1	G	22	ALA	2.2
1	K	285	ALA	2.2
1	H	334	GLU	2.2
1	M	319	ASP	2.2
1	K	276	THR	2.2
1	M	276	THR	2.2
1	H	279	LEU	2.2
1	K	334	GLU	2.2
1	J	332	GLY	2.2
1	J	326	LEU	2.2
1	K	329	VAL	2.2
1	K	336	LYS	2.2
1	H	288	VAL	2.2
1	H	337	THR	2.2
1	K	14	GLU	2.1
1	K	278	ASP	2.1
1	B	333	VAL	2.1
1	K	283	ALA	2.1
1	J	288	VAL	2.1
1	K	19	THR	2.1
1	M	323	THR	2.1
1	M	274	GLY	2.1
1	M	314	GLY	2.1
1	L	294	VAL	2.1
1	J	22	ALA	2.1
1	E	291	GLN	2.1
1	M	309	TRP	2.1
1	M	273	GLN	2.1
1	M	283	ALA	2.1
1	M	20	LEU	2.1
1	K	297	ARG	2.1
1	H	287	VAL	2.1
1	H	323	THR	2.1
1	I	283	ALA	2.1
1	L	270	ALA	2.1
1	F	22	ALA	2.1
1	K	330	GLN	2.1
1	M	299	ILE	2.1
1	M	328	PHE	2.1
1	H	14	GLU	2.1

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Mol	Chain	Res	Type	RSRZ
1	J	325	GLY	2.1
1	K	294	VAL	2.1
1	I	330	GLN	2.1
1	G	285	ALA	2.1
1	G	338	VAL	2.0
1	I	271	PRO	2.0
1	H	270	ALA	2.0
1	H	294	VAL	2.0
1	E	283	ALA	2.0
1	H	285	ALA	2.0
1	M	292	ASN	2.0
1	K	331	PRO	2.0
1	M	327	GLN	2.0
1	M	294	VAL	2.0

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

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	RSR	LLDF	B-factors(Å ²)	Q<0.9
2	SO4	E	1340	5/5	0.21	-0.33	50,60,69,87	0
2	SO4	M	1340	5/5	0.20	-0.50	65,69,92,99	0
2	SO4	B	1340	5/5	0.19	-0.87	65,78,84,95	0
2	SO4	A	1260	5/5	0.13	-1.22	70,77,101,103	0
2	SO4	F	1340	5/5	0.14	-1.30	62,76,97,97	0
2	SO4	B	1341	5/5	0.17	-1.45	70,75,95,101	0
2	SO4	A	1261	5/5	0.17	-1.61	62,66,94,95	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
2	SO4	C	1340	5/5	0.12	-2.24	71,71,77,85	0
2	SO4	L	1340	5/5	0.17	-2.70	42,44,72,73	0
2	SO4	J	1340	5/5	0.15	-3.10	44,50,70,76	0
2	SO4	G	1340	5/5	0.08	-3.17	87,89,108,112	0
2	SO4	K	1340	5/5	0.17	-3.37	34,34,58,60	0
2	SO4	F	1341	5/5	0.12	-3.37	67,75,92,100	0
2	SO4	H	1340	5/5	0.15	-3.40	54,57,74,79	0
2	SO4	E	1341	5/5	0.13	-3.76	43,52,59,68	0
2	SO4	I	1340	5/5	0.13	-4.06	55,56,72,87	0

6.5 Other polymers ⓘ

There are no such residues in this entry.