Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 06:30 AM GMT

PDB ID	:	2XA7
Title	:	AP2 CLATHRIN ADAPTOR CORE IN ACTIVE COMPLEX WITH CARGO PEPTIDES
Authors	:	Jackson, L.P.; Kelly, B.T.; Mccoy, A.J.; Evans, P.R.; Owen, D.J.
Deposited on	:	2010-03-29
Resolution	:	3.10 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 (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

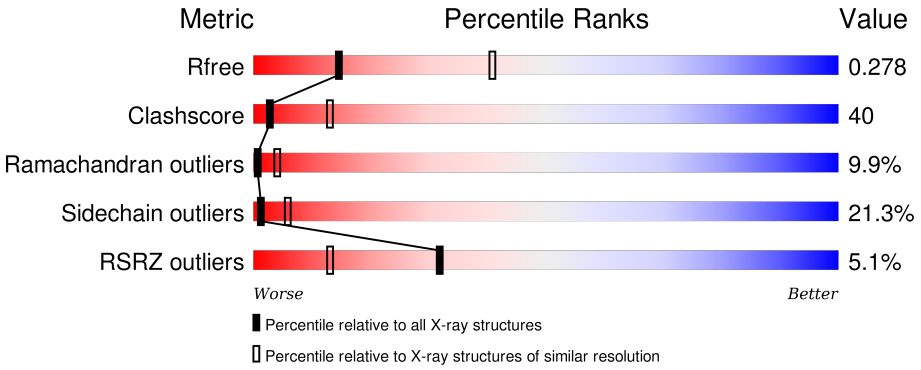
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.10 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	1114 (3.14-3.06)
Clashscore	102246	1222 (3.14-3.06)
Ramachandran outliers	100387	1174 (3.14-3.06)
Sidechain outliers	100360	1174 (3.14-3.06)
RSRZ outliers	91569	1119 (3.14-3.06)

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 <=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	621	4% 37% 45% 16%
2	B	592	32% 44% 19%
3	M	446	14% 36% 40% 18%
4	P	6	17% 33% 67%
5	S	142	% 28% 53% 19%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 14137 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 ADAPTOR-RELATED PROTEIN COMPLEX 2, ALPHA 2 SUBUNIT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	613	4836	3081	833	901	21	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	579	4596	2928	763	880	25	0	0	0

- Molecule 3 is a protein called AP-2 COMPLEX SUBUNIT MU,.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	M	428	3423	2192	591	621	19	0	0	0

There are 11 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
M	237	MET	-	INSERTION	UNP P84092
M	238	GLU	-	INSERTION	UNP P84092
M	239	GLN	-	INSERTION	UNP P84092
M	240	LYS	-	INSERTION	UNP P84092
M	241	LEU	-	INSERTION	UNP P84092
M	242	ILE	-	INSERTION	UNP P84092
M	243	SER	-	INSERTION	UNP P84092
M	244	GLU	-	INSERTION	UNP P84092
M	245	GLU	-	INSERTION	UNP P84092
M	246	ASP	-	INSERTION	UNP P84092
M	247	LEU	-	INSERTION	UNP P84092

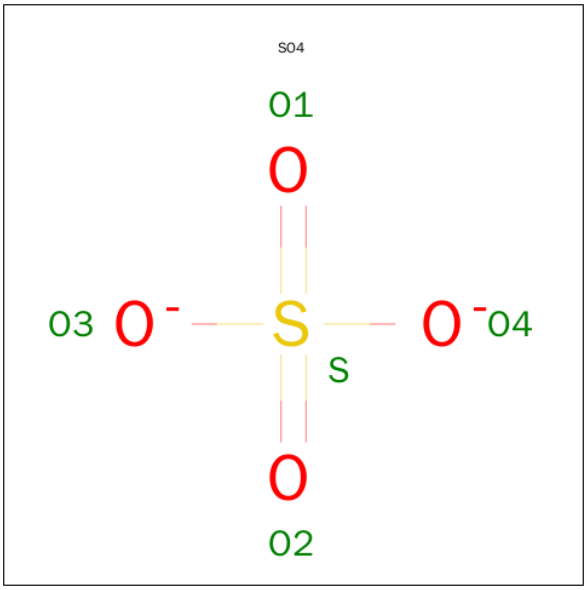
- Molecule 4 is a protein called TGN38 CARGO PEPTIDE.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	P	6	Total	C	N	O	0	0	0
			57	34	11	12			

- Molecule 5 is a protein called AP-2 COMPLEX SUBUNIT SIGMA.

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

- Molecule 6 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



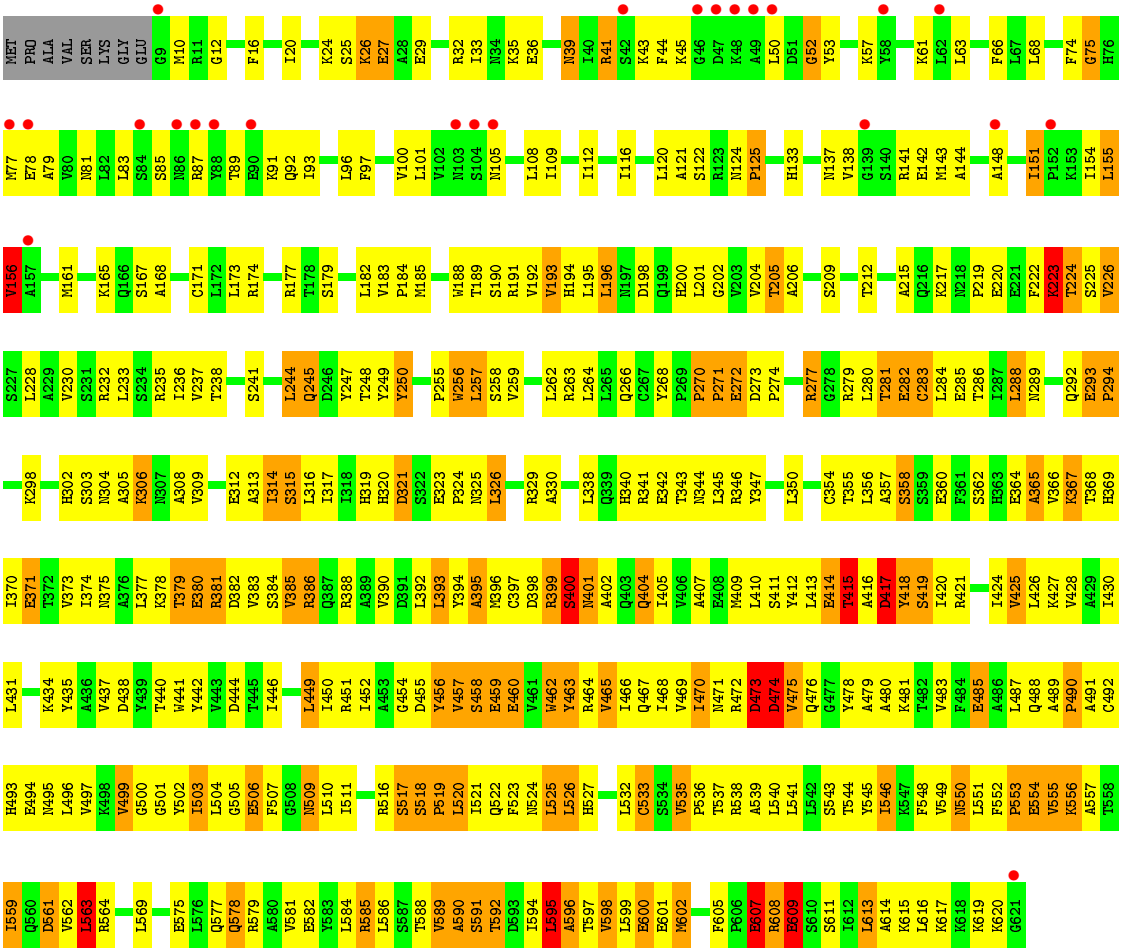
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	O	S	0	0
			5	4	1		
6	A	1	Total	O	S	0	0
			5	4	1		
6	A	1	Total	O	S	0	0
			5	4	1		
6	S	1	Total	O	S	0	0
			5	4	1		
6	S	1	Total	O	S	0	0
			5	4	1		

3 Residue-property plots (i)

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.

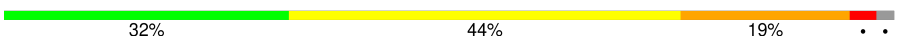
- Molecule 1: ADAPTOR-RELATED PROTEIN COMPLEX 2, ALPHA 2 SUBUNIT

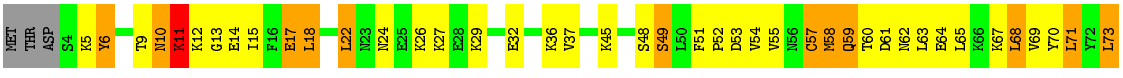
Chain A:

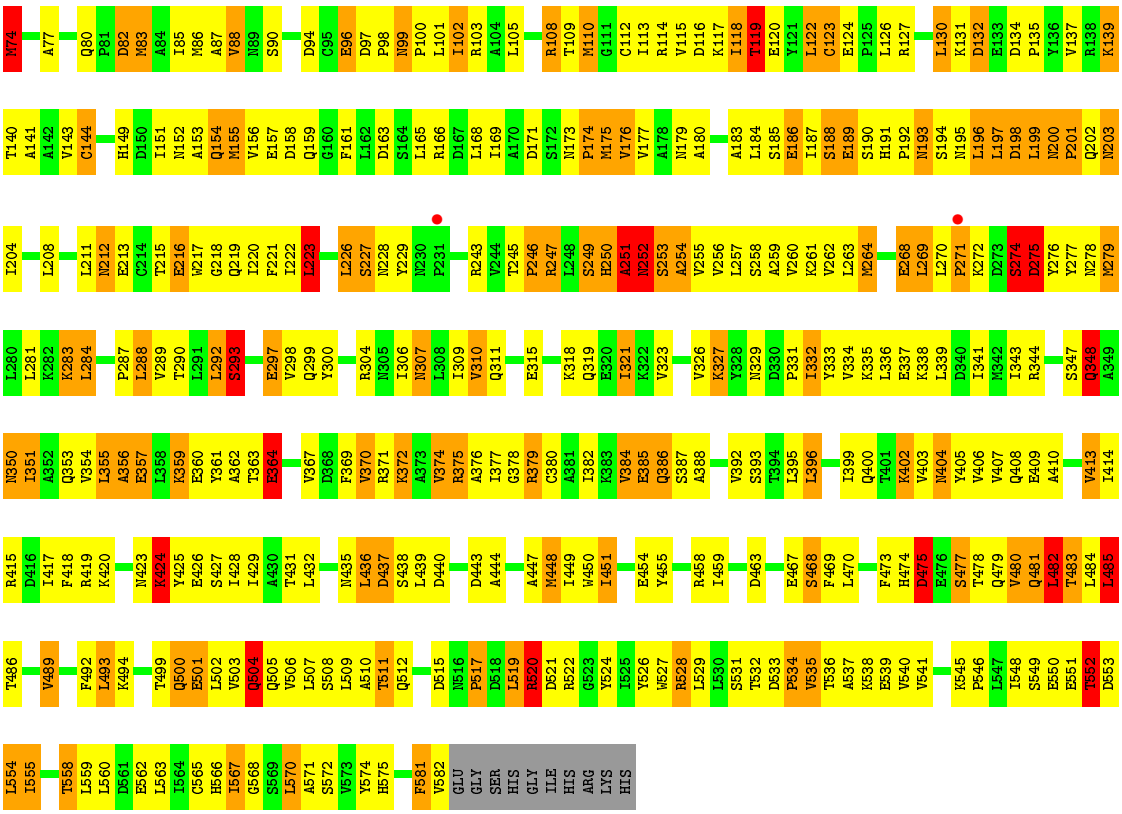


- Molecule 2: AP-2 COMPLEX SUBUNIT BETA

Chain B:

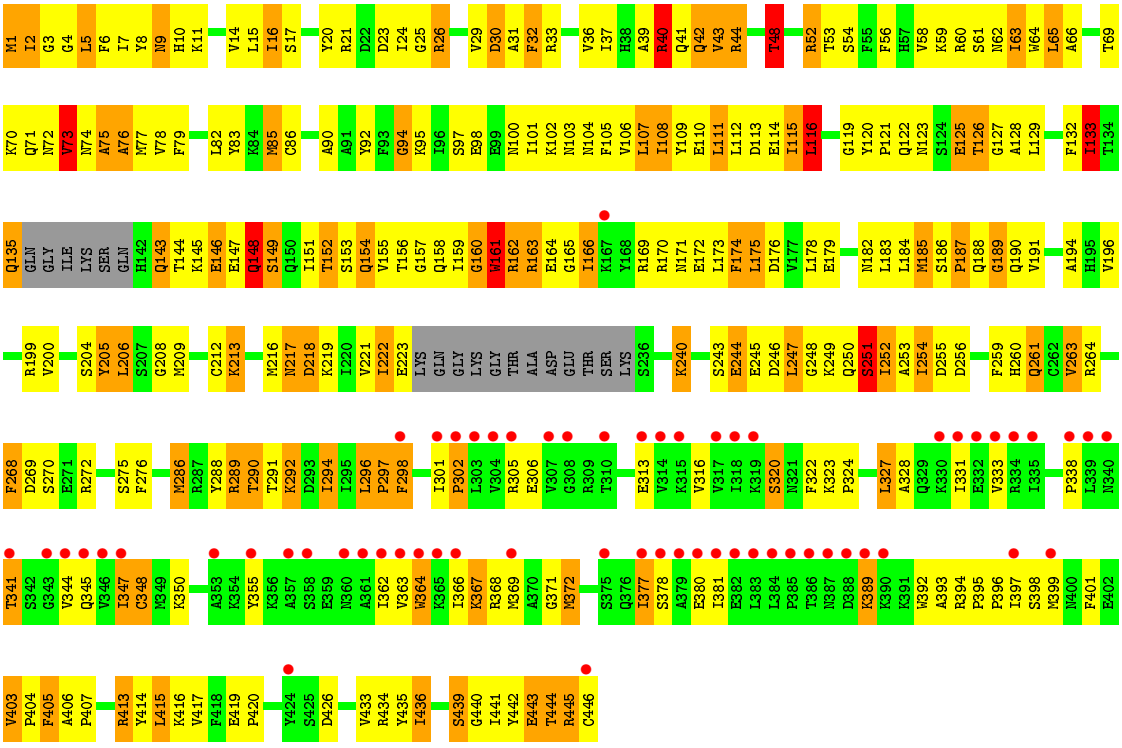






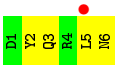
• Molecule 3: AP-2 COMPLEX SUBUNIT MU,

Chain M:



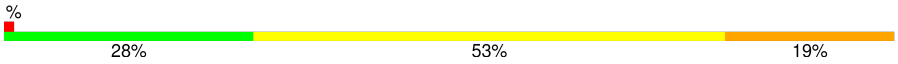
• Molecule 4: TGN38 CARGO PEPTIDE

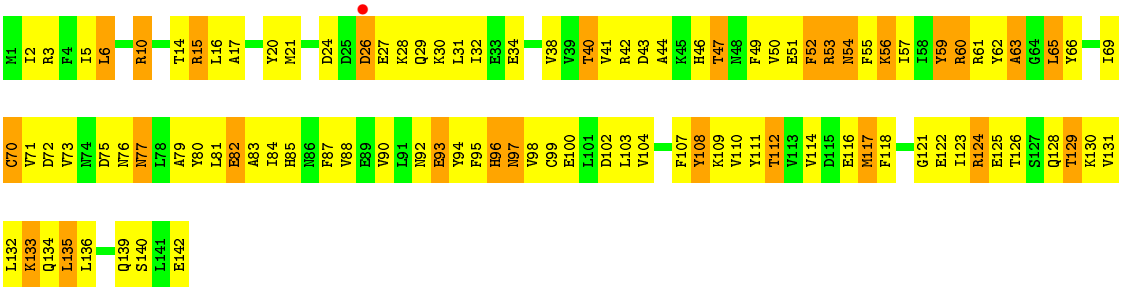
Chain P:



• Molecule 5: AP-2 COMPLEX SUBUNIT SIGMA

Chain S:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	H 3	Depositor
Cell constants a, b, c, α, β, γ	255.32Å 255.32Å 156.75Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	127.88 – 3.10 42.63 – 3.10	Depositor EDS
% Data completeness (in resolution range)	96.2 (127.88-3.10) 96.2 (42.63-3.10)	Depositor EDS
R_{merge}	0.20	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.77 (at 3.12Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.236 , 0.285 0.231 , 0.278	Depositor DCC
R_{free} test set	3378 reflections (5.35%)	DCC
Wilson B-factor (Å^2)	83.6	Xtriage
Anisotropy	0.500	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 82.8	EDS
Estimated twinning fraction	0.027 for -1/3*h+1/3*k+4/3*l,-k,2/3*h+1/3*k+1/3*l 0.018 for -2/3*h-1/3*k-4/3*l,-1/3*h-2/3*k+4/3*l,-1/3*h+1/3*k+1/3*l 0.028 for -h,1/3*h-1/3*k-4/3*l,-1/3*h-2/3*k+1/3*l 0.022 for -1/3*h-2/3*k+4/3*l,-2/3*h-1/3*k-4/3*l,1/3*h-1/3*k-1/3*l 0.024 for -h,2/3*h+1/3*k+4/3*l,1/3*h+2/3*k-1/3*l 0.026 for 1/3*h+2/3*k-4/3*l,-k,-2/3*h-1/3*k-1/3*l 0.043 for h,-h-k,-l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.44$, $< L^2 > = 0.26$	Xtriage
Outliers	0 of 66521 reflections	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	14137	wwPDB-VP
Average B, all atoms (Å^2)	112.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.60% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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

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	1.01	12/4921 (0.2%)	1.05	14/6669 (0.2%)
2	B	0.83	2/4668 (0.0%)	0.97	10/6331 (0.2%)
3	M	0.81	0/3488	0.91	2/4701 (0.0%)
4	P	0.63	0/57	0.82	0/74
5	S	0.85	0/1224	0.89	0/1650
All	All	0.89	14/14358 (0.1%)	0.98	26/19425 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	3
2	B	0	5
3	M	0	2
All	All	0	10

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	607	GLU	CB-CG	11.97	1.74	1.52
1	A	607	GLU	CG-CD	11.27	1.68	1.51
1	A	492	CYS	CB-SG	-8.39	1.68	1.82
1	A	85	SER	C-N	6.45	1.48	1.34
1	A	400	SER	C-O	6.22	1.35	1.23
1	A	463	TYR	CE2-CZ	6.08	1.46	1.38
2	B	57	CYS	CB-SG	-5.62	1.72	1.81
2	B	74	MET	C-O	5.52	1.33	1.23
1	A	469	VAL	CB-CG2	-5.43	1.41	1.52
1	A	417	ASP	CB-CG	5.40	1.63	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	459	GLU	CB-CG	5.40	1.62	1.52
1	A	399	ARG	C-O	5.31	1.33	1.23
1	A	462	TRP	CB-CG	-5.17	1.41	1.50
1	A	441	TRP	CB-CG	-5.05	1.41	1.50

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	595	LEU	CA-CB-CG	8.76	135.44	115.30
1	A	456	TYR	N-CA-C	-7.51	90.72	111.00
1	A	458	SER	N-CA-C	-7.25	91.43	111.00
2	B	196	LEU	CA-CB-CG	7.17	131.78	115.30
1	A	399	ARG	NE-CZ-NH1	7.06	123.83	120.30
1	A	415	THR	N-CA-C	6.97	129.81	111.00
1	A	607	GLU	CB-CA-C	6.69	123.78	110.40
2	B	528	ARG	NE-CZ-NH2	-6.67	116.97	120.30
2	B	519	LEU	CB-CG-CD2	-6.38	100.15	111.00
1	A	551	LEU	CA-CB-CG	6.38	129.97	115.30
2	B	223	LEU	CA-CB-CG	6.32	129.83	115.30
3	M	3	GLY	N-CA-C	-6.29	97.36	113.10
2	B	252	ASN	CB-CA-C	6.04	122.47	110.40
2	B	570	LEU	CA-CB-CG	5.89	128.85	115.30
1	A	520	LEU	CA-CB-CG	5.80	128.65	115.30
2	B	485	LEU	CA-CB-CG	5.67	128.35	115.30
2	B	520	ARG	NE-CZ-NH1	5.66	123.13	120.30
1	A	400	SER	N-CA-CB	-5.46	102.32	110.50
1	A	563	LEU	CA-CB-CG	5.32	127.55	115.30
2	B	226	LEU	CA-CB-CG	-5.28	103.17	115.30
1	A	196	LEU	CA-CB-CG	5.18	127.21	115.30
2	B	71	LEU	CA-CB-CG	5.16	127.16	115.30
1	A	399	ARG	NE-CZ-NH2	-5.15	117.72	120.30
1	A	444	ASP	CB-CG-OD1	-5.15	113.67	118.30
1	A	393	LEU	CB-CG-CD1	-5.11	102.31	111.00
3	M	73	VAL	CB-CA-C	-5.04	101.82	111.40

There are no chirality outliers.

All (10) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	381	ARG	Peptide
1	A	401	ASN	Peptide
1	A	456	TYR	Peptide

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Mol	Chain	Res	Type	Group
2	B	249	SER	Peptide
2	B	251	ALA	Peptide
2	B	274	SER	Peptide
2	B	275	ASP	Peptide
2	B	550	GLU	Peptide
3	M	443	GLU	Peptide
3	M	48	THR	Peptide

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	4836	0	4952	403	0
2	B	4596	0	4715	435	0
3	M	3423	0	3485	260	0
4	P	57	0	53	4	0
5	S	1200	0	1195	120	0
6	A	15	0	0	0	0
6	S	10	0	0	2	0
All	All	14137	0	14400	1144	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 40.

All (1144) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:607:GLU:CB	1:A:607:GLU:CG	1.74	1.56
2:B:155:MET:HB2	2:B:158:ASP:CB	1.67	1.24
1:A:457:VAL:HG13	1:A:458:SER:O	1.41	1.19
3:M:320:SER:HB2	3:M:322:PHE:HE1	1.03	1.17
5:S:57:ILE:HG22	5:S:70:CYS:HB2	1.29	1.15
2:B:189:GLU:HA	2:B:189:GLU:OE1	1.45	1.14
3:M:320:SER:HB2	3:M:322:PHE:CE1	1.83	1.13
1:A:472:ARG:HB2	1:A:475:VAL:HG21	1.31	1.13
1:A:416:ALA:HB1	1:A:420:ILE:HD12	1.21	1.12

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:417:ASP:CG	1:A:418:TYR:H	1.54	1.11
2:B:200:ASN:HB2	2:B:201:PRO:HD2	1.32	1.09
1:A:472:ARG:HB2	1:A:475:VAL:CG2	1.84	1.07
3:M:323:LYS:HG2	3:M:324:PRO:HD2	1.30	1.07
2:B:249:SER:O	2:B:252:ASN:ND2	1.86	1.07
1:A:371:GLU:HA	1:A:371:GLU:OE1	1.47	1.07
2:B:10:ASN:O	2:B:11:LYS:HB2	1.54	1.05
3:M:144:THR:HG22	3:M:145:LYS:H	1.17	1.04
1:A:53:TYR:O	1:A:57:LYS:HB2	1.55	1.04
2:B:515:ASP:O	2:B:517:PRO:HD3	1.56	1.04
2:B:155:MET:HB2	2:B:158:ASP:HB2	1.03	1.03
2:B:166:ARG:HH21	2:B:197:LEU:HG	1.20	1.02
2:B:582:VAL:H	3:M:52:ARG:HH11	1.02	1.01
1:A:377:LEU:CD1	1:A:390:VAL:HG22	1.90	1.01
5:S:2:ILE:HA	5:S:71:VAL:HG12	1.43	1.00
1:A:377:LEU:HD11	1:A:390:VAL:HG22	1.41	0.98
1:A:397:CYS:HA	1:A:401:ASN:HD22	1.28	0.98
2:B:203:ASN:H	2:B:203:ASN:HD22	1.01	0.97
1:A:417:ASP:CG	1:A:418:TYR:N	2.10	0.97
2:B:492:PHE:HD1	2:B:499:THR:HB	1.25	0.96
1:A:457:VAL:HG13	1:A:458:SER:H	1.27	0.95
3:M:347:ILE:HG23	3:M:378:SER:HB2	1.48	0.95
2:B:321:ILE:HG21	2:B:350:ASN:HD22	1.28	0.95
2:B:250:HIS:C	2:B:252:ASN:H	1.68	0.95
2:B:385:GLU:O	2:B:388:ALA:N	1.98	0.95
1:A:535:VAL:HG23	1:A:536:PRO:HD3	1.46	0.95
2:B:58:MET:HB3	2:B:69:VAL:HG11	1.48	0.95
1:A:470:ILE:HD11	1:A:605:PHE:HD1	1.31	0.94
5:S:49:PHE:CE2	5:S:77:ASN:HB3	2.02	0.94
2:B:18:LEU:HD12	2:B:37:VAL:HG23	1.49	0.94
2:B:321:ILE:HG21	2:B:350:ASN:ND2	1.82	0.93
2:B:155:MET:CB	2:B:158:ASP:HB2	1.96	0.93
3:M:161:TRP:O	3:M:162:ARG:HB2	1.67	0.93
1:A:354:CYS:CA	1:A:392:LEU:HD13	1.97	0.93
1:A:354:CYS:HA	1:A:392:LEU:CD1	1.99	0.92
3:M:5:LEU:HD12	3:M:5:LEU:C	1.90	0.92
2:B:247:ARG:HA	2:B:249:SER:OG	1.69	0.91
2:B:261:LYS:HG3	2:B:567:ILE:HB	1.50	0.91
3:M:42:GLN:O	3:M:44:ARG:HG3	1.70	0.91
1:A:460:GLU:N	1:A:460:GLU:OE1	2.03	0.91
1:A:317:ILE:HG12	1:A:326:LEU:HD12	1.49	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:327:LYS:HG2	3:M:441:ILE:HG21	1.52	0.91
2:B:581:PHE:HA	3:M:52:ARG:HG2	1.50	0.90
5:S:108:TYR:HD2	5:S:108:TYR:H	1.18	0.90
1:A:133:HIS:O	1:A:137:ASN:HB2	1.70	0.89
1:A:417:ASP:OD2	1:A:418:TYR:N	2.05	0.88
3:M:135:GLN:HE21	3:M:135:GLN:HA	1.37	0.88
3:M:320:SER:CB	3:M:322:PHE:HE1	1.86	0.88
1:A:354:CYS:HA	1:A:392:LEU:HD13	1.52	0.88
2:B:199:LEU:HD13	2:B:229:TYR:HD1	1.37	0.87
2:B:203:ASN:HD22	2:B:203:ASN:N	1.72	0.87
3:M:53:THR:OG1	3:M:70:LYS:HE2	1.75	0.86
3:M:348:CYS:HB2	3:M:364:TRP:HE1	1.40	0.86
2:B:571:ALA:H	3:M:72:ASN:HD21	1.18	0.86
2:B:154:GLN:HG3	2:B:155:MET:N	1.89	0.86
1:A:32:ARG:HH12	1:A:36:GLU:HG2	1.40	0.86
1:A:271:PRO:HD2	1:A:320:HIS:NE2	1.91	0.85
2:B:379:ARG:HB3	2:B:552:THR:HB	1.56	0.85
1:A:527:HIS:HD2	1:A:545:TYR:OH	1.59	0.85
2:B:251:ALA:HB3	2:B:255:VAL:HG23	1.57	0.84
1:A:483:VAL:HG11	1:A:500:GLY:HA2	1.56	0.84
1:A:293:GLU:HB3	1:A:294:PRO:CD	2.07	0.84
1:A:457:VAL:CG1	1:A:458:SER:O	2.25	0.83
2:B:203:ASN:H	2:B:203:ASN:ND2	1.77	0.83
2:B:245:THR:O	2:B:247:ARG:N	2.11	0.83
1:A:380:GLU:HG2	1:A:385:VAL:HG11	1.58	0.83
3:M:32:PHE:CE2	3:M:36:VAL:HB	2.14	0.83
1:A:585:ARG:NH1	1:A:589:VAL:HG21	1.94	0.82
1:A:457:VAL:HG13	1:A:458:SER:N	1.93	0.82
3:M:417:VAL:O	3:M:417:VAL:HG12	1.78	0.82
2:B:327:LYS:HG2	3:M:441:ILE:CG2	2.10	0.82
3:M:268:PHE:CD2	3:M:268:PHE:C	2.53	0.81
2:B:511:THR:HG23	2:B:512:GLN:HE21	1.45	0.81
5:S:42:ARG:HD3	5:S:59:TYR:CZ	2.15	0.81
2:B:343:ILE:CD1	2:B:376:ALA:HB1	2.11	0.81
2:B:155:MET:O	2:B:158:ASP:HB3	1.81	0.81
1:A:417:ASP:OD2	1:A:420:ILE:HG12	1.80	0.80
1:A:323:GLU:HB3	1:A:326:LEU:HB2	1.63	0.80
3:M:132:PHE:HB3	3:M:151:ILE:HD13	1.63	0.80
3:M:125:GLU:HG2	3:M:161:TRP:HA	1.60	0.80
5:S:42:ARG:HD3	5:S:59:TYR:CE2	2.15	0.80
1:A:417:ASP:OD2	1:A:420:ILE:CG1	2.30	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:32:ARG:HH12	1:A:36:GLU:CG	1.94	0.80
2:B:252:ASN:O	2:B:253:SER:C	2.19	0.80
1:A:289:ASN:O	1:A:292:GLN:HB2	1.82	0.80
2:B:64:GLU:O	2:B:68:LEU:HD13	1.81	0.80
1:A:511:ILE:HG13	1:A:517:SER:OG	1.82	0.80
2:B:250:HIS:C	2:B:252:ASN:N	2.35	0.80
5:S:90:VAL:HG23	5:S:128:GLN:HE21	1.48	0.79
2:B:261:LYS:HD2	2:B:567:ILE:H	1.47	0.79
1:A:509:ASN:H	1:A:509:ASN:HD22	1.28	0.79
2:B:250:HIS:O	2:B:252:ASN:N	2.11	0.79
2:B:297:GLU:HB2	3:M:83:TYR:OH	1.82	0.79
5:S:42:ARG:HD3	5:S:59:TYR:OH	1.83	0.78
1:A:579:ARG:HG2	2:B:522:ARG:NH1	1.98	0.78
2:B:250:HIS:HD2	3:M:261:GLN:HA	1.48	0.78
2:B:68:LEU:HD11	3:M:106:VAL:HG13	1.64	0.78
1:A:464:ARG:HE	1:A:468:ILE:HD11	1.48	0.78
1:A:598:VAL:HA	2:B:528:ARG:HB3	1.65	0.77
2:B:166:ARG:NH2	2:B:197:LEU:HG	2.00	0.77
2:B:492:PHE:CD1	2:B:499:THR:HB	2.15	0.77
2:B:200:ASN:HB2	2:B:201:PRO:CD	2.14	0.77
5:S:24:ASP:HB2	5:S:27:GLU:HB3	1.66	0.77
1:A:292:GLN:HE21	1:A:329:ARG:HH22	1.33	0.77
5:S:96:HIS:O	5:S:97:ASN:HB2	1.84	0.77
3:M:108:ILE:O	3:M:112:LEU:HD23	1.85	0.76
2:B:11:LYS:HE2	5:S:61:ARG:HB3	1.68	0.76
1:A:470:ILE:HD11	1:A:605:PHE:CD1	2.20	0.76
3:M:127:GLY:HA3	3:M:162:ARG:HG3	1.66	0.76
5:S:16:LEU:CD1	5:S:111:TYR:CE1	2.69	0.76
2:B:155:MET:CB	2:B:158:ASP:CB	2.59	0.76
1:A:53:TYR:O	1:A:57:LYS:CB	2.32	0.76
3:M:44:ARG:CB	3:M:44:ARG:HH11	1.98	0.76
3:M:44:ARG:HH11	3:M:44:ARG:CG	1.97	0.76
5:S:87:PHE:CZ	5:S:114:VAL:HG23	2.21	0.76
4:P:5:LEU:O	4:P:6:ASN:HB2	1.85	0.76
2:B:582:VAL:H	3:M:52:ARG:NH1	1.82	0.76
1:A:483:VAL:CG1	1:A:500:GLY:HA2	2.16	0.75
3:M:144:THR:CG2	3:M:145:LYS:H	1.98	0.75
3:M:32:PHE:C	3:M:32:PHE:HD2	1.90	0.75
5:S:57:ILE:HG22	5:S:70:CYS:CB	2.12	0.75
5:S:49:PHE:CD2	5:S:77:ASN:HB3	2.21	0.75
2:B:395:LEU:O	2:B:399:ILE:HD12	1.87	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:426:LEU:HD21	1:A:615:LYS:HD3	1.67	0.75
1:A:209:SER:HB3	5:S:122:GLU:OE1	1.87	0.75
2:B:343:ILE:HD11	2:B:376:ALA:HB1	1.68	0.74
3:M:132:PHE:O	3:M:133:ILE:HD12	1.87	0.74
3:M:5:LEU:C	3:M:5:LEU:CD1	2.56	0.74
2:B:261:LYS:CG	2:B:567:ILE:HB	2.17	0.74
1:A:154:ILE:HG22	1:A:155:LEU:HD13	1.69	0.74
1:A:598:VAL:HG22	2:B:528:ARG:O	1.88	0.74
2:B:186:GLU:OE1	3:M:21:ARG:NH2	2.20	0.74
1:A:602:MET:HE1	2:B:524:TYR:HB2	1.69	0.74
1:A:284:LEU:O	1:A:288:LEU:HD12	1.88	0.74
1:A:377:LEU:CD1	1:A:390:VAL:CG2	2.65	0.73
1:A:380:GLU:HG2	1:A:385:VAL:CG1	2.18	0.73
1:A:548:PHE:O	1:A:552:PHE:HB2	1.88	0.73
1:A:262:LEU:O	1:A:266:GLN:HG3	1.89	0.73
1:A:489:ALA:HB1	1:A:490:PRO:HD2	1.70	0.73
2:B:256:VAL:O	2:B:259:ALA:HB3	1.89	0.73
1:A:466:ILE:HD11	1:A:499:VAL:HA	1.70	0.73
3:M:331:ILE:HB	3:M:366:ILE:HB	1.71	0.73
1:A:266:GLN:HE22	1:A:315:SER:HB2	1.52	0.72
1:A:442:TYR:CE2	1:A:465:VAL:HG23	2.24	0.72
3:M:164:GLU:HG2	3:M:165:GLY:H	1.54	0.72
2:B:250:HIS:CD2	3:M:261:GLN:HG2	2.25	0.72
5:S:62:TYR:O	5:S:65:LEU:HB2	1.90	0.72
2:B:6:TYR:C	2:B:6:TYR:CD2	2.63	0.72
2:B:306:ILE:O	2:B:309:ILE:N	2.23	0.72
2:B:555:ILE:CG2	2:B:560:LEU:HB2	2.19	0.72
5:S:16:LEU:HD13	5:S:111:TYR:CE1	2.25	0.72
3:M:174:PHE:N	3:M:174:PHE:HD1	1.87	0.72
2:B:6:TYR:HD2	2:B:6:TYR:C	1.92	0.72
3:M:268:PHE:C	3:M:268:PHE:HD2	1.93	0.71
2:B:250:HIS:CD2	3:M:261:GLN:HA	2.26	0.71
2:B:378:GLY:HA3	2:B:413:VAL:HG11	1.71	0.71
1:A:249:TYR:CE2	5:S:82:GLU:HG3	2.26	0.71
3:M:144:THR:HG22	3:M:145:LYS:N	2.01	0.71
3:M:135:GLN:NE2	3:M:135:GLN:HA	2.05	0.71
1:A:382:ASP:O	1:A:386:ARG:HD2	1.91	0.71
3:M:173:LEU:C	3:M:174:PHE:HD1	1.94	0.71
1:A:89:THR:OG1	5:S:142:GLU:HG3	1.91	0.71
5:S:136:LEU:HA	5:S:139:GLN:HB2	1.73	0.71
5:S:93:GLU:HA	5:S:93:GLU:OE1	1.89	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:100:PRO:HD2	3:M:148:GLN:HG2	1.73	0.70
3:M:1:MET:H2	3:M:71:GLN:NE2	1.89	0.70
1:A:464:ARG:HE	1:A:468:ILE:CD1	2.04	0.70
1:A:377:LEU:HD12	1:A:390:VAL:CG2	2.21	0.70
3:M:174:PHE:CD1	3:M:174:PHE:N	2.59	0.70
1:A:442:TYR:HE2	1:A:465:VAL:HG23	1.56	0.70
2:B:70:TYR:CG	2:B:109:THR:HG21	2.27	0.70
2:B:440:ASP:N	2:B:440:ASP:OD2	2.20	0.70
5:S:59:TYR:CD1	5:S:59:TYR:O	2.45	0.70
1:A:527:HIS:CD2	1:A:545:TYR:OH	2.45	0.69
2:B:73:LEU:O	2:B:77:ALA:HB2	1.91	0.69
2:B:260:VAL:O	2:B:264:MET:HB2	1.92	0.69
2:B:385:GLU:O	2:B:388:ALA:HB3	1.91	0.69
2:B:407:VAL:O	2:B:410:ALA:HB3	1.92	0.69
3:M:32:PHE:C	3:M:32:PHE:CD2	2.64	0.69
1:A:493:HIS:CD2	1:A:495:ASN:H	2.11	0.69
1:A:451:ARG:HB3	1:A:451:ARG:NH1	2.07	0.69
2:B:226:LEU:O	2:B:228:ASN:N	2.23	0.69
2:B:18:LEU:CD1	2:B:37:VAL:HG23	2.22	0.69
1:A:493:HIS:HD2	1:A:495:ASN:H	1.39	0.69
2:B:292:LEU:N	2:B:292:LEU:HD13	2.08	0.69
3:M:445:ARG:O	3:M:446:CYS:SG	2.50	0.69
3:M:107:LEU:O	3:M:108:ILE:C	2.31	0.69
3:M:1:MET:HA	3:M:73:VAL:HG12	1.75	0.68
1:A:92:GLN:HE21	5:S:112:THR:HB	1.57	0.68
1:A:506:GLU:O	1:A:506:GLU:HG3	1.94	0.68
1:A:585:ARG:HB3	2:B:540:VAL:HG22	1.75	0.68
1:A:394:TYR:CD1	1:A:431:LEU:HD21	2.29	0.68
1:A:504:LEU:HD21	1:A:522:GLN:OE1	1.94	0.68
2:B:221:PHE:HZ	3:M:121:PRO:HD2	1.58	0.68
3:M:1:MET:N	3:M:71:GLN:NE2	2.41	0.68
2:B:154:GLN:HG3	2:B:155:MET:H	1.57	0.68
5:S:57:ILE:CG2	5:S:70:CYS:HB2	2.18	0.68
5:S:93:GLU:CB	5:S:132:LEU:HD11	2.24	0.68
5:S:65:LEU:C	5:S:66:TYR:HD1	1.97	0.68
2:B:250:HIS:HD2	3:M:261:GLN:HG2	1.60	0.67
3:M:44:ARG:HH11	3:M:44:ARG:HG3	1.59	0.67
5:S:59:TYR:CG	5:S:59:TYR:O	2.47	0.67
2:B:117:LYS:O	2:B:120:GLU:HG3	1.94	0.67
2:B:571:ALA:N	3:M:72:ASN:HD21	1.92	0.67
2:B:73:LEU:O	2:B:77:ALA:CB	2.42	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:451:ARG:HB3	1:A:451:ARG:HH11	1.59	0.67
2:B:347:SER:O	2:B:351:ILE:HG13	1.93	0.67
1:A:105:ASN:O	1:A:109:ILE:HD13	1.94	0.67
2:B:307:ASN:HD22	2:B:307:ASN:C	1.97	0.67
3:M:184:LEU:HD13	3:M:443:GLU:OE1	1.94	0.67
2:B:388:ALA:O	2:B:392:VAL:HG23	1.95	0.67
1:A:589:VAL:HG12	1:A:590:ALA:H	1.59	0.67
1:A:552:PHE:O	1:A:553:PRO:C	2.31	0.67
2:B:251:ALA:CB	2:B:255:VAL:HG23	2.24	0.67
2:B:187:ILE:C	2:B:189:GLU:H	1.98	0.66
2:B:168:LEU:O	2:B:171:ASP:HB2	1.95	0.66
3:M:222:ILE:HD11	3:M:247:LEU:HA	1.76	0.66
3:M:44:ARG:NH1	3:M:44:ARG:HB2	2.10	0.66
2:B:376:ALA:HA	2:B:379:ARG:HG3	1.77	0.66
1:A:416:ALA:HB1	1:A:420:ILE:CD1	2.13	0.66
5:S:42:ARG:CD	5:S:59:TYR:CE2	2.79	0.66
1:A:591:SER:OG	1:A:594:ILE:HG22	1.96	0.66
2:B:572:SER:O	2:B:575:HIS:HD2	1.79	0.65
1:A:262:LEU:CD2	1:A:313:ALA:HA	2.26	0.65
1:A:487:LEU:HD23	1:A:496:LEU:HD23	1.78	0.65
2:B:139:LYS:HG3	2:B:179:ASN:ND2	2.11	0.65
3:M:56:PHE:HD1	3:M:56:PHE:N	1.94	0.65
3:M:56:PHE:CD1	3:M:56:PHE:N	2.64	0.65
1:A:411:SER:O	1:A:414:GLU:N	2.29	0.65
2:B:194:SER:O	2:B:197:LEU:HD13	1.97	0.65
2:B:58:MET:CB	2:B:69:VAL:HG11	2.23	0.65
2:B:226:LEU:C	2:B:228:ASN:H	2.00	0.65
2:B:562:GLU:HA	2:B:565:CYS:SG	2.35	0.65
3:M:255:ASP:HB2	3:M:289:ARG:O	1.96	0.65
2:B:336:LEU:HD23	2:B:369:PHE:HD1	1.61	0.65
1:A:392:LEU:O	1:A:395:ALA:HB3	1.97	0.65
5:S:38:VAL:O	5:S:41:VAL:HG12	1.96	0.65
1:A:263:ARG:HH12	5:S:75:ASP:HA	1.61	0.65
3:M:26:ARG:NE	3:M:26:ARG:H	1.93	0.65
1:A:377:LEU:HD12	1:A:390:VAL:HG22	1.73	0.65
1:A:77:MET:C	1:A:79:ALA:H	2.00	0.65
1:A:379:THR:HG22	1:A:380:GLU:N	2.10	0.65
1:A:555:VAL:HG13	1:A:559:ILE:HG13	1.76	0.65
5:S:90:VAL:HG23	5:S:128:GLN:NE2	2.12	0.65
5:S:129:THR:O	5:S:132:LEU:N	2.30	0.64
5:S:95:PHE:CD2	5:S:102:ASP:HB3	2.32	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:249:TYR:HE2	5:S:82:GLU:HG3	1.61	0.64
5:S:82:GLU:HA	5:S:82:GLU:OE1	1.98	0.64
2:B:99:ASN:HD22	2:B:101:LEU:H	1.46	0.64
1:A:262:LEU:HD22	1:A:313:ALA:HA	1.79	0.64
1:A:247:TYR:OH	5:S:125:GLU:OE2	2.09	0.64
2:B:505:GLN:O	2:B:509:LEU:HG	1.98	0.64
2:B:425:TYR:HB3	2:B:428:ILE:HD11	1.79	0.64
1:A:381:ARG:HG2	1:A:386:ARG:NH2	2.13	0.64
1:A:520:LEU:CD1	1:A:521:ILE:HD13	2.28	0.64
1:A:490:PRO:HG2	1:A:491:ALA:H	1.62	0.64
1:A:519:PRO:HG3	1:A:552:PHE:CE1	2.33	0.64
2:B:436:LEU:C	2:B:438:SER:H	2.00	0.64
2:B:533:ASP:HB2	2:B:535:VAL:HB	1.79	0.64
2:B:567:ILE:HG22	2:B:568:GLY:N	2.13	0.64
2:B:85:ILE:O	2:B:88:VAL:HG22	1.98	0.64
1:A:462:TRP:HB2	1:A:499:VAL:HG23	1.79	0.63
2:B:403:VAL:O	2:B:406:VAL:HG12	1.96	0.63
2:B:82:ASP:O	2:B:85:ILE:HG13	1.97	0.63
1:A:430:ILE:HD13	1:A:613:LEU:HD12	1.78	0.63
2:B:155:MET:HB2	2:B:158:ASP:HB3	1.72	0.63
1:A:356:LEU:O	1:A:358:SER:N	2.31	0.63
3:M:153:SER:HA	3:M:156:THR:HG22	1.80	0.63
2:B:385:GLU:O	2:B:388:ALA:CB	2.45	0.63
1:A:520:LEU:HD12	1:A:521:ILE:HD13	1.81	0.63
2:B:52:PRO:HB3	2:B:83:MET:HE1	1.81	0.63
2:B:110:MET:HE2	2:B:122:LEU:HB2	1.81	0.63
3:M:444:THR:CG2	3:M:445:ARG:N	2.62	0.63
1:A:471:ASN:HD21	1:A:605:PHE:HB2	1.64	0.63
1:A:517:SER:O	1:A:518:SER:O	2.17	0.63
3:M:217:ASN:N	3:M:217:ASN:OD1	2.32	0.63
1:A:457:VAL:CG1	1:A:458:SER:N	2.62	0.63
2:B:223:LEU:HD12	2:B:259:ALA:N	2.14	0.63
2:B:572:SER:O	2:B:575:HIS:CD2	2.52	0.63
2:B:276:TYR:HA	2:B:279:MET:HE3	1.79	0.63
1:A:417:ASP:O	1:A:418:TYR:CD2	2.52	0.63
2:B:189:GLU:OE1	2:B:189:GLU:CA	2.33	0.62
3:M:160:GLY:O	3:M:162:ARG:N	2.25	0.62
2:B:261:LYS:HA	2:B:567:ILE:HD13	1.81	0.62
2:B:114:ARG:NH2	2:B:151:ILE:HB	2.14	0.62
1:A:555:VAL:CG1	1:A:559:ILE:HG13	2.29	0.62
1:A:417:ASP:OD2	1:A:420:ILE:HG13	1.99	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:M:111:LEU:O	3:M:114:GLU:N	2.32	0.62
5:S:87:PHE:CE1	5:S:114:VAL:HG23	2.33	0.62
5:S:24:ASP:H	5:S:27:GLU:CD	2.03	0.62
3:M:268:PHE:HD2	3:M:269:ASP:N	1.97	0.62
2:B:582:VAL:O	2:B:582:VAL:HG12	1.99	0.62
2:B:139:LYS:HD2	3:M:122:GLN:OE1	1.99	0.62
3:M:44:ARG:HH11	3:M:44:ARG:HB2	1.63	0.62
1:A:485:GLU:O	1:A:488:GLN:HG2	1.99	0.62
2:B:503:VAL:O	2:B:507:LEU:HB2	1.99	0.62
2:B:74:MET:CE	2:B:109:THR:HG22	2.30	0.62
2:B:261:LYS:HA	2:B:567:ILE:CD1	2.29	0.62
1:A:472:ARG:HB2	1:A:475:VAL:HG22	1.77	0.62
2:B:428:ILE:O	2:B:431:THR:HB	2.00	0.62
3:M:125:GLU:HG2	3:M:161:TRP:CA	2.28	0.62
5:S:59:TYR:CD1	5:S:59:TYR:C	2.73	0.62
1:A:602:MET:HE1	2:B:524:TYR:CB	2.29	0.62
1:A:539:ALA:HB1	1:A:579:ARG:NH1	2.15	0.61
2:B:534:PRO:HA	2:B:537:ALA:HB3	1.82	0.61
1:A:417:ASP:H	1:A:420:ILE:HD11	1.65	0.61
2:B:18:LEU:O	2:B:22:LEU:HB2	1.99	0.61
1:A:462:TRP:O	1:A:466:ILE:HG12	2.00	0.61
1:A:87:ARG:NH1	5:S:142:GLU:OE2	2.33	0.61
2:B:484:LEU:C	2:B:484:LEU:HD23	2.20	0.61
3:M:196:VAL:HG12	3:M:290:THR:O	2.00	0.61
1:A:564:ARG:O	1:A:569:LEU:HD12	2.00	0.61
1:A:228:LEU:O	1:A:232:ARG:HG2	2.00	0.61
1:A:473:ASP:O	1:A:476:GLN:N	2.33	0.61
2:B:582:VAL:N	3:M:52:ARG:HH11	1.86	0.61
1:A:188:TRP:O	1:A:192:VAL:HG23	2.00	0.61
1:A:494:GLU:O	1:A:497:VAL:N	2.32	0.61
1:A:397:CYS:SG	1:A:402:ALA:HA	2.40	0.61
1:A:539:ALA:HB1	1:A:579:ARG:CZ	2.30	0.61
2:B:404:ASN:O	2:B:407:VAL:HB	2.00	0.61
1:A:451:ARG:HH11	1:A:451:ARG:CB	2.14	0.61
1:A:460:GLU:OE2	1:A:615:LYS:HD2	2.00	0.61
1:A:156:VAL:HG12	1:A:188:TRP:HB3	1.83	0.61
2:B:436:LEU:O	2:B:438:SER:N	2.34	0.61
1:A:344:ASN:HB3	5:S:49:PHE:HE1	1.63	0.61
1:A:589:VAL:HG12	1:A:590:ALA:N	2.15	0.61
1:A:245:GLN:H	1:A:245:GLN:NE2	1.99	0.61
2:B:555:ILE:HG22	2:B:560:LEU:HB2	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:282:GLU:O	1:A:285:GLU:HB2	2.01	0.60
2:B:548:ILE:HB	2:B:551:GLU:OE1	2.01	0.60
1:A:519:PRO:HB3	1:A:552:PHE:CE1	2.36	0.60
1:A:343:THR:OG1	1:A:346:ARG:NH2	2.27	0.60
2:B:155:MET:C	2:B:158:ASP:HB3	2.22	0.60
1:A:417:ASP:N	1:A:420:ILE:HD11	2.16	0.60
2:B:288:LEU:HD22	2:B:306:ILE:HG12	1.84	0.60
2:B:18:LEU:HD12	2:B:37:VAL:CG2	2.28	0.60
2:B:479:GLN:O	2:B:483:THR:HB	2.00	0.60
2:B:290:THR:HG22	3:M:289:ARG:HH11	1.66	0.60
3:M:128:ALA:HB1	3:M:155:VAL:HG22	1.84	0.60
1:A:247:TYR:HE1	5:S:130:LYS:NZ	1.99	0.60
2:B:191:HIS:HA	2:B:195:ASN:OD1	2.02	0.60
1:A:317:ILE:CG1	1:A:326:LEU:HD12	2.26	0.60
5:S:117:MET:O	5:S:118:PHE:CD2	2.55	0.59
1:A:413:LEU:C	1:A:415:THR:N	2.54	0.59
2:B:474:HIS:O	2:B:475:ASP:C	2.40	0.59
5:S:108:TYR:N	5:S:108:TYR:CD2	2.66	0.59
1:A:591:SER:O	1:A:592:THR:HB	2.02	0.59
5:S:24:ASP:HB2	5:S:27:GLU:CB	2.32	0.59
1:A:356:LEU:HD21	1:A:362:SER:OG	2.02	0.59
1:A:381:ARG:HG2	1:A:386:ARG:CZ	2.33	0.59
3:M:149:SER:O	3:M:152:THR:HG22	2.03	0.59
1:A:264:LEU:O	1:A:264:LEU:HG	2.02	0.59
1:A:354:CYS:N	1:A:392:LEU:HD13	2.17	0.59
2:B:517:PRO:O	2:B:521:ASP:HB2	2.02	0.59
5:S:47:THR:HG1	5:S:49:PHE:HD1	1.51	0.59
1:A:585:ARG:HH12	1:A:589:VAL:HG21	1.65	0.59
2:B:74:MET:CE	2:B:109:THR:CG2	2.81	0.59
1:A:314:ILE:HG12	1:A:330:ALA:HB1	1.85	0.58
5:S:116:GLU:O	5:S:124:ARG:HD3	2.03	0.58
2:B:10:ASN:HB2	2:B:45:LYS:HE3	1.85	0.58
2:B:297:GLU:HG2	3:M:79:PHE:CE2	2.39	0.58
5:S:93:GLU:HG3	5:S:132:LEU:HD11	1.85	0.58
2:B:478:THR:O	2:B:482:LEU:HB2	2.02	0.58
2:B:566:HIS:HB3	2:B:571:ALA:HB3	1.86	0.58
2:B:511:THR:CG2	2:B:512:GLN:HE21	2.14	0.58
2:B:570:LEU:HD12	2:B:574:TYR:CE2	2.39	0.58
2:B:99:ASN:ND2	2:B:101:LEU:H	2.01	0.58
3:M:125:GLU:O	3:M:126:THR:HB	2.04	0.58
5:S:42:ARG:HE	5:S:46:HIS:HB3	1.68	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:577:GLN:O	1:A:578:GLN:C	2.42	0.58
2:B:247:ARG:CA	2:B:249:SER:OG	2.48	0.58
2:B:382:ILE:HD11	2:B:417:ILE:HG12	1.86	0.58
1:A:417:ASP:OD2	1:A:419:SER:N	2.36	0.58
2:B:348:GLN:O	2:B:351:ILE:HD11	2.04	0.58
2:B:108:ARG:HH11	3:M:113:ASP:CG	2.07	0.58
2:B:187:ILE:O	2:B:189:GLU:N	2.37	0.57
3:M:323:LYS:CG	3:M:324:PRO:HD2	2.19	0.57
3:M:205:TYR:HD2	3:M:205:TYR:N	2.02	0.57
3:M:191:VAL:CG2	3:M:194:ALA:HB2	2.34	0.57
3:M:333:VAL:HG22	3:M:399:MET:HG2	1.86	0.57
2:B:188:SER:HB3	2:B:196:LEU:H	1.69	0.57
2:B:223:LEU:HB2	2:B:258:SER:HB3	1.87	0.57
1:A:247:TYR:HE1	5:S:130:LYS:HZ2	1.51	0.57
2:B:372:LYS:O	2:B:375:ARG:HB3	2.04	0.57
3:M:186:SER:HB2	3:M:187:PRO:HD2	1.86	0.57
2:B:55:VAL:O	2:B:58:MET:HG2	2.04	0.57
2:B:52:PRO:HB3	2:B:83:MET:CE	2.33	0.57
3:M:30:ASP:O	3:M:31:ALA:C	2.42	0.57
2:B:392:VAL:O	2:B:396:LEU:HD12	2.03	0.57
3:M:123:ASN:HD22	3:M:155:VAL:HG13	1.68	0.57
2:B:11:LYS:CE	5:S:61:ARG:HB3	2.34	0.57
1:A:390:VAL:HG21	1:A:412:TYR:CE2	2.40	0.57
1:A:354:CYS:CB	1:A:392:LEU:HD13	2.35	0.57
1:A:460:GLU:CD	1:A:460:GLU:H	2.07	0.57
1:A:506:GLU:OE2	1:A:601:GLU:O	2.22	0.57
5:S:62:TYR:CE1	5:S:88:VAL:HG21	2.40	0.57
1:A:420:ILE:O	1:A:424:ILE:HG13	2.05	0.57
3:M:205:TYR:N	3:M:205:TYR:CD2	2.73	0.57
1:A:66:PHE:CD1	1:A:101:LEU:HD21	2.40	0.57
2:B:500:GLN:HA	2:B:500:GLN:HE21	1.70	0.57
2:B:290:THR:O	2:B:293:SER:HB2	2.05	0.57
3:M:135:GLN:NE2	3:M:135:GLN:CA	2.67	0.57
3:M:106:VAL:O	3:M:110:GLU:CG	2.53	0.57
1:A:533:CYS:SG	1:A:537:THR:HG21	2.44	0.57
3:M:1:MET:HA	3:M:73:VAL:CG1	2.35	0.56
2:B:374:VAL:HG11	2:B:406:VAL:HG23	1.86	0.56
3:M:205:TYR:O	3:M:206:LEU:HD23	2.05	0.56
2:B:195:ASN:O	2:B:196:LEU:HB3	2.05	0.56
2:B:149:HIS:HA	2:B:153:ALA:HB3	1.85	0.56
2:B:424:LYS:HB3	2:B:425:TYR:CD1	2.40	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:74:MET:HE1	2:B:109:THR:HG22	1.87	0.56
5:S:50:VAL:HG13	5:S:57:ILE:HG12	1.86	0.56
1:A:562:VAL:C	1:A:564:ARG:H	2.08	0.56
1:A:417:ASP:HB3	1:A:420:ILE:HD11	1.88	0.56
1:A:270:PRO:HA	1:A:320:HIS:CD2	2.40	0.56
3:M:32:PHE:HD2	3:M:32:PHE:O	1.88	0.56
2:B:489:VAL:HG11	2:B:526:TYR:CD1	2.41	0.56
2:B:287:PRO:HG2	2:B:288:LEU:H	1.71	0.56
1:A:12:GLY:HA3	1:A:57:LYS:HD2	1.88	0.56
3:M:5:LEU:HD12	3:M:6:PHE:N	2.19	0.56
2:B:570:LEU:CD2	3:M:73:VAL:HG23	2.36	0.56
2:B:351:ILE:HG22	2:B:355:LEU:HD12	1.88	0.56
2:B:417:ILE:O	2:B:420:LYS:N	2.39	0.56
3:M:263:VAL:HA	3:M:276:PHE:HB3	1.88	0.56
1:A:92:GLN:NE2	5:S:112:THR:HB	2.20	0.56
2:B:385:GLU:O	2:B:388:ALA:CA	2.54	0.55
3:M:32:PHE:CE1	3:M:66:ALA:HB2	2.41	0.55
1:A:493:HIS:HD2	1:A:495:ASN:N	2.03	0.55
1:A:608:ARG:HD3	2:B:515:ASP:OD2	2.06	0.55
2:B:396:LEU:HD21	2:B:428:ILE:HG23	1.87	0.55
1:A:464:ARG:NE	1:A:468:ILE:HD11	2.19	0.55
1:A:26:LYS:O	1:A:29:GLU:HB3	2.06	0.55
2:B:58:MET:HG3	2:B:59:GLN:N	2.20	0.55
2:B:335:LYS:HB3	2:B:369:PHE:CE1	2.40	0.55
1:A:397:CYS:HA	1:A:401:ASN:ND2	2.11	0.55
3:M:60:ARG:O	3:M:63:ILE:HB	2.07	0.55
1:A:466:ILE:CD1	1:A:499:VAL:HG22	2.36	0.55
1:A:393:LEU:O	1:A:394:TYR:C	2.42	0.55
2:B:103:ARG:HH21	2:B:137:VAL:HG21	1.70	0.55
5:S:81:LEU:O	5:S:84:ILE:HB	2.07	0.55
1:A:174:ARG:O	1:A:177:ARG:HB3	2.06	0.55
1:A:535:VAL:O	1:A:538:ARG:N	2.38	0.55
3:M:42:GLN:O	3:M:44:ARG:NH1	2.40	0.55
3:M:133:ILE:O	3:M:133:ILE:HG22	2.06	0.55
3:M:212:CYS:HA	3:M:416:LYS:O	2.07	0.55
2:B:253:SER:OG	2:B:298:VAL:HB	2.06	0.55
3:M:152:THR:CG2	3:M:153:SER:N	2.69	0.55
2:B:357:GLU:HG2	2:B:361:TYR:OH	2.07	0.55
1:A:41:ARG:NH2	1:A:74:PHE:HB2	2.22	0.55
3:M:125:GLU:CG	3:M:161:TRP:HA	2.33	0.55
1:A:578:GLN:HG3	1:A:582:GLU:OE2	2.05	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:586:LEU:O	1:A:590:ALA:HB3	2.06	0.54
3:M:163:ARG:HG2	3:M:209:MET:SD	2.47	0.54
2:B:115:VAL:HG23	2:B:118:ILE:HB	1.90	0.54
3:M:32:PHE:HE2	3:M:37:ILE:HG13	1.72	0.54
1:A:519:PRO:O	1:A:520:LEU:C	2.44	0.54
1:A:427:LYS:O	1:A:428:VAL:C	2.46	0.54
2:B:402:LYS:NZ	2:B:435:ASN:ND2	2.56	0.54
2:B:199:LEU:HD13	2:B:229:TYR:CD1	2.29	0.54
2:B:554:LEU:HD23	2:B:555:ILE:H	1.71	0.54
2:B:114:ARG:CZ	2:B:151:ILE:HB	2.37	0.54
2:B:277:TYR:HD2	2:B:278:ASN:HD22	1.54	0.54
1:A:417:ASP:O	1:A:418:TYR:HD2	1.91	0.54
3:M:417:VAL:O	3:M:417:VAL:CG1	2.51	0.54
1:A:504:LEU:CD2	1:A:522:GLN:OE1	2.56	0.54
3:M:191:VAL:HG22	3:M:194:ALA:HB2	1.88	0.54
2:B:292:LEU:N	2:B:292:LEU:CD1	2.70	0.54
1:A:615:LYS:HE3	1:A:619:LYS:HE2	1.90	0.54
2:B:470:LEU:HD21	2:B:484:LEU:HD21	1.88	0.54
2:B:74:MET:HE1	2:B:109:THR:CG2	2.37	0.54
1:A:272:GLU:O	1:A:273:ASP:C	2.46	0.54
2:B:511:THR:HG21	2:B:527:TRP:CZ3	2.42	0.54
5:S:15:ARG:HD2	5:S:100:GLU:OE2	2.08	0.54
3:M:191:VAL:HG13	3:M:191:VAL:O	2.08	0.54
2:B:203:ASN:ND2	2:B:203:ASN:N	2.44	0.54
2:B:304:ARG:HH21	2:B:575:HIS:CD2	2.26	0.54
1:A:356:LEU:C	1:A:356:LEU:HD23	2.28	0.54
2:B:382:ILE:CD1	2:B:417:ILE:HG12	2.38	0.54
1:A:434:LYS:HD2	1:A:435:TYR:CZ	2.43	0.54
1:A:609:GLU:OE2	1:A:609:GLU:O	2.26	0.54
2:B:511:THR:HG21	2:B:527:TRP:HZ3	1.73	0.53
3:M:102:LYS:O	3:M:104:ASN:N	2.39	0.53
3:M:14:VAL:HG12	3:M:15:LEU:N	2.23	0.53
1:A:473:ASP:O	1:A:475:VAL:N	2.42	0.53
1:A:602:MET:HA	1:A:602:MET:HE2	1.91	0.53
2:B:105:LEU:O	2:B:109:THR:OG1	2.17	0.53
3:M:178:LEU:HD23	3:M:436:ILE:HB	1.89	0.53
1:A:559:ILE:HG22	1:A:563:LEU:CD2	2.39	0.53
2:B:70:TYR:CD1	2:B:109:THR:HG21	2.44	0.53
2:B:110:MET:CE	2:B:122:LEU:HB2	2.38	0.53
1:A:400:SER:O	1:A:401:ASN:C	2.45	0.53
1:A:344:ASN:OD1	5:S:49:PHE:CE1	2.61	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:144:ALA:O	1:A:148:ALA:HB2	2.09	0.53
1:A:200:HIS:O	1:A:204:VAL:HG23	2.08	0.53
2:B:493:LEU:HD11	2:B:537:ALA:HB1	1.89	0.53
1:A:226:VAL:O	1:A:230:VAL:HG23	2.09	0.53
2:B:343:ILE:HD12	2:B:376:ALA:HB1	1.90	0.53
1:A:559:ILE:O	1:A:563:LEU:HD23	2.09	0.53
5:S:93:GLU:HG3	5:S:132:LEU:CD1	2.38	0.53
2:B:264:MET:CE	2:B:264:MET:HA	2.39	0.53
2:B:219:GLN:O	2:B:222:ILE:N	2.43	0.52
1:A:608:ARG:CD	2:B:515:ASP:OD2	2.58	0.52
3:M:183:LEU:N	3:M:441:ILE:O	2.33	0.52
2:B:351:ILE:HG22	2:B:355:LEU:CD1	2.40	0.52
1:A:483:VAL:CG1	1:A:500:GLY:CA	2.86	0.52
5:S:99:CYS:O	5:S:102:ASP:HB2	2.09	0.52
2:B:11:LYS:HG2	2:B:12:LYS:H	1.73	0.52
3:M:106:VAL:O	3:M:110:GLU:HG3	2.09	0.52
2:B:186:GLU:CD	3:M:21:ARG:HH22	2.13	0.52
3:M:345:GLN:HB2	3:M:380:GLU:HB2	1.91	0.52
1:A:518:SER:O	1:A:522:GLN:HG3	2.09	0.52
2:B:139:LYS:HG3	2:B:179:ASN:HD22	1.72	0.52
1:A:460:GLU:HB3	1:A:611:SER:OG	2.09	0.52
2:B:551:GLU:O	2:B:552:THR:C	2.47	0.52
1:A:151:ILE:O	1:A:154:ILE:HB	2.10	0.52
3:M:90:ALA:O	3:M:94:GLY:N	2.31	0.52
3:M:433:VAL:HG21	4:P:5:LEU:HD13	1.91	0.52
1:A:449:LEU:O	1:A:450:ILE:C	2.46	0.52
3:M:302:PRO:HG2	3:M:445:ARG:HA	1.91	0.52
2:B:336:LEU:HD23	2:B:369:PHE:CD1	2.44	0.52
2:B:402:LYS:HZ3	2:B:435:ASN:ND2	2.08	0.52
1:A:190:SER:HB3	1:A:191:ARG:HH12	1.74	0.52
3:M:296:LEU:HD22	3:M:297:PRO:HD3	1.92	0.52
2:B:332:ILE:O	2:B:335:LYS:HB2	2.10	0.52
2:B:149:HIS:HE1	2:B:190:SER:HB3	1.75	0.52
2:B:570:LEU:O	2:B:571:ALA:C	2.49	0.52
2:B:379:ARG:HE	2:B:552:THR:CB	2.23	0.52
2:B:485:LEU:O	2:B:486:THR:C	2.45	0.52
5:S:40:THR:HA	5:S:66:TYR:HE2	1.74	0.52
2:B:217:TRP:HA	2:B:220:ILE:HD12	1.91	0.52
1:A:283:CYS:O	1:A:286:THR:HB	2.10	0.51
3:M:355:TYR:HD1	3:M:362:ILE:HG12	1.75	0.51
1:A:338:LEU:HD22	1:A:350:LEU:CD2	2.40	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:151:ILE:HA	1:A:154:ILE:HD12	1.92	0.51
1:A:594:ILE:HG23	1:A:595:LEU:H	1.75	0.51
1:A:413:LEU:O	1:A:415:THR:N	2.43	0.51
3:M:252:ILE:HD13	3:M:253:ALA:H	1.75	0.51
2:B:287:PRO:O	2:B:290:THR:N	2.44	0.51
1:A:314:ILE:O	1:A:317:ILE:HB	2.11	0.51
1:A:379:THR:O	1:A:380:GLU:C	2.48	0.51
3:M:9:ASN:C	3:M:9:ASN:OD1	2.48	0.51
2:B:215:THR:HG23	2:B:218:GLY:H	1.74	0.51
2:B:200:ASN:O	2:B:204:ILE:HB	2.10	0.51
2:B:515:ASP:O	2:B:517:PRO:CD	2.46	0.51
5:S:42:ARG:CD	5:S:59:TYR:HE2	2.23	0.51
2:B:68:LEU:H	2:B:68:LEU:HD13	1.75	0.51
1:A:466:ILE:HD11	1:A:499:VAL:HG22	1.93	0.51
2:B:139:LYS:HD3	2:B:175:MET:HG2	1.92	0.51
2:B:94:ASP:C	2:B:96:GLU:H	2.13	0.51
2:B:119:THR:HG21	2:B:155:MET:HE3	1.92	0.51
1:A:467:GLN:HE22	1:A:608:ARG:HG3	1.74	0.51
1:A:535:VAL:CG2	1:A:536:PRO:HD3	2.30	0.51
2:B:571:ALA:O	2:B:575:HIS:N	2.42	0.51
1:A:292:GLN:HE21	1:A:329:ARG:NH2	2.05	0.51
2:B:110:MET:HG2	2:B:122:LEU:HD22	1.93	0.51
2:B:200:ASN:CB	2:B:201:PRO:HD2	2.18	0.51
3:M:213:LYS:HB2	3:M:416:LYS:HB2	1.92	0.51
2:B:429:ILE:HG21	2:B:459:ILE:HD11	1.93	0.51
3:M:341:THR:HG21	3:M:344:VAL:HG22	1.93	0.51
2:B:289:VAL:O	2:B:292:LEU:HD22	2.10	0.50
3:M:161:TRP:O	3:M:162:ARG:CB	2.48	0.50
1:A:546:ILE:HG23	1:A:599:LEU:HD11	1.92	0.50
1:A:293:GLU:HB3	1:A:294:PRO:HD3	1.89	0.50
2:B:32:GLU:O	2:B:36:LYS:HG3	2.10	0.50
2:B:208:LEU:O	2:B:211:LEU:N	2.43	0.50
1:A:366:VAL:O	1:A:368:THR:N	2.44	0.50
3:M:154:GLN:HG3	3:M:155:VAL:N	2.25	0.50
3:M:109:TYR:O	3:M:110:GLU:C	2.50	0.50
5:S:93:GLU:CG	5:S:132:LEU:HD11	2.41	0.50
2:B:74:MET:HE2	2:B:113:ILE:CD1	2.40	0.50
2:B:414:ILE:HA	2:B:417:ILE:HD12	1.94	0.50
2:B:510:ALA:O	2:B:520:ARG:HA	2.10	0.50
1:A:401:ASN:HB3	1:A:405:ILE:CD1	2.41	0.50
1:A:249:TYR:O	1:A:250:TYR:C	2.49	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:52:GLY:HA3	1:A:87:ARG:NH1	2.26	0.50
2:B:54:VAL:O	2:B:57:CYS:HB2	2.11	0.50
1:A:555:VAL:O	1:A:557:ALA:N	2.44	0.50
3:M:164:GLU:HG2	3:M:165:GLY:N	2.25	0.50
1:A:87:ARG:O	1:A:91:LYS:HG3	2.11	0.50
2:B:468:SER:OG	2:B:469:PHE:N	2.44	0.50
2:B:252:ASN:O	2:B:253:SER:O	2.28	0.50
2:B:350:ASN:O	2:B:354:VAL:HG23	2.12	0.50
2:B:558:THR:O	2:B:559:LEU:C	2.49	0.50
3:M:75:ALA:O	3:M:76:ALA:C	2.49	0.50
2:B:115:VAL:CG2	2:B:118:ILE:HB	2.42	0.50
5:S:50:VAL:CG1	5:S:57:ILE:HG12	2.42	0.50
1:A:463:TYR:O	1:A:467:GLN:HG3	2.11	0.50
2:B:549:SER:N	2:B:551:GLU:OE1	2.45	0.50
1:A:586:LEU:CD2	2:B:540:VAL:HG21	2.41	0.50
2:B:511:THR:HG23	2:B:512:GLN:NE2	2.19	0.50
2:B:131:LYS:O	2:B:132:ASP:HB2	2.11	0.50
2:B:288:LEU:HD22	2:B:306:ILE:CG1	2.40	0.50
1:A:364:GLU:O	1:A:365:ALA:C	2.50	0.50
1:A:414:GLU:HG3	1:A:452:ILE:HG12	1.94	0.49
3:M:26:ARG:CD	3:M:26:ARG:H	2.25	0.49
3:M:69:THR:HG21	3:M:73:VAL:HG22	1.93	0.49
2:B:503:VAL:HA	2:B:506:VAL:HG12	1.95	0.49
1:A:105:ASN:CB	1:A:108:LEU:HD12	2.41	0.49
3:M:163:ARG:CZ	3:M:166:ILE:HD12	2.42	0.49
1:A:579:ARG:HH21	2:B:482:LEU:HD21	1.76	0.49
1:A:52:GLY:HA3	1:A:87:ARG:HH12	1.77	0.49
2:B:74:MET:HE3	2:B:109:THR:CG2	2.41	0.49
2:B:108:ARG:NH1	3:M:113:ASP:OD1	2.46	0.49
5:S:3:ARG:HD2	5:S:55:PHE:CZ	2.48	0.49
1:A:581:VAL:HG21	2:B:545:LYS:HG2	1.93	0.49
1:A:598:VAL:HA	2:B:528:ARG:CB	2.37	0.49
2:B:367:VAL:HG13	2:B:405:TYR:CZ	2.48	0.49
3:M:392:TRP:CZ2	3:M:395:PRO:HD3	2.47	0.49
1:A:201:LEU:HD11	1:A:244:LEU:HD13	1.92	0.49
1:A:344:ASN:CB	5:S:49:PHE:HE1	2.24	0.49
1:A:459:GLU:HG2	1:A:460:GLU:OE1	2.13	0.49
1:A:266:GLN:HG2	1:A:316:LEU:CD1	2.43	0.49
3:M:394:ARG:NH1	3:M:445:ARG:O	2.45	0.49
2:B:51:PHE:N	2:B:52:PRO:HD2	2.28	0.49
2:B:299:GLN:O	2:B:300:TYR:C	2.50	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:338:LYS:O	2:B:339:LEU:C	2.50	0.49
1:A:44:PHE:HE1	1:A:75:GLY:HA3	1.77	0.49
1:A:509:ASN:H	1:A:509:ASN:ND2	2.04	0.49
1:A:579:ARG:HG2	2:B:522:ARG:HH12	1.75	0.49
5:S:92:ASN:OD1	5:S:98:VAL:HG12	2.12	0.49
2:B:227:SER:OG	2:B:227:SER:O	2.21	0.49
5:S:69:ILE:HG22	5:S:71:VAL:HG13	1.94	0.49
3:M:37:ILE:HG12	3:M:64:TRP:CE2	2.48	0.49
1:A:520:LEU:HD12	1:A:521:ILE:CD1	2.42	0.49
2:B:118:ILE:CG2	2:B:119:THR:N	2.75	0.49
2:B:425:TYR:O	2:B:428:ILE:HG13	2.12	0.49
1:A:493:HIS:CD2	1:A:494:GLU:N	2.81	0.49
2:B:501:GLU:O	2:B:505:GLN:HG2	2.12	0.49
5:S:43:ASP:HB2	6:S:1143:SO4:O2	2.13	0.49
1:A:39:ASN:O	1:A:43:LYS:HB2	2.12	0.49
2:B:310:VAL:HG11	2:B:344:ARG:CB	2.42	0.49
3:M:260:HIS:CG	3:M:261:GLN:N	2.81	0.49
2:B:55:VAL:HG13	2:B:58:MET:CE	2.43	0.49
5:S:87:PHE:HD1	5:S:117:MET:SD	2.36	0.49
1:A:575:GLU:OE1	2:B:482:LEU:HD22	2.13	0.49
5:S:66:TYR:N	5:S:66:TYR:CD1	2.81	0.49
2:B:174:PRO:O	2:B:177:VAL:HG12	2.12	0.49
1:A:375:ASN:O	1:A:379:THR:HB	2.13	0.48
3:M:24:ILE:HG22	3:M:25:GLY:N	2.28	0.48
2:B:10:ASN:O	2:B:11:LYS:CB	2.40	0.48
2:B:22:LEU:HD11	2:B:54:VAL:CG2	2.43	0.48
1:A:92:GLN:HE21	5:S:112:THR:CB	2.23	0.48
2:B:279:MET:O	2:B:283:LYS:HB2	2.12	0.48
2:B:506:VAL:HG13	2:B:507:LEU:N	2.27	0.48
2:B:507:LEU:O	2:B:511:THR:HB	2.13	0.48
1:A:602:MET:HA	1:A:602:MET:CE	2.44	0.48
2:B:359:LYS:HG2	2:B:360:GLU:N	2.28	0.48
2:B:581:PHE:CD2	2:B:581:PHE:N	2.81	0.48
1:A:367:LYS:HD2	1:A:398:ASP:OD2	2.12	0.48
1:A:262:LEU:HD13	1:A:312:GLU:HB3	1.94	0.48
1:A:546:ILE:HA	1:A:549:VAL:HG23	1.95	0.48
3:M:106:VAL:O	3:M:110:GLU:HG2	2.12	0.48
5:S:93:GLU:HB3	5:S:132:LEU:HD11	1.95	0.48
5:S:95:PHE:CE2	5:S:102:ASP:HB3	2.49	0.48
1:A:466:ILE:HD13	1:A:503:ILE:HD13	1.95	0.48
2:B:226:LEU:C	2:B:228:ASN:N	2.63	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:M:405:PHE:HD1	3:M:406:ALA:H	1.60	0.48
2:B:245:THR:HB	2:B:246:PRO:HD3	1.94	0.48
3:M:127:GLY:CA	3:M:162:ARG:HG3	2.41	0.48
5:S:131:VAL:O	5:S:135:LEU:HB2	2.13	0.48
3:M:397:ILE:HB	3:M:444:THR:O	2.13	0.48
1:A:281:THR:O	1:A:285:GLU:HG3	2.14	0.48
2:B:270:LEU:HD23	2:B:271:PRO:HD2	1.95	0.48
1:A:63:LEU:HD13	1:A:97:PHE:HA	1.96	0.48
3:M:434:ARG:NH2	4:P:2:TYR:OH	2.46	0.48
3:M:10:HIS:NE2	3:M:11:LYS:HE3	2.29	0.48
3:M:1:MET:N	3:M:71:GLN:HE22	2.11	0.48
1:A:271:PRO:CD	1:A:320:HIS:NE2	2.72	0.48
1:A:585:ARG:NH1	1:A:589:VAL:CG2	2.72	0.48
2:B:63:LEU:HD21	2:B:102:ILE:CD1	2.44	0.48
3:M:179:GLU:OE2	3:M:288:TYR:OH	2.31	0.48
1:A:364:GLU:OE1	1:A:367:LYS:HE2	2.14	0.48
1:A:200:HIS:HD2	1:A:202:GLY:H	1.60	0.48
1:A:209:SER:O	1:A:212:THR:HB	2.14	0.48
5:S:66:TYR:HD1	5:S:66:TYR:N	2.11	0.48
2:B:250:HIS:HA	2:B:252:ASN:ND2	2.29	0.48
1:A:32:ARG:HH12	1:A:36:GLU:HG3	1.77	0.48
2:B:548:ILE:HG22	2:B:551:GLU:HG3	1.96	0.48
1:A:478:TYR:O	1:A:479:ALA:C	2.52	0.48
2:B:382:ILE:N	2:B:382:ILE:HD12	2.28	0.48
2:B:11:LYS:HD3	5:S:63:ALA:O	2.14	0.48
1:A:383:VAL:C	1:A:385:VAL:N	2.65	0.48
3:M:25:GLY:HA2	3:M:26:ARG:NH2	2.28	0.48
3:M:20:TYR:CE2	3:M:116:LEU:O	2.67	0.48
3:M:44:ARG:NH1	3:M:44:ARG:HG3	2.27	0.47
1:A:550:ASN:HB3	1:A:599:LEU:HD12	1.96	0.47
1:A:585:ARG:HH22	2:B:539:GLU:HG3	1.79	0.47
1:A:586:LEU:HD23	2:B:540:VAL:HG21	1.96	0.47
1:A:600:GLU:OE2	1:A:601:GLU:N	2.47	0.47
3:M:222:ILE:O	3:M:223:GLU:CB	2.62	0.47
2:B:276:TYR:HA	2:B:279:MET:CE	2.44	0.47
2:B:275:ASP:HB3	2:B:278:ASN:HB2	1.96	0.47
1:A:369:HIS:O	1:A:370:ILE:C	2.53	0.47
5:S:28:LYS:HA	5:S:31:LEU:HD12	1.96	0.47
2:B:123:CYS:HB3	2:B:157:GLU:OE1	2.13	0.47
1:A:393:LEU:HB3	1:A:405:ILE:HG23	1.95	0.47
1:A:470:ILE:CD1	1:A:605:PHE:CD1	2.94	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:M:182:ASN:OD1	3:M:441:ILE:HB	2.14	0.47
3:M:444:THR:HG23	3:M:445:ARG:N	2.29	0.47
1:A:478:TYR:O	1:A:481:LYS:N	2.48	0.47
3:M:219:LYS:HE3	3:M:219:LYS:HB3	1.76	0.47
3:M:260:HIS:CG	3:M:261:GLN:H	2.32	0.47
2:B:300:TYR:HB2	2:B:333:TYR:CD1	2.50	0.47
2:B:448:MET:HE2	2:B:451:ILE:HB	1.95	0.47
2:B:60:THR:HG21	2:B:65:LEU:HD23	1.97	0.47
3:M:406:ALA:HB2	3:M:435:TYR:HD2	1.80	0.47
2:B:259:ALA:O	2:B:263:LEU:HB2	2.14	0.47
5:S:24:ASP:N	5:S:27:GLU:OE1	2.38	0.47
4:P:5:LEU:O	4:P:6:ASN:CB	2.57	0.47
2:B:74:MET:HE3	2:B:109:THR:HG22	1.96	0.47
1:A:562:VAL:O	1:A:564:ARG:N	2.47	0.47
3:M:20:TYR:HE2	3:M:116:LEU:O	1.97	0.47
3:M:159:ILE:O	3:M:159:ILE:HG22	2.14	0.47
3:M:132:PHE:CG	3:M:132:PHE:O	2.68	0.47
2:B:165:LEU:O	2:B:168:LEU:HB2	2.14	0.47
2:B:277:TYR:HE2	2:B:281:LEU:HD11	1.80	0.47
3:M:107:LEU:O	3:M:110:GLU:N	2.48	0.47
1:A:601:GLU:O	1:A:602:MET:CB	2.63	0.47
1:A:105:ASN:HB3	1:A:108:LEU:HD12	1.97	0.47
3:M:252:ILE:HD13	3:M:253:ALA:N	2.30	0.47
1:A:472:ARG:O	1:A:473:ASP:CB	2.63	0.47
3:M:398:SER:HA	3:M:442:TYR:O	2.14	0.47
5:S:76:ASN:O	5:S:79:ALA:HB3	2.14	0.47
1:A:329:ARG:HB3	1:A:329:ARG:HE	1.43	0.47
2:B:268:GLU:OE2	2:B:269:LEU:HG	2.15	0.47
2:B:289:VAL:HG13	2:B:323:VAL:HG11	1.97	0.46
3:M:247:LEU:H	3:M:247:LEU:HD12	1.80	0.46
5:S:54:ASN:O	5:S:55:PHE:CD2	2.68	0.46
1:A:222:PHE:O	1:A:225:SER:N	2.47	0.46
2:B:155:MET:CB	2:B:158:ASP:HB3	2.41	0.46
2:B:204:ILE:HD11	2:B:229:TYR:CG	2.50	0.46
1:A:460:GLU:N	1:A:460:GLU:CD	2.68	0.46
2:B:274:SER:O	2:B:276:TYR:N	2.37	0.46
2:B:353:GLN:O	2:B:356:ALA:HB3	2.15	0.46
2:B:415:ARG:HD3	2:B:447:ALA:CB	2.45	0.46
3:M:143:GLN:HG3	3:M:147:GLU:HB2	1.97	0.46
2:B:309:ILE:O	2:B:310:VAL:C	2.52	0.46
3:M:183:LEU:O	3:M:442:TYR:HA	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:M:32:PHE:O	3:M:33:ARG:C	2.54	0.46
3:M:301:ILE:HA	3:M:302:PRO:HD3	1.69	0.46
2:B:369:PHE:O	2:B:370:VAL:C	2.53	0.46
1:A:434:LYS:HD2	1:A:435:TYR:CE1	2.50	0.46
1:A:255:PRO:HD2	1:A:256:TRP:CE3	2.49	0.46
1:A:124:ASN:HB2	1:A:125:PRO:HD2	1.98	0.46
2:B:563:LEU:HD23	2:B:563:LEU:HA	1.70	0.46
2:B:126:LEU:HD23	2:B:161:PHE:CE1	2.50	0.46
2:B:289:VAL:O	2:B:290:THR:C	2.54	0.46
3:M:32:PHE:CE2	3:M:37:ILE:HG13	2.50	0.46
1:A:188:TRP:CE3	1:A:192:VAL:HG21	2.50	0.46
1:A:190:SER:HB3	1:A:191:ARG:NH1	2.30	0.46
3:M:292:LYS:HA	3:M:292:LYS:HD3	1.78	0.46
2:B:198:ASP:OD2	2:B:198:ASP:N	2.48	0.46
3:M:401:PHE:H	3:M:439:SER:HB2	1.79	0.46
2:B:258:SER:O	2:B:262:VAL:HG23	2.16	0.46
2:B:264:MET:SD	2:B:309:ILE:HG23	2.55	0.46
1:A:383:VAL:O	1:A:384:SER:C	2.52	0.46
1:A:493:HIS:CD2	1:A:494:GLU:H	2.33	0.46
1:A:226:VAL:HG22	1:A:268:TYR:CD2	2.51	0.46
3:M:264:ARG:HG2	3:M:275:SER:O	2.15	0.46
3:M:322:PHE:CZ	3:M:328:ALA:HB2	2.50	0.46
3:M:364:TRP:CG	3:M:377:ILE:HD12	2.50	0.46
2:B:551:GLU:N	2:B:551:GLU:OE2	2.49	0.46
1:A:487:LEU:HD23	1:A:496:LEU:CD2	2.46	0.46
3:M:107:LEU:O	3:M:109:TYR:N	2.49	0.46
2:B:348:GLN:CD	2:B:348:GLN:H	2.17	0.46
1:A:100:VAL:HG12	1:A:101:LEU:HD12	1.98	0.46
5:S:15:ARG:HD3	5:S:104:VAL:HG22	1.96	0.46
1:A:552:PHE:O	1:A:554:GLU:N	2.48	0.46
2:B:481:GLN:O	2:B:482:LEU:C	2.54	0.46
1:A:188:TRP:HE3	1:A:192:VAL:HG21	1.81	0.46
2:B:307:ASN:HD21	2:B:311:GLN:NE2	2.14	0.46
2:B:176:VAL:HG12	2:B:177:VAL:N	2.31	0.46
1:A:245:GLN:H	1:A:245:GLN:HE21	1.64	0.46
5:S:95:PHE:O	5:S:97:ASN:N	2.49	0.46
1:A:155:LEU:HD11	1:A:165:LYS:HG2	1.98	0.46
2:B:169:ILE:HA	2:B:177:VAL:HG23	1.97	0.46
5:S:52:PHE:O	5:S:52:PHE:CD2	2.68	0.46
1:A:526:LEU:HD22	1:A:541:LEU:HD23	1.98	0.46
2:B:519:LEU:HD12	2:B:519:LEU:HA	1.69	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:277:ARG:HH11	1:A:277:ARG:HB3	1.81	0.46
2:B:484:LEU:O	2:B:484:LEU:HD23	2.15	0.46
1:A:89:THR:HG23	5:S:142:GLU:HA	1.98	0.46
2:B:55:VAL:HG11	2:B:86:MET:HB3	1.98	0.46
3:M:1:MET:HB3	3:M:2:ILE:H	1.46	0.46
5:S:90:VAL:CG2	5:S:128:GLN:HE21	2.25	0.46
1:A:493:HIS:CG	1:A:494:GLU:N	2.84	0.46
1:A:502:TYR:CE1	2:B:517:PRO:HB3	2.51	0.45
2:B:175:MET:O	2:B:176:VAL:C	2.54	0.45
1:A:338:LEU:HD22	1:A:350:LEU:HD21	1.97	0.45
1:A:472:ARG:C	1:A:473:ASP:OD1	2.55	0.45
2:B:284:LEU:O	2:B:288:LEU:HB2	2.16	0.45
1:A:404:GLN:O	1:A:405:ILE:C	2.53	0.45
3:M:440:GLY:O	3:M:441:ILE:HG13	2.16	0.45
5:S:129:THR:HG22	5:S:130:LYS:N	2.31	0.45
2:B:191:HIS:ND1	2:B:195:ASN:OD1	2.49	0.45
3:M:254:ILE:HD12	3:M:254:ILE:HA	1.78	0.45
1:A:266:GLN:HG2	1:A:316:LEU:HD12	1.99	0.45
2:B:404:ASN:O	2:B:408:GLN:HG3	2.16	0.45
2:B:208:LEU:HB3	2:B:243:ARG:HE	1.80	0.45
2:B:338:LYS:O	2:B:341:ILE:N	2.50	0.45
3:M:208:GLY:HA3	3:M:419:GLU:OE2	2.16	0.45
2:B:192:PRO:O	2:B:194:SER:N	2.36	0.45
1:A:393:LEU:O	1:A:396:MET:N	2.48	0.45
2:B:68:LEU:HD13	2:B:68:LEU:N	2.32	0.45
1:A:600:GLU:CA	1:A:600:GLU:OE2	2.63	0.45
2:B:449:ILE:HD11	2:B:469:PHE:CE2	2.51	0.45
1:A:25:SER:O	1:A:27:GLU:N	2.50	0.45
2:B:256:VAL:O	2:B:260:VAL:HG23	2.15	0.45
5:S:117:MET:HE3	5:S:131:VAL:HG21	1.98	0.45
2:B:533:ASP:HA	2:B:534:PRO:HD2	1.58	0.45
1:A:16:PHE:O	1:A:20:ILE:HD13	2.16	0.45
5:S:26:ASP:N	5:S:26:ASP:OD2	2.49	0.45
2:B:529:LEU:HD12	2:B:529:LEU:HA	1.32	0.45
5:S:52:PHE:CE2	5:S:55:PHE:HB2	2.52	0.45
5:S:6:LEU:HD11	5:S:32:ILE:HG12	1.97	0.45
1:A:600:GLU:HB2	2:B:528:ARG:NH1	2.32	0.45
2:B:67:LYS:O	2:B:70:TYR:HB2	2.17	0.45
5:S:90:VAL:O	5:S:93:GLU:HB2	2.17	0.45
1:A:446:ILE:HD13	1:A:449:LEU:HD23	1.97	0.45
3:M:444:THR:HG23	3:M:445:ARG:H	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:255:PRO:HD2	1:A:256:TRP:CZ3	2.52	0.45
3:M:199:ARG:HA	3:M:286:MET:O	2.17	0.45
3:M:294:ILE:HG13	3:M:294:ILE:H	1.43	0.45
5:S:95:PHE:HB2	5:S:98:VAL:HB	1.98	0.45
1:A:446:ILE:HG21	1:A:465:VAL:HB	1.99	0.45
2:B:67:LYS:HD2	2:B:67:LYS:O	2.16	0.45
2:B:110:MET:HE3	2:B:122:LEU:CB	2.47	0.45
2:B:190:SER:O	2:B:192:PRO:HD3	2.17	0.45
2:B:287:PRO:CG	2:B:288:LEU:H	2.29	0.45
2:B:423:ASN:O	2:B:424:LYS:HE3	2.16	0.45
2:B:221:PHE:CZ	3:M:121:PRO:HD2	2.46	0.45
3:M:347:ILE:HG13	3:M:348:CYS:N	2.32	0.44
3:M:5:LEU:CD1	3:M:6:PHE:N	2.78	0.44
2:B:83:MET:HE3	2:B:83:MET:HB3	1.74	0.44
3:M:14:VAL:CG1	3:M:15:LEU:N	2.80	0.44
3:M:256:ASP:O	3:M:288:TYR:HA	2.18	0.44
1:A:312:GLU:HB2	5:S:76:ASN:ND2	2.32	0.44
1:A:262:LEU:HD21	1:A:313:ALA:HA	1.98	0.44
3:M:173:LEU:C	3:M:174:PHE:CD1	2.83	0.44
1:A:41:ARG:HH21	1:A:74:PHE:HB2	1.82	0.44
2:B:363:THR:HB	3:M:393:ALA:CB	2.47	0.44
1:A:540:LEU:HD23	1:A:540:LEU:HA	1.53	0.44
2:B:216:GLU:H	3:M:261:GLN:NE2	2.15	0.44
2:B:292:LEU:H	2:B:292:LEU:HD13	1.78	0.44
3:M:125:GLU:CB	3:M:161:TRP:HA	2.47	0.44
1:A:601:GLU:O	1:A:602:MET:HG2	2.16	0.44
2:B:374:VAL:HG22	2:B:409:GLU:HG3	1.99	0.44
1:A:594:ILE:HG23	1:A:595:LEU:N	2.32	0.44
1:A:414:GLU:O	1:A:415:THR:HG23	2.17	0.44
1:A:273:ASP:OD1	1:A:274:PRO:HD2	2.18	0.44
5:S:43:ASP:OD2	5:S:44:ALA:N	2.50	0.44
1:A:256:TRP:CE3	5:S:126:THR:HG21	2.52	0.44
1:A:501:GLY:HA2	1:A:526:LEU:HD21	1.99	0.44
1:A:388:ARG:HD3	1:A:388:ARG:HA	1.74	0.44
1:A:188:TRP:HE3	1:A:192:VAL:CG2	2.30	0.44
2:B:169:ILE:O	2:B:171:ASP:N	2.50	0.44
2:B:108:ARG:NH1	3:M:113:ASP:CG	2.70	0.44
3:M:291:THR:O	3:M:294:ILE:CG1	2.65	0.44
1:A:189:THR:O	1:A:193:VAL:HG22	2.17	0.44
3:M:170:ARG:HB3	3:M:170:ARG:HH11	1.82	0.44
2:B:247:ARG:HA	2:B:249:SER:HG	1.79	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:517:PRO:O	2:B:521:ASP:CB	2.65	0.44
2:B:533:ASP:N	2:B:533:ASP:OD2	2.50	0.44
5:S:30:LYS:O	5:S:31:LEU:C	2.56	0.44
3:M:371:GLY:O	3:M:372:MET:HB2	2.18	0.44
3:M:8:TYR:CD1	3:M:8:TYR:N	2.86	0.44
3:M:338:PRO:HD2	3:M:381:ILE:HD13	1.98	0.44
1:A:420:ILE:O	1:A:421:ARG:C	2.51	0.44
3:M:259:PHE:CZ	3:M:268:PHE:CE1	3.06	0.44
3:M:316:VAL:HB	3:M:377:ILE:HG23	2.00	0.44
1:A:545:TYR:O	1:A:549:VAL:HG23	2.18	0.44
1:A:517:SER:C	1:A:518:SER:O	2.55	0.44
2:B:67:LYS:C	2:B:67:LYS:HD2	2.38	0.44
2:B:168:LEU:HD22	2:B:176:VAL:HG13	1.99	0.44
2:B:436:LEU:HD23	2:B:437:ASP:N	2.33	0.44
2:B:63:LEU:HD21	2:B:102:ILE:HD11	1.98	0.44
1:A:215:ALA:HB2	1:A:222:PHE:CD1	2.52	0.44
2:B:119:THR:HG21	2:B:155:MET:CE	2.47	0.44
2:B:155:MET:CA	2:B:158:ASP:HB3	2.48	0.44
2:B:18:LEU:HD22	2:B:18:LEU:HA	1.78	0.44
1:A:459:GLU:CG	1:A:460:GLU:OE1	2.66	0.44
2:B:327:LYS:HG2	3:M:441:ILE:HG23	1.96	0.44
3:M:53:THR:HG1	3:M:70:LYS:HE2	1.80	0.44
1:A:487:LEU:HB3	1:A:525:LEU:HD21	2.00	0.44
1:A:496:LEU:HG	1:A:496:LEU:O	2.17	0.44
3:M:92:TYR:CE1	3:M:111:LEU:HD21	2.52	0.44
1:A:509:ASN:N	1:A:509:ASN:HD22	2.06	0.44
2:B:470:LEU:HD21	2:B:484:LEU:CD2	2.48	0.44
2:B:361:TYR:O	2:B:364:GLU:HB2	2.16	0.44
2:B:331:PRO:HD2	2:B:334:VAL:HB	1.99	0.44
5:S:14:THR:HG21	5:S:17:ALA:HB2	1.98	0.44
3:M:7:ILE:HD12	3:M:16:ILE:HG12	1.99	0.44
2:B:408:GLN:NE2	2:B:439:LEU:HA	2.33	0.44
2:B:99:ASN:ND2	2:B:101:LEU:HB2	2.32	0.44
3:M:74:ASN:OD1	3:M:74:ASN:C	2.56	0.44
1:A:470:ILE:CD1	1:A:605:PHE:HD1	2.15	0.44
1:A:525:LEU:C	1:A:527:HIS:N	2.71	0.44
2:B:480:VAL:HG12	2:B:481:GLN:N	2.33	0.44
2:B:188:SER:HA	2:B:195:ASN:HD22	1.83	0.44
3:M:313:GLU:HG2	3:M:380:GLU:HG2	2.00	0.44
3:M:328:ALA:HB3	3:M:369:MET:HB3	2.00	0.43
2:B:216:GLU:O	2:B:219:GLN:HB2	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:370:ILE:HG23	1:A:371:GLU:N	2.33	0.43
1:A:32:ARG:HA	1:A:35:LYS:HD2	2.00	0.43
3:M:107:LEU:HA	3:M:110:GLU:HG3	2.00	0.43
2:B:532:THR:HB	2:B:533:ASP:H	1.66	0.43
2:B:382:ILE:CG2	2:B:382:ILE:O	2.65	0.43
5:S:94:TYR:CE2	5:S:109:LYS:HD3	2.53	0.43
1:A:506:GLU:OE1	1:A:602:MET:HG2	2.19	0.43
1:A:601:GLU:O	1:A:602:MET:HB2	2.18	0.43
2:B:185:SER:O	2:B:186:GLU:C	2.56	0.43
3:M:327:LEU:HB2	3:M:368:ARG:HH12	1.83	0.43
2:B:134:ASP:HA	2:B:135:PRO:HD3	1.75	0.43
1:A:473:ASP:HB2	1:A:474:ASP:H	1.62	0.43
1:A:371:GLU:OE1	1:A:371:GLU:CA	2.38	0.43
2:B:10:ASN:OD1	5:S:10:ARG:NH1	2.51	0.43
2:B:485:LEU:HA	2:B:506:VAL:HG21	1.99	0.43
3:M:152:THR:HG23	3:M:153:SER:N	2.33	0.43
1:A:281:THR:O	1:A:282:GLU:C	2.57	0.43
2:B:126:LEU:CD1	2:B:144:CYS:HB3	2.48	0.43
3:M:170:ARG:NH1	3:M:170:ARG:HB3	2.33	0.43
3:M:127:GLY:HA3	3:M:162:ARG:HA	2.01	0.43
5:S:90:VAL:HG11	5:S:131:VAL:HG11	2.00	0.43
2:B:371:ARG:O	2:B:372:LYS:C	2.56	0.43
2:B:139:LYS:O	2:B:143:VAL:HG23	2.18	0.43
2:B:509:LEU:HA	2:B:509:LEU:HD23	1.73	0.43
2:B:110:MET:CE	2:B:122:LEU:CB	2.96	0.43
1:A:173:LEU:O	1:A:177:ARG:HB2	2.19	0.43
3:M:403:VAL:HG22	3:M:405:PHE:H	1.83	0.43
3:M:39:ALA:C	3:M:41:GLN:N	2.71	0.43
2:B:386:GLN:O	2:B:387:SER:C	2.56	0.43
1:A:473:ASP:O	1:A:474:ASP:C	2.57	0.43
1:A:155:LEU:O	1:A:156:VAL:O	2.36	0.43
5:S:62:TYR:CZ	5:S:88:VAL:HG21	2.53	0.43
2:B:74:MET:CE	2:B:109:THR:HG23	2.47	0.43
3:M:222:ILE:O	3:M:223:GLU:HB3	2.18	0.43
2:B:562:GLU:HG2	2:B:562:GLU:O	2.18	0.43
1:A:356:LEU:CD2	1:A:356:LEU:C	2.86	0.43
3:M:196:VAL:CG1	3:M:290:THR:HG22	2.48	0.43
2:B:449:ILE:HD11	2:B:469:PHE:CD2	2.53	0.43
1:A:167:SER:O	1:A:171:CYS:HB2	2.18	0.43
3:M:77:MET:HE2	3:M:78:VAL:HA	2.00	0.43
2:B:257:LEU:HD23	2:B:257:LEU:HA	1.93	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:250:HIS:HD2	3:M:261:GLN:CG	2.29	0.43
1:A:316:LEU:HG	1:A:320:HIS:HD1	1.83	0.43
1:A:281:THR:O	1:A:283:CYS:N	2.51	0.43
2:B:417:ILE:O	2:B:418:PHE:C	2.56	0.43
3:M:297:PRO:O	3:M:298:PHE:CD1	2.72	0.43
2:B:212:ASN:ND2	2:B:243:ARG:HH22	2.16	0.43
2:B:384:VAL:O	2:B:387:SER:HB2	2.18	0.43
1:A:374:ILE:O	1:A:378:LYS:HB2	2.18	0.43
5:S:60:ARG:HG2	6:S:1144:SO4:O3	2.19	0.43
2:B:154:GLN:CG	2:B:155:MET:N	2.73	0.43
2:B:192:PRO:C	2:B:194:SER:H	2.17	0.43
2:B:473:PHE:CZ	2:B:481:GLN:HB3	2.53	0.43
1:A:165:LYS:O	1:A:168:ALA:HB3	2.19	0.43
2:B:74:MET:HE1	2:B:109:THR:O	2.19	0.43
1:A:413:LEU:O	1:A:414:GLU:C	2.52	0.43
1:A:481:LYS:HE3	1:A:485:GLU:OE1	2.18	0.43
1:A:569:LEU:O	1:A:577:GLN:NE2	2.50	0.43
2:B:356:ALA:O	2:B:357:GLU:C	2.57	0.43
3:M:419:GLU:OE1	3:M:420:PRO:HD2	2.18	0.43
1:A:355:THR:O	1:A:355:THR:HG22	2.15	0.43
3:M:259:PHE:CE1	3:M:268:PHE:CE1	3.07	0.43
1:A:519:PRO:HG3	1:A:552:PHE:CD1	2.53	0.43
1:A:200:HIS:NE2	5:S:130:LYS:HD3	2.33	0.43
2:B:139:LYS:HG2	2:B:140:THR:N	2.33	0.43
1:A:283:CYS:O	1:A:286:THR:N	2.52	0.43
1:A:33:ILE:HD11	1:A:68:LEU:HD13	1.99	0.43
2:B:189:GLU:O	2:B:190:SER:C	2.58	0.43
2:B:22:LEU:HD11	2:B:54:VAL:HG22	2.01	0.43
3:M:355:TYR:CD1	3:M:362:ILE:HG12	2.53	0.43
3:M:108:ILE:O	3:M:111:LEU:HB2	2.19	0.43
1:A:555:VAL:CG1	1:A:556:LYS:N	2.80	0.43
5:S:82:GLU:CA	5:S:82:GLU:OE1	2.67	0.43
3:M:146:GLU:HB3	3:M:147:GLU:H	1.67	0.43
3:M:175:LEU:HD21	3:M:415:LEU:HD22	2.00	0.43
1:A:183:VAL:HA	1:A:184:PRO:HD2	1.86	0.43
1:A:195:LEU:HA	1:A:198:ASP:HB2	2.00	0.43
1:A:112:ILE:O	1:A:116:ILE:HG13	2.19	0.43
2:B:288:LEU:CD2	2:B:306:ILE:HG12	2.49	0.42
2:B:310:VAL:HG11	2:B:344:ARG:HB3	2.00	0.42
3:M:348:CYS:HB2	3:M:364:TRP:NE1	2.19	0.42
1:A:354:CYS:HB2	1:A:392:LEU:HD13	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:89:THR:O	1:A:93:ILE:HB	2.18	0.42
3:M:249:LYS:C	3:M:251:SER:H	2.22	0.42
1:A:373:VAL:HG12	1:A:393:LEU:HD21	2.01	0.42
1:A:410:LEU:HD21	1:A:428:VAL:HG11	2.01	0.42
5:S:2:ILE:HB	5:S:121:GLY:HA2	2.00	0.42
1:A:519:PRO:CG	1:A:552:PHE:CD1	3.02	0.42
2:B:73:LEU:HD22	2:B:77:ALA:HB2	2.01	0.42
2:B:436:LEU:C	2:B:438:SER:N	2.70	0.42
5:S:83:ALA:O	5:S:84:ILE:C	2.57	0.42
1:A:63:LEU:CD2	1:A:96:LEU:HD23	2.49	0.42
3:M:185:MET:SD	3:M:189:GLY:HA2	2.59	0.42
3:M:97:SER:O	3:M:101:ILE:N	2.48	0.42
2:B:51:PHE:CD2	2:B:51:PHE:C	2.93	0.42
3:M:367:LYS:HD3	3:M:367:LYS:H	1.85	0.42
5:S:47:THR:OG1	5:S:49:PHE:HD1	2.01	0.42
1:A:250:TYR:O	1:A:302:HIS:HB2	2.20	0.42
2:B:173:ASN:ND2	2:B:175:MET:N	2.67	0.42
3:M:85:MET:O	3:M:86:CYS:C	2.57	0.42
1:A:205:THR:O	1:A:206:ALA:C	2.57	0.42
3:M:240:LYS:H	3:M:240:LYS:HG3	1.48	0.42
1:A:472:ARG:O	1:A:473:ASP:HB2	2.19	0.42
3:M:111:LEU:HD23	3:M:129:LEU:HD13	2.00	0.42
5:S:92:ASN:HA	5:S:98:VAL:HG12	2.02	0.42
1:A:493:HIS:CG	1:A:494:GLU:H	2.37	0.42
1:A:77:MET:C	1:A:79:ALA:N	2.70	0.42
2:B:191:HIS:CD2	2:B:193:ASN:HA	2.55	0.42
1:A:523:PHE:O	1:A:524:ASN:C	2.58	0.42
2:B:183:ALA:HA	3:M:120:TYR:OH	2.20	0.42
3:M:42:GLN:O	3:M:43:VAL:C	2.57	0.42
2:B:570:LEU:HB2	3:M:72:ASN:HD22	1.85	0.42
1:A:266:GLN:HA	1:A:319:HIS:CD2	2.54	0.42
2:B:507:LEU:HA	2:B:507:LEU:HD23	1.85	0.42
2:B:395:LEU:HD23	2:B:395:LEU:HA	1.84	0.42
2:B:374:VAL:HA	2:B:377:ILE:HD12	2.00	0.42
5:S:20:TYR:O	5:S:21:MET:HG3	2.19	0.42
3:M:40:ARG:HG3	3:M:40:ARG:H	1.57	0.42
1:A:233:LEU:O	1:A:236:ILE:N	2.53	0.42
1:A:404:GLN:O	1:A:407:ALA:N	2.53	0.42
5:S:135:LEU:O	5:S:139:GLN:HG2	2.20	0.42
1:A:602:MET:CE	2:B:524:TYR:CB	2.98	0.42
2:B:404:ASN:CG	2:B:405:TYR:N	2.73	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:277:TYR:HD2	2:B:278:ASN:ND2	2.18	0.42
2:B:281:LEU:HD23	2:B:281:LEU:HA	1.74	0.42
2:B:270:LEU:O	2:B:272:LYS:N	2.52	0.42
1:A:304:ASN:O	1:A:305:ALA:C	2.57	0.42
3:M:48:THR:O	3:M:54:SER:HA	2.20	0.42
1:A:595:LEU:HD13	1:A:596:ALA:N	2.34	0.42
1:A:413:LEU:CD1	1:A:425:VAL:HG23	2.49	0.42
3:M:97:SER:OG	3:M:98:GLU:N	2.52	0.42
3:M:413:ARG:HB3	3:M:413:ARG:HE	1.39	0.42
1:A:489:ALA:HB1	1:A:490:PRO:CD	2.45	0.42
2:B:417:ILE:C	2:B:419:ARG:N	2.69	0.42
1:A:505:GLY:HA2	1:A:544:THR:HG23	2.01	0.42
1:A:366:VAL:O	1:A:367:LYS:C	2.58	0.42
1:A:401:ASN:O	1:A:402:ALA:C	2.58	0.42
2:B:503:VAL:O	2:B:504:GLN:O	2.38	0.42
1:A:455:ASP:OD1	1:A:493:HIS:HE1	2.03	0.42
3:M:394:ARG:HA	3:M:395:PRO:HD3	1.90	0.42
1:A:179:SER:HB3	1:A:182:LEU:HB2	2.01	0.42
1:A:377:LEU:HD13	1:A:393:LEU:HD11	2.02	0.41
3:M:69:THR:HG21	3:M:73:VAL:CG2	2.50	0.41
1:A:525:LEU:O	1:A:527:HIS:N	2.52	0.41
2:B:130:LEU:HG	2:B:141:ALA:HB1	2.02	0.41
2:B:253:SER:O	2:B:256:VAL:N	2.52	0.41
3:M:256:ASP:HB3	3:M:289:ARG:NH1	2.36	0.41
2:B:55:VAL:HG13	2:B:58:MET:HE2	2.00	0.41
5:S:16:LEU:HD12	5:S:111:TYR:CE1	2.52	0.41
2:B:409:GLU:O	2:B:413:VAL:HG23	2.20	0.41
2:B:455:TYR:O	2:B:459:ILE:HG13	2.20	0.41
5:S:133:LYS:O	5:S:134:GLN:C	2.58	0.41
1:A:507:PHE:HB3	1:A:510:LEU:HD12	2.01	0.41
3:M:144:THR:CG2	3:M:145:LYS:N	2.71	0.41
3:M:71:GLN:N	3:M:71:GLN:OE1	2.53	0.41
1:A:519:PRO:O	1:A:522:GLN:N	2.53	0.41
2:B:336:LEU:CD2	2:B:369:PHE:HD1	2.31	0.41
5:S:84:ILE:HG22	5:S:85:HIS:N	2.34	0.41
1:A:340:HIS:ND1	1:A:342:GLU:HB3	2.35	0.41
2:B:287:PRO:HG2	2:B:288:LEU:N	2.33	0.41
1:A:398:ASP:H	1:A:401:ASN:ND2	2.18	0.41
3:M:2:ILE:O	3:M:119:GLY:HA3	2.20	0.41
2:B:87:ALA:O	2:B:88:VAL:C	2.59	0.41
1:A:562:VAL:C	1:A:564:ARG:N	2.74	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:17:GLU:OE1	2:B:17:GLU:HA	2.19	0.41
3:M:4:GLY:HA3	3:M:6:PHE:CZ	2.56	0.41
2:B:261:LYS:HA	2:B:567:ILE:HD12	2.00	0.41
2:B:174:PRO:HG3	3:M:158:GLN:HG3	2.02	0.41
1:A:141:ARG:O	1:A:144:ALA:N	2.53	0.41
1:A:68:LEU:O	1:A:68:LEU:HD23	2.21	0.41
1:A:120:LEU:O	1:A:122:SER:N	2.46	0.41
2:B:61:ASP:OD2	2:B:61:ASP:N	2.54	0.41
1:A:204:VAL:HB	1:A:257:LEU:HD11	2.02	0.41
3:M:79:PHE:O	3:M:82:LEU:N	2.54	0.41
5:S:65:LEU:HD22	5:S:65:LEU:HA	1.73	0.41
2:B:177:VAL:HA	2:B:180:ALA:HB3	2.03	0.41
1:A:350:LEU:HA	1:A:350:LEU:HD23	1.40	0.41
3:M:403:VAL:HA	3:M:404:PRO:HD3	1.83	0.41
1:A:305:ALA:O	1:A:306:LYS:C	2.58	0.41
2:B:450:TRP:CZ2	2:B:454:GLU:HG3	2.56	0.41
1:A:223:LYS:O	1:A:223:LYS:HG2	2.20	0.41
1:A:424:ILE:HD13	1:A:424:ILE:HG21	1.82	0.41
1:A:519:PRO:CG	1:A:552:PHE:CE1	3.03	0.41
2:B:481:GLN:O	2:B:484:LEU:N	2.53	0.41
3:M:259:PHE:HB3	3:M:260:HIS:H	1.73	0.41
1:A:377:LEU:HD12	1:A:390:VAL:HG23	1.98	0.41
1:A:394:TYR:CD1	1:A:427:LYS:HB3	2.56	0.41
5:S:2:ILE:HG12	5:S:80:TYR:HE2	1.86	0.41
3:M:125:GLU:O	3:M:126:THR:CB	2.68	0.41
1:A:611:SER:O	1:A:614:ALA:HB3	2.20	0.41
1:A:270:PRO:HA	1:A:271:PRO:HD2	1.47	0.41
2:B:377:ILE:O	2:B:380:CYS:HB2	2.21	0.41
2:B:375:ARG:HD2	2:B:409:GLU:OE1	2.20	0.41
3:M:24:ILE:HG22	3:M:25:GLY:H	1.86	0.41
2:B:437:ASP:OD2	2:B:437:ASP:N	2.51	0.41
1:A:480:ALA:O	1:A:481:LYS:C	2.57	0.41
2:B:94:ASP:C	2:B:96:GLU:N	2.74	0.41
2:B:444:ALA:O	2:B:448:MET:HB2	2.21	0.41
3:M:7:ILE:HG12	3:M:65:LEU:HG	2.02	0.41
3:M:39:ALA:C	3:M:41:GLN:H	2.24	0.41
2:B:424:LYS:HB3	2:B:425:TYR:CE1	2.56	0.41
2:B:382:ILE:HD11	2:B:417:ILE:HA	2.03	0.41
1:A:308:ALA:O	1:A:309:VAL:C	2.59	0.41
5:S:47:THR:HG1	5:S:49:PHE:H	1.67	0.40
1:A:553:PRO:O	1:A:555:VAL:N	2.54	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:371:ARG:HA	2:B:374:VAL:HG13	2.03	0.40
1:A:478:TYR:C	1:A:478:TYR:CD2	2.95	0.40
1:A:345:LEU:O	1:A:346:ARG:C	2.59	0.40
2:B:382:ILE:HG22	2:B:382:ILE:O	2.20	0.40
3:M:244:GLU:O	3:M:245:GLU:HB3	2.20	0.40
2:B:200:ASN:H	2:B:203:ASN:HB2	1.86	0.40
2:B:68:LEU:CD1	2:B:68:LEU:N	2.84	0.40
2:B:99:ASN:HD21	2:B:101:LEU:HD12	1.86	0.40
1:A:66:PHE:CD2	1:A:101:LEU:HD11	2.57	0.40
3:M:406:ALA:HB2	3:M:435:TYR:CD2	2.56	0.40
1:A:63:LEU:HD23	5:S:107:PHE:HE1	1.85	0.40
5:S:56:LYS:HE3	5:S:77:ASN:ND2	2.36	0.40
1:A:151:ILE:HG23	1:A:154:ILE:HD12	2.03	0.40
5:S:52:PHE:HE2	5:S:55:PHE:HB2	1.86	0.40
1:A:222:PHE:O	1:A:224:THR:N	2.55	0.40
3:M:291:THR:O	3:M:294:ILE:HG13	2.22	0.40
3:M:185:MET:HB3	3:M:185:MET:HE3	1.96	0.40
3:M:305:ARG:HG2	3:M:306:GLU:H	1.86	0.40
3:M:323:LYS:HG2	3:M:324:PRO:CD	2.23	0.40
1:A:385:VAL:O	1:A:386:ARG:C	2.59	0.40
1:A:519:PRO:HG3	1:A:552:PHE:HE1	1.84	0.40
1:A:596:ALA:O	1:A:597:THR:C	2.59	0.40
3:M:205:TYR:C	3:M:206:LEU:HD23	2.42	0.40
2:B:264:MET:HA	2:B:264:MET:HE3	2.04	0.40
1:A:57:LYS:HG2	1:A:61:LYS:HZ1	1.87	0.40
2:B:254:ALA:O	2:B:255:VAL:C	2.59	0.40
2:B:226:LEU:HD23	2:B:226:LEU:HA	1.87	0.40
3:M:217:ASN:O	3:M:218:ASP:CG	2.59	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	611/621 (98%)	429 (70%)	120 (20%)	62 (10%)	1 4
2	B	577/592 (98%)	380 (66%)	139 (24%)	58 (10%)	1 4
3	M	422/446 (95%)	307 (73%)	72 (17%)	43 (10%)	1 4
4	P	4/6 (67%)	4 (100%)	0	0	100 100
5	S	140/142 (99%)	106 (76%)	24 (17%)	10 (7%)	1 8
All	All	1754/1807 (97%)	1226 (70%)	355 (20%)	173 (10%)	1 4

All (173) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	125	PRO
1	A	156	VAL
1	A	223	LYS
1	A	226	VAL
1	A	270	PRO
1	A	293	GLU
1	A	294	PRO
1	A	357	ALA
1	A	417	ASP
1	A	474	ASP
1	A	553	PRO
1	A	554	GLU
1	A	556	LYS
1	A	590	ALA
1	A	592	THR
1	A	602	MET
1	A	608	ARG
2	B	11	LYS
2	B	155	MET
2	B	176	VAL
2	B	199	LEU
2	B	216	GLU
2	B	246	PRO
2	B	251	ALA
2	B	252	ASN
2	B	253	SER
2	B	254	ALA
2	B	271	PRO
2	B	370	VAL
2	B	437	ASP
2	B	504	GLN

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Mol	Chain	Res	Type
3	M	52	ARG
3	M	75	ALA
3	M	115	ILE
3	M	125	GLU
3	M	126	THR
3	M	143	GLN
3	M	146	GLU
3	M	161	TRP
3	M	162	ARG
3	M	187	PRO
3	M	247	LEU
3	M	248	GLY
3	M	297	PRO
3	M	298	PHE
3	M	372	MET
5	S	96	HIS
5	S	97	ASN
5	S	129	THR
5	S	133	LYS
1	A	75	GLY
1	A	78	GLU
1	A	250	TYR
1	A	367	LYS
1	A	380	GLU
1	A	395	ALA
1	A	454	GLY
1	A	473	ASP
1	A	490	PRO
1	A	526	LEU
1	A	561	ASP
1	A	589	VAL
1	A	591	SER
1	A	596	ALA
2	B	5	LYS
2	B	9	THR
2	B	49	SER
2	B	82	ASP
2	B	98	PRO
2	B	200	ASN
2	B	213	GLU
2	B	227	SER
2	B	275	ASP

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Mol	Chain	Res	Type
2	B	283	LYS
2	B	293	SER
2	B	348	GLN
2	B	362	ALA
2	B	481	GLN
2	B	552	THR
3	M	43	VAL
3	M	76	ALA
3	M	103	ASN
3	M	105	PHE
3	M	108	ILE
3	M	160	GLY
3	M	439	SER
3	M	445	ARG
5	S	140	SER
1	A	26	LYS
1	A	45	LYS
1	A	81	ASN
1	A	121	ALA
1	A	272	GLU
1	A	282	GLU
1	A	321	ASP
1	A	414	GLU
1	A	457	VAL
2	B	59	GLN
2	B	123	CYS
2	B	130	LEU
2	B	174	PRO
2	B	188	SER
2	B	193	ASN
2	B	197	LEU
2	B	201	PRO
2	B	212	ASN
2	B	274	SER
2	B	297	GLU
2	B	364	GLU
2	B	424	LYS
2	B	475	ASP
2	B	477	SER
3	M	40	ARG
3	M	107	LEU
3	M	116	LEU

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Mol	Chain	Res	Type
3	M	148	GLN
3	M	218	ASP
3	M	243	SER
3	M	302	PRO
3	M	389	LYS
3	M	426	ASP
3	M	444	THR
5	S	72	ASP
5	S	77	ASN
1	A	83	LEU
1	A	205	THR
1	A	241	SER
1	A	518	SER
1	A	563	LEU
1	A	588	THR
1	A	609	GLU
2	B	88	VAL
2	B	119	THR
2	B	482	LEU
3	M	244	GLU
3	M	251	SER
5	S	53	ARG
5	S	63	ALA
1	A	50	LEU
1	A	138	VAL
1	A	220	GLU
1	A	365	ALA
1	A	418	TYR
1	A	578	GLN
1	A	598	VAL
2	B	13	GLY
2	B	356	ALA
2	B	535	VAL
3	M	42	GLN
3	M	157	GLY
3	M	250	GLN
3	M	407	PRO
1	A	400	SER
2	B	132	ASP
2	B	198	ASP
2	B	310	VAL
3	M	133	ILE

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Mol	Chain	Res	Type
1	A	52	GLY
1	A	219	PRO
1	A	271	PRO
1	A	519	PRO
2	B	541	VAL
2	B	546	PRO
3	M	189	GLY
5	S	110	VAL
1	A	193	VAL
1	A	324	PRO
1	A	385	VAL
2	B	480	VAL
3	M	94	GLY
2	B	451	ILE
2	B	534	PRO
3	M	396	PRO

5.3.2 Protein sidechains (i)

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	537/543 (99%)	445 (83%)	92 (17%)	2 11
2	B	522/533 (98%)	394 (76%)	128 (24%)	1 3
3	M	378/398 (95%)	291 (77%)	87 (23%)	1 4
4	P	6/6 (100%)	5 (83%)	1 (17%)	3 11
5	S	131/131 (100%)	103 (79%)	28 (21%)	1 5
All	All	1574/1611 (98%)	1238 (79%)	336 (21%)	1 6

All (336) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10	MET
1	A	24	LYS
1	A	27	GLU

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Mol	Chain	Res	Type
1	A	39	ASN
1	A	41	ARG
1	A	142	GLU
1	A	143	MET
1	A	151	ILE
1	A	155	LEU
1	A	156	VAL
1	A	161	MET
1	A	185	MET
1	A	194	HIS
1	A	196	LEU
1	A	217	LYS
1	A	223	LYS
1	A	224	THR
1	A	235	ARG
1	A	237	VAL
1	A	238	THR
1	A	244	LEU
1	A	245	GLN
1	A	248	THR
1	A	256	TRP
1	A	257	LEU
1	A	258	SER
1	A	259	VAL
1	A	277	ARG
1	A	279	ARG
1	A	280	LEU
1	A	281	THR
1	A	283	CYS
1	A	288	LEU
1	A	298	LYS
1	A	303	SER
1	A	306	LYS
1	A	314	ILE
1	A	315	SER
1	A	321	ASP
1	A	325	ASN
1	A	326	LEU
1	A	341	ARG
1	A	347	TYR
1	A	358	SER
1	A	360	GLU

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Mol	Chain	Res	Type
1	A	371	GLU
1	A	379	THR
1	A	386	ARG
1	A	399	ARG
1	A	404	GLN
1	A	409	MET
1	A	415	THR
1	A	417	ASP
1	A	419	SER
1	A	425	VAL
1	A	437	VAL
1	A	438	ASP
1	A	440	THR
1	A	449	LEU
1	A	460	GLU
1	A	465	VAL
1	A	470	ILE
1	A	473	ASP
1	A	474	ASP
1	A	475	VAL
1	A	485	GLU
1	A	499	VAL
1	A	503	ILE
1	A	506	GLU
1	A	509	ASN
1	A	516	ARG
1	A	517	SER
1	A	525	LEU
1	A	532	LEU
1	A	533	CYS
1	A	535	VAL
1	A	543	SER
1	A	546	ILE
1	A	550	ASN
1	A	555	VAL
1	A	559	ILE
1	A	561	ASP
1	A	584	LEU
1	A	585	ARG
1	A	595	LEU
1	A	600	GLU
1	A	607	GLU

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Mol	Chain	Res	Type
1	A	609	GLU
1	A	613	LEU
1	A	616	LEU
1	A	617	LYS
1	A	620	LYS
2	B	6	TYR
2	B	10	ASN
2	B	11	LYS
2	B	14	GLU
2	B	15	ILE
2	B	17	GLU
2	B	18	LEU
2	B	22	LEU
2	B	24	ASN
2	B	26	LYS
2	B	27	LYS
2	B	29	LYS
2	B	48	SER
2	B	49	SER
2	B	53	ASP
2	B	58	MET
2	B	62	ASN
2	B	68	LEU
2	B	71	LEU
2	B	73	LEU
2	B	74	MET
2	B	80	GLN
2	B	83	MET
2	B	90	SER
2	B	96	GLU
2	B	97	ASP
2	B	99	ASN
2	B	102	ILE
2	B	108	ARG
2	B	110	MET
2	B	112	CYS
2	B	116	ASP
2	B	118	ILE
2	B	119	THR
2	B	122	LEU
2	B	124	GLU
2	B	127	ARG

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Mol	Chain	Res	Type
2	B	139	LYS
2	B	144	CYS
2	B	152	ASN
2	B	154	GLN
2	B	156	VAL
2	B	159	GLN
2	B	163	ASP
2	B	175	MET
2	B	184	LEU
2	B	186	GLU
2	B	189	GLU
2	B	202	GLN
2	B	203	ASN
2	B	223	LEU
2	B	247	ARG
2	B	250	HIS
2	B	264	MET
2	B	268	GLU
2	B	269	LEU
2	B	279	MET
2	B	284	LEU
2	B	288	LEU
2	B	292	LEU
2	B	293	SER
2	B	307	ASN
2	B	315	GLU
2	B	318	LYS
2	B	319	GLN
2	B	321	ILE
2	B	326	VAL
2	B	327	LYS
2	B	329	ASN
2	B	332	ILE
2	B	337	GLU
2	B	348	GLN
2	B	350	ASN
2	B	351	ILE
2	B	355	LEU
2	B	357	GLU
2	B	359	LYS
2	B	364	GLU
2	B	372	LYS

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Mol	Chain	Res	Type
2	B	374	VAL
2	B	375	ARG
2	B	379	ARG
2	B	384	VAL
2	B	385	GLU
2	B	386	GLN
2	B	393	SER
2	B	396	LEU
2	B	400	GLN
2	B	402	LYS
2	B	404	ASN
2	B	413	VAL
2	B	424	LYS
2	B	426	GLU
2	B	427	SER
2	B	432	LEU
2	B	436	LEU
2	B	443	ASP
2	B	448	MET
2	B	458	ARG
2	B	463	ASP
2	B	467	GLU
2	B	468	SER
2	B	475	ASP
2	B	477	SER
2	B	482	LEU
2	B	483	THR
2	B	485	LEU
2	B	489	VAL
2	B	493	LEU
2	B	494	LYS
2	B	500	GLN
2	B	501	GLU
2	B	502	LEU
2	B	504	GLN
2	B	508	SER
2	B	511	THR
2	B	517	PRO
2	B	520	ARG
2	B	531	SER
2	B	536	THR
2	B	538	LYS

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Mol	Chain	Res	Type
2	B	552	THR
2	B	553	ASP
2	B	554	LEU
2	B	555	ILE
2	B	558	THR
2	B	567	ILE
2	B	581	PHE
3	M	1	MET
3	M	2	ILE
3	M	5	LEU
3	M	9	ASN
3	M	16	ILE
3	M	17	SER
3	M	23	ASP
3	M	26	ARG
3	M	29	VAL
3	M	30	ASP
3	M	32	PHE
3	M	40	ARG
3	M	44	ARG
3	M	48	THR
3	M	58	VAL
3	M	59	LYS
3	M	61	SER
3	M	62	ASN
3	M	63	ILE
3	M	65	LEU
3	M	73	VAL
3	M	85	MET
3	M	95	LYS
3	M	100	ASN
3	M	111	LEU
3	M	115	ILE
3	M	116	LEU
3	M	133	ILE
3	M	135	GLN
3	M	148	GLN
3	M	149	SER
3	M	152	THR
3	M	154	GLN
3	M	161	TRP
3	M	163	ARG

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Mol	Chain	Res	Type
3	M	166	ILE
3	M	169	ARG
3	M	171	ASN
3	M	172	GLU
3	M	174	PHE
3	M	175	LEU
3	M	176	ASP
3	M	185	MET
3	M	188	GLN
3	M	190	GLN
3	M	200	VAL
3	M	204	SER
3	M	205	TYR
3	M	206	LEU
3	M	213	LYS
3	M	216	MET
3	M	217	ASN
3	M	221	VAL
3	M	222	ILE
3	M	240	LYS
3	M	246	ASP
3	M	251	SER
3	M	252	ILE
3	M	254	ILE
3	M	261	GLN
3	M	263	VAL
3	M	268	PHE
3	M	270	SER
3	M	272	ARG
3	M	286	MET
3	M	289	ARG
3	M	290	THR
3	M	292	LYS
3	M	294	ILE
3	M	296	LEU
3	M	320	SER
3	M	327	LEU
3	M	341	THR
3	M	347	ILE
3	M	348	CYS
3	M	350	LYS
3	M	363	VAL

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Mol	Chain	Res	Type
3	M	364	TRP
3	M	367	LYS
3	M	377	ILE
3	M	389	LYS
3	M	403	VAL
3	M	405	PHE
3	M	413	ARG
3	M	414	TYR
3	M	415	LEU
3	M	436	ILE
4	P	3	GLN
5	S	5	ILE
5	S	6	LEU
5	S	10	ARG
5	S	15	ARG
5	S	26	ASP
5	S	29	GLN
5	S	34	GLU
5	S	40	THR
5	S	47	THR
5	S	51	GLU
5	S	52	PHE
5	S	53	ARG
5	S	54	ASN
5	S	56	LYS
5	S	59	TYR
5	S	60	ARG
5	S	65	LEU
5	S	70	CYS
5	S	73	VAL
5	S	82	GLU
5	S	93	GLU
5	S	103	LEU
5	S	108	TYR
5	S	112	THR
5	S	117	MET
5	S	123	ILE
5	S	124	ARG
5	S	135	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (48) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	39	ASN
1	A	199	GLN
1	A	218	ASN
1	A	245	GLN
1	A	266	GLN
1	A	289	ASN
1	A	292	GLN
1	A	333	GLN
1	A	369	HIS
1	A	387	GLN
1	A	401	ASN
1	A	467	GLN
1	A	493	HIS
1	A	495	ASN
1	A	509	ASN
1	A	527	HIS
1	A	531	HIS
1	A	550	ASN
1	A	578	GLN
2	B	62	ASN
2	B	89	ASN
2	B	99	ASN
2	B	149	HIS
2	B	152	ASN
2	B	173	ASN
2	B	203	ASN
2	B	205	ASN
2	B	278	ASN
2	B	307	ASN
2	B	348	GLN
2	B	404	ASN
2	B	435	ASN
2	B	500	GLN
2	B	512	GLN
2	B	575	HIS
3	M	49	ASN
3	M	71	GLN
3	M	72	ASN
3	M	100	ASN
3	M	135	GLN
3	M	158	GLN
3	M	261	GLN
4	P	3	GLN

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Mol	Chain	Res	Type
4	P	6	ASN
5	S	48	ASN
5	S	54	ASN
5	S	85	HIS
5	S	128	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

5 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	1622	-	4,4,4	0.12	0	6,6,6	0.29	0
6	SO4	A	1623	-	4,4,4	0.20	0	6,6,6	0.40	0
6	SO4	A	1624	-	4,4,4	0.09	0	6,6,6	0.32	0
6	SO4	S	1143	-	4,4,4	0.40	0	6,6,6	0.39	0
6	SO4	S	1144	-	4,4,4	0.09	0	6,6,6	0.43	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	1622	-	-	0/0/0/0	0/0/0/0
6	SO4	A	1623	-	-	0/0/0/0	0/0/0/0
6	SO4	A	1624	-	-	0/0/0/0	0/0/0/0
6	SO4	S	1143	-	-	0/0/0/0	0/0/0/0
6	SO4	S	1144	-	-	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.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	S	1143	SO4	1	0
6	S	1144	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, 95^{th} 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	613/621 (98%)	-0.14	24 (3%) 43 21	40, 94, 189, 206	0
2	B	579/592 (97%)	-0.28	2 (0%) 94 88	57, 101, 139, 157	0
3	M	428/446 (95%)	0.53	62 (14%) 3 1	62, 118, 216, 252	0
4	P	6/6 (100%)	0.67	1 (16%) 2 1	121, 124, 129, 129	0
5	S	142/142 (100%)	-0.27	1 (0%) 89 78	70, 106, 149, 184	0
All	All	1768/1807 (97%)	-0.03	90 (5%) 32 13	40, 105, 188, 252	0

All (90) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	M	387	ASN	7.5
3	M	379	ALA	7.4
3	M	385	PRO	7.2
3	M	315	LYS	6.1
3	M	386	THR	6.0
3	M	314	VAL	5.5
3	M	318	ILE	5.5
1	A	42	SER	5.4
3	M	317	VAL	5.3
3	M	364	TRP	5.1
1	A	47	ASP	4.9
3	M	366	ILE	4.8
3	M	388	ASP	4.7
3	M	347	ILE	4.6
3	M	341	THR	4.6
3	M	340	ASN	4.6
3	M	362	ILE	4.5
3	M	335	ILE	4.5
3	M	308	GLY	4.4
1	A	49	ALA	4.3

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Mol	Chain	Res	Type	RSRZ
3	M	380	GLU	4.3
3	M	381	ILE	4.1
3	M	384	LEU	4.1
3	M	344	VAL	4.0
1	A	148	ALA	4.0
3	M	303	LEU	4.0
3	M	363	VAL	4.0
1	A	46	GLY	3.9
3	M	357	ALA	3.9
3	M	307	VAL	3.9
3	M	302	PRO	3.8
3	M	353	ALA	3.7
3	M	378	SER	3.7
1	A	139	GLY	3.7
1	A	78	GLU	3.6
3	M	355	TYR	3.6
3	M	399	MET	3.6
3	M	301	ILE	3.5
3	M	358	SER	3.5
3	M	346	VAL	3.5
1	A	9	GLY	3.4
3	M	345	GLN	3.2
3	M	310	THR	3.2
3	M	375	SER	3.2
3	M	389	LYS	3.2
3	M	334	ARG	3.1
1	A	103	ASN	3.1
1	A	77	MET	3.1
3	M	332	GLU	3.1
3	M	319	LYS	3.0
3	M	167	LYS	3.0
3	M	343	GLY	3.0
3	M	313	GLU	3.0
1	A	58	TYR	3.0
3	M	382	GLU	2.9
2	B	271	PRO	2.9
3	M	377	ILE	2.8
3	M	424	TYR	2.8
1	A	104	SER	2.8
3	M	383	LEU	2.8
3	M	390	LYS	2.7
1	A	86	ASN	2.7

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Mol	Chain	Res	Type	RSRZ
3	M	360	ASN	2.7
1	A	48	LYS	2.7
1	A	157	ALA	2.7
3	M	331	ILE	2.6
3	M	361	ALA	2.6
3	M	446	CYS	2.5
3	M	305	ARG	2.5
1	A	105	ASN	2.5
1	A	621	GLY	2.4
1	A	62	LEU	2.4
1	A	50	LEU	2.4
3	M	298	PHE	2.4
4	P	5	LEU	2.4
3	M	333	VAL	2.4
1	A	84	SER	2.3
3	M	365	LYS	2.3
3	M	330	LYS	2.3
1	A	88	TYR	2.2
2	B	231	PRO	2.2
3	M	338	PRO	2.2
1	A	152	PRO	2.1
3	M	369	MET	2.1
1	A	90	GLU	2.1
5	S	26	ASP	2.1
3	M	397	ILE	2.0
3	M	339	LEU	2.0
3	M	304	VAL	2.0
1	A	87	ARG	2.0

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

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

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron

density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95^{th} 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
6	SO4	A	1623	5/5	0.98	0.16	-0.45	77,78,79,79	0
6	SO4	S	1143	5/5	0.97	0.16	-0.84	83,85,86,86	0
6	SO4	A	1622	5/5	0.88	0.13	-1.80	162,162,163,163	0
6	SO4	A	1624	5/5	0.93	0.14	-	122,122,123,123	0
6	SO4	S	1144	5/5	0.95	0.13	-	104,105,107,108	0

6.5 Other polymers (i)

There are no such residues in this entry.