



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 03:00 AM GMT

PDB ID : 2JKR
Title : AP2 CLATHRIN ADAPTOR CORE with Dileucine peptide
RM(phosphoS)QIKRLLSE
Authors : Owen, D.J.; Mccoy, A.J.; Kelly, B.T.; Evans, P.R.
Deposited on : 2008-08-29
Resolution : 2.98 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

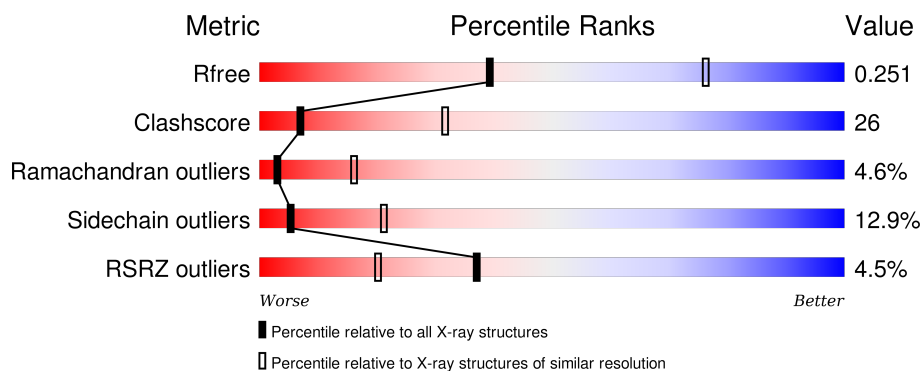
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.98 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	1992 (3.00-2.96)
Clashscore	102246	2349 (3.00-2.96)
Ramachandran outliers	100387	2274 (3.00-2.96)
Sidechain outliers	100360	2277 (3.00-2.96)
RSRZ outliers	91569	2007 (3.00-2.96)

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	623	<div> <div>5%</div> <div>51% 40% 8%</div> </div>
1	L	623	<div> <div>4%</div> <div>53% 38% 8%</div> </div>
2	B	591	<div> <div>5%</div> <div>39% 45% 12%</div> </div>
2	E	591	<div> <div>5%</div> <div>40% 45% 11%</div> </div>
3	I	142	<div> <div></div> <div>55% 40% 5%</div> </div>

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Mol	Chain	Length	Quality of chain
3	S	142	
4	M	435	
4	U	435	
5	P	11	
5	Q	11	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
6	SO4	A	1624	-	-	X	-
6	SO4	A	1625	-	-	X	-
6	SO4	A	1629	-	-	-	X
6	SO4	A	1630	-	-	-	X
6	SO4	E	1587	-	-	X	-
6	SO4	L	1627	-	-	-	X
6	SO4	U	1437	-	-	-	X

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 28120 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 AP-2 COMPLEX SUBUNIT ALPHA-2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	621	Total	C	N	O	S	0	0	0
			4885	3109	842	913	21			
1	L	621	Total	C	N	O	S	0	0	0
			4885	3109	842	913	21			

- Molecule 2 is a protein called AP-2 COMPLEX SUBUNIT BETA-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	571	Total	C	N	O	S	0	0	0
			4527	2883	752	867	25			
2	E	571	Total	C	N	O	S	0	0	0
			4527	2883	752	867	25			

- Molecule 3 is a protein called AP-2 COMPLEX SUBUNIT SIGMA-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	I	142	Total	C	N	O	S	0	0	0
			1200	778	200	215	7			
3	S	142	Total	C	N	O	S	0	0	0
			1200	778	200	215	7			

- Molecule 4 is a protein called AP-2 COMPLEX SUBUNIT MU-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	M	409	Total	C	N	O	S	0	0	0
			3288	2111	573	585	19			
4	U	409	Total	C	N	O	S	0	0	0
			3288	2111	573	585	19			

- Molecule 5 is a protein called CD4 PEPTIDE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	P	9	Total	C	N	O	S	0	0	0
			73	46	14	12	1			
5	Q	9	Total	C	N	O	S	0	0	0
			73	46	14	12	1			

- Molecule 6 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	O	S	0	0
			5	4	1		
6	A	1	Total	O	S	0	0
			5	4	1		
6	A	1	Total	O	S	0	0
			5	4	1		
6	A	1	Total	O	S	0	0
			5	4	1		
6	A	1	Total	O	S	0	0
			5	4	1		
6	A	1	Total	O	S	0	0
			5	4	1		
6	B	1	Total	O	S	0	0
			5	4	1		
6	B	1	Total	O	S	0	0
			5	4	1		
6	B	1	Total	O	S	0	0
			5	4	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	B	1	Total	O	S	0	0
			5	4	1		
6	E	1	Total	O	S	0	0
			5	4	1		
6	E	1	Total	O	S	0	0
			5	4	1		
6	E	1	Total	O	S	0	0
			5	4	1		
6	E	1	Total	O	S	0	0
			5	4	1		
6	E	1	Total	O	S	0	0
			5	4	1		
6	L	1	Total	O	S	0	0
			5	4	1		
6	L	1	Total	O	S	0	0
			5	4	1		
6	L	1	Total	O	S	0	0
			5	4	1		
6	L	1	Total	O	S	0	0
			5	4	1		
6	L	1	Total	O	S	0	0
			5	4	1		
6	L	1	Total	O	S	0	0
			5	4	1		
6	L	1	Total	O	S	0	0
			5	4	1		
6	M	1	Total	O	S	0	0
			5	4	1		
6	M	1	Total	O	S	0	0
			5	4	1		
6	M	1	Total	O	S	0	0
			5	4	1		
6	U	1	Total	O	S	0	0
			5	4	1		
6	U	1	Total	O	S	0	0
			5	4	1		
6	U	1	Total	O	S	0	0
			5	4	1		
6	U	1	Total	O	S	0	0
			5	4	1		

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	3	Total 3	O 3	0	0
7	B	3	Total 3	O 3	0	0
7	E	3	Total 3	O 3	0	0
7	I	2	Total 2	O 2	0	0
7	L	3	Total 3	O 3	0	0
7	M	3	Total 3	O 3	0	0
7	S	1	Total 1	O 1	0	0
7	U	1	Total 1	O 1	0	0

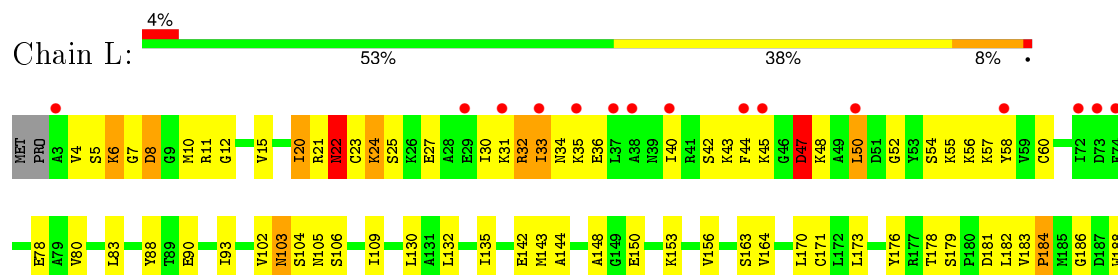
3 Residue-property plots

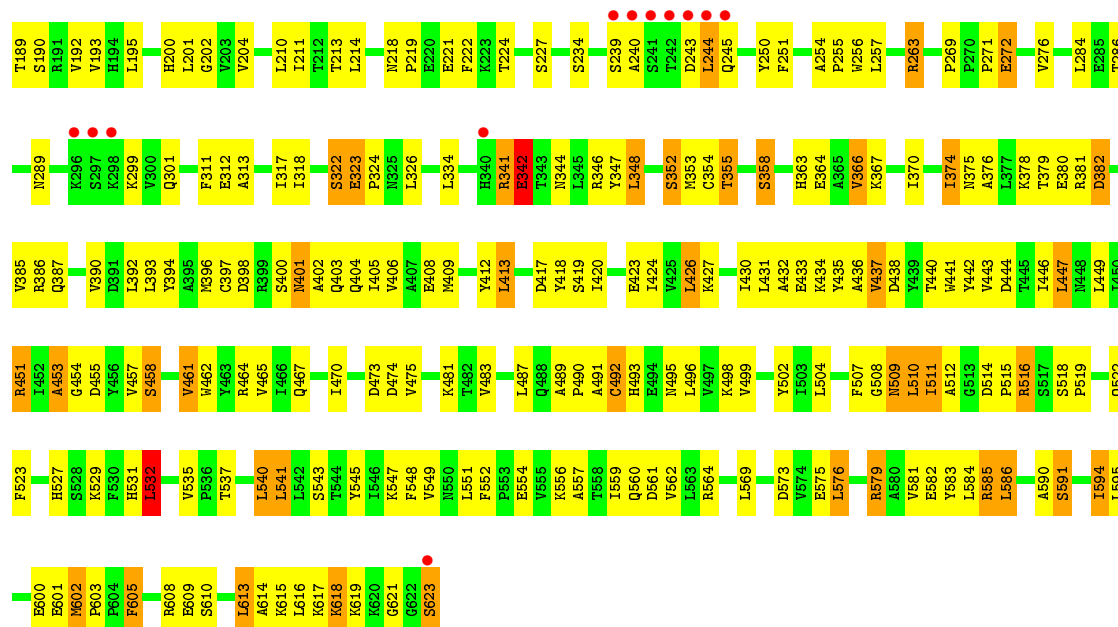
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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: AP-2 COMPLEX SUBUNIT ALPHA-2

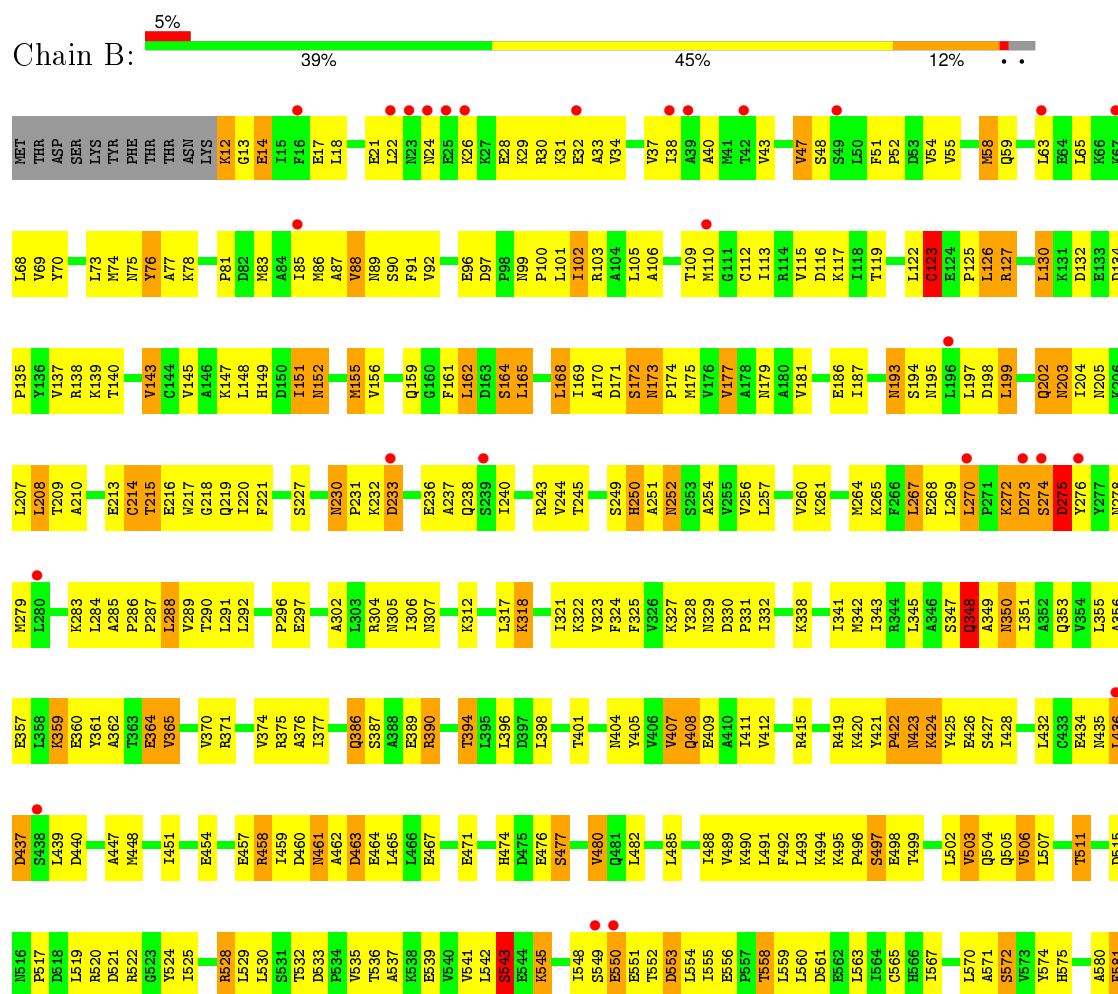


• Molecule 1: AP-2 COMPLEX SUBUNIT ALPHA-2



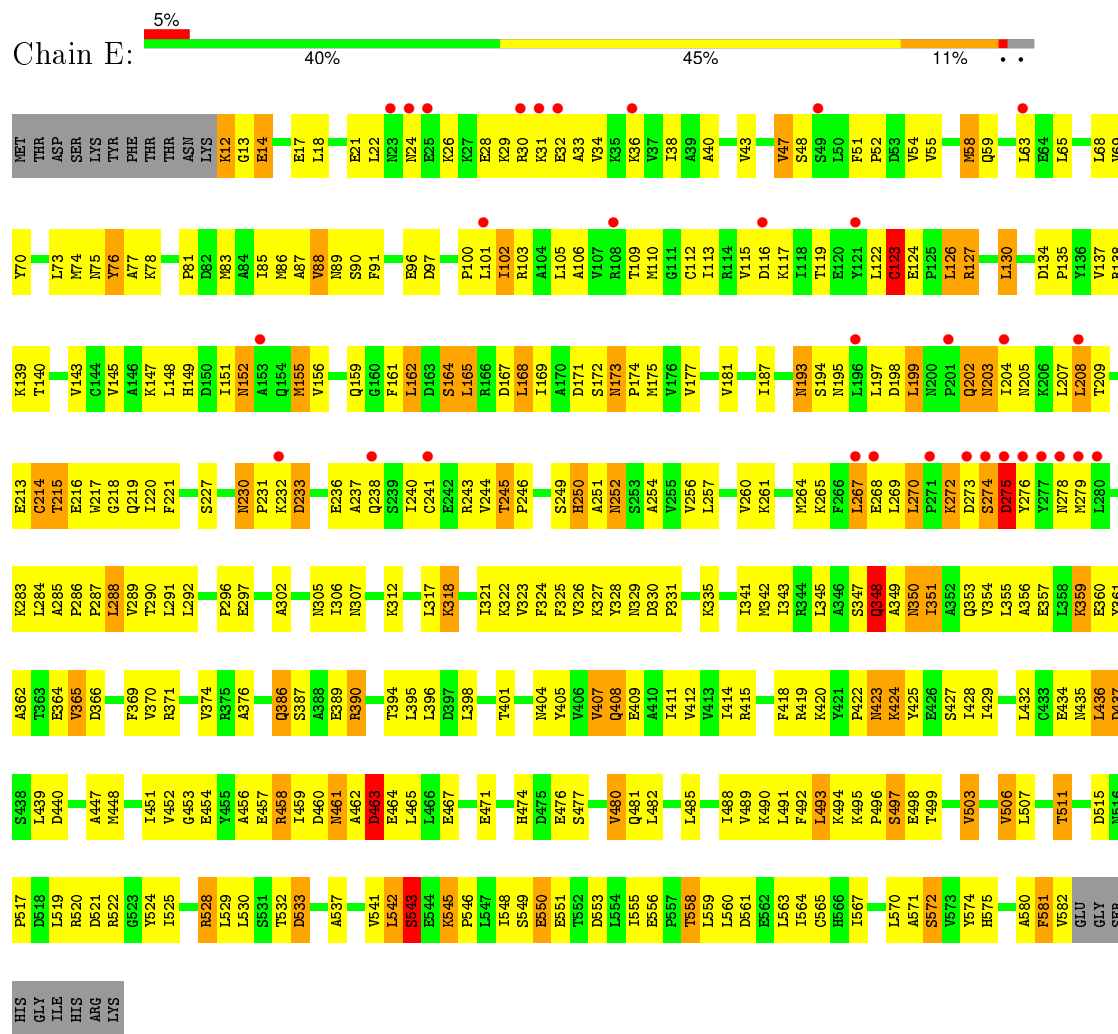


• Molecule 2: AP-2 COMPLEX SUBUNIT BETA-1



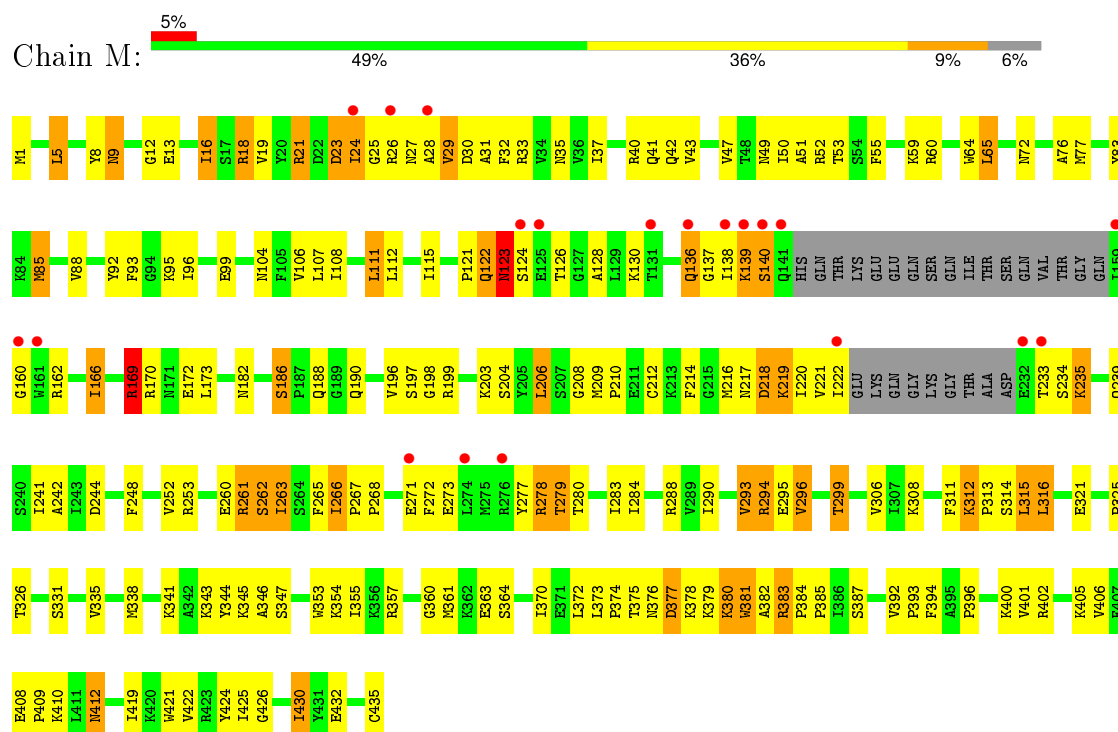
V582	GLU
	GLY
	SER
	HIS
	GLY
	ILE
	HIS
	ARG
	LYS

• Molecule 2: AP-2 COMPLEX SUBUNIT BETA-1

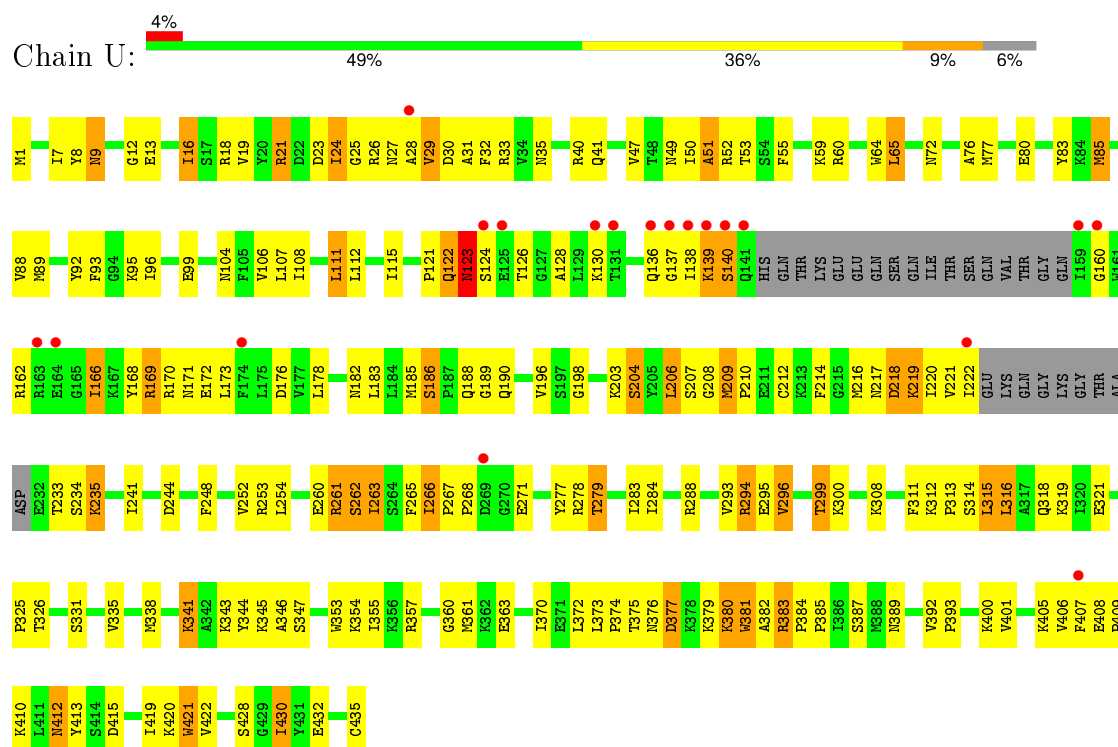




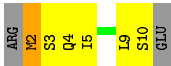
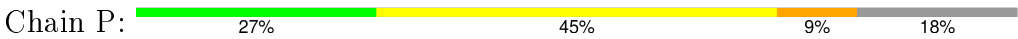
• Molecule 4: AP-2 COMPLEX SUBUNIT MU-1



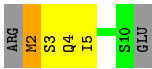
• Molecule 4: AP-2 COMPLEX SUBUNIT MU-1



• Molecule 5: CD4 PEPTIDE



● Molecule 5: CD4 PEPTIDE



4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α , β , γ	169.90 Å 169.90 Å 321.70 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.95 – 2.98 50.96 – 2.98	Depositor EDS
% Data completeness (in resolution range)	99.9 (50.95-2.98) 99.9 (50.96-2.98)	Depositor EDS
R_{merge}	0.20	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.76 (at 2.96 Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.199 , 0.260 0.188 , 0.251	Depositor DCC
R_{free} test set	4813 reflections (4.99%)	DCC
Wilson B-factor (Å ²)	60.2	Xtriage
Anisotropy	0.043	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 75.1	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Outliers	0 of 96579 reflections	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	28120	wwPDB-VP
Average B, all atoms (Å ²)	81.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.76% 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

5.1 Standard geometry

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

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	0.50	0/4970	0.69	1/6734 (0.0%)
1	L	0.49	0/4970	0.69	2/6734 (0.0%)
2	B	0.46	0/4597	0.66	0/6236
2	E	0.46	0/4597	0.67	0/6236
3	I	0.52	0/1224	0.66	0/1650
3	S	0.50	0/1224	0.67	0/1650
4	M	0.54	0/3353	0.72	0/4513
4	U	0.55	0/3353	0.72	0/4513
5	P	0.40	0/65	0.61	0/82
5	Q	0.41	0/65	0.68	0/82
All	All	0.50	0/28418	0.69	3/38430 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	586	LEU	CA-CB-CG	5.97	129.03	115.30
1	L	586	LEU	CA-CB-CG	5.79	128.62	115.30
1	L	540	LEU	CA-CB-CG	5.08	126.97	115.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4885	0	4999	251	0
1	L	4885	0	4999	245	0
2	B	4527	0	4646	310	0
2	E	4527	0	4646	306	0
3	I	1200	0	1195	58	0
3	S	1200	0	1195	69	0
4	M	3288	0	3382	180	0
4	U	3288	0	3382	176	0
5	P	73	0	83	8	0
5	Q	73	0	83	5	0
6	A	35	0	0	7	0
6	B	20	0	0	2	0
6	E	25	0	0	2	0
6	L	40	0	0	1	0
6	M	15	0	0	1	0
6	U	20	0	0	0	0
7	A	3	0	0	0	0
7	B	3	0	0	0	0
7	E	3	0	0	0	0
7	I	2	0	0	0	0
7	L	3	0	0	1	0
7	M	3	0	0	0	0
7	S	1	0	0	0	0
7	U	1	0	0	0	0
All	All	28120	0	28610	1501	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 26.

All (1501) 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)
2:B:434:GLU:HG3	2:B:435:ASN:HD22	1.19	1.08
2:E:434:GLU:HG3	2:E:435:ASN:HD22	1.17	1.08
1:L:579:ARG:HG2	1:L:579:ARG:HH11	1.16	1.07
1:L:516:ARG:HH11	1:L:516:ARG:HG3	1.14	1.05
1:A:516:ARG:HG3	1:A:516:ARG:HH11	1.15	1.04
3:S:86:ASN:HB2	3:S:128:GLN:HE21	1.25	1.00
1:A:579:ARG:HG2	1:A:579:ARG:HH11	1.23	0.99
2:E:55:VAL:O	2:E:58:MET:HB2	1.65	0.97
2:B:55:VAL:O	2:B:58:MET:HB2	1.65	0.97
3:I:86:ASN:HB2	3:I:128:GLN:HE21	1.30	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:M:21:ARG:HH11	4:M:21:ARG:HB2	1.34	0.93
4:M:115:ILE:HD13	4:M:124:SER:HB2	1.51	0.92
4:U:21:ARG:HH11	4:U:21:ARG:HB2	1.32	0.92
4:U:166:ILE:H	4:U:166:ILE:HD13	1.35	0.90
4:U:115:ILE:HD13	4:U:124:SER:HB2	1.53	0.90
2:E:127:ARG:HH11	2:E:127:ARG:HG2	1.35	0.89
4:M:88:VAL:HG11	4:M:111:LEU:HD11	1.53	0.89
2:E:174:PRO:HB3	2:E:214:CYS:HA	1.53	0.88
2:B:127:ARG:HG2	2:B:127:ARG:HH11	1.37	0.88
1:A:380:GLU:O	1:A:386:ARG:HD2	1.74	0.87
1:L:20:ILE:HD11	1:L:33:ILE:CD1	2.04	0.87
1:A:20:ILE:HD11	1:A:33:ILE:HD11	1.57	0.87
1:A:20:ILE:HD11	1:A:33:ILE:CD1	2.04	0.87
2:B:390:ARG:HB3	2:B:390:ARG:HH11	1.39	0.87
1:L:508:GLY:H	1:L:510:LEU:HD12	1.36	0.87
4:U:1:MET:HE1	4:U:121:PRO:HD2	1.57	0.86
1:L:20:ILE:HD11	1:L:33:ILE:HD11	1.56	0.86
2:E:390:ARG:HH11	2:E:390:ARG:HB3	1.38	0.86
4:M:166:ILE:HD13	4:M:166:ILE:H	1.40	0.86
1:A:200:HIS:CD2	1:A:202:GLY:H	1.92	0.86
1:L:437:VAL:HG21	7:L:2002:HOH:O	1.74	0.86
1:L:380:GLU:O	1:L:386:ARG:HD2	1.75	0.85
4:M:26:ARG:HH22	4:M:33:ARG:HH21	1.23	0.85
2:E:434:GLU:HG3	2:E:435:ASN:ND2	1.91	0.85
1:L:200:HIS:CD2	1:L:202:GLY:H	1.95	0.85
4:U:26:ARG:HH22	4:U:33:ARG:HH21	1.24	0.85
1:A:381:ARG:O	1:A:382:ASP:HB3	1.76	0.84
1:L:458:SER:O	1:L:461:VAL:HG23	1.77	0.84
4:U:186:SER:HB3	4:U:190:GLN:HB2	1.59	0.84
4:U:374:PRO:O	4:U:375:THR:HG22	1.77	0.84
4:U:88:VAL:HG11	4:U:111:LEU:HD11	1.59	0.84
2:B:174:PRO:HB3	2:B:214:CYS:HA	1.58	0.84
2:B:286:PRO:O	2:B:290:THR:HG23	1.77	0.84
1:L:358:SER:HB3	4:U:295:GLU:HB3	1.59	0.84
1:A:614:ALA:HA	1:A:623:SER:HB3	1.60	0.83
1:A:318:ILE:HD13	1:A:355:THR:HG22	1.61	0.83
1:A:457:VAL:HG13	1:A:495:ASN:HD22	1.44	0.83
1:A:200:HIS:HD2	1:A:202:GLY:H	1.27	0.82
3:S:19:TRP:CZ2	3:S:28:LYS:HG3	2.14	0.82
1:A:458:SER:O	1:A:461:VAL:HG23	1.80	0.81
1:A:12:GLY:HA3	1:A:57:LYS:HE3	1.62	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:434:GLU:HG3	2:B:435:ASN:ND2	1.94	0.81
1:L:508:GLY:H	1:L:510:LEU:CD1	1.92	0.81
3:S:19:TRP:CE2	3:S:28:LYS:HG3	2.15	0.81
2:E:156:VAL:HG12	2:E:162:LEU:HD23	1.62	0.81
1:A:609:GLU:OE1	1:L:610:SER:HB2	1.80	0.81
4:U:59:LYS:HE3	4:U:64:TRP:CZ2	2.16	0.81
4:M:21:ARG:HB2	4:M:21:ARG:NH1	1.95	0.81
1:L:12:GLY:HA3	1:L:57:LYS:HE3	1.60	0.81
4:U:21:ARG:HB2	4:U:21:ARG:NH1	1.94	0.81
2:B:78:LYS:HE3	2:B:112:CYS:SG	2.21	0.81
4:U:182:ASN:ND2	4:U:430:ILE:H	1.79	0.80
4:M:186:SER:HB3	4:M:190:GLN:HB2	1.64	0.80
4:U:261:ARG:O	4:U:263:ILE:N	2.13	0.80
3:S:86:ASN:HB2	3:S:128:GLN:NE2	1.97	0.80
4:M:182:ASN:ND2	4:M:430:ILE:H	1.79	0.80
1:A:358:SER:HB3	4:M:295:GLU:HB3	1.63	0.80
1:L:457:VAL:HG13	1:L:495:ASN:HD22	1.46	0.80
4:M:261:ARG:O	4:M:263:ILE:N	2.15	0.79
4:M:1:MET:HE1	4:M:121:PRO:HD2	1.65	0.79
1:L:381:ARG:O	1:L:382:ASP:HB3	1.79	0.79
1:L:614:ALA:HA	1:L:623:SER:HB3	1.63	0.79
2:E:78:LYS:HE3	2:E:112:CYS:SG	2.23	0.79
4:M:59:LYS:HE3	4:M:64:TRP:CZ2	2.18	0.79
2:E:63:LEU:HD21	2:E:101:LEU:HD12	1.64	0.79
2:B:581:PHE:HA	4:M:52:ARG:HG2	1.65	0.79
1:A:317:ILE:HD13	1:A:326:LEU:HB3	1.63	0.79
2:B:63:LEU:HD21	2:B:101:LEU:HD12	1.64	0.79
1:A:7:GLY:O	1:A:8:ASP:HB2	1.81	0.79
1:A:40:ILE:HG23	1:A:58:TYR:HB3	1.65	0.79
4:U:1:MET:CE	4:U:121:PRO:HD2	2.13	0.78
4:M:374:PRO:O	4:M:375:THR:HG22	1.82	0.78
1:L:370:ILE:HG12	1:L:396:MET:HE3	1.65	0.78
1:L:200:HIS:HD2	1:L:202:GLY:H	1.32	0.78
4:M:385:PRO:HB2	4:M:432:GLU:HB3	1.66	0.78
1:L:317:ILE:HD13	1:L:326:LEU:HB3	1.65	0.78
2:E:285:ALA:HB3	2:E:286:PRO:HD3	1.66	0.78
4:U:385:PRO:HB2	4:U:432:GLU:HB3	1.66	0.78
2:E:318:LYS:O	2:E:318:LYS:HE3	1.83	0.78
2:B:156:VAL:HG12	2:B:162:LEU:HD23	1.66	0.77
3:I:19:TRP:CZ2	3:I:28:LYS:HG3	2.18	0.77
1:L:318:ILE:HD13	1:L:355:THR:HG22	1.66	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:U:222:ILE:HD12	4:U:222:ILE:H	1.47	0.77
3:I:19:TRP:CE2	3:I:28:LYS:HG3	2.19	0.77
1:A:381:ARG:HD2	3:S:45:LYS:HD2	1.64	0.77
2:E:286:PRO:O	2:E:290:THR:HG23	1.84	0.77
1:A:516:ARG:NH1	1:A:516:ARG:HG3	1.94	0.76
4:M:222:ILE:H	4:M:222:ILE:HD12	1.48	0.76
1:A:508:GLY:H	1:A:510:LEU:HD12	1.48	0.76
2:B:312:LYS:HE2	2:B:561:ASP:OD1	1.85	0.76
3:S:92:ASN:HD22	3:S:98:VAL:H	1.33	0.76
3:S:49:PHE:CE2	3:S:77:ASN:HB3	2.19	0.76
4:M:293:VAL:HG22	4:M:294:ARG:H	1.51	0.76
1:A:200:HIS:HD2	1:A:202:GLY:N	1.84	0.76
4:M:1:MET:CE	4:M:121:PRO:HD2	2.16	0.75
1:A:508:GLY:H	1:A:510:LEU:CD1	1.99	0.75
2:E:218:GLY:HA2	2:E:221:PHE:CD1	2.22	0.75
3:I:102:ASP:O	3:I:106:ASN:HB2	1.86	0.75
1:L:516:ARG:NH1	1:L:516:ARG:HG3	1.94	0.75
1:L:40:ILE:HG23	1:L:58:TYR:HB3	1.69	0.75
1:L:7:GLY:O	1:L:8:ASP:HB2	1.86	0.75
1:A:602:MET:HE1	2:B:521:ASP:HA	1.67	0.75
2:E:482:LEU:HD21	1:L:579:ARG:HH21	1.50	0.74
2:B:218:GLY:HA2	2:B:221:PHE:CD1	2.22	0.74
4:U:293:VAL:HG22	4:U:294:ARG:H	1.51	0.74
1:A:603:PRO:O	2:B:520:ARG:NH2	2.20	0.74
2:E:296:PRO:HB3	2:E:331:PRO:HG3	1.69	0.74
2:B:296:PRO:HB3	2:B:331:PRO:HG3	1.67	0.74
1:L:200:HIS:HD2	1:L:202:GLY:N	1.85	0.74
4:M:331:SER:HB3	4:M:373:LEU:HG	1.70	0.74
3:I:86:ASN:HB2	3:I:128:GLN:NE2	2.01	0.74
2:B:119:THR:HG21	2:B:152:ASN:HD22	1.52	0.74
4:M:40:ARG:HB2	6:M:1437:SO4:O4	1.88	0.74
3:I:49:PHE:CE2	3:I:77:ASN:HB3	2.22	0.73
2:E:264:MET:HA	2:E:267:LEU:HD23	1.69	0.73
1:A:619:LYS:HD3	2:E:471:GLU:OE1	1.89	0.73
2:E:28:GLU:O	2:E:32:GLU:HG2	1.89	0.73
1:A:512:ALA:HB1	1:A:519:PRO:HD3	1.69	0.73
1:A:610:SER:HB2	1:L:609:GLU:OE1	1.89	0.73
3:S:92:ASN:HD21	3:S:97:ASN:HA	1.54	0.73
2:B:264:MET:HA	2:B:267:LEU:HD23	1.69	0.73
2:B:40:ALA:HA	2:B:43:VAL:HG22	1.69	0.73
2:E:74:MET:SD	2:E:109:THR:HG22	2.29	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:549:VAL:HG13	1:A:556:LYS:HG3	1.71	0.72
2:B:285:ALA:HB3	2:B:286:PRO:HD3	1.72	0.72
1:A:318:ILE:HG21	1:A:355:THR:CG2	2.20	0.72
2:E:215:THR:O	2:E:219:GLN:HG3	1.90	0.72
2:B:28:GLU:O	2:B:32:GLU:HG2	1.89	0.72
2:E:103:ARG:HH11	2:E:137:VAL:HG21	1.55	0.72
2:E:312:LYS:HE2	2:E:561:ASP:OD1	1.89	0.72
2:B:215:THR:O	2:B:219:GLN:HG3	1.89	0.72
1:A:218:ASN:N	1:A:219:PRO:HD3	2.04	0.72
2:E:119:THR:HG21	2:E:152:ASN:HD22	1.52	0.72
1:L:618:LYS:O	1:L:619:LYS:HG2	1.89	0.72
2:E:40:ALA:HA	2:E:43:VAL:HG22	1.71	0.72
2:B:408:GLN:NE2	2:B:439:LEU:HA	2.05	0.72
4:U:343:LYS:HE2	4:U:345:LYS:CE	2.20	0.72
3:I:116:LEU:HD21	3:I:114:VAL:HG21	1.71	0.72
2:E:581:PHE:HA	4:U:52:ARG:HG2	1.71	0.72
2:B:249:SER:O	2:B:251:ALA:N	2.18	0.72
1:L:591:SER:HB2	1:L:594:ILE:H	1.53	0.72
2:E:570:LEU:HB2	4:U:72:ASN:HD22	1.55	0.71
2:E:249:SER:O	2:E:251:ALA:N	2.19	0.71
3:I:8:GLN:HE22	3:I:36:HIS:HB2	1.53	0.71
1:A:498:LYS:HE3	1:A:537:THR:OG1	1.90	0.71
2:E:31:LYS:HA	2:E:65:LEU:HD13	1.70	0.71
4:U:169:ARG:HB3	4:U:169:ARG:HH11	1.54	0.71
4:U:331:SER:HB3	4:U:373:LEU:HG	1.71	0.71
2:B:292:LEU:HD12	2:B:323:VAL:HG12	1.73	0.71
2:E:423:ASN:O	2:E:425:TYR:N	2.24	0.71
4:U:379:LYS:C	4:U:381:TRP:H	1.94	0.71
1:A:272:GLU:CD	1:A:272:GLU:H	1.93	0.71
1:A:591:SER:HB2	1:A:594:ILE:H	1.56	0.71
2:B:423:ASN:O	2:B:425:TYR:N	2.24	0.70
3:I:138:LEU:O	3:I:139:GLN:HB3	1.89	0.70
1:L:192:VAL:O	1:L:195:LEU:HB2	1.90	0.70
1:L:318:ILE:HG21	1:L:355:THR:HG22	1.72	0.70
2:E:115:VAL:HG12	2:E:117:LYS:H	1.55	0.70
2:B:31:LYS:HA	2:B:65:LEU:HD13	1.72	0.70
1:A:263:ARG:NH2	3:S:75:ASP:HA	2.05	0.70
4:M:169:ARG:HH11	4:M:169:ARG:HB3	1.55	0.70
2:B:325:PHE:HA	2:B:342:MET:HE1	1.73	0.70
1:L:579:ARG:CG	1:L:579:ARG:HH11	1.99	0.70
4:M:293:VAL:HG13	4:M:294:ARG:N	2.05	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:318:ILE:HG21	1:L:355:THR:CG2	2.21	0.70
2:B:115:VAL:HG12	2:B:117:LYS:H	1.55	0.70
1:A:11:ARG:HB3	6:A:1625:SO4:O2	1.90	0.70
2:B:492:PHE:CD1	2:B:503:VAL:HG21	2.27	0.70
4:U:31:ALA:O	4:U:35:ASN:HB2	1.92	0.69
1:L:239:SER:HB2	1:L:243:ASP:OD2	1.92	0.69
1:A:370:ILE:HG12	1:A:396:MET:HE1	1.72	0.69
1:L:218:ASN:N	1:L:219:PRO:HD3	2.06	0.69
2:B:85:ILE:O	2:B:88:VAL:HG22	1.92	0.69
1:L:250:TYR:CD2	1:L:301:GLN:HB2	2.28	0.69
2:E:193:ASN:HD22	2:E:194:SER:H	1.39	0.69
2:E:193:ASN:HD22	2:E:194:SER:N	1.91	0.69
2:E:127:ARG:HH11	2:E:127:ARG:CG	2.05	0.69
2:E:464:GLU:HA	2:E:467:GLU:HB3	1.75	0.69
2:B:398:LEU:O	2:B:401:THR:HG23	1.92	0.69
1:L:272:GLU:H	1:L:272:GLU:CD	1.93	0.69
2:E:521:ASP:HA	1:L:602:MET:HE1	1.74	0.69
5:Q:2:MET:SD	5:Q:2:MET:N	2.65	0.69
3:S:138:LEU:O	3:S:139:GLN:HB3	1.91	0.69
3:S:16:LEU:HD21	3:S:114:VAL:HG21	1.74	0.69
2:B:217:TRP:HE1	4:M:123:ASN:HA	1.58	0.68
3:S:102:ASP:O	3:S:106:ASN:HB2	1.91	0.68
2:B:97:ASP:OD2	2:B:102:ILE:HD11	1.93	0.68
4:M:379:LYS:C	4:M:381:TRP:H	1.95	0.68
3:S:8:GLN:HE22	3:S:36:HIS:HB2	1.56	0.68
3:I:92:ASN:HD22	3:I:98:VAL:H	1.39	0.68
4:M:343:LYS:HE2	4:M:345:LYS:CE	2.24	0.68
1:L:189:THR:HG21	1:L:221:GLU:HG3	1.73	0.68
1:A:413:LEU:HD21	1:A:453:ALA:HB2	1.76	0.68
1:A:509:ASN:HB3	1:A:551:LEU:HD23	1.76	0.68
1:L:549:VAL:HG13	1:L:556:LYS:HG3	1.76	0.68
1:A:192:VAL:O	1:A:195:LEU:HB2	1.92	0.67
4:M:241:ILE:HD13	3:S:23:PHE:CE2	2.28	0.67
2:E:103:ARG:NH1	2:E:137:VAL:HG21	2.08	0.67
2:E:520:ARG:HD3	1:L:605:PHE:CZ	2.28	0.67
2:E:495:LYS:O	2:E:499:THR:HG22	1.94	0.67
4:U:203:LYS:HG3	4:U:271:GLU:HB2	1.74	0.67
1:L:512:ALA:HB1	1:L:519:PRO:HD3	1.75	0.67
1:A:189:THR:HG21	1:A:221:GLU:HG3	1.75	0.67
2:B:127:ARG:CG	2:B:127:ARG:HH11	2.07	0.67
2:E:357:GLU:HG3	2:E:361:TYR:CZ	2.29	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:328:TYR:CE1	2:B:329:ASN:HB3	2.30	0.67
2:E:97:ASP:OD2	2:E:102:ILE:HD11	1.95	0.67
4:U:26:ARG:HH22	4:U:33:ARG:NH2	1.92	0.67
2:B:464:GLU:HA	2:B:467:GLU:HB3	1.76	0.67
2:E:327:LYS:HE2	2:E:330:ASP:OD2	1.95	0.67
1:L:413:LEU:HD21	1:L:453:ALA:HB2	1.77	0.67
2:B:495:LYS:O	2:B:499:THR:HG22	1.94	0.67
2:B:208:LEU:HD13	2:B:243:ARG:HE	1.60	0.66
4:M:88:VAL:CG1	4:M:111:LEU:HD11	2.25	0.66
1:L:617:LYS:HE3	1:L:623:SER:HB2	1.76	0.66
2:B:408:GLN:HE22	2:B:440:ASP:H	1.44	0.66
2:B:193:ASN:HD22	2:B:194:SER:N	1.93	0.66
1:A:510:LEU:H	1:A:510:LEU:HD12	1.60	0.66
2:E:83:MET:O	2:E:86:MET:HE2	1.95	0.66
2:B:193:ASN:HD22	2:B:194:SER:H	1.41	0.66
2:E:322:LYS:HE2	2:E:353:GLN:NE2	2.11	0.66
2:B:571:ALA:H	4:M:72:ASN:HD21	1.42	0.66
1:A:318:ILE:HG21	1:A:355:THR:HG22	1.77	0.66
2:B:268:GLU:O	2:B:269:LEU:HG	1.96	0.66
2:E:208:LEU:HD13	2:E:243:ARG:HE	1.61	0.66
4:M:26:ARG:HH22	4:M:33:ARG:NH2	1.92	0.66
3:I:75:ASP:HA	1:L:263:ARG:NH2	2.10	0.66
2:E:174:PRO:HB3	2:E:214:CYS:CA	2.24	0.66
1:A:464:ARG:NH1	1:A:467:GLN:HE21	1.94	0.66
2:E:292:LEU:HD12	2:E:323:VAL:HG12	1.77	0.66
2:E:492:PHE:CD1	2:E:503:VAL:HG21	2.31	0.66
2:B:318:LYS:HE3	2:B:318:LYS:O	1.95	0.66
1:L:103:ASN:O	1:L:109:ILE:HD11	1.96	0.65
4:U:343:LYS:HE2	4:U:345:LYS:HE3	1.76	0.65
4:U:261:ARG:O	4:U:262:SER:C	2.33	0.65
2:B:103:ARG:HH11	2:B:137:VAL:HG21	1.62	0.65
2:B:420:LYS:NZ	2:B:550:GLU:OE2	2.29	0.65
4:M:31:ALA:O	4:M:35:ASN:HB2	1.97	0.65
1:A:250:TYR:CD2	1:A:301:GLN:HB2	2.32	0.65
1:L:561:ASP:HB3	1:L:564:ARG:HE	1.62	0.65
5:P:5:ILE:HD12	3:S:99:CYS:SG	2.37	0.65
2:E:408:GLN:NE2	2:E:439:LEU:HA	2.12	0.65
2:E:232:LYS:O	2:E:233:ASP:HB2	1.96	0.65
1:L:380:GLU:HG3	1:L:385:VAL:HG11	1.79	0.64
1:A:380:GLU:HG3	1:A:385:VAL:HG11	1.79	0.64
1:L:509:ASN:HB3	1:L:551:LEU:HD23	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:582:VAL:O	2:B:582:VAL:HG12	1.95	0.64
1:A:239:SER:HB2	1:A:243:ASP:OD2	1.97	0.64
2:B:324:PHE:CD2	2:B:341:ILE:HG21	2.32	0.64
2:E:520:ARG:NH2	1:L:603:PRO:O	2.29	0.64
3:I:92:ASN:HD21	3:I:97:ASN:HA	1.62	0.64
4:U:9:ASN:C	4:U:9:ASN:HD22	2.01	0.64
2:B:274:SER:O	2:B:276:TYR:N	2.29	0.64
5:P:2:MET:SD	5:P:2:MET:N	2.70	0.64
2:E:559:LEU:HG	2:E:559:LEU:O	1.98	0.64
1:L:590:ALA:HB1	1:L:594:ILE:HG22	1.78	0.64
2:E:328:TYR:CE1	2:E:329:ASN:HB3	2.32	0.64
2:E:85:ILE:O	2:E:88:VAL:HG22	1.98	0.64
1:L:491:ALA:O	1:L:492:CYS:O	2.16	0.64
2:E:343:ILE:HD11	2:E:376:ALA:HB1	1.79	0.63
2:B:74:MET:SD	2:B:109:THR:HG22	2.38	0.63
1:A:381:ARG:O	1:A:382:ASP:CB	2.45	0.63
2:B:471:GLU:OE1	1:L:619:LYS:HD3	1.97	0.63
1:L:437:VAL:HG23	1:L:438:ASP:H	1.64	0.63
1:L:381:ARG:O	1:L:382:ASP:CB	2.47	0.63
3:I:126:THR:HG21	1:L:256:TRP:HB2	1.81	0.63
1:A:437:VAL:HG23	1:A:438:ASP:H	1.62	0.63
2:E:297:GLU:HB2	4:U:83:TYR:OH	1.99	0.63
1:L:516:ARG:CG	1:L:516:ARG:HH11	2.00	0.63
4:U:344:TYR:CE2	4:U:346:ALA:HB2	2.33	0.63
2:B:327:LYS:HE2	2:B:330:ASP:OD2	1.99	0.62
1:L:464:ARG:NH1	1:L:467:GLN:HE21	1.97	0.62
1:A:442:TYR:CE2	1:A:465:VAL:HG12	2.34	0.62
2:B:343:ILE:HD11	2:B:376:ALA:HB1	1.80	0.62
2:E:237:ALA:O	2:E:240:ILE:HG22	2.00	0.62
1:A:491:ALA:O	1:A:492:CYS:O	2.17	0.62
2:E:347:SER:C	2:E:349:ALA:H	2.02	0.62
1:L:250:TYR:HD2	1:L:301:GLN:HB2	1.64	0.62
1:A:561:ASP:HB3	1:A:564:ARG:HE	1.64	0.62
1:A:618:LYS:O	1:A:619:LYS:HG2	2.00	0.62
2:B:347:SER:C	2:B:349:ALA:H	2.03	0.62
1:L:341:ARG:CZ	1:L:341:ARG:O	2.47	0.62
1:A:579:ARG:CG	1:A:579:ARG:HH11	2.05	0.62
2:E:268:GLU:O	2:E:269:LEU:HG	1.99	0.62
2:B:570:LEU:HB2	4:M:72:ASN:HD22	1.63	0.62
2:E:305:ASN:ND2	2:E:567:ILE:O	2.33	0.62
4:U:216:MET:H	4:U:261:ARG:CB	2.12	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:344:ASN:HD21	3:S:48:ASN:ND2	1.96	0.62
2:E:524:TYR:O	2:E:528:ARG:HG3	1.99	0.62
4:U:312:LYS:HG3	4:U:313:PRO:CD	2.30	0.62
2:E:507:LEU:O	2:E:511:THR:HB	1.98	0.62
2:B:476:GLU:HB3	2:B:480:VAL:HG22	1.80	0.62
4:M:9:ASN:C	4:M:9:ASN:HD22	2.04	0.62
1:L:442:TYR:CE2	1:L:465:VAL:HG12	2.35	0.62
1:L:470:ILE:HD11	1:L:502:TYR:HE2	1.64	0.62
2:B:145:VAL:HG11	2:B:165:LEU:HD22	1.81	0.62
1:L:617:LYS:O	1:L:619:LYS:N	2.31	0.61
2:B:232:LYS:O	2:B:233:ASP:HB2	1.99	0.61
2:B:292:LEU:HD12	2:B:323:VAL:CG1	2.30	0.61
2:E:408:GLN:HE22	2:E:440:ASP:H	1.49	0.61
2:B:26:LYS:HD2	2:B:29:LYS:HD2	1.83	0.61
2:B:174:PRO:HB3	2:B:214:CYS:CA	2.29	0.61
1:A:605:PHE:CZ	2:B:520:ARG:HD3	2.35	0.61
1:A:574:VAL:HG12	2:B:419:ARG:CZ	2.29	0.61
2:E:420:LYS:NZ	2:E:550:GLU:OE2	2.33	0.61
1:A:342:GLU:O	1:A:346:ARG:HD3	2.01	0.61
2:E:273:ASP:O	2:E:274:SER:O	2.17	0.61
4:M:162:ARG:NH2	4:M:166:ILE:HG13	2.16	0.61
1:A:284:LEU:HD23	1:A:313:ALA:HB1	1.81	0.61
1:A:470:ILE:HD11	1:A:502:TYR:HE2	1.65	0.61
2:E:362:ALA:HA	2:E:370:VAL:HG13	1.82	0.61
3:S:19:TRP:CE2	3:S:28:LYS:CG	2.82	0.61
2:B:103:ARG:NH1	2:B:137:VAL:HG21	2.14	0.61
2:B:83:MET:O	2:B:86:MET:HE2	2.01	0.61
2:E:217:TRP:HE1	4:U:123:ASN:HA	1.66	0.61
1:A:617:LYS:O	1:A:619:LYS:N	2.33	0.61
2:B:325:PHE:HA	2:B:342:MET:CE	2.30	0.61
4:M:343:LYS:HE2	4:M:345:LYS:HE3	1.82	0.61
2:B:70:TYR:HD2	2:B:109:THR:HG21	1.66	0.61
4:M:203:LYS:HG3	4:M:271:GLU:HB2	1.80	0.61
1:L:481:LYS:HG3	1:L:511:ILE:HD11	1.82	0.61
2:B:85:ILE:HG12	2:B:113:ILE:HG21	1.83	0.61
2:E:325:PHE:HA	2:E:342:MET:CE	2.31	0.61
2:E:398:LEU:O	2:E:401:THR:HG23	2.00	0.61
1:L:379:THR:OG1	1:L:380:GLU:N	2.34	0.60
4:U:353:TRP:CZ2	4:U:355:ILE:HD11	2.35	0.60
1:A:103:ASN:O	1:A:109:ILE:HD11	2.01	0.60
2:E:348:GLN:CB	2:E:386:GLN:HE22	2.14	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:270:LEU:C	2:E:270:LEU:HD23	2.22	0.60
2:E:274:SER:O	2:E:276:TYR:N	2.33	0.60
1:A:467:GLN:HG3	1:A:605:PHE:CG	2.35	0.60
4:U:50:ILE:O	4:U:51:ALA:HB3	2.00	0.60
4:U:1:MET:HE3	4:U:77:MET:SD	2.41	0.60
3:I:45:LYS:HD2	1:L:381:ARG:HD2	1.83	0.60
1:A:531:HIS:O	1:A:532:LEU:HB3	2.01	0.60
4:M:32:PHE:HB2	4:M:55:PHE:CE2	2.36	0.60
2:E:51:PHE:O	2:E:55:VAL:HG23	2.01	0.60
1:L:510:LEU:H	1:L:510:LEU:HD12	1.67	0.60
2:E:491:LEU:HD11	2:E:495:LYS:HD2	1.83	0.60
2:E:325:PHE:HA	2:E:342:MET:HE1	1.84	0.60
4:U:162:ARG:NH2	4:U:166:ILE:HG13	2.17	0.60
2:B:237:ALA:O	2:B:240:ILE:HG22	2.01	0.60
1:L:156:VAL:HG11	1:L:188:TRP:HB2	1.83	0.60
1:A:334:LEU:HB3	1:A:353:MET:HE2	1.83	0.60
2:B:51:PHE:O	2:B:55:VAL:HG23	2.02	0.60
1:A:50:LEU:H	1:A:50:LEU:HD12	1.67	0.60
2:B:231:PRO:HB3	2:B:236:GLU:HB3	1.84	0.60
4:U:32:PHE:HB2	4:U:55:PHE:CE2	2.37	0.59
2:B:507:LEU:O	2:B:511:THR:HB	2.02	0.59
2:E:371:ARG:HG2	2:E:409:GLU:HG3	1.84	0.59
1:A:579:ARG:HH21	2:B:482:LEU:HD21	1.66	0.59
2:E:582:VAL:O	2:E:582:VAL:HG12	2.02	0.59
1:L:189:THR:HG21	1:L:221:GLU:CG	2.32	0.59
1:L:556:LYS:O	1:L:560:GLN:HB2	2.03	0.59
1:A:516:ARG:CG	1:A:516:ARG:HH11	2.01	0.59
2:E:85:ILE:HG12	2:E:113:ILE:HG21	1.84	0.59
2:B:348:GLN:CB	2:B:386:GLN:HE22	2.15	0.59
2:B:51:PHE:HB3	2:B:52:PRO:HD3	1.85	0.59
1:A:379:THR:OG1	1:A:380:GLU:N	2.36	0.59
3:I:19:TRP:CE2	3:I:28:LYS:CG	2.85	0.59
4:U:32:PHE:HB2	4:U:55:PHE:CD2	2.38	0.59
2:B:307:ASN:HD22	2:B:575:HIS:CE1	2.21	0.59
2:E:51:PHE:HB3	2:E:52:PRO:HD3	1.85	0.59
2:E:26:LYS:HD2	2:E:29:LYS:HD2	1.85	0.59
2:B:305:ASN:ND2	2:B:567:ILE:O	2.35	0.59
4:M:24:ILE:HG22	4:M:25:GLY:N	2.17	0.59
1:A:440:THR:O	1:A:444:ASP:HB2	2.03	0.59
2:B:371:ARG:HG2	2:B:409:GLU:HG3	1.85	0.59
1:A:189:THR:HG21	1:A:221:GLU:CG	2.32	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:M:261:ARG:O	4:M:262:SER:C	2.41	0.59
2:E:78:LYS:NZ	6:E:1587:SO4:O4	2.23	0.59
2:B:496:PRO:O	2:B:497:SER:CB	2.51	0.59
2:E:307:ASN:HD22	2:E:575:HIS:CE1	2.21	0.59
1:A:341:ARG:CZ	1:A:341:ARG:O	2.50	0.59
2:B:273:ASP:O	2:B:274:SER:O	2.21	0.59
1:L:31:LYS:O	1:L:35:LYS:HG3	2.03	0.59
2:B:529:LEU:HD21	2:B:537:ALA:HA	1.84	0.59
1:A:556:LYS:O	1:A:560:GLN:HB2	2.03	0.58
1:A:487:LEU:HD23	1:A:496:LEU:HD23	1.83	0.58
4:M:261:ARG:O	4:M:263:ILE:HD13	2.03	0.58
1:A:590:ALA:HB1	1:A:594:ILE:HG22	1.84	0.58
2:E:476:GLU:HB3	2:E:480:VAL:HG22	1.86	0.58
4:M:308:LYS:HG3	4:M:363:GLU:HG2	1.85	0.58
2:E:482:LEU:HD12	2:E:519:LEU:HD13	1.86	0.58
4:M:216:MET:H	4:M:261:ARG:CB	2.17	0.58
2:E:496:PRO:O	2:E:497:SER:CB	2.51	0.58
2:E:292:LEU:HD12	2:E:323:VAL:CG1	2.34	0.58
4:M:312:LYS:HG3	4:M:313:PRO:CD	2.33	0.58
2:E:571:ALA:H	4:U:72:ASN:HD21	1.50	0.58
1:L:182:LEU:O	1:L:184:PRO:HD3	2.04	0.58
1:L:579:ARG:NH1	1:L:579:ARG:HG2	1.97	0.58
2:B:284:LEU:O	2:B:288:LEU:HD22	2.03	0.58
2:B:581:PHE:HA	4:M:52:ARG:CG	2.33	0.58
1:A:603:PRO:HG2	2:B:524:TYR:CZ	2.38	0.58
1:A:256:TRP:HB2	3:S:126:THR:HG21	1.86	0.58
2:B:491:LEU:HD11	2:B:495:LYS:HD2	1.84	0.58
1:A:481:LYS:HG3	1:A:511:ILE:HD11	1.85	0.58
1:L:508:GLY:N	1:L:510:LEU:HD12	2.13	0.58
2:E:307:ASN:HD22	2:E:575:HIS:HE1	1.52	0.58
2:B:304:ARG:NH2	6:B:1583:SO4:O1	2.37	0.58
1:A:527:HIS:HE1	6:A:1624:SO4:O2	1.86	0.58
2:E:435:ASN:C	2:E:437:ASP:H	2.07	0.58
4:U:385:PRO:CB	4:U:432:GLU:HB3	2.34	0.58
2:E:87:ALA:HB3	2:E:91:PHE:CE2	2.39	0.58
2:E:231:PRO:HB3	2:E:236:GLU:HB3	1.85	0.58
2:E:493:LEU:HD13	2:E:541:VAL:HG21	1.85	0.58
2:B:390:ARG:O	2:B:394:THR:HG23	2.04	0.58
1:L:50:LEU:H	1:L:50:LEU:HD12	1.69	0.58
4:M:32:PHE:HB2	4:M:55:PHE:CD2	2.39	0.58
2:B:322:LYS:HE2	2:B:353:GLN:NE2	2.19	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:559:LEU:HG	2:B:559:LEU:O	2.02	0.58
2:E:130:LEU:HD23	2:E:168:LEU:HD21	1.85	0.57
4:M:312:LYS:HG3	4:M:313:PRO:HD2	1.86	0.57
2:B:297:GLU:HB2	4:M:83:TYR:OH	2.03	0.57
2:B:362:ALA:HA	2:B:370:VAL:HG13	1.86	0.57
3:S:10:ARG:HE	3:S:64:GLY:HA2	1.69	0.57
2:E:356:ALA:O	2:E:359:LYS:HB3	2.04	0.57
4:M:162:ARG:O	4:M:209:MET:HE1	2.05	0.57
1:L:531:HIS:O	1:L:532:LEU:HB3	2.03	0.57
2:E:265:LYS:HE3	2:E:565:CYS:SG	2.45	0.57
4:M:85:MET:CE	4:M:112:LEU:HD21	2.34	0.57
1:A:430:ILE:HG22	1:A:431:LEU:N	2.17	0.57
3:I:27:GLU:HG2	4:U:241:ILE:HB	1.85	0.57
1:A:31:LYS:O	1:A:35:LYS:HG3	2.05	0.57
2:E:522:ARG:HG2	2:E:522:ARG:HH11	1.68	0.57
4:U:380:LYS:O	4:U:382:ALA:N	2.36	0.57
1:L:498:LYS:HE3	1:L:537:THR:OG1	2.05	0.57
1:A:47:ASP:OD2	1:A:48:LYS:N	2.31	0.57
4:M:408:GLU:O	4:M:412:ASN:HA	2.04	0.57
1:A:618:LYS:HD2	6:A:1627:SO4:O4	2.04	0.57
1:A:218:ASN:N	1:A:219:PRO:CD	2.67	0.57
2:B:328:TYR:CE2	4:M:405:LYS:HD2	2.40	0.57
2:E:436:LEU:CD2	2:E:448:MET:HG2	2.34	0.57
2:E:145:VAL:HG11	2:E:165:LEU:HD22	1.86	0.57
4:U:99:GLU:HA	4:U:99:GLU:OE2	2.04	0.57
2:E:284:LEU:O	2:E:288:LEU:HD22	2.04	0.57
4:M:380:LYS:O	4:M:382:ALA:N	2.35	0.57
1:L:103:ASN:HD22	1:L:103:ASN:C	2.08	0.57
4:U:312:LYS:HG3	4:U:313:PRO:HD2	1.85	0.57
1:A:156:VAL:HG11	1:A:188:TRP:HB2	1.86	0.57
2:B:130:LEU:HD23	2:B:168:LEU:HD21	1.87	0.57
2:B:488:ILE:HG21	2:B:506:VAL:HG21	1.87	0.57
2:E:530:LEU:HD23	2:E:537:ALA:HB1	1.87	0.57
2:B:256:VAL:O	2:B:260:VAL:HG23	2.05	0.57
2:E:17:GLU:O	2:E:21:GLU:HG3	2.05	0.57
1:A:266:GLN:O	4:M:380:LYS:HE3	2.05	0.57
1:L:523:PHE:CE1	1:L:559:ILE:HG12	2.40	0.57
1:A:56:LYS:HG3	1:A:93:ILE:HD12	1.87	0.57
1:L:178:THR:HG22	1:L:179:SER:OG	2.04	0.57
1:L:487:LEU:HD23	1:L:496:LEU:HD23	1.87	0.57
4:M:99:GLU:OE2	4:M:99:GLU:HA	2.05	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:36:LYS:HE2	1:L:24:LYS:HE2	1.86	0.56
2:E:432:LEU:C	2:E:434:GLU:H	2.07	0.56
2:E:135:PRO:HG3	2:E:138:ARG:NH2	2.20	0.56
2:E:307:ASN:ND2	2:E:575:HIS:HE1	2.03	0.56
2:E:218:GLY:HA2	2:E:221:PHE:HD1	1.68	0.56
1:L:36:GLU:O	1:L:40:ILE:HG13	2.04	0.56
2:B:218:GLY:HA2	2:B:221:PHE:HD1	1.68	0.56
4:U:293:VAL:HG13	4:U:294:ARG:N	2.19	0.56
2:E:570:LEU:HB2	4:U:72:ASN:ND2	2.20	0.56
4:U:296:VAL:HG22	4:U:296:VAL:O	2.05	0.56
2:B:265:LYS:HE3	2:B:565:CYS:SG	2.46	0.56
2:B:270:LEU:C	2:B:270:LEU:HD23	2.26	0.56
2:B:489:VAL:O	2:B:493:LEU:HD12	2.05	0.56
1:L:250:TYR:CD2	1:L:301:GLN:CB	2.89	0.56
2:B:348:GLN:HB2	2:B:386:GLN:HE22	1.71	0.56
3:I:10:ARG:HE	3:I:64:GLY:HA2	1.70	0.56
4:U:308:LYS:HG3	4:U:363:GLU:HG2	1.87	0.56
1:A:581:VAL:O	1:A:585:ARG:HB2	2.04	0.56
4:U:85:MET:CE	4:U:112:LEU:HD21	2.34	0.56
1:A:464:ARG:HH11	1:A:467:GLN:HE21	1.52	0.56
4:M:41:GLN:HG3	4:M:284:ILE:HD12	1.88	0.56
2:B:493:LEU:HD13	2:B:541:VAL:HG21	1.87	0.56
2:E:457:GLU:OE1	2:E:494:LYS:HE2	2.06	0.56
2:B:432:LEU:C	2:B:434:GLU:H	2.09	0.56
2:B:524:TYR:O	2:B:528:ARG:HG3	2.05	0.56
2:B:407:VAL:HG12	2:B:408:GLN:N	2.19	0.56
4:U:344:TYR:HE2	4:U:346:ALA:HB2	1.68	0.56
4:M:9:ASN:HD21	4:M:13:GLU:H	1.54	0.56
2:E:256:VAL:O	2:E:260:VAL:HG23	2.06	0.56
2:B:307:ASN:HD22	2:B:575:HIS:HE1	1.50	0.56
4:U:24:ILE:HG22	4:U:25:GLY:N	2.21	0.56
2:B:54:VAL:HG12	2:B:69:VAL:HG13	1.86	0.56
2:E:126:LEU:HD23	2:E:161:PHE:CE2	2.41	0.56
2:B:522:ARG:HH11	2:B:522:ARG:HG2	1.70	0.56
1:L:156:VAL:HG11	1:L:188:TRP:CB	2.36	0.56
2:E:488:ILE:HG21	2:E:506:VAL:HG21	1.88	0.56
2:B:435:ASN:C	2:B:437:ASP:H	2.10	0.56
4:U:92:TYR:HB3	4:U:107:LEU:HD21	1.87	0.56
4:M:241:ILE:HG12	3:S:31:LEU:HD13	1.87	0.56
2:E:581:PHE:HA	4:U:52:ARG:CG	2.35	0.56
4:U:408:GLU:O	4:U:412:ASN:HA	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:M:266:ILE:N	4:M:266:ILE:HD12	2.21	0.56
1:A:200:HIS:CD2	1:A:202:GLY:N	2.64	0.55
2:B:135:PRO:HG3	2:B:138:ARG:NH2	2.21	0.55
4:M:59:LYS:NZ	4:M:218:ASP:OD2	2.32	0.55
1:L:601:GLU:O	1:L:602:MET:O	2.24	0.55
2:B:357:GLU:HG3	2:B:361:TYR:CZ	2.40	0.55
2:E:302:ALA:O	2:E:306:ILE:HG12	2.06	0.55
3:S:127:SER:O	3:S:131:VAL:HG12	2.07	0.55
2:E:177:VAL:HB	2:E:214:CYS:SG	2.46	0.55
1:L:398:ASP:H	1:L:401:ASN:HD21	1.54	0.55
1:A:103:ASN:C	1:A:103:ASN:HD22	2.10	0.55
1:L:342:GLU:O	1:L:346:ARG:HD3	2.06	0.55
1:L:581:VAL:O	1:L:585:ARG:HB2	2.06	0.55
1:L:334:LEU:HB3	1:L:353:MET:HE2	1.87	0.55
1:A:178:THR:HG22	1:A:179:SER:OG	2.06	0.55
4:U:208:GLY:O	4:U:210:PRO:HD3	2.07	0.55
1:L:467:GLN:HG3	1:L:605:PHE:CG	2.41	0.55
2:B:272:LYS:NZ	2:B:278:ASN:HD21	2.05	0.55
4:M:379:LYS:O	4:M:381:TRP:N	2.38	0.55
1:A:442:TYR:CZ	1:A:465:VAL:HG12	2.42	0.55
2:E:273:ASP:CG	2:E:274:SER:H	2.10	0.55
1:L:613:LEU:HG	4:U:335:VAL:HG13	1.88	0.55
4:M:198:GLY:HA3	4:M:277:TYR:CE1	2.42	0.55
1:A:286:THR:O	1:A:289:ASN:HB2	2.07	0.55
2:B:177:VAL:HB	2:B:214:CYS:SG	2.46	0.55
2:E:489:VAL:O	2:E:493:LEU:HD12	2.07	0.55
4:M:344:TYR:CE2	4:M:346:ALA:HB2	2.41	0.55
1:L:374:ILE:HG12	1:L:408:GLU:HG2	1.87	0.55
4:M:162:ARG:NH2	4:M:206:LEU:O	2.38	0.55
1:L:440:THR:O	1:L:444:ASP:HB2	2.07	0.55
2:B:457:GLU:OE1	2:B:494:LYS:HE2	2.07	0.55
1:L:200:HIS:CD2	1:L:202:GLY:N	2.65	0.55
1:A:374:ILE:HG12	1:A:408:GLU:HG2	1.87	0.55
1:A:602:MET:CE	2:B:521:ASP:HA	2.37	0.55
3:S:138:LEU:O	3:S:139:GLN:CB	2.55	0.55
1:A:173:LEU:HD13	1:A:210:LEU:HD12	1.89	0.55
4:U:376:ASN:O	4:U:377:ASP:HB3	2.07	0.55
1:A:579:ARG:NH1	1:A:579:ARG:HG2	2.03	0.54
2:B:302:ALA:O	2:B:306:ILE:HG12	2.07	0.54
1:A:617:LYS:HB2	6:A:1629:SO4:O2	2.07	0.54
2:E:312:LYS:HB2	2:E:560:LEU:HD21	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:397:CYS:SG	1:A:431:LEU:HD13	2.47	0.54
2:E:161:PHE:HA	2:E:164:SER:HB2	1.90	0.54
1:L:455:ASP:HA	1:L:493:HIS:CE1	2.42	0.54
1:L:286:THR:O	1:L:289:ASN:HB2	2.07	0.54
4:M:29:VAL:HG13	4:M:30:ASP:H	1.73	0.54
1:L:464:ARG:HH11	1:L:467:GLN:HE21	1.54	0.54
3:I:92:ASN:ND2	3:I:98:VAL:H	2.05	0.54
2:E:70:TYR:HD2	2:E:109:THR:HG21	1.72	0.54
1:L:370:ILE:HG23	1:L:396:MET:CE	2.37	0.54
2:E:423:ASN:C	2:E:425:TYR:H	2.10	0.54
2:B:307:ASN:ND2	2:B:575:HIS:HE1	2.05	0.54
2:B:436:LEU:CD2	2:B:448:MET:HG2	2.36	0.54
1:A:44:PHE:CD1	1:A:78:GLU:HG2	2.42	0.54
4:U:59:LYS:NZ	4:U:218:ASP:OD2	2.37	0.54
2:B:273:ASP:CG	2:B:274:SER:H	2.11	0.54
2:B:440:ASP:HB3	4:M:316:LEU:HD12	1.89	0.54
2:E:564:ILE:O	2:E:567:ILE:HG13	2.08	0.54
2:E:365:VAL:HG13	4:U:401:VAL:HG12	1.90	0.54
4:M:92:TYR:HB3	4:M:107:LEU:HD21	1.88	0.54
4:U:430:ILE:HG12	4:U:430:ILE:O	2.07	0.54
2:E:127:ARG:NH1	2:E:127:ARG:CG	2.70	0.54
2:B:220:ILE:HD13	4:M:77:MET:HG3	1.90	0.54
1:A:617:LYS:HE3	1:A:623:SER:HB2	1.89	0.54
2:B:81:PRO:HB2	2:B:115:VAL:HG23	1.90	0.54
4:U:88:VAL:CG1	4:U:111:LEU:HD11	2.35	0.54
4:M:385:PRO:CB	4:M:432:GLU:HB3	2.35	0.54
1:A:36:GLU:O	1:A:40:ILE:HG13	2.08	0.54
2:E:81:PRO:HB2	2:E:115:VAL:HG23	1.90	0.54
1:A:243:ASP:O	1:A:244:LEU:C	2.45	0.54
1:A:455:ASP:HA	1:A:493:HIS:CE1	2.43	0.54
2:E:138:ARG:NH1	2:E:171:ASP:OD2	2.39	0.54
2:E:390:ARG:O	2:E:394:THR:HG23	2.08	0.54
1:L:454:GLY:O	1:L:457:VAL:HG12	2.08	0.54
2:E:272:LYS:NZ	2:E:278:ASN:HD21	2.06	0.54
2:B:126:LEU:HD23	2:B:161:PHE:CE2	2.43	0.54
2:E:202:GLN:HG3	2:E:203:ASN:N	2.22	0.54
4:M:208:GLY:O	4:M:210:PRO:HD3	2.08	0.53
2:B:65:LEU:O	2:B:65:LEU:HG	2.07	0.53
2:B:149:HIS:NE2	2:B:187:ILE:HG23	2.23	0.53
4:U:343:LYS:HE2	4:U:345:LYS:HE2	1.90	0.53
2:B:549:SER:O	2:B:550:GLU:O	2.27	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:M:353:TRP:CZ2	4:M:355:ILE:HD11	2.43	0.53
1:A:182:LEU:O	1:A:184:PRO:HD3	2.07	0.53
2:E:522:ARG:HD2	1:L:579:ARG:CZ	2.38	0.53
1:A:454:GLY:O	1:A:457:VAL:HG12	2.09	0.53
4:U:379:LYS:O	4:U:381:TRP:N	2.39	0.53
1:A:601:GLU:O	1:A:602:MET:O	2.27	0.53
4:M:139:LYS:O	4:M:140:SER:HB2	2.07	0.53
2:E:77:ALA:HB1	2:E:113:ILE:HG12	1.91	0.53
1:L:243:ASP:O	1:L:244:LEU:C	2.46	0.53
4:U:266:ILE:N	4:U:266:ILE:HD12	2.23	0.53
1:L:313:ALA:O	1:L:317:ILE:HG13	2.09	0.53
2:E:31:LYS:HA	2:E:65:LEU:CD1	2.38	0.53
4:U:28:ALA:HB1	4:U:55:PHE:CZ	2.44	0.53
2:B:138:ARG:NH1	2:B:171:ASP:OD2	2.42	0.53
2:E:349:ALA:O	2:E:350:ASN:HB3	2.09	0.53
4:M:296:VAL:HG22	4:M:296:VAL:O	2.09	0.53
4:M:40:ARG:HB3	4:M:284:ILE:HD13	1.91	0.53
2:B:423:ASN:C	2:B:425:TYR:H	2.11	0.53
2:E:324:PHE:CD2	2:E:341:ILE:HG21	2.43	0.53
4:U:166:ILE:N	4:U:166:ILE:HD13	2.16	0.53
4:U:182:ASN:HD22	4:U:430:ILE:H	1.52	0.53
2:E:521:ASP:HA	1:L:602:MET:CE	2.39	0.53
4:M:376:ASN:O	4:M:377:ASP:HB3	2.09	0.53
1:A:464:ARG:HH11	1:A:467:GLN:NE2	2.06	0.53
1:L:430:ILE:HG22	1:L:431:LEU:N	2.24	0.53
2:B:202:GLN:HG3	2:B:203:ASN:N	2.24	0.53
2:B:216:GLU:HB3	2:B:250:HIS:CE1	2.44	0.52
2:E:216:GLU:HB3	2:E:250:HIS:CE1	2.43	0.52
1:L:56:LYS:HG3	1:L:93:ILE:HD12	1.91	0.52
2:B:312:LYS:HB2	2:B:560:LEU:HD21	1.90	0.52
2:B:77:ALA:HB1	2:B:113:ILE:HG12	1.91	0.52
4:M:343:LYS:HE2	4:M:345:LYS:HE2	1.91	0.52
2:E:348:GLN:HB2	2:E:386:GLN:HE22	1.74	0.52
4:U:172:GLU:HB3	4:U:419:ILE:HB	1.90	0.52
3:I:107:PHE:CG	3:I:108:TYR:N	2.77	0.52
4:M:419:ILE:HD13	4:M:419:ILE:N	2.23	0.52
2:B:127:ARG:CG	2:B:127:ARG:NH1	2.71	0.52
1:A:398:ASP:H	1:A:401:ASN:HD21	1.58	0.52
2:B:420:LYS:O	2:B:420:LYS:HG3	2.09	0.52
2:E:420:LYS:HG3	2:E:420:LYS:O	2.08	0.52
4:U:16:ILE:HD12	4:U:108:ILE:HG21	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:U:59:LYS:HE3	4:U:64:TRP:CE2	2.44	0.52
2:E:318:LYS:HE3	2:E:318:LYS:C	2.28	0.52
2:B:268:GLU:C	2:B:269:LEU:HG	2.30	0.52
1:A:413:LEU:HD21	1:A:453:ALA:CB	2.40	0.52
2:E:149:HIS:NE2	2:E:187:ILE:HG23	2.25	0.52
1:A:33:ILE:HG22	1:A:34:ASN:N	2.24	0.52
4:M:1:MET:HE3	4:M:77:MET:SD	2.49	0.52
2:E:461:ASN:HB3	2:E:465:LEU:HG	1.89	0.52
4:M:104:ASN:O	4:M:108:ILE:HG13	2.09	0.52
4:U:198:GLY:HA3	4:U:277:TYR:CE1	2.45	0.52
4:U:196:VAL:HG23	4:U:283:ILE:HG12	1.91	0.52
2:E:22:LEU:O	2:E:30:ARG:HG2	2.10	0.52
2:E:515:ASP:O	2:E:517:PRO:HD3	2.09	0.52
2:B:288:LEU:HD23	2:B:289:VAL:N	2.25	0.52
3:S:92:ASN:ND2	3:S:98:VAL:H	2.03	0.52
1:L:442:TYR:CZ	1:L:465:VAL:HG12	2.45	0.52
2:B:17:GLU:O	2:B:21:GLU:HG3	2.10	0.52
4:M:196:VAL:HG23	4:M:283:ILE:HG12	1.92	0.52
4:M:50:ILE:O	4:M:51:ALA:HB3	2.10	0.52
3:S:107:PHE:CG	3:S:108:TYR:N	2.78	0.52
4:M:107:LEU:O	4:M:111:LEU:HB2	2.09	0.52
1:A:313:ALA:O	1:A:317:ILE:HG13	2.10	0.52
2:E:288:LEU:HD22	2:E:288:LEU:H	1.74	0.52
2:E:530:LEU:HD23	2:E:537:ALA:CB	2.39	0.52
4:M:85:MET:HE1	4:M:112:LEU:HD21	1.90	0.52
2:E:251:ALA:O	2:E:252:ASN:C	2.48	0.52
2:E:545:LYS:HG3	1:L:581:VAL:HG21	1.92	0.52
2:B:436:LEU:HD12	2:B:465:LEU:HD22	1.92	0.52
3:I:48:ASN:ND2	1:L:344:ASN:HD21	2.08	0.52
1:A:267:CYS:O	4:M:378:LYS:NZ	2.37	0.52
1:A:447:LEU:O	1:A:451:ARG:HB2	2.09	0.52
4:U:21:ARG:HH11	4:U:21:ARG:CB	2.15	0.52
4:M:166:ILE:HD11	4:M:208:GLY:O	2.10	0.52
1:A:509:ASN:HA	1:A:552:PHE:HZ	1.74	0.52
2:E:322:LYS:HE2	2:E:353:GLN:HE22	1.74	0.52
4:M:172:GLU:HB3	4:M:419:ILE:HB	1.91	0.52
3:I:55:PHE:HB3	3:I:71:VAL:O	2.10	0.52
2:E:268:GLU:C	2:E:269:LEU:HG	2.29	0.51
2:E:407:VAL:HG12	2:E:408:GLN:N	2.25	0.51
2:B:530:LEU:HD23	2:B:537:ALA:CB	2.41	0.51
1:L:387:GLN:OE1	4:U:188:GLN:HG2	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:18:LEU:HD13	2:B:37:VAL:HG22	1.92	0.51
2:B:505:GLN:NE2	1:L:619:LYS:O	2.37	0.51
1:L:464:ARG:HH11	1:L:467:GLN:NE2	2.07	0.51
2:B:451:ILE:O	2:B:454:GLU:O	2.28	0.51
1:A:509:ASN:HA	1:A:552:PHE:CZ	2.46	0.51
1:L:446:ILE:HG21	1:L:465:VAL:HG11	1.93	0.51
4:U:139:LYS:O	4:U:140:SER:HB2	2.10	0.51
2:B:390:ARG:CB	2:B:390:ARG:HH11	2.19	0.51
4:U:123:ASN:O	4:U:123:ASN:ND2	2.43	0.51
1:A:527:HIS:CE1	6:A:1624:SO4:O2	2.63	0.51
4:M:234:SER:O	4:M:235:LYS:C	2.47	0.51
2:B:78:LYS:NZ	4:M:18:ARG:NH1	2.57	0.51
2:E:496:PRO:O	2:E:497:SER:OG	2.22	0.51
1:A:250:TYR:CD2	1:A:301:GLN:CB	2.94	0.51
1:L:470:ILE:HD11	1:L:502:TYR:CE2	2.44	0.51
1:A:470:ILE:HD11	1:A:502:TYR:CE2	2.45	0.51
4:M:424:TYR:O	4:M:425:ILE:HD13	2.09	0.51
2:E:54:VAL:HG12	2:E:69:VAL:HG13	1.91	0.51
3:I:127:SER:O	3:I:131:VAL:HG12	2.11	0.51
3:I:86:ASN:CB	3:I:128:GLN:HE21	2.15	0.51
2:E:173:ASN:HD21	2:E:175:MET:HB3	1.76	0.51
1:L:434:LYS:HE2	1:L:435:TYR:CZ	2.46	0.51
2:B:208:LEU:HD13	2:B:243:ARG:NE	2.25	0.51
2:E:436:LEU:HD21	2:E:448:MET:SD	2.50	0.51
3:S:86:ASN:CB	3:S:128:GLN:HE21	2.11	0.51
2:E:288:LEU:HA	2:E:291:LEU:HB2	1.92	0.51
2:B:267:LEU:C	2:B:269:LEU:H	2.14	0.51
1:L:218:ASN:N	1:L:219:PRO:CD	2.72	0.51
2:E:522:ARG:NH2	1:L:582:GLU:OE1	2.41	0.51
2:E:390:ARG:HH11	2:E:390:ARG:CB	2.18	0.51
2:B:580:ALA:C	2:B:581:PHE:HD2	2.13	0.51
2:B:251:ALA:O	2:B:252:ASN:C	2.48	0.51
1:A:250:TYR:HD2	1:A:301:GLN:HB2	1.73	0.51
4:U:234:SER:O	4:U:235:LYS:C	2.49	0.51
4:U:29:VAL:HG13	4:U:30:ASP:H	1.76	0.51
4:M:220:ILE:HG22	4:M:221:VAL:N	2.25	0.51
1:L:393:LEU:HD22	1:L:405:ILE:HG12	1.92	0.51
4:M:26:ARG:HG3	4:M:26:ARG:O	2.11	0.50
2:B:78:LYS:HZ3	4:M:18:ARG:NH1	2.09	0.50
2:B:31:LYS:HA	2:B:65:LEU:CD1	2.39	0.50
3:S:16:LEU:HD12	3:S:17:ALA:N	2.26	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:305:ASN:HD21	2:E:572:SER:HB3	1.75	0.50
1:L:44:PHE:CD1	1:L:78:GLU:HG2	2.46	0.50
1:A:549:VAL:CG1	1:A:556:LYS:HG3	2.38	0.50
3:I:138:LEU:O	3:I:139:GLN:CB	2.54	0.50
2:E:85:ILE:HD11	2:E:115:VAL:HB	1.93	0.50
3:I:72:ASP:HB2	3:I:75:ASP:OD2	2.12	0.50
4:M:28:ALA:HB1	4:M:55:PHE:CZ	2.46	0.50
4:U:9:ASN:HD21	4:U:13:GLU:H	1.60	0.50
1:L:23:CYS:C	1:L:25:SER:H	2.14	0.50
3:I:34:GLU:O	3:I:38:VAL:HG23	2.11	0.50
4:M:123:ASN:ND2	4:M:123:ASN:O	2.44	0.50
2:B:274:SER:O	2:B:275:ASP:C	2.49	0.50
1:L:447:LEU:O	1:L:451:ARG:HB2	2.12	0.50
2:B:47:VAL:HG12	2:B:48:SER:N	2.27	0.50
4:U:65:LEU:N	4:U:65:LEU:HD23	2.26	0.50
1:L:33:ILE:HG22	1:L:34:ASN:N	2.26	0.50
2:B:408:GLN:HE22	2:B:439:LEU:HA	1.75	0.50
1:A:516:ARG:NH1	1:A:516:ARG:CG	2.68	0.50
1:L:367:LYS:O	1:L:370:ILE:HG13	2.12	0.50
2:B:85:ILE:HD11	2:B:115:VAL:HB	1.93	0.50
4:M:16:ILE:HD12	4:M:108:ILE:HG21	1.93	0.50
2:E:198:ASP:OD2	2:E:199:LEU:N	2.45	0.50
1:A:434:LYS:HE2	1:A:435:TYR:CZ	2.47	0.50
4:U:41:GLN:HG3	4:U:284:ILE:HD12	1.94	0.50
4:M:430:ILE:O	4:M:430:ILE:HG12	2.10	0.50
4:M:182:ASN:HD22	4:M:430:ILE:H	1.54	0.50
4:M:59:LYS:HE3	4:M:64:TRP:CE2	2.46	0.50
2:E:208:LEU:HD13	2:E:243:ARG:NE	2.26	0.50
3:I:23:PHE:CE2	4:U:241:ILE:HD13	2.46	0.50
2:B:356:ALA:O	2:B:359:LYS:HB3	2.12	0.50
2:B:556:GLU:HG2	2:B:558:THR:H	1.77	0.50
2:B:482:LEU:HD12	2:B:519:LEU:HD13	1.94	0.50
1:L:413:LEU:HD21	1:L:453:ALA:CB	2.42	0.50
2:E:549:SER:O	2:E:550:GLU:O	2.30	0.50
4:U:353:TRP:CE2	4:U:355:ILE:HD11	2.47	0.50
1:A:156:VAL:HG11	1:A:188:TRP:CB	2.41	0.50
1:L:204:VAL:HG12	1:L:257:LEU:HD11	1.94	0.50
5:P:4:GLN:HB3	3:S:100:GLU:CB	2.42	0.50
2:E:12:LYS:HD2	2:E:12:LYS:N	2.27	0.50
2:B:12:LYS:N	2:B:12:LYS:HD2	2.26	0.50
2:B:530:LEU:HD23	2:B:537:ALA:HB1	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:U:419:ILE:HD13	4:U:419:ILE:N	2.27	0.50
2:B:18:LEU:O	2:B:22:LEU:HG	2.11	0.50
4:M:12:GLY:O	4:M:33:ARG:NH1	2.45	0.49
1:A:535:VAL:HG11	1:A:573:ASP:OD1	2.11	0.49
1:L:27:GLU:HA	1:L:30:ILE:HG13	1.94	0.49
4:U:12:GLY:O	4:U:33:ARG:NH1	2.44	0.49
2:B:288:LEU:HA	2:B:291:LEU:HB2	1.93	0.49
1:L:509:ASN:HA	1:L:552:PHE:HZ	1.77	0.49
1:L:173:LEU:HD13	1:L:210:LEU:HD12	1.94	0.49
4:M:321:GLU:HG2	4:M:354:LYS:HG2	1.94	0.49
2:B:305:ASN:HD21	2:B:572:SER:HB3	1.76	0.49
1:A:173:LEU:HD11	1:A:213:THR:HB	1.94	0.49
2:E:522:ARG:HG2	2:E:522:ARG:NH1	2.25	0.49
2:B:173:ASN:HD21	2:B:175:MET:HB3	1.77	0.49
2:E:267:LEU:C	2:E:269:LEU:H	2.15	0.49
3:I:115:ASP:HA	3:I:118:PHE:O	2.12	0.49
2:E:582:VAL:H	4:U:52:ARG:HG2	1.77	0.49
5:Q:2:MET:O	5:Q:3:SEP:C	2.60	0.49
4:M:9:ASN:ND2	4:M:13:GLU:H	2.10	0.49
1:L:418:TYR:HD1	1:L:418:TYR:N	2.10	0.49
1:A:393:LEU:HD22	1:A:405:ILE:HG12	1.93	0.49
2:B:257:LEU:HD12	4:M:76:ALA:HB2	1.94	0.49
5:P:5:ILE:O	5:P:5:ILE:HG13	2.10	0.49
2:B:161:PHE:HA	2:B:164:SER:HB2	1.95	0.49
4:M:33:ARG:O	4:M:37:ILE:HB	2.13	0.49
2:E:288:LEU:HD23	2:E:289:VAL:N	2.28	0.49
2:B:145:VAL:HG11	2:B:165:LEU:CD2	2.43	0.49
1:A:322:SER:O	1:A:323:GLU:O	2.30	0.49
4:M:326:THR:HG22	4:M:370:ILE:HD13	1.93	0.49
3:I:8:GLN:HE22	3:I:36:HIS:CB	2.22	0.49
4:M:28:ALA:HA	4:M:31:ALA:HB3	1.95	0.49
2:B:149:HIS:CD2	2:B:187:ILE:HG23	2.47	0.49
2:B:274:SER:C	2:B:276:TYR:N	2.64	0.49
2:E:328:TYR:CE2	4:U:405:LYS:HD2	2.48	0.49
1:A:363:HIS:O	1:A:364:GLU:HB2	2.13	0.49
4:U:107:LEU:O	4:U:111:LEU:HB2	2.13	0.49
2:E:218:GLY:CA	2:E:221:PHE:CD1	2.94	0.49
4:M:344:TYR:HE2	4:M:346:ALA:HB2	1.77	0.49
4:M:173:LEU:O	4:M:173:LEU:HD12	2.13	0.49
1:A:40:ILE:CG2	1:A:58:TYR:HB3	2.40	0.49
1:L:284:LEU:HD23	1:L:313:ALA:HB1	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:M:316:LEU:HD13	4:M:357:ARG:HB2	1.94	0.49
2:E:265:LYS:HA	2:E:265:LYS:HD3	1.58	0.49
3:S:55:PHE:HB3	3:S:71:VAL:O	2.13	0.49
1:A:347:TYR:CD2	1:A:347:TYR:C	2.86	0.49
4:U:162:ARG:HD2	4:U:267:PRO:O	2.13	0.48
1:L:481:LYS:HA	1:L:511:ILE:HD12	1.94	0.48
1:A:375:ASN:O	1:A:376:ALA:C	2.52	0.48
1:A:510:LEU:HD12	1:A:510:LEU:N	2.20	0.48
4:M:28:ALA:HB2	4:M:53:THR:HG21	1.95	0.48
1:A:481:LYS:HA	1:A:511:ILE:HD12	1.94	0.48
2:B:522:ARG:NH1	2:B:522:ARG:HG2	2.28	0.48
1:A:514:ASP:CG	1:A:516:ARG:HB2	2.34	0.48
4:M:166:ILE:CD1	4:M:166:ILE:H	2.17	0.48
3:S:49:PHE:HD2	3:S:58:ILE:HD12	1.78	0.48
3:I:49:PHE:HD2	3:I:58:ILE:HD12	1.78	0.48
1:L:250:TYR:HD1	1:L:250:TYR:N	2.11	0.48
2:B:318:LYS:HE3	2:B:318:LYS:C	2.33	0.48
2:B:477:SER:OG	2:B:480:VAL:HG13	2.13	0.48
1:A:23:CYS:C	1:A:25:SER:H	2.16	0.48
1:L:449:LEU:H	1:L:449:LEU:HD12	1.79	0.48
4:U:379:LYS:C	4:U:381:TRP:N	2.64	0.48
3:S:7:ILE:HD11	3:S:16:LEU:HD23	1.95	0.48
1:L:109:ILE:HG21	1:L:142:GLU:HG2	1.96	0.48
1:A:518:SER:O	1:A:522:GLN:HG3	2.13	0.48
1:L:322:SER:O	1:L:323:GLU:O	2.32	0.48
2:B:218:GLY:CA	2:B:221:PHE:CD1	2.95	0.48
2:B:40:ALA:CA	2:B:43:VAL:HG22	2.43	0.48
2:E:428:ILE:O	2:E:432:LEU:HD13	2.14	0.48
2:E:177:VAL:O	2:E:181:VAL:HG23	2.14	0.48
2:E:495:LYS:HD3	2:E:498:GLU:OE2	2.14	0.48
1:L:509:ASN:HA	1:L:552:PHE:CZ	2.49	0.48
1:A:442:TYR:CZ	1:A:468:ILE:HD12	2.49	0.48
4:M:346:ALA:O	4:M:347:SER:C	2.52	0.48
2:B:461:ASN:HB3	2:B:465:LEU:HG	1.94	0.48
2:E:135:PRO:HB3	2:E:173:ASN:OD1	2.14	0.48
2:E:169:ILE:O	2:E:177:VAL:HG13	2.13	0.48
2:E:387:SER:O	2:E:390:ARG:HG2	2.14	0.48
4:M:162:ARG:HB3	4:M:209:MET:HE1	1.96	0.48
2:B:106:ALA:O	2:B:110:MET:HB2	2.14	0.48
1:A:394:TYR:CE2	4:M:294:ARG:HD3	2.49	0.48
2:E:412:VAL:O	2:E:415:ARG:HB3	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:447:ALA:O	2:E:451:ILE:HG13	2.13	0.48
1:A:613:LEU:HG	4:M:335:VAL:HG13	1.95	0.48
3:S:41:VAL:O	3:S:41:VAL:HG22	2.14	0.48
4:U:166:ILE:HD11	4:U:208:GLY:O	2.14	0.48
4:U:28:ALA:HA	4:U:31:ALA:HB3	1.96	0.48
3:S:16:LEU:HD12	3:S:17:ALA:H	1.79	0.48
1:A:204:VAL:HG12	1:A:257:LEU:HD11	1.96	0.48
1:A:271:PRO:HB3	1:A:276:VAL:HG12	1.96	0.48
2:B:543:SER:O	2:B:545:LYS:HE3	2.13	0.48
3:I:65:LEU:HD21	3:I:100:GLU:HG2	1.96	0.48
2:B:38:ILE:HD12	2:B:68:LEU:HD22	1.96	0.47
2:E:580:ALA:C	2:E:581:PHE:HD2	2.17	0.47
3:S:72:ASP:HB2	3:S:75:ASP:OD2	2.14	0.47
5:P:2:MET:O	5:P:3:SEP:C	2.62	0.47
2:E:305:ASN:ND2	2:E:572:SER:HB3	2.29	0.47
2:E:529:LEU:HD21	2:E:537:ALA:HA	1.95	0.47
1:A:354:CYS:HA	1:A:392:LEU:HD13	1.96	0.47
4:U:26:ARG:O	4:U:26:ARG:HG3	2.12	0.47
2:B:288:LEU:HD22	2:B:288:LEU:H	1.79	0.47
1:L:250:TYR:N	1:L:250:TYR:CD1	2.82	0.47
2:B:13:GLY:O	2:B:14:GLU:HB3	2.14	0.47
1:A:88:TYR:HB2	3:S:141:LEU:HD13	1.96	0.47
2:B:428:ILE:O	2:B:432:LEU:HD13	2.14	0.47
2:E:174:PRO:HB3	2:E:214:CYS:N	2.28	0.47
4:U:430:ILE:CG1	4:U:430:ILE:O	2.62	0.47
4:M:182:ASN:ND2	4:M:430:ILE:N	2.58	0.47
1:L:173:LEU:HD11	1:L:213:THR:HB	1.96	0.47
1:L:403:GLN:HG2	1:L:441:TRP:CE2	2.49	0.47
4:M:360:GLY:O	4:M:361:MET:HB2	2.14	0.47
4:U:162:ARG:HB3	4:U:209:MET:HE1	1.95	0.47
2:E:497:SER:C	2:E:499:THR:H	2.18	0.47
1:L:569:LEU:HD22	1:L:581:VAL:HG22	1.96	0.47
4:M:353:TRP:CE2	4:M:355:ILE:HD11	2.49	0.47
2:E:197:LEU:O	2:E:198:ASP:CG	2.53	0.47
4:U:316:LEU:HD13	4:U:357:ARG:HB2	1.96	0.47
4:U:171:ASN:ND2	4:U:413:TYR:CZ	2.83	0.47
1:L:510:LEU:HD12	1:L:510:LEU:N	2.29	0.47
2:B:135:PRO:HB3	2:B:173:ASN:OD1	2.14	0.47
4:M:216:MET:HG3	4:M:217:ASN:O	2.15	0.47
2:E:274:SER:C	2:E:276:TYR:N	2.67	0.47
2:E:543:SER:O	2:E:545:LYS:HE3	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:412:VAL:O	2:B:415:ARG:HB3	2.14	0.47
3:I:99:CYS:SG	5:Q:5:ILE:HD12	2.54	0.47
3:I:41:VAL:HG22	3:I:41:VAL:O	2.14	0.47
1:A:314:ILE:HG12	1:A:330:ALA:HB1	1.96	0.47
4:U:85:MET:HE1	4:U:112:LEU:HD21	1.95	0.47
4:U:186:SER:CB	4:U:190:GLN:HB2	2.37	0.47
4:U:217:ASN:O	4:U:218:ASP:O	2.31	0.47
3:S:92:ASN:ND2	3:S:97:ASN:HA	2.27	0.47
3:I:87:PHE:CZ	3:I:114:VAL:HG23	2.49	0.47
1:A:446:ILE:HG21	1:A:465:VAL:HG11	1.95	0.47
2:E:231:PRO:HG2	2:E:237:ALA:HB2	1.96	0.47
2:B:265:LYS:HA	2:B:265:LYS:HD3	1.56	0.47
2:B:22:LEU:O	2:B:30:ARG:HG2	2.15	0.47
1:A:543:SER:O	1:A:547:LYS:HG3	2.15	0.47
1:A:367:LYS:O	1:A:370:ILE:HG13	2.15	0.47
2:E:149:HIS:CD2	2:E:187:ILE:HG23	2.49	0.47
2:E:18:LEU:O	2:E:22:LEU:HG	2.14	0.47
1:L:418:TYR:CD1	1:L:418:TYR:N	2.81	0.47
2:E:220:ILE:HD13	4:U:77:MET:HG3	1.97	0.47
4:U:169:ARG:CG	4:U:170:ARG:H	2.28	0.47
2:E:347:SER:C	2:E:349:ALA:N	2.68	0.47
2:E:451:ILE:O	2:E:454:GLU:O	2.32	0.47
2:E:480:VAL:O	2:E:481:GLN:C	2.52	0.47
2:B:54:VAL:CG1	2:B:69:VAL:HG13	2.45	0.47
4:U:41:GLN:CG	4:U:284:ILE:HD12	2.45	0.47
1:L:535:VAL:HG11	1:L:573:ASP:OD1	2.15	0.47
1:A:252:VAL:HG12	1:A:255:PRO:HG3	1.96	0.47
3:S:94:TYR:OH	3:S:109:LYS:HD2	2.15	0.47
2:E:139:LYS:NZ	4:U:122:GLN:HG3	2.30	0.47
4:U:204:SER:OG	4:U:204:SER:O	2.33	0.47
1:A:618:LYS:O	1:A:618:LYS:HG2	2.15	0.47
2:B:220:ILE:HD11	2:B:254:ALA:HB3	1.97	0.47
1:L:54:SER:O	1:L:58:TYR:CD1	2.68	0.47
3:S:8:GLN:HE22	3:S:36:HIS:CB	2.27	0.47
2:B:26:LYS:O	2:B:29:LYS:N	2.47	0.47
2:E:73:LEU:HD13	2:E:91:PHE:CZ	2.50	0.47
1:L:363:HIS:O	1:L:364:GLU:HB2	2.15	0.47
1:L:42:SER:HA	1:L:45:LYS:HB3	1.97	0.47
3:S:42:ARG:HH21	3:S:47:THR:H	1.63	0.47
4:U:360:GLY:O	4:U:361:MET:HB2	2.15	0.47
2:E:245:THR:HG22	2:E:246:PRO:HD3	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:177:VAL:O	2:B:181:VAL:HG23	2.15	0.46
2:B:496:PRO:O	2:B:497:SER:OG	2.28	0.46
2:B:447:ALA:O	2:B:451:ILE:HG13	2.15	0.46
1:L:432:ALA:O	1:L:436:ALA:HB2	2.14	0.46
2:E:47:VAL:HG12	2:E:48:SER:N	2.30	0.46
4:U:212:CYS:HB3	4:U:406:VAL:HA	1.97	0.46
2:B:365:VAL:HG13	4:M:401:VAL:HG12	1.97	0.46
3:S:7:ILE:CD1	3:S:16:LEU:HD23	2.45	0.46
1:A:189:THR:HG22	1:A:190:SER:N	2.30	0.46
3:S:65:LEU:HD21	3:S:100:GLU:HG2	1.97	0.46
1:L:375:ASN:O	1:L:376:ALA:C	2.52	0.46
1:A:418:TYR:N	1:A:418:TYR:HD1	2.13	0.46
2:B:204:ILE:CG2	2:B:205:ASN:N	2.78	0.46
1:L:516:ARG:CG	1:L:516:ARG:NH1	2.67	0.46
1:L:20:ILE:CD1	1:L:33:ILE:HD11	2.38	0.46
2:B:213:GLU:HB2	2:B:214:CYS:H	1.53	0.46
2:B:306:ILE:HG23	2:B:317:LEU:HD12	1.96	0.46
1:L:618:LYS:HG2	1:L:618:LYS:O	2.16	0.46
1:A:508:GLY:N	1:A:510:LEU:HD12	2.23	0.46
2:B:497:SER:OG	2:B:498:GLU:N	2.48	0.46
2:B:347:SER:C	2:B:349:ALA:N	2.68	0.46
2:B:305:ASN:ND2	2:B:572:SER:HB3	2.29	0.46
2:E:106:ALA:O	2:E:110:MET:HB2	2.15	0.46
2:E:321:ILE:HG13	2:E:345:LEU:HB2	1.96	0.46
1:A:42:SER:HA	1:A:45:LYS:HB3	1.96	0.46
2:E:147:LYS:HB2	2:E:147:LYS:HE2	1.65	0.46
2:E:74:MET:HE2	6:E:1587:SO4:O4	2.16	0.46
1:L:36:GLU:HG3	1:L:40:ILE:HD11	1.96	0.46
1:L:43:LYS:HB3	1:L:50:LEU:HD21	1.98	0.46
2:B:497:SER:C	2:B:499:THR:H	2.18	0.46
2:B:305:ASN:OD1	2:B:572:SER:HB2	2.16	0.46
2:B:461:ASN:O	2:B:462:ALA:C	2.53	0.46
3:I:94:TYR:OH	3:I:109:LYS:HD2	2.14	0.46
1:A:80:VAL:HA	1:A:83:LEU:HD12	1.98	0.46
1:L:32:ARG:O	1:L:32:ARG:HD2	2.16	0.46
2:B:521:ASP:O	2:B:525:ILE:HD12	2.16	0.46
2:B:420:LYS:HD2	2:B:548:ILE:O	2.15	0.46
2:E:436:LEU:HD12	2:E:465:LEU:HD22	1.97	0.46
2:B:436:LEU:CD1	2:B:465:LEU:HD22	2.46	0.46
5:Q:5:ILE:O	5:Q:5:ILE:HG13	2.15	0.46
1:L:135:ILE:CG2	1:L:171:CYS:SG	3.04	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:S:34:GLU:O	3:S:38:VAL:HG23	2.15	0.46
4:U:252:VAL:HA	4:U:265:PHE:HB3	1.96	0.46
2:B:332:ILE:HG21	4:M:402:ARG:NH2	2.29	0.46
2:E:395:LEU:HD13	2:E:414:ILE:HG12	1.97	0.46
3:S:95:PHE:O	3:S:96:HIS:O	2.34	0.46
2:B:127:ARG:HG2	2:B:127:ARG:NH1	2.17	0.46
1:A:36:GLU:HG3	1:A:40:ILE:HD11	1.97	0.46
1:L:40:ILE:CG2	1:L:58:TYR:HB3	2.43	0.46
4:U:293:VAL:HG22	4:U:294:ARG:N	2.25	0.46
2:E:306:ILE:HG23	2:E:317:LEU:HD12	1.97	0.46
2:B:155:MET:HE3	2:B:161:PHE:HE1	1.81	0.46
1:A:27:GLU:HA	1:A:30:ILE:HG13	1.98	0.46
2:B:169:ILE:O	2:B:177:VAL:HG13	2.16	0.46
2:B:250:HIS:O	2:B:251:ALA:HB3	2.16	0.46
3:S:83:ALA:O	3:S:84:ILE:C	2.53	0.46
2:E:404:ASN:O	2:E:405:TYR:C	2.53	0.46
1:A:420:ILE:HD13	1:A:420:ILE:N	2.30	0.46
2:E:454:GLU:OE2	2:E:490:LYS:NZ	2.49	0.46
2:E:274:SER:O	2:E:275:ASP:C	2.53	0.46
2:B:38:ILE:CD1	2:B:68:LEU:HB3	2.46	0.46
3:S:109:LYS:HA	3:S:112:THR:HG23	1.98	0.46
2:E:556:GLU:HG2	2:E:558:THR:H	1.80	0.46
2:E:213:GLU:HB2	2:E:214:CYS:H	1.56	0.46
2:B:515:ASP:O	2:B:517:PRO:HD3	2.15	0.46
2:B:216:GLU:HB3	2:B:250:HIS:HE1	1.80	0.46
2:E:65:LEU:O	2:E:65:LEU:HG	2.15	0.46
2:E:408:GLN:HE22	2:E:439:LEU:HA	1.80	0.46
2:B:26:LYS:HB2	2:B:29:LYS:HB2	1.96	0.46
2:B:13:GLY:HA2	2:B:17:GLU:HG3	1.97	0.46
1:A:418:TYR:N	1:A:418:TYR:CD1	2.84	0.46
1:A:387:GLN:OE1	4:M:188:GLN:HG2	2.15	0.46
3:I:58:ILE:N	3:I:58:ILE:HD13	2.31	0.46
3:S:1:MET:HB3	3:S:72:ASP:OD2	2.16	0.46
2:B:454:GLU:OE2	2:B:490:LYS:NZ	2.48	0.46
1:A:22:ASN:HB3	1:A:23:CYS:H	1.40	0.46
1:A:144:ALA:O	1:A:148:ALA:HB2	2.16	0.46
3:I:119:LEU:O	3:I:120:ALA:HB3	2.16	0.46
1:L:518:SER:O	1:L:522:GLN:HG3	2.16	0.46
4:U:218:ASP:HB3	4:U:219:LYS:H	1.50	0.45
2:E:419:ARG:NH2	2:E:548:ILE:HG21	2.31	0.45
1:L:523:PHE:CD1	1:L:559:ILE:HG12	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:216:GLU:HB3	2:E:250:HIS:HE1	1.81	0.45
1:L:412:TYR:CD2	1:L:424:ILE:HD11	2.51	0.45
4:U:408:GLU:HA	4:U:409:PRO:HD3	1.62	0.45
4:M:268:PRO:HD2	4:M:272:PHE:CE2	2.51	0.45
1:L:354:CYS:HA	1:L:392:LEU:HD13	1.97	0.45
2:B:574:TYR:CE1	4:M:49:ASN:HB2	2.51	0.45
2:B:197:LEU:HB3	2:B:199:LEU:HD22	1.97	0.45
2:E:458:ARG:HA	2:E:458:ARG:HD2	1.69	0.45
4:M:112:LEU:HA	4:M:115:ILE:HG22	1.97	0.45
2:E:156:VAL:CG1	2:E:162:LEU:HD23	2.40	0.45
1:A:43:LYS:HB3	1:A:50:LEU:HD21	1.98	0.45
1:L:54:SER:O	1:L:58:TYR:HD1	1.99	0.45
4:M:41:GLN:CG	4:M:284:ILE:HD12	2.45	0.45
1:L:590:ALA:HB1	1:L:594:ILE:CG2	2.45	0.45
2:E:524:TYR:CZ	1:L:603:PRO:HG2	2.50	0.45
4:U:296:VAL:HG13	4:U:300:LYS:O	2.17	0.45
2:B:123:CYS:SG	2:B:159:GLN:HG3	2.56	0.45
1:A:403:GLN:HG2	1:A:441:TRP:CE2	2.51	0.45
3:I:128:GLN:HA	3:I:131:VAL:CG1	2.47	0.45
2:E:174:PRO:HA	2:E:177:VAL:HG23	1.97	0.45
1:L:618:LYS:C	1:L:619:LYS:HG2	2.37	0.45
2:B:570:LEU:HB2	4:M:72:ASN:ND2	2.31	0.45
2:B:355:LEU:O	2:B:356:ALA:C	2.55	0.45
2:B:12:LYS:CD	2:B:12:LYS:N	2.80	0.45
2:B:198:ASP:OD2	2:B:199:LEU:N	2.49	0.45
2:E:204:ILE:CG2	2:E:205:ASN:N	2.79	0.45
2:B:580:ALA:C	2:B:581:PHE:CD2	2.90	0.45
1:L:334:LEU:CD1	1:L:352:SER:HB3	2.46	0.45
1:A:252:VAL:CG1	1:A:255:PRO:HG3	2.46	0.45
4:U:299:THR:O	4:U:372:LEU:HB2	2.17	0.45
1:A:483:VAL:HG12	1:A:484:PHE:N	2.32	0.45
1:L:347:TYR:C	1:L:347:TYR:CD2	2.89	0.45
1:A:616:LEU:HD12	1:A:616:LEU:HA	1.47	0.45
1:A:375:ASN:O	1:A:378:LYS:N	2.50	0.45
4:M:263:ILE:HD12	4:M:263:ILE:HA	1.65	0.45
1:A:263:ARG:HD3	1:A:312:GLU:OE2	2.15	0.45
4:M:288:ARG:HG3	4:M:288:ARG:HH11	1.81	0.45
3:S:101:LEU:HA	3:S:101:LEU:HD23	1.72	0.45
4:U:107:LEU:HD22	4:U:137:GLY:HA2	1.97	0.45
4:U:382:ALA:O	4:U:383:ARG:C	2.54	0.45
4:M:9:ASN:HD21	4:M:13:GLU:HG3	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:24:ASN:ND2	2:B:29:LYS:HD2	2.31	0.45
2:B:436:LEU:HD21	2:B:448:MET:SD	2.56	0.45
4:U:214:PHE:HE2	4:U:401:VAL:HG13	1.82	0.45
4:M:104:ASN:HD21	4:M:138:ILE:H	1.65	0.45
1:L:135:ILE:HG22	1:L:171:CYS:SG	2.56	0.45
4:M:42:GLN:HA	4:M:42:GLN:HE21	1.82	0.45
2:B:100:PRO:CB	2:B:134:ASP:OD2	2.65	0.45
2:E:197:LEU:HB3	2:E:199:LEU:HD22	1.98	0.45
2:E:38:ILE:CD1	2:E:68:LEU:HB3	2.47	0.45
1:L:489:ALA:HA	1:L:490:PRO:HD3	1.75	0.45
3:S:16:LEU:HD22	3:S:110:VAL:CG1	2.46	0.45
2:E:322:LYS:CE	2:E:353:GLN:NE2	2.80	0.45
1:L:532:LEU:HD23	1:L:532:LEU:C	2.37	0.45
1:L:543:SER:HA	1:L:583:TYR:CE2	2.51	0.45
4:M:299:THR:O	4:M:372:LEU:HB2	2.17	0.45
1:A:523:PHE:CE1	1:A:559:ILE:HG12	2.52	0.45
1:L:130:LEU:HA	1:L:130:LEU:HD23	1.78	0.45
3:S:114:VAL:HG12	3:S:115:ASP:N	2.31	0.45
3:I:109:LYS:HA	3:I:112:THR:HG23	1.98	0.45
1:L:514:ASP:CG	1:L:516:ARG:HB2	2.38	0.44
4:U:85:MET:HE3	4:U:112:LEU:CD2	2.47	0.44
2:B:143:VAL:HG12	2:B:179:ASN:HB3	1.99	0.44
2:B:174:PRO:HB3	2:B:214:CYS:N	2.32	0.44
1:L:394:TYR:CE2	4:U:294:ARG:HD3	2.51	0.44
1:L:239:SER:CB	1:L:243:ASP:OD2	2.63	0.44
2:B:230:ASN:HA	2:B:231:PRO:HD3	1.84	0.44
1:A:432:ALA:O	1:A:436:ALA:HB2	2.17	0.44
2:B:532:THR:O	2:B:533:ASP:HB2	2.17	0.44
1:L:426:LEU:O	1:L:427:LYS:C	2.54	0.44
2:E:220:ILE:HD11	2:E:254:ALA:HB3	1.99	0.44
2:B:286:PRO:N	2:B:287:PRO:CD	2.80	0.44
4:M:430:ILE:HG13	4:M:432:GLU:HG3	1.98	0.44
4:M:379:LYS:C	4:M:381:TRP:N	2.65	0.44
1:L:189:THR:HG22	1:L:190:SER:N	2.31	0.44
2:E:355:LEU:O	2:E:356:ALA:C	2.56	0.44
2:E:12:LYS:CD	2:E:12:LYS:N	2.80	0.44
3:I:42:ARG:HH21	3:I:47:THR:H	1.65	0.44
2:E:435:ASN:C	2:E:437:ASP:N	2.71	0.44
1:L:32:ARG:NH1	1:L:36:GLU:HB2	2.33	0.44
3:I:138:LEU:C	3:I:140:SER:H	2.20	0.44
2:B:495:LYS:HD3	2:B:498:GLU:OE2	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:541:VAL:HG23	2:E:542:LEU:HD23	2.00	0.44
2:B:488:ILE:HD12	2:B:506:VAL:CG2	2.48	0.44
2:B:488:ILE:HG21	2:B:506:VAL:CG2	2.47	0.44
1:L:80:VAL:HA	1:L:83:LEU:HD12	2.00	0.44
1:L:402:ALA:O	1:L:406:VAL:HG23	2.17	0.44
4:M:5:LEU:HA	4:M:5:LEU:HD12	1.73	0.44
4:U:288:ARG:HG3	4:U:288:ARG:HH11	1.82	0.44
4:M:107:LEU:HD22	4:M:137:GLY:HA2	1.98	0.44
4:U:85:MET:HE3	4:U:112:LEU:HD21	1.99	0.44
2:B:139:LYS:HE3	2:B:175:MET:HG2	1.99	0.44
3:S:58:ILE:N	3:S:58:ILE:HD13	2.32	0.44
4:U:241:ILE:N	4:U:241:ILE:HD12	2.33	0.44
2:E:461:ASN:O	2:E:462:ALA:C	2.56	0.44
2:E:13:GLY:O	2:E:14:GLU:HB3	2.17	0.44
2:E:488:ILE:HG21	2:E:506:VAL:CG2	2.47	0.44
2:E:546:PRO:HG2	1:L:569:LEU:HB3	1.98	0.44
4:U:40:ARG:HB3	4:U:284:ILE:HD13	1.99	0.44
3:I:95:PHE:O	3:I:96:HIS:O	2.35	0.44
4:U:248:PHE:CD1	4:U:254:LEU:HD21	2.52	0.44
4:U:185:MET:HE3	4:U:189:GLY:O	2.17	0.44
1:L:367:LYS:NZ	1:L:398:ASP:HB3	2.32	0.44
1:A:11:ARG:O	1:A:15:VAL:HG23	2.17	0.44
2:B:349:ALA:O	2:B:350:ASN:HB3	2.18	0.44
3:I:21:MET:HG3	3:I:23:PHE:CE1	2.52	0.44
2:E:13:GLY:HA2	2:E:17:GLU:HG3	1.98	0.44
1:A:426:LEU:O	1:A:427:LYS:C	2.55	0.44
1:A:265:LEU:HD13	1:A:280:LEU:HD13	2.00	0.44
5:P:9:LEU:HB3	5:P:10:SER:H	1.52	0.44
4:U:173:LEU:HD12	4:U:173:LEU:O	2.17	0.44
1:A:344:ASN:ND2	3:S:48:ASN:ND2	2.65	0.44
1:L:397:CYS:SG	1:L:431:LEU:HD13	2.57	0.44
3:I:119:LEU:HB3	1:L:170:LEU:HD12	2.00	0.44
1:L:143:MET:O	1:L:144:ALA:C	2.54	0.44
2:B:147:LYS:HE2	2:B:147:LYS:HB2	1.63	0.44
2:B:284:LEU:O	2:B:287:PRO:HD2	2.17	0.44
1:A:367:LYS:NZ	1:A:398:ASP:HB3	2.32	0.44
2:E:342:MET:HE1	2:E:361:TYR:OH	2.18	0.44
1:A:250:TYR:O	1:A:251:PHE:HB2	2.17	0.44
1:A:379:THR:O	1:A:380:GLU:C	2.56	0.44
4:M:430:ILE:CG1	4:M:430:ILE:O	2.66	0.44
2:E:524:TYR:CD1	1:L:602:MET:HE3	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:99:ASN:HB3	2:B:102:ILE:CD1	2.48	0.44
2:E:34:VAL:O	2:E:38:ILE:HG13	2.18	0.44
2:E:68:LEU:HA	2:E:68:LEU:HD23	1.89	0.44
1:L:420:ILE:HD13	1:L:420:ILE:N	2.32	0.44
4:M:65:LEU:N	4:M:65:LEU:HD23	2.33	0.44
2:E:482:LEU:HD23	1:L:575:GLU:OE1	2.18	0.44
1:L:508:GLY:H	1:L:510:LEU:HD11	1.80	0.44
4:U:261:ARG:O	4:U:263:ILE:HD13	2.18	0.44
1:A:508:GLY:H	1:A:510:LEU:HD11	1.82	0.44
1:L:556:LYS:HG2	1:L:560:GLN:OE1	2.18	0.44
3:I:141:LEU:HB3	1:L:88:TYR:HB3	2.00	0.44
2:B:284:LEU:C	2:B:287:PRO:HD2	2.38	0.43
3:S:137:MET:C	3:S:138:LEU:O	2.52	0.43
1:L:543:SER:O	1:L:547:LYS:HG3	2.18	0.43
1:L:11:ARG:O	1:L:15:VAL:HG23	2.18	0.43
2:E:100:PRO:CB	2:E:134:ASP:OD2	2.66	0.43
2:E:574:TYR:CE1	4:U:49:ASN:HB2	2.53	0.43
2:E:532:THR:O	2:E:533:ASP:HB2	2.18	0.43
1:L:379:THR:O	1:L:380:GLU:C	2.56	0.43
2:B:139:LYS:CE	2:B:175:MET:HG2	2.49	0.43
1:A:618:LYS:C	1:A:619:LYS:HG2	2.38	0.43
2:B:581:PHE:CD2	2:B:581:PHE:N	2.86	0.43
2:E:284:LEU:C	2:E:287:PRO:HD2	2.38	0.43
4:U:325:PRO:CB	4:U:384:PRO:HG2	2.49	0.43
1:A:401:ASN:HD22	1:A:401:ASN:C	2.21	0.43
2:B:324:PHE:O	2:B:338:LYS:HD2	2.18	0.43
4:M:29:VAL:HG13	4:M:30:ASP:N	2.33	0.43
1:L:375:ASN:O	1:L:378:LYS:N	2.48	0.43
3:I:101:LEU:HD23	3:I:101:LEU:HA	1.70	0.43
3:S:128:GLN:HA	3:S:131:VAL:CG1	2.48	0.43
1:L:382:ASP:OD2	1:L:385:VAL:HG23	2.18	0.43
2:E:286:PRO:N	2:E:287:PRO:CD	2.81	0.43
1:A:250:TYR:CD1	1:A:250:TYR:N	2.86	0.43
4:U:346:ALA:O	4:U:347:SER:C	2.56	0.43
2:E:550:GLU:HG2	2:E:551:GLU:N	2.33	0.43
2:E:541:VAL:HG23	2:E:542:LEU:CD2	2.48	0.43
1:L:22:ASN:HB3	1:L:23:CYS:H	1.38	0.43
3:I:100:GLU:CB	5:Q:4:GLN:HB3	2.48	0.43
4:M:214:PHE:HE2	4:M:401:VAL:HG13	1.84	0.43
4:U:321:GLU:HG2	4:U:354:LYS:HG2	2.01	0.43
1:L:4:VAL:HG12	1:L:5:SER:N	2.34	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:M:21:ARG:HH11	4:M:21:ARG:CB	2.18	0.43
1:A:32:ARG:HD2	1:A:32:ARG:O	2.18	0.43
1:A:603:PRO:HG2	2:B:524:TYR:OH	2.19	0.43
2:E:497:SER:OG	2:E:498:GLU:N	2.51	0.43
2:E:357:GLU:CG	2:E:361:TYR:OH	2.67	0.43
2:B:570:LEU:HA	2:B:570:LEU:HD23	1.74	0.43
2:B:419:ARG:NH2	2:B:548:ILE:HG21	2.33	0.43
2:B:421:TYR:O	2:B:422:PRO:C	2.55	0.43
2:E:240:ILE:CG2	2:E:241:CYS:N	2.81	0.43
2:E:436:LEU:HD21	2:E:448:MET:HG2	1.99	0.43
4:M:198:GLY:HA3	4:M:277:TYR:CZ	2.53	0.43
1:A:543:SER:HA	1:A:583:TYR:CE2	2.52	0.43
4:M:222:ILE:HD12	4:M:222:ILE:N	2.26	0.43
4:M:293:VAL:HG22	4:M:294:ARG:N	2.26	0.43
3:S:115:ASP:HA	3:S:118:PHE:O	2.17	0.43
4:M:383:ARG:HA	4:M:384:PRO:HD2	1.73	0.43
2:E:83:MET:O	2:E:86:MET:CE	2.66	0.43
2:B:274:SER:C	2:B:276:TYR:H	2.22	0.43
2:B:227:SER:OG	2:B:261:LYS:HE3	2.19	0.43
4:U:162:ARG:NH2	4:U:206:LEU:O	2.45	0.43
2:B:387:SER:O	2:B:390:ARG:HG2	2.19	0.43
1:L:380:GLU:O	1:L:386:ARG:CD	2.58	0.43
3:S:19:TRP:CZ3	3:S:31:LEU:HD23	2.54	0.43
1:A:54:SER:O	1:A:58:TYR:CD1	2.72	0.43
4:M:382:ALA:O	4:M:383:ARG:C	2.55	0.43
1:L:549:VAL:CG1	1:L:556:LYS:HG3	2.44	0.43
1:A:250:TYR:HD1	1:A:250:TYR:N	2.16	0.43
1:A:151:ILE:HB	1:A:152:PRO:HD3	2.01	0.43
1:L:616:LEU:HA	1:L:616:LEU:HD12	1.44	0.43
2:E:348:GLN:HB3	2:E:386:GLN:HE22	1.83	0.43
2:E:26:LYS:O	2:E:29:LYS:N	2.52	0.43
4:U:104:ASN:O	4:U:108:ILE:HG13	2.19	0.43
3:I:69:ILE:HG22	3:I:71:VAL:HG13	2.01	0.43
2:B:87:ALA:HB3	2:B:91:PHE:CE2	2.53	0.43
2:B:389:GLU:OE2	2:B:424:LYS:HE2	2.19	0.43
2:B:321:ILE:HG13	2:B:345:LEU:HB2	1.99	0.43
4:U:421:TRP:N	4:U:421:TRP:CD1	2.86	0.43
2:E:173:ASN:HA	2:E:174:PRO:HD3	1.77	0.43
4:M:212:CYS:SG	4:M:267:PRO:HG3	2.58	0.43
2:B:504:GLN:NE2	4:U:375:THR:HA	2.33	0.43
1:L:594:ILE:CG2	1:L:595:LEU:N	2.82	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:U:169:ARG:HG3	4:U:170:ARG:H	1.83	0.43
2:B:122:LEU:O	2:B:123:CYS:C	2.57	0.43
2:B:73:LEU:HD13	2:B:91:PHE:CZ	2.53	0.43
1:L:176:TYR:HA	1:L:183:VAL:HG21	2.01	0.43
1:A:209:SER:HB3	3:S:122:GLU:HG3	2.00	0.43
4:M:241:ILE:HB	3:S:27:GLU:HG2	1.99	0.43
1:L:615:LYS:N	1:L:623:SER:HB3	2.34	0.43
2:B:550:GLU:HG2	2:B:551:GLU:N	2.33	0.43
2:E:529:LEU:HG	2:E:537:ALA:HB2	2.00	0.43
2:E:155:MET:HE3	2:E:161:PHE:HE1	1.83	0.43
4:U:376:ASN:O	4:U:377:ASP:CB	2.66	0.43
1:A:254:ALA:N	1:A:255:PRO:HD3	2.34	0.43
4:M:239:GLN:HB3	3:S:21:MET:HE1	2.01	0.43
1:L:47:ASP:OD2	1:L:48:LYS:N	2.35	0.43
2:B:552:THR:O	2:B:553:ASP:HB2	2.19	0.43
1:A:602:MET:HA	1:A:603:PRO:HD3	1.79	0.43
3:S:87:PHE:CZ	3:S:114:VAL:HG23	2.54	0.43
4:U:203:LYS:HA	4:U:271:GLU:HA	2.01	0.43
2:B:436:LEU:HD21	2:B:448:MET:HG2	2.00	0.43
2:B:555:ILE:HG22	2:B:556:GLU:O	2.19	0.43
1:A:122:SER:C	1:A:124:ASN:H	2.22	0.43
1:L:348:LEU:HD12	1:L:348:LEU:HA	1.73	0.43
2:B:169:ILE:HD12	2:B:170:ALA:N	2.34	0.42
1:L:57:LYS:CE	6:L:1625:SO4:O3	2.66	0.42
1:A:32:ARG:NH1	1:A:36:GLU:HB2	2.34	0.42
2:B:477:SER:CB	2:B:480:VAL:HG13	2.49	0.42
2:B:231:PRO:HG2	2:B:237:ALA:HB2	2.00	0.42
2:E:145:VAL:HG11	2:E:165:LEU:CD2	2.47	0.42
4:U:196:VAL:HB	4:U:279:THR:HG23	2.01	0.42
5:P:4:GLN:HB3	3:S:100:GLU:HB3	2.01	0.42
2:B:364:GLU:HB3	2:B:365:VAL:H	1.59	0.42
2:E:555:ILE:CG2	2:E:556:GLU:N	2.82	0.42
1:L:311:PHE:CZ	1:L:348:LEU:HB3	2.54	0.42
1:A:615:LYS:HZ3	4:U:341:LYS:HZ2	1.67	0.42
2:B:375:ARG:NH2	6:B:1586:SO4:O4	2.46	0.42
4:U:392:VAL:HA	4:U:393:PRO:HD3	1.74	0.42
4:U:85:MET:O	4:U:89:MET:HB2	2.19	0.42
1:L:618:LYS:O	1:L:619:LYS:CG	2.65	0.42
1:A:605:PHE:HE2	2:B:515:ASP:HA	1.83	0.42
2:B:548:ILE:HG13	2:B:548:ILE:O	2.19	0.42
1:A:239:SER:CB	1:A:243:ASP:OD2	2.67	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:173:LEU:HD13	1:A:210:LEU:HA	2.01	0.42
1:A:88:TYR:CG	3:S:141:LEU:HD12	2.54	0.42
2:B:404:ASN:O	2:B:405:TYR:C	2.57	0.42
1:A:607:GLU:O	1:A:608:ARG:C	2.57	0.42
2:B:408:GLN:HE22	2:B:440:ASP:N	2.13	0.42
4:M:169:ARG:CG	4:M:170:ARG:H	2.32	0.42
1:A:44:PHE:CE1	1:A:78:GLU:HG2	2.54	0.42
3:I:65:LEU:HD23	3:I:65:LEU:HA	1.82	0.42
2:E:139:LYS:HE2	4:U:122:GLN:OE1	2.19	0.42
4:M:381:TRP:CE3	4:M:383:ARG:HB3	2.54	0.42
2:E:564:ILE:HD13	2:E:564:ILE:HA	1.80	0.42
4:U:50:ILE:O	4:U:51:ALA:CB	2.66	0.42
1:A:88:TYR:HB3	3:S:141:LEU:HB3	2.00	0.42
2:B:197:LEU:O	2:B:198:ASP:CG	2.58	0.42
1:A:135:ILE:HG22	1:A:171:CYS:SG	2.59	0.42
2:B:435:ASN:C	2:B:437:ASP:N	2.73	0.42
2:B:254:ALA:HA	4:M:76:ALA:HB3	2.02	0.42
2:B:267:LEU:HD12	2:B:267:LEU:O	2.20	0.42
3:I:75:ASP:HA	1:L:263:ARG:HH22	1.84	0.42
2:E:305:ASN:OD1	2:E:572:SER:HB2	2.20	0.42
4:M:312:LYS:O	4:M:315:LEU:HD12	2.19	0.42
1:A:493:HIS:CD2	1:A:494:GLU:H	2.36	0.42
2:E:555:ILE:HG22	2:E:556:GLU:O	2.20	0.42
3:I:83:ALA:O	3:I:84:ILE:C	2.57	0.42
3:S:35:VAL:HG22	3:S:57:ILE:HD11	2.01	0.42
2:B:210:ALA:O	2:B:214:CYS:HB2	2.19	0.42
2:E:581:PHE:N	2:E:581:PHE:CD2	2.87	0.42
1:L:556:LYS:O	1:L:557:ALA:C	2.58	0.42
1:A:577:GLN:O	1:A:581:VAL:HG23	2.18	0.42
2:E:272:LYS:CE	2:E:278:ASN:HD21	2.33	0.42
1:A:412:TYR:CD2	1:A:424:ILE:HD11	2.54	0.42
4:M:242:ALA:O	4:M:280:THR:HG21	2.19	0.42
1:L:367:LYS:O	1:L:370:ILE:CG1	2.68	0.42
2:E:284:LEU:O	2:E:287:PRO:HD2	2.19	0.42
2:B:408:GLN:HE21	2:B:439:LEU:HA	1.81	0.42
2:E:580:ALA:C	2:E:581:PHE:CD2	2.93	0.42
3:S:7:ILE:HG13	3:S:16:LEU:HB3	2.01	0.42
2:B:421:TYR:O	2:B:422:PRO:O	2.38	0.42
3:S:69:ILE:HG22	3:S:71:VAL:HG13	2.02	0.42
1:L:271:PRO:HB3	1:L:276:VAL:HG12	2.00	0.42
1:A:473:ASP:C	1:A:475:VAL:H	2.23	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:214:LEU:HB3	1:L:222:PHE:CE1	2.55	0.42
1:L:132:LEU:HD11	1:L:164:VAL:HG13	2.01	0.42
1:L:150:GLU:O	1:L:153:LYS:HB2	2.20	0.42
1:A:380:GLU:O	1:A:386:ARG:CD	2.58	0.42
2:E:81:PRO:O	2:E:85:ILE:HG13	2.20	0.42
1:A:53:TYR:HE2	6:A:1625:SO4:O4	2.03	0.42
2:E:357:GLU:HG3	2:E:361:TYR:OH	2.19	0.42
1:A:433:GLU:HB3	1:A:442:TYR:HE1	1.84	0.42
2:E:415:ARG:O	2:E:419:ARG:HG3	2.20	0.42
1:L:269:PRO:HA	4:U:377:ASP:OD2	2.19	0.42
4:M:376:ASN:O	4:M:377:ASP:CB	2.68	0.42
2:B:21:GLU:HB3	2:B:33:ALA:HB1	2.02	0.42
4:U:248:PHE:N	4:U:248:PHE:CD1	2.87	0.42
1:A:265:LEU:HD23	1:A:265:LEU:HA	1.87	0.42
4:M:392:VAL:HG22	4:M:426:GLY:O	2.20	0.42
1:A:214:LEU:HB3	1:A:222:PHE:CE1	2.55	0.42
4:U:267:PRO:C	4:U:268:PRO:O	2.54	0.42
4:U:112:LEU:HA	4:U:115:ILE:HG22	2.01	0.42
1:A:376:ALA:O	1:A:380:GLU:HB2	2.20	0.42
2:E:524:TYR:CD1	1:L:602:MET:CE	3.03	0.42
5:P:2:MET:HE1	3:S:9:ASN:HB2	2.02	0.42
1:A:286:THR:O	1:A:289:ASN:N	2.53	0.42
4:M:85:MET:HE3	4:M:112:LEU:CD2	2.50	0.42
2:B:156:VAL:CG1	2:B:162:LEU:HD23	2.41	0.42
4:U:381:TRP:CE3	4:U:383:ARG:HB3	2.55	0.42
4:U:383:ARG:HA	4:U:384:PRO:HD2	1.72	0.42
4:M:203:LYS:HA	4:M:271:GLU:HA	2.02	0.42
1:A:341:ARG:HD3	1:A:341:ARG:H	1.85	0.42
2:E:389:GLU:OE2	2:E:424:LYS:HE2	2.20	0.42
2:E:463:ASP:N	2:E:463:ASP:OD1	2.52	0.42
2:E:230:ASN:N	2:E:230:ASN:OD1	2.52	0.42
1:A:54:SER:O	1:A:58:TYR:HD1	2.02	0.41
2:B:81:PRO:O	2:B:85:ILE:HG13	2.20	0.41
1:L:250:TYR:O	1:L:251:PHE:HB2	2.19	0.41
2:B:97:ASP:HB3	2:B:102:ILE:HG13	2.02	0.41
1:A:16:PHE:HE2	1:A:65:ILE:HG13	1.84	0.41
2:E:435:ASN:O	2:E:437:ASP:N	2.53	0.41
4:M:21:ARG:HG2	4:M:23:ASP:OD2	2.20	0.41
3:I:43:ASP:C	3:I:45:LYS:H	2.24	0.41
3:I:114:VAL:HG12	3:I:115:ASP:N	2.34	0.41
1:A:594:ILE:HA	1:A:594:ILE:HD12	1.62	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:367:LYS:HZ1	1:A:398:ASP:HB3	1.85	0.41
4:U:9:ASN:ND2	4:U:13:GLU:H	2.17	0.41
2:B:305:ASN:ND2	2:B:567:ILE:HG23	2.34	0.41
1:A:286:THR:HG22	1:A:287:ILE:N	2.34	0.41
4:U:376:ASN:HB3	4:U:377:ASP:OD1	2.20	0.41
4:M:252:VAL:HA	4:M:265:PHE:HB3	2.02	0.41
1:A:132:LEU:HA	1:A:132:LEU:HD23	1.76	0.41
1:A:311:PHE:CZ	1:A:348:LEU:HB3	2.54	0.41
2:E:351:ILE:HA	2:E:354:VAL:HB	2.02	0.41
2:E:174:PRO:HA	2:E:177:VAL:CG2	2.49	0.41
2:B:285:ALA:HB3	2:B:286:PRO:CD	2.48	0.41
2:E:497:SER:C	2:E:499:THR:N	2.73	0.41
1:A:83:LEU:HD11	1:A:98:ILE:HD13	2.03	0.41
1:A:61:LYS:NZ	6:A:1626:SO4:O2	2.50	0.41
1:L:473:ASP:C	1:L:475:VAL:H	2.24	0.41
2:E:123:CYS:SG	2:E:159:GLN:HG3	2.60	0.41
2:E:257:LEU:HD12	4:U:76:ALA:HB2	2.01	0.41
2:E:76:TYR:O	2:E:76:TYR:CD2	2.73	0.41
2:B:179:ASN:ND2	4:M:122:GLN:OE1	2.39	0.41
2:E:101:LEU:O	2:E:105:LEU:HB2	2.20	0.41
2:E:307:ASN:ND2	2:E:575:HIS:CE1	2.84	0.41
2:B:488:ILE:HD12	2:B:506:VAL:HG22	2.02	0.41
4:U:168:TYR:H	4:U:207:SER:HB3	1.85	0.41
1:L:504:LEU:O	1:L:548:PHE:HE1	2.03	0.41
1:A:77:MET:SD	1:A:108:LEU:HD21	2.60	0.41
1:A:497:VAL:HG22	1:A:529:LYS:HD3	2.02	0.41
2:B:288:LEU:HG	2:B:306:ILE:HD13	2.01	0.41
1:A:40:ILE:O	1:A:43:LYS:HB2	2.20	0.41
1:L:366:VAL:HG12	1:L:367:LYS:N	2.36	0.41
2:E:40:ALA:CA	2:E:43:VAL:HG22	2.44	0.41
2:E:325:PHE:HA	2:E:342:MET:HE2	2.02	0.41
2:B:419:ARG:CZ	2:B:548:ILE:HG21	2.50	0.41
1:A:109:ILE:HG21	1:A:142:GLU:HG2	2.03	0.41
2:E:26:LYS:HB2	2:E:29:LYS:HB2	2.01	0.41
2:E:21:GLU:HB3	2:E:33:ALA:HB1	2.02	0.41
4:M:392:VAL:HA	4:M:393:PRO:HD3	1.68	0.41
4:M:290:ILE:HB	4:M:306:VAL:HB	2.02	0.41
1:A:462:TRP:HB2	1:A:499:VAL:CG2	2.50	0.41
1:A:310:LEU:HA	1:A:310:LEU:HD12	1.74	0.41
3:I:31:LEU:HD12	3:I:31:LEU:HA	1.78	0.41
3:S:43:ASP:C	3:S:45:LYS:H	2.23	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:S:23:PHE:HB2	3:S:28:LYS:HD3	2.02	0.41
2:B:151:ILE:O	2:B:152:ASN:HB2	2.19	0.41
2:E:521:ASP:O	2:E:525:ILE:HD12	2.20	0.41
1:L:442:TYR:O	1:L:443:VAL:C	2.59	0.41
2:E:541:VAL:HG23	2:E:542:LEU:N	2.34	0.41
2:B:34:VAL:O	2:B:38:ILE:HG13	2.20	0.41
3:I:84:ILE:HG21	3:I:84:ILE:HD13	1.71	0.41
2:E:122:LEU:O	2:E:123:CYS:C	2.58	0.41
2:E:335:LYS:HB3	2:E:369:PHE:CE1	2.56	0.41
4:M:136:GLN:HG2	4:M:136:GLN:H	1.67	0.41
1:L:584:LEU:O	1:L:584:LEU:HD12	2.21	0.41
4:M:212:CYS:HB3	4:M:406:VAL:HA	2.03	0.41
1:L:602:MET:HA	1:L:603:PRO:HD3	1.80	0.41
4:M:325:PRO:CB	4:M:384:PRO:HG2	2.51	0.41
2:E:86:MET:HB2	2:E:86:MET:HE2	1.72	0.41
1:L:263:ARG:HD3	1:L:312:GLU:OE2	2.21	0.41
2:E:24:ASN:ND2	2:E:29:LYS:HD2	2.36	0.41
2:B:529:LEU:CD2	2:B:537:ALA:HA	2.48	0.41
2:B:322:LYS:HE2	2:B:353:GLN:HE22	1.85	0.41
4:M:266:ILE:CD1	4:M:266:ILE:N	2.83	0.41
2:E:250:HIS:O	2:E:250:HIS:ND1	2.54	0.41
4:U:220:ILE:HG22	4:U:221:VAL:N	2.35	0.41
2:B:426:GLU:OE1	2:B:458:ARG:HG2	2.21	0.41
3:I:29:GLN:HA	3:I:29:GLN:NE2	2.36	0.41
4:M:166:ILE:HG12	4:M:208:GLY:H	1.86	0.41
4:M:218:ASP:HB3	4:M:219:LYS:H	1.50	0.41
4:U:28:ALA:HB2	4:U:53:THR:HG21	2.02	0.41
2:E:488:ILE:HD12	2:E:506:VAL:HG22	2.03	0.41
1:L:144:ALA:O	1:L:148:ALA:HB2	2.20	0.41
1:A:526:LEU:HA	1:A:526:LEU:HD23	1.93	0.41
3:S:43:ASP:O	3:S:45:LYS:N	2.51	0.41
2:B:101:LEU:O	2:B:105:LEU:HB2	2.21	0.41
2:E:288:LEU:CD2	2:E:288:LEU:H	2.33	0.41
4:M:40:ARG:HB3	4:M:284:ILE:CD1	2.51	0.41
1:A:556:LYS:O	1:A:557:ALA:C	2.58	0.41
1:L:594:ILE:HA	1:L:594:ILE:HD12	1.66	0.41
4:U:312:LYS:O	4:U:315:LEU:HD12	2.21	0.41
2:E:453:GLY:C	2:E:454:GLU:O	2.57	0.41
2:E:217:TRP:HE1	4:U:123:ASN:CA	2.30	0.41
1:A:341:ARG:N	1:A:341:ARG:HD3	2.36	0.41
4:M:408:GLU:HA	4:M:409:PRO:HD3	1.61	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:183:VAL:HA	1:A:184:PRO:HD3	1.84	0.41
4:U:104:ASN:HD21	4:U:138:ILE:H	1.69	0.41
1:A:253:PRO:O	1:A:254:ALA:C	2.59	0.41
2:E:555:ILE:HG22	2:E:556:GLU:N	2.36	0.41
1:L:412:TYR:CE2	1:L:424:ILE:HD11	2.56	0.41
4:U:183:LEU:HD11	4:U:185:MET:HB2	2.03	0.41
3:S:18:LYS:HG2	3:S:20:TYR:OH	2.21	0.41
2:B:536:THR:HA	2:B:539:GLU:HB2	2.03	0.41
1:L:193:VAL:HA	1:L:211:ILE:HD11	2.01	0.41
1:L:254:ALA:N	1:L:255:PRO:HD3	2.36	0.41
2:E:452:VAL:O	2:E:456:ALA:HB2	2.21	0.41
4:U:389:ASN:HA	4:U:428:SER:OG	2.21	0.41
2:E:227:SER:OG	2:E:261:LYS:HE3	2.21	0.41
4:M:394:PHE:O	4:M:396:PRO:HD3	2.21	0.41
1:A:521:ILE:HD13	1:A:521:ILE:HA	1.80	0.41
1:L:576:LEU:HA	1:L:576:LEU:HD12	1.86	0.41
1:L:201:LEU:HA	1:L:201:LEU:HD23	1.77	0.41
1:A:110:ARG:CZ	1:A:110:ARG:HB3	2.48	0.41
4:U:222:ILE:HD12	4:U:222:ILE:N	2.25	0.41
2:B:330:ASP:HA	2:B:331:PRO:HD2	1.95	0.41
1:A:594:ILE:CG2	1:A:595:LEU:N	2.83	0.41
1:A:353:MET:HG2	1:A:366:VAL:HG22	2.03	0.41
2:E:54:VAL:CG1	2:E:69:VAL:HG13	2.49	0.41
1:A:615:LYS:NZ	4:U:341:LYS:NZ	2.68	0.41
1:L:527:HIS:HA	1:L:545:TYR:OH	2.21	0.41
4:U:80:GLU:OE1	4:U:80:GLU:HA	2.21	0.41
1:L:541:LEU:HA	1:L:541:LEU:HD12	1.82	0.41
1:A:264:LEU:O	1:A:264:LEU:HG	2.20	0.41
1:L:514:ASP:HA	1:L:515:PRO:HD3	1.91	0.40
2:B:139:LYS:NZ	4:M:122:GLN:HG3	2.35	0.40
4:U:430:ILE:HG13	4:U:432:GLU:HG3	2.02	0.40
1:L:367:LYS:HZ1	1:L:398:ASP:HB3	1.85	0.40
4:M:373:LEU:HD23	4:M:373:LEU:HA	1.90	0.40
2:B:497:SER:C	2:B:499:THR:N	2.73	0.40
2:B:103:ARG:NH1	2:B:132:ASP:OD1	2.54	0.40
2:E:420:LYS:HD2	2:E:548:ILE:O	2.21	0.40
4:U:241:ILE:N	4:U:241:ILE:CD1	2.84	0.40
2:B:13:GLY:O	2:B:14:GLU:CB	2.68	0.40
2:B:47:VAL:HG12	2:B:48:SER:H	1.86	0.40
4:M:173:LEU:C	4:M:173:LEU:HD12	2.41	0.40
1:A:428:VAL:HG11	1:A:449:LEU:HD11	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:92:VAL:HG13	2:B:125:PRO:HG3	2.03	0.40
4:M:197:SER:OG	4:M:278:ARG:NH1	2.54	0.40
2:E:124:GLU:HG3	2:E:127:ARG:HH12	1.86	0.40
2:B:173:ASN:HA	2:B:174:PRO:HD3	1.80	0.40
4:M:217:ASN:O	4:M:218:ASP:O	2.39	0.40
3:I:92:ASN:ND2	3:I:97:ASN:HA	2.34	0.40
2:E:488:ILE:HD12	2:E:506:VAL:CG2	2.51	0.40
1:L:55:LYS:O	1:L:56:LYS:C	2.60	0.40
4:U:29:VAL:HG13	4:U:30:ASP:N	2.36	0.40
4:U:7:ILE:HG23	4:U:65:LEU:HB3	2.02	0.40
1:A:135:ILE:CG2	1:A:171:CYS:SG	3.09	0.40
1:A:575:GLU:OE1	2:B:482:LEU:HD23	2.21	0.40
4:M:186:SER:CB	4:M:190:GLN:HB2	2.44	0.40
1:L:40:ILE:O	1:L:43:LYS:HB2	2.21	0.40
2:E:524:TYR:O	2:E:528:ARG:CG	2.67	0.40
1:L:5:SER:OG	1:L:6:LYS:N	2.55	0.40
2:B:458:ARG:HD2	2:B:458:ARG:HA	1.75	0.40
4:U:326:THR:HG22	4:U:370:ILE:HD13	2.02	0.40
1:A:112:ILE:O	1:A:116:ILE:HG13	2.22	0.40
2:E:418:PHE:CE2	2:E:429:ILE:HD11	2.56	0.40
2:B:554:LEU:H	2:B:554:LEU:HD12	1.86	0.40
1:A:597:THR:OG1	1:L:324:PRO:HG2	2.21	0.40
1:L:507:PHE:HB3	1:L:510:LEU:HD11	2.04	0.40
2:B:134:ASP:HA	2:B:135:PRO:HD3	1.95	0.40
2:B:306:ILE:HG23	2:B:317:LEU:CD1	2.51	0.40
1:L:401:ASN:HD22	1:L:401:ASN:C	2.25	0.40
2:E:581:PHE:O	2:E:582:VAL:HG23	2.22	0.40
2:B:420:LYS:O	2:B:421:TYR:CD2	2.75	0.40
2:E:415:ARG:NH1	2:E:447:ALA:HA	2.36	0.40
2:E:366:ASP:O	2:E:370:VAL:HG23	2.21	0.40
2:B:18:LEU:HA	2:B:18:LEU:HD23	1.89	0.40
4:U:173:LEU:HD12	4:U:173:LEU:C	2.41	0.40
4:U:318:GLN:O	4:U:319:LYS:C	2.59	0.40
4:U:415:ASP:OD2	4:U:420:LYS:NZ	2.55	0.40
1:A:193:VAL:HA	1:A:211:ILE:HD11	2.02	0.40
1:A:489:ALA:HA	1:A:490:PRO:HD3	1.78	0.40
1:A:540:LEU:HD12	1:A:540:LEU:O	2.21	0.40
4:M:88:VAL:HG21	4:M:124:SER:OG	2.22	0.40
1:L:20:ILE:HG22	1:L:21:ARG:N	2.37	0.40
4:M:162:ARG:HD2	4:M:267:PRO:O	2.21	0.40
1:A:573:ASP:OD2	1:A:574:VAL:N	2.54	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:551:LEU:HB3	1:L:552:PHE:CE2	2.57	0.40
4:U:9:ASN:C	4:U:9:ASN:ND2	2.73	0.40
2:E:436:LEU:HD21	2:E:448:MET:CG	2.52	0.40
2:B:502:LEU:O	2:B:506:VAL:HG23	2.21	0.40
4:U:16:ILE:HD12	4:U:108:ILE:CG2	2.52	0.40
4:M:196:VAL:HB	4:M:279:THR:HG23	2.04	0.40
2:B:355:LEU:HD22	2:B:377:ILE:HG23	2.03	0.40
2:E:326:VAL:HG13	2:E:335:LYS:HG2	2.04	0.40
1:A:268:TYR:HB3	1:A:269:PRO:CD	2.52	0.40
1:L:52:GLY:HA3	1:L:90:GLU:OE2	2.21	0.40
1:L:462:TRP:HB2	1:L:499:VAL:CG2	2.52	0.40
4:U:176:ASP:HB3	4:U:178:LEU:HD21	2.04	0.40
2:B:76:TYR:O	2:B:76:TYR:CD2	2.74	0.40
4:M:248:PHE:N	4:M:248:PHE:CD1	2.89	0.40
3:I:78:LEU:HA	3:I:78:LEU:HD23	1.91	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	619/623 (99%)	532 (86%)	64 (10%)	23 (4%)	4	21
1	L	619/623 (99%)	534 (86%)	63 (10%)	22 (4%)	4	22
2	B	569/591 (96%)	469 (82%)	67 (12%)	33 (6%)	2	11
2	E	569/591 (96%)	469 (82%)	68 (12%)	32 (6%)	2	11
3	I	140/142 (99%)	119 (85%)	19 (14%)	2 (1%)	14	50
3	S	140/142 (99%)	118 (84%)	20 (14%)	2 (1%)	14	50
4	M	403/435 (93%)	321 (80%)	58 (14%)	24 (6%)	2	10
4	U	403/435 (93%)	325 (81%)	55 (14%)	23 (6%)	2	11

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	P	6/11 (54%)	4 (67%)	2 (33%)	0	100	100
5	Q	6/11 (54%)	5 (83%)	1 (17%)	0	100	100
All	All	3474/3604 (96%)	2896 (83%)	417 (12%)	161 (5%)	3	16

All (161) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	22	ASN
1	A	47	ASP
1	A	240	ALA
1	A	453	ALA
1	A	492	CYS
1	A	532	LEU
1	A	602	MET
1	A	618	LYS
2	B	47	VAL
2	B	233	ASP
2	B	250	HIS
2	B	274	SER
2	B	350	ASN
2	B	422	PRO
2	B	424	LYS
2	B	497	SER
2	B	550	GLU
2	E	47	VAL
2	E	233	ASP
2	E	250	HIS
2	E	274	SER
2	E	350	ASN
2	E	422	PRO
2	E	424	LYS
2	E	497	SER
2	E	550	GLU
3	I	96	HIS
1	L	22	ASN
1	L	47	ASP
1	L	240	ALA
1	L	382	ASP
1	L	453	ALA
1	L	492	CYS
1	L	532	LEU

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Mol	Chain	Res	Type
1	L	602	MET
1	L	618	LYS
4	M	24	ILE
4	M	27	ASN
4	M	29	VAL
4	M	123	ASN
4	M	136	GLN
4	M	218	ASP
4	M	262	SER
4	M	377	ASP
4	M	381	TRP
3	S	96	HIS
4	U	27	ASN
4	U	29	VAL
4	U	123	ASN
4	U	136	GLN
4	U	218	ASP
4	U	235	LYS
4	U	262	SER
4	U	377	ASP
4	U	381	TRP
1	A	8	ASP
1	A	24	LYS
1	A	323	GLU
1	A	382	ASP
1	A	600	GLU
1	A	608	ARG
1	A	621	GLY
2	B	14	GLU
2	B	59	GLN
2	B	76	TYR
2	B	152	ASN
2	B	215	THR
2	B	252	ASN
2	B	272	LYS
2	B	275	ASP
2	E	14	GLU
2	E	59	GLN
2	E	152	ASN
2	E	215	THR
2	E	252	ASN
2	E	272	LYS

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Mol	Chain	Res	Type
2	E	275	ASP
2	E	436	LEU
1	L	8	ASP
1	L	24	LYS
1	L	474	ASP
1	L	600	GLU
1	L	608	ARG
1	L	621	GLY
4	M	160	GLY
4	M	235	LYS
4	M	294	ARG
4	M	412	ASN
4	U	24	ILE
4	U	160	GLY
4	U	412	ASN
1	A	342	GLU
1	A	451	ARG
1	A	474	ASP
2	B	172	SER
2	B	177	VAL
2	B	348	GLN
2	B	364	GLU
2	B	436	LEU
2	B	437	ASP
2	E	76	TYR
2	E	172	SER
2	E	348	GLN
2	E	437	ASP
2	E	463	ASP
3	I	44	ALA
1	L	342	GLU
1	L	451	ARG
4	M	93	PHE
4	M	126	THR
4	M	128	ALA
4	M	338	MET
4	U	93	PHE
4	U	338	MET
1	A	244	LEU
2	B	123	CYS
2	B	199	LEU
2	B	270	LEU

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Mol	Chain	Res	Type
2	B	273	ASP
2	B	461	ASN
2	B	463	ASP
2	B	543	SER
2	B	553	ASP
2	E	199	LEU
2	E	270	LEU
2	E	553	ASP
1	L	323	GLU
4	M	260	GLU
4	M	380	LYS
4	M	383	ARG
3	S	44	ALA
4	U	51	ALA
4	U	128	ALA
4	U	260	GLU
4	U	294	ARG
4	U	380	LYS
4	U	383	ARG
1	A	184	PRO
2	B	542	LEU
2	E	123	CYS
2	E	364	GLU
2	E	407	VAL
2	E	461	ASN
2	E	542	LEU
1	L	105	ASN
1	L	184	PRO
1	L	244	LEU
4	M	140	SER
4	M	169	ARG
4	M	199	ARG
4	M	261	ARG
4	U	126	THR
4	U	140	SER
4	U	261	ARG
1	A	105	ASN
1	A	380	GLU
2	E	543	SER
2	B	407	VAL
2	E	533	ASP
1	L	186	GLY

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Mol	Chain	Res	Type
1	A	186	GLY

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	542/544 (100%)	474 (88%)	68 (12%)	6	22
1	L	542/544 (100%)	476 (88%)	66 (12%)	6	24
2	B	514/532 (97%)	438 (85%)	76 (15%)	4	16
2	E	514/532 (97%)	440 (86%)	74 (14%)	4	17
3	I	131/131 (100%)	124 (95%)	7 (5%)	28	66
3	S	131/131 (100%)	123 (94%)	8 (6%)	23	60
4	M	364/387 (94%)	312 (86%)	52 (14%)	4	17
4	U	364/387 (94%)	316 (87%)	48 (13%)	5	20
5	P	8/10 (80%)	7 (88%)	1 (12%)	6	22
5	Q	8/10 (80%)	7 (88%)	1 (12%)	6	22
All	All	3118/3208 (97%)	2717 (87%)	401 (13%)	5	21

All (401) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	LYS
1	A	10	MET
1	A	20	ILE
1	A	22	ASN
1	A	32	ARG
1	A	47	ASP
1	A	50	LEU
1	A	60	CYS
1	A	102	VAL
1	A	103	ASN
1	A	104	SER
1	A	106	SER

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Mol	Chain	Res	Type
1	A	114	ASN
1	A	163	SER
1	A	181	ASP
1	A	224	THR
1	A	234	SER
1	A	245	GLN
1	A	263	ARG
1	A	272	GLU
1	A	280	LEU
1	A	299	LYS
1	A	300	VAL
1	A	322	SER
1	A	341	ARG
1	A	342	GLU
1	A	348	LEU
1	A	352	SER
1	A	355	THR
1	A	358	SER
1	A	366	VAL
1	A	374	ILE
1	A	379	THR
1	A	390	VAL
1	A	400	SER
1	A	401	ASN
1	A	404	GLN
1	A	409	MET
1	A	413	LEU
1	A	417	ASP
1	A	419	SER
1	A	423	GLU
1	A	426	LEU
1	A	433	GLU
1	A	437	VAL
1	A	447	LEU
1	A	458	SER
1	A	461	VAL
1	A	467	GLN
1	A	483	VAL
1	A	509	ASN
1	A	510	LEU
1	A	511	ILE
1	A	516	ARG

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Mol	Chain	Res	Type
1	A	529	LYS
1	A	532	LEU
1	A	540	LEU
1	A	541	LEU
1	A	554	GLU
1	A	576	LEU
1	A	579	ARG
1	A	585	ARG
1	A	586	LEU
1	A	591	SER
1	A	594	ILE
1	A	605	PHE
1	A	613	LEU
1	A	623	SER
2	B	12	LYS
2	B	58	MET
2	B	75	ASN
2	B	88	VAL
2	B	89	ASN
2	B	90	SER
2	B	96	GLU
2	B	102	ILE
2	B	116	ASP
2	B	123	CYS
2	B	126	LEU
2	B	127	ARG
2	B	130	LEU
2	B	140	THR
2	B	143	VAL
2	B	148	LEU
2	B	151	ILE
2	B	155	MET
2	B	162	LEU
2	B	164	SER
2	B	165	LEU
2	B	168	LEU
2	B	172	SER
2	B	173	ASN
2	B	186	GLU
2	B	193	ASN
2	B	195	ASN
2	B	202	GLN

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Mol	Chain	Res	Type
2	B	203	ASN
2	B	207	LEU
2	B	208	LEU
2	B	209	THR
2	B	214	CYS
2	B	230	ASN
2	B	238	GLN
2	B	244	VAL
2	B	245	THR
2	B	267	LEU
2	B	275	ASP
2	B	279	MET
2	B	283	LYS
2	B	288	LEU
2	B	318	LYS
2	B	348	GLN
2	B	351	ILE
2	B	359	LYS
2	B	360	GLU
2	B	365	VAL
2	B	374	VAL
2	B	386	GLN
2	B	390	ARG
2	B	394	THR
2	B	396	LEU
2	B	408	GLN
2	B	411	ILE
2	B	423	ASN
2	B	427	SER
2	B	458	ARG
2	B	459	ILE
2	B	460	ASP
2	B	463	ASP
2	B	474	HIS
2	B	477	SER
2	B	480	VAL
2	B	485	LEU
2	B	503	VAL
2	B	506	VAL
2	B	511	THR
2	B	528	ARG
2	B	535	VAL

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Mol	Chain	Res	Type
2	B	543	SER
2	B	545	LYS
2	B	558	THR
2	B	563	LEU
2	B	572	SER
2	B	581	PHE
2	E	12	LYS
2	E	58	MET
2	E	75	ASN
2	E	88	VAL
2	E	89	ASN
2	E	90	SER
2	E	96	GLU
2	E	102	ILE
2	E	116	ASP
2	E	123	CYS
2	E	126	LEU
2	E	127	ARG
2	E	130	LEU
2	E	140	THR
2	E	143	VAL
2	E	148	LEU
2	E	151	ILE
2	E	155	MET
2	E	162	LEU
2	E	164	SER
2	E	165	LEU
2	E	167	ASP
2	E	168	LEU
2	E	173	ASN
2	E	193	ASN
2	E	195	ASN
2	E	202	GLN
2	E	203	ASN
2	E	207	LEU
2	E	208	LEU
2	E	209	THR
2	E	214	CYS
2	E	230	ASN
2	E	238	GLN
2	E	244	VAL
2	E	245	THR

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Mol	Chain	Res	Type
2	E	267	LEU
2	E	275	ASP
2	E	279	MET
2	E	283	LYS
2	E	288	LEU
2	E	318	LYS
2	E	348	GLN
2	E	351	ILE
2	E	359	LYS
2	E	360	GLU
2	E	365	VAL
2	E	374	VAL
2	E	386	GLN
2	E	390	ARG
2	E	396	LEU
2	E	408	GLN
2	E	411	ILE
2	E	423	ASN
2	E	427	SER
2	E	458	ARG
2	E	459	ILE
2	E	460	ASP
2	E	463	ASP
2	E	474	HIS
2	E	477	SER
2	E	480	VAL
2	E	485	LEU
2	E	493	LEU
2	E	503	VAL
2	E	506	VAL
2	E	511	THR
2	E	528	ARG
2	E	543	SER
2	E	545	LYS
2	E	558	THR
2	E	563	LEU
2	E	572	SER
2	E	581	PHE
3	I	28	LYS
3	I	31	LEU
3	I	86	ASN
3	I	102	ASP

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Mol	Chain	Res	Type
3	I	112	THR
3	I	114	VAL
3	I	130	LYS
1	L	6	LYS
1	L	10	MET
1	L	20	ILE
1	L	22	ASN
1	L	32	ARG
1	L	33	ILE
1	L	47	ASP
1	L	50	LEU
1	L	60	CYS
1	L	102	VAL
1	L	103	ASN
1	L	104	SER
1	L	106	SER
1	L	163	SER
1	L	181	ASP
1	L	224	THR
1	L	227	SER
1	L	234	SER
1	L	245	GLN
1	L	263	ARG
1	L	272	GLU
1	L	299	LYS
1	L	322	SER
1	L	341	ARG
1	L	342	GLU
1	L	348	LEU
1	L	352	SER
1	L	355	THR
1	L	358	SER
1	L	366	VAL
1	L	374	ILE
1	L	390	VAL
1	L	400	SER
1	L	401	ASN
1	L	404	GLN
1	L	409	MET
1	L	413	LEU
1	L	417	ASP
1	L	419	SER

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Mol	Chain	Res	Type
1	L	423	GLU
1	L	426	LEU
1	L	433	GLU
1	L	437	VAL
1	L	447	LEU
1	L	458	SER
1	L	461	VAL
1	L	483	VAL
1	L	509	ASN
1	L	510	LEU
1	L	511	ILE
1	L	516	ARG
1	L	529	LYS
1	L	532	LEU
1	L	540	LEU
1	L	541	LEU
1	L	554	GLU
1	L	562	VAL
1	L	576	LEU
1	L	579	ARG
1	L	585	ARG
1	L	586	LEU
1	L	591	SER
1	L	594	ILE
1	L	605	PHE
1	L	613	LEU
1	L	623	SER
4	M	5	LEU
4	M	8	TYR
4	M	9	ASN
4	M	16	ILE
4	M	18	ARG
4	M	19	VAL
4	M	21	ARG
4	M	23	ASP
4	M	43	VAL
4	M	47	VAL
4	M	60	ARG
4	M	65	LEU
4	M	85	MET
4	M	95	LYS
4	M	96	ILE

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Mol	Chain	Res	Type
4	M	106	VAL
4	M	111	LEU
4	M	122	GLN
4	M	123	ASN
4	M	130	LYS
4	M	139	LYS
4	M	166	ILE
4	M	169	ARG
4	M	186	SER
4	M	204	SER
4	M	206	LEU
4	M	219	LYS
4	M	233	THR
4	M	244	ASP
4	M	253	ARG
4	M	263	ILE
4	M	266	ILE
4	M	273	GLU
4	M	278	ARG
4	M	279	THR
4	M	293	VAL
4	M	296	VAL
4	M	299	THR
4	M	311	PHE
4	M	312	LYS
4	M	314	SER
4	M	315	LEU
4	M	316	LEU
4	M	341	LYS
4	M	364	SER
4	M	387	SER
4	M	400	LYS
4	M	410	LYS
4	M	421	TRP
4	M	422	VAL
4	M	430	ILE
4	M	435	CYS
5	P	2	MET
5	Q	2	MET
3	S	6	LEU
3	S	28	LYS
3	S	31	LEU

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Mol	Chain	Res	Type
3	S	86	ASN
3	S	102	ASP
3	S	112	THR
3	S	114	VAL
3	S	130	LYS
4	U	8	TYR
4	U	9	ASN
4	U	16	ILE
4	U	18	ARG
4	U	19	VAL
4	U	21	ARG
4	U	23	ASP
4	U	47	VAL
4	U	60	ARG
4	U	65	LEU
4	U	85	MET
4	U	95	LYS
4	U	96	ILE
4	U	106	VAL
4	U	111	LEU
4	U	122	GLN
4	U	123	ASN
4	U	130	LYS
4	U	139	LYS
4	U	166	ILE
4	U	169	ARG
4	U	186	SER
4	U	204	SER
4	U	206	LEU
4	U	209	MET
4	U	219	LYS
4	U	233	THR
4	U	244	ASP
4	U	253	ARG
4	U	263	ILE
4	U	266	ILE
4	U	278	ARG
4	U	279	THR
4	U	296	VAL
4	U	299	THR
4	U	311	PHE
4	U	314	SER

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Mol	Chain	Res	Type
4	U	315	LEU
4	U	316	LEU
4	U	341	LYS
4	U	387	SER
4	U	400	LYS
4	U	407	PHE
4	U	410	LYS
4	U	421	TRP
4	U	422	VAL
4	U	430	ILE
4	U	435	CYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (95) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	103	ASN
1	A	200	HIS
1	A	301	GLN
1	A	319	HIS
1	A	320	HIS
1	A	401	ASN
1	A	467	GLN
1	A	488	GLN
1	A	495	ASN
1	A	509	ASN
1	A	527	HIS
1	A	550	ASN
1	A	568	GLN
2	B	152	ASN
2	B	191	HIS
2	B	193	ASN
2	B	228	ASN
2	B	278	ASN
2	B	305	ASN
2	B	307	ASN
2	B	311	GLN
2	B	319	GLN
2	B	348	GLN
2	B	353	GLN
2	B	386	GLN
2	B	408	GLN
2	B	435	ASN

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Mol	Chain	Res	Type
2	B	481	GLN
2	B	504	GLN
2	B	512	GLN
2	B	575	HIS
2	E	152	ASN
2	E	191	HIS
2	E	193	ASN
2	E	228	ASN
2	E	278	ASN
2	E	305	ASN
2	E	307	ASN
2	E	311	GLN
2	E	319	GLN
2	E	348	GLN
2	E	353	GLN
2	E	386	GLN
2	E	408	GLN
2	E	435	ASN
2	E	481	GLN
2	E	504	GLN
2	E	512	GLN
2	E	575	HIS
3	I	8	GLN
3	I	29	GLN
3	I	36	HIS
3	I	48	ASN
3	I	86	ASN
3	I	92	ASN
3	I	128	GLN
1	L	103	ASN
1	L	200	HIS
1	L	301	GLN
1	L	319	HIS
1	L	320	HIS
1	L	401	ASN
1	L	467	GLN
1	L	488	GLN
1	L	495	ASN
1	L	509	ASN
1	L	527	HIS
1	L	550	ASN
1	L	568	GLN

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Mol	Chain	Res	Type
4	M	9	ASN
4	M	42	GLN
4	M	72	ASN
4	M	100	ASN
4	M	104	ASN
4	M	141	GLN
4	M	182	ASN
4	M	318	GLN
4	M	349	ASN
5	P	4	GLN
5	Q	4	GLN
3	S	8	GLN
3	S	29	GLN
3	S	48	ASN
3	S	92	ASN
3	S	128	GLN
4	U	9	ASN
4	U	42	GLN
4	U	72	ASN
4	U	100	ASN
4	U	104	ASN
4	U	135	GLN
4	U	141	GLN
4	U	182	ASN
4	U	318	GLN
4	U	349	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

2 non-standard protein/DNA/RNA residues 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	$\# Z > 2$
5	SEP	P	3	5	4,5,10	0.56	0	2,5,14	0.92	0
5	SEP	Q	3	5	4,5,10	0.50	0	2,5,14	0.72	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
5	SEP	P	3	5	-	0/2/4/10	0/0/0/0
5	SEP	Q	3	5	-	0/2/4/10	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.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	P	3	SEP	1	0
5	Q	3	SEP	1	0

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

31 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
6	SO4	A	1624	-	4,4,4	0.39	0	6,6,6	0.13	0
6	SO4	A	1625	-	4,4,4	0.22	0	6,6,6	0.24	0
6	SO4	A	1626	-	4,4,4	0.16	0	6,6,6	0.39	0
6	SO4	A	1627	-	4,4,4	0.22	0	6,6,6	0.33	0
6	SO4	A	1628	-	4,4,4	0.11	0	6,6,6	0.22	0
6	SO4	A	1629	-	4,4,4	0.20	0	6,6,6	0.25	0
6	SO4	A	1630	-	4,4,4	0.17	0	6,6,6	0.19	0
6	SO4	B	1583	-	4,4,4	0.22	0	6,6,6	0.20	0
6	SO4	B	1584	-	4,4,4	0.13	0	6,6,6	0.10	0
6	SO4	B	1585	-	4,4,4	0.10	0	6,6,6	0.12	0
6	SO4	B	1586	-	4,4,4	0.21	0	6,6,6	0.08	0
6	SO4	E	1583	-	4,4,4	0.19	0	6,6,6	0.20	0
6	SO4	E	1584	-	4,4,4	0.17	0	6,6,6	0.20	0
6	SO4	E	1585	-	4,4,4	0.21	0	6,6,6	0.32	0
6	SO4	E	1586	-	4,4,4	0.15	0	6,6,6	0.15	0
6	SO4	E	1587	-	4,4,4	0.27	0	6,6,6	0.32	0
6	SO4	L	1624	-	4,4,4	0.19	0	6,6,6	0.28	0
6	SO4	L	1625	-	4,4,4	0.15	0	6,6,6	0.20	0
6	SO4	L	1626	-	4,4,4	0.15	0	6,6,6	0.32	0
6	SO4	L	1627	-	4,4,4	0.17	0	6,6,6	0.24	0
6	SO4	L	1628	-	4,4,4	0.17	0	6,6,6	0.25	0
6	SO4	L	1629	-	4,4,4	0.19	0	6,6,6	0.38	0
6	SO4	L	1630	-	4,4,4	0.18	0	6,6,6	0.10	0
6	SO4	L	1631	-	4,4,4	0.12	0	6,6,6	0.11	0
6	SO4	M	1436	-	4,4,4	0.28	0	6,6,6	0.22	0
6	SO4	M	1437	-	4,4,4	0.15	0	6,6,6	0.39	0
6	SO4	M	1438	-	4,4,4	0.16	0	6,6,6	0.33	0
6	SO4	U	1436	-	4,4,4	0.26	0	6,6,6	0.18	0
6	SO4	U	1437	-	4,4,4	0.13	0	6,6,6	0.14	0
6	SO4	U	1438	-	4,4,4	0.21	0	6,6,6	0.67	0
6	SO4	U	1439	-	4,4,4	0.14	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
6	SO4	A	1624	-	-	0/0/0/0	0/0/0/0
6	SO4	A	1625	-	-	0/0/0/0	0/0/0/0
6	SO4	A	1626	-	-	0/0/0/0	0/0/0/0
6	SO4	A	1627	-	-	0/0/0/0	0/0/0/0
6	SO4	A	1628	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	SO4	A	1629	-	-	0/0/0/0	0/0/0/0
6	SO4	A	1630	-	-	0/0/0/0	0/0/0/0
6	SO4	B	1583	-	-	0/0/0/0	0/0/0/0
6	SO4	B	1584	-	-	0/0/0/0	0/0/0/0
6	SO4	B	1585	-	-	0/0/0/0	0/0/0/0
6	SO4	B	1586	-	-	0/0/0/0	0/0/0/0
6	SO4	E	1583	-	-	0/0/0/0	0/0/0/0
6	SO4	E	1584	-	-	0/0/0/0	0/0/0/0
6	SO4	E	1585	-	-	0/0/0/0	0/0/0/0
6	SO4	E	1586	-	-	0/0/0/0	0/0/0/0
6	SO4	E	1587	-	-	0/0/0/0	0/0/0/0
6	SO4	L	1624	-	-	0/0/0/0	0/0/0/0
6	SO4	L	1625	-	-	0/0/0/0	0/0/0/0
6	SO4	L	1626	-	-	0/0/0/0	0/0/0/0
6	SO4	L	1627	-	-	0/0/0/0	0/0/0/0
6	SO4	L	1628	-	-	0/0/0/0	0/0/0/0
6	SO4	L	1629	-	-	0/0/0/0	0/0/0/0
6	SO4	L	1630	-	-	0/0/0/0	0/0/0/0
6	SO4	L	1631	-	-	0/0/0/0	0/0/0/0
6	SO4	M	1436	-	-	0/0/0/0	0/0/0/0
6	SO4	M	1437	-	-	0/0/0/0	0/0/0/0
6	SO4	M	1438	-	-	0/0/0/0	0/0/0/0
6	SO4	U	1436	-	-	0/0/0/0	0/0/0/0
6	SO4	U	1437	-	-	0/0/0/0	0/0/0/0
6	SO4	U	1438	-	-	0/0/0/0	0/0/0/0
6	SO4	U	1439	-	-	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.

10 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	1624	SO4	2	0
6	A	1625	SO4	2	0
6	A	1626	SO4	1	0
6	A	1627	SO4	1	0
6	A	1629	SO4	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	B	1583	SO4	1	0
6	B	1586	SO4	1	0
6	E	1587	SO4	2	0
6	L	1625	SO4	1	0
6	M	1437	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	621/623 (99%)	0.11	30 (4%) 34 19	37, 70, 125, 219	0
1	L	621/623 (99%)	0.07	27 (4%) 39 21	36, 70, 127, 220	0
2	B	571/591 (96%)	0.18	27 (4%) 35 19	38, 82, 147, 231	0
2	E	571/591 (96%)	0.22	32 (5%) 28 14	42, 82, 149, 229	0
3	I	142/142 (100%)	-0.29	0 100 100	39, 63, 107, 136	0
3	S	142/142 (100%)	-0.34	1 (0%) 89 75	43, 66, 106, 138	0
4	M	409/435 (94%)	0.17	20 (4%) 33 18	41, 72, 139, 216	0
4	U	409/435 (94%)	0.17	19 (4%) 36 19	40, 72, 140, 216	0
5	P	8/11 (72%)	0.16	0 100 100	62, 87, 119, 121	0
5	Q	8/11 (72%)	0.18	0 100 100	60, 89, 118, 121	0
All	All	3502/3604 (97%)	0.11	156 (4%) 37 20	36, 73, 136, 231	0

All (156) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	L	240	ALA	9.8
4	M	159	ILE	9.2
1	A	240	ALA	8.7
1	A	242	THR	7.4
1	A	241	SER	7.4
4	U	159	ILE	6.9
4	U	141	GLN	6.5
2	B	25	GLU	6.3
1	L	241	SER	6.3
1	A	243	ASP	5.8
4	U	139	LYS	5.1
1	L	242	THR	5.1
2	B	42	THR	5.0

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Mol	Chain	Res	Type	RSRZ
1	L	243	ASP	4.9
1	A	24	LYS	4.8
2	E	201	PRO	4.4
2	E	204	ILE	4.3
4	M	233	THR	4.3
2	E	278	ASN	4.2
4	M	141	GLN	4.2
2	E	24	ASN	4.2
4	M	160	GLY	4.2
4	M	232	GLU	4.1
2	E	232	LYS	4.1
1	A	35	LYS	4.1
4	M	140	SER	4.0
1	L	44	PHE	4.0
2	E	271	PRO	3.9
2	E	30	ARG	3.9
2	E	32	GLU	3.9
2	B	549	SER	3.8
4	U	124	SER	3.8
4	U	138	ILE	3.8
2	E	121	TYR	3.8
4	M	138	ILE	3.8
2	E	49	SER	3.8
1	L	239	SER	3.7
1	L	33	ILE	3.6
4	U	125	GLU	3.6
4	U	163	ARG	3.6
1	A	244	LEU	3.6
2	B	24	ASN	3.5
2	B	274	SER	3.4
3	S	45	LYS	3.4
1	A	3	ALA	3.3
2	B	23	ASN	3.3
1	L	74	PHE	3.3
2	E	196	LEU	3.3
2	B	280	LEU	3.3
1	L	623	SER	3.3
1	A	37	LEU	3.3
4	M	125	GLU	3.2
4	M	131	THR	3.2
2	B	22	LEU	3.2
2	E	63	LEU	3.1

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Mol	Chain	Res	Type	RSRZ
4	U	222	ILE	3.1
1	A	44	PHE	3.1
1	L	3	ALA	3.0
2	B	49	SER	3.0
2	B	550	GLU	3.0
1	L	50	LEU	3.0
4	U	131	THR	3.0
4	U	136	GLN	3.0
1	A	25	SER	3.0
2	B	436	LEU	2.9
2	E	275	ASP	2.9
2	B	273	ASP	2.9
1	A	104	SER	2.9
1	L	73	ASP	2.9
1	L	45	LYS	2.9
4	U	140	SER	2.8
2	E	277	TYR	2.8
1	L	244	LEU	2.8
2	E	280	LEU	2.8
4	M	136	GLN	2.8
4	U	160	GLY	2.7
2	B	438	SER	2.7
2	B	63	LEU	2.7
1	A	45	LYS	2.7
2	B	270	LEU	2.7
2	E	274	SER	2.7
2	E	31	LYS	2.6
2	B	67	LYS	2.6
2	E	276	TYR	2.6
2	E	267	LEU	2.6
1	L	72	ILE	2.6
4	M	139	LYS	2.6
4	M	28	ALA	2.6
2	E	25	GLU	2.6
1	A	30	ILE	2.6
2	E	36	LYS	2.6
4	M	24	ILE	2.6
4	M	222	ILE	2.5
1	L	37	LEU	2.5
2	E	273	ASP	2.5
1	A	70	HIS	2.5
2	E	241	CYS	2.5

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Mol	Chain	Res	Type	RSRZ
2	B	239	SER	2.5
1	A	239	SER	2.4
1	L	35	LYS	2.4
1	L	40	ILE	2.4
2	B	38	ILE	2.4
4	U	28	ALA	2.4
4	U	164	GLU	2.4
1	A	74	PHE	2.4
4	M	274	LEU	2.4
4	U	130	LYS	2.4
2	B	196	LEU	2.4
4	M	124	SER	2.4
4	M	161	TRP	2.4
1	A	296	LYS	2.4
1	A	417	ASP	2.4
1	L	31	LYS	2.3
4	U	174	PHE	2.3
2	B	16	PHE	2.3
1	A	188	TRP	2.3
1	A	38	ALA	2.3
1	L	298	LYS	2.3
2	E	208	LEU	2.3
2	E	23	ASN	2.2
4	U	407	PHE	2.2
1	A	623	SER	2.2
1	A	4	VAL	2.2
1	A	237	VAL	2.2
4	M	271	GLU	2.2
1	A	297	SER	2.2
2	E	108	ARG	2.2
2	E	153	ALA	2.2
4	M	26	ARG	2.2
2	B	110	MET	2.2
2	E	101	LEU	2.2
1	A	41	ARG	2.2
1	A	341	ARG	2.2
2	B	85	ILE	2.2
2	B	39	ALA	2.2
2	B	276	TYR	2.2
2	B	233	ASP	2.1
1	L	297	SER	2.1
1	L	38	ALA	2.1

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Mol	Chain	Res	Type	RSRZ
2	E	116	ASP	2.1
1	L	296	LYS	2.1
2	B	32	GLU	2.1
2	E	268	GLU	2.1
1	L	58	TYR	2.1
4	M	276	ARG	2.1
1	L	245	GLN	2.1
2	E	238	GLN	2.1
1	L	340	HIS	2.1
2	B	26	LYS	2.1
4	U	137	GLY	2.1
1	A	343	THR	2.0
4	U	269	ASP	2.0
1	L	29	GLU	2.0
2	E	279	MET	2.0
1	A	298	LYS	2.0
1	A	339	GLN	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [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(Å ²)	Q<0.9
5	SEP	Q	3	6/11	0.95	0.12	-	71,84,108,126	0
5	SEP	P	3	6/11	0.91	0.13	-	70,95,107,128	0

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
6	SO4	A	1630	5/5	0.86	0.44	10.64	164,169,180,186	0
6	SO4	A	1629	5/5	0.91	0.58	6.64	117,151,174,187	0
6	SO4	U	1437	5/5	0.93	0.26	4.35	92,110,143,154	0
6	SO4	L	1627	5/5	0.87	0.29	3.90	101,106,135,154	0
6	SO4	L	1626	5/5	0.93	0.21	1.08	87,99,139,170	0
6	SO4	L	1624	5/5	0.96	0.18	0.68	57,89,118,119	0
6	SO4	M	1436	5/5	0.98	0.16	0.55	49,55,73,75	0
6	SO4	A	1626	5/5	0.90	0.31	0.51	112,115,148,158	0
6	SO4	M	1438	5/5	0.90	0.20	0.41	75,104,141,151	0
6	SO4	B	1586	5/5	0.95	0.17	-0.04	126,127,129,137	0
6	SO4	A	1625	5/5	0.94	0.18	-0.07	87,115,156,158	0
6	SO4	E	1586	5/5	0.95	0.16	-0.23	93,121,144,157	0
6	SO4	U	1436	5/5	0.99	0.14	-0.69	54,56,72,82	0
6	SO4	L	1625	5/5	0.91	0.21	-0.76	110,116,139,144	0
6	SO4	E	1587	5/5	0.96	0.15	-0.83	93,98,159,161	0
6	SO4	U	1439	5/5	0.95	0.14	-0.91	88,108,134,139	0
6	SO4	A	1624	5/5	0.98	0.14	-1.40	50,75,94,102	0
6	SO4	M	1437	5/5	0.92	0.17	-	90,90,124,130	0
6	SO4	A	1627	5/5	0.72	0.21	-	101,120,184,186	0
6	SO4	U	1438	5/5	0.96	0.17	-	64,77,130,145	0
6	SO4	B	1584	5/5	0.82	0.26	-	123,130,155,171	0
6	SO4	L	1628	5/5	0.84	0.22	-	123,136,161,174	0
6	SO4	E	1583	5/5	0.93	0.19	-	72,100,119,132	0
6	SO4	L	1629	5/5	0.82	0.38	-	118,137,168,169	0
6	SO4	E	1584	5/5	0.90	0.18	-	105,132,143,151	0
6	SO4	B	1583	5/5	0.95	0.11	-	51,107,130,133	0
6	SO4	L	1631	5/5	0.89	0.18	-	111,118,126,128	0
6	SO4	L	1630	5/5	0.83	0.19	-	126,137,152,172	0
6	SO4	B	1585	5/5	0.89	0.17	-	95,117,144,156	0
6	SO4	E	1585	5/5	0.90	0.24	-	100,123,136,157	0
6	SO4	A	1628	5/5	0.97	0.13	-	94,110,133,155	0

6.5 Other polymers

There are no such residues in this entry.