Full wwPDB X-ray Structure Validation Report (i)

Jan 24, 2017 – 09:06 PM EST

PDB ID	:	1KK7
Title	:	SCALLOP MYOSIN IN THE NEAR RIGOR CONFORMATION
Authors	:	Himmel, D.M.; Gourinath, S.; Reshetnikova, L.; Shen, Y.; Szent-Gyorgyi, A.G.; Cohen, C.
Deposited on	:	2001-12-06
Resolution	:	3.20 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

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

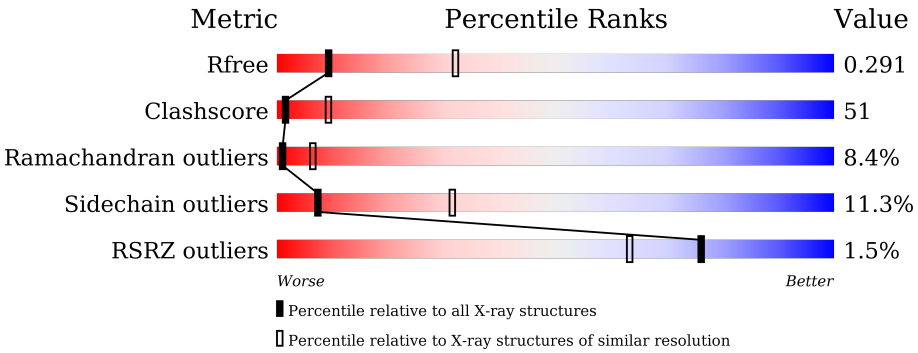
MolProbity	:	4.02b-467
Mogul	:	unknown
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20028442
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20028442

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.20 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	1124 (3.24-3.16)
Clashscore	102246	1024 (3.22-3.18)
Ramachandran outliers	100387	1004 (3.22-3.18)
Sidechain outliers	100360	1003 (3.22-3.18)
RSRZ outliers	91569	1129 (3.24-3.16)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	837	36% 49% 10%
2	Y	156	7% 35% 44% 13% 8%
3	Z	156	% 35% 53% 10%

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
4	SO4	A	995	-	-	-	X
6	CA	Z	998	-	-	-	X

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 8147 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 MYOSIN HEAVY CHAIN, STRIATED MUSCLE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	803	Total	C	N	O	S	5	0	0
			5985	3802	1020	1130	33			

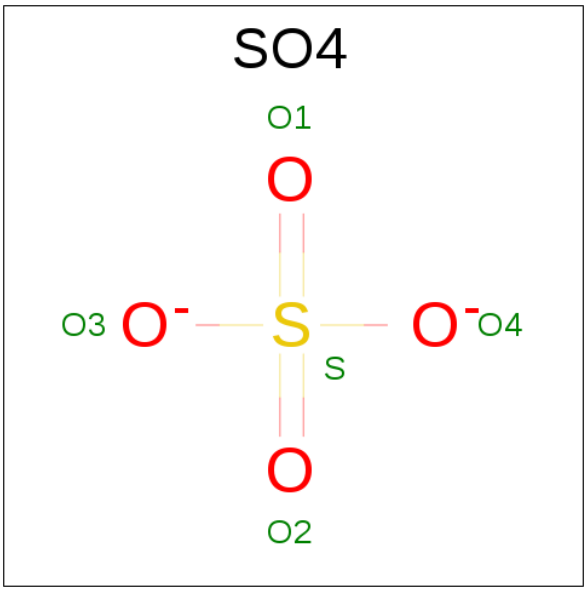
- Molecule 2 is a protein called MYOSIN REGULATORY LIGHT CHAIN, STRIATED ADDUCTOR MUSCLE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	Y	144	Total	C	N	O	S	0	0	0
			1011	638	162	203	8			

- Molecule 3 is a protein called MYOSIN ESSENTIAL LIGHT CHAIN, STRIATED ADDUCTOR MUSCLE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	Z	154	Total	C	N	O	S	0	0	0
			1133	720	182	224	7			

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



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

- Molecule 5 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total Mg 1 1	0	0
5	Y	1	Total Mg 1 1	0	0

- Molecule 6 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	Z	1	Total Ca 1 1	0	0

- Molecule 7 is water.

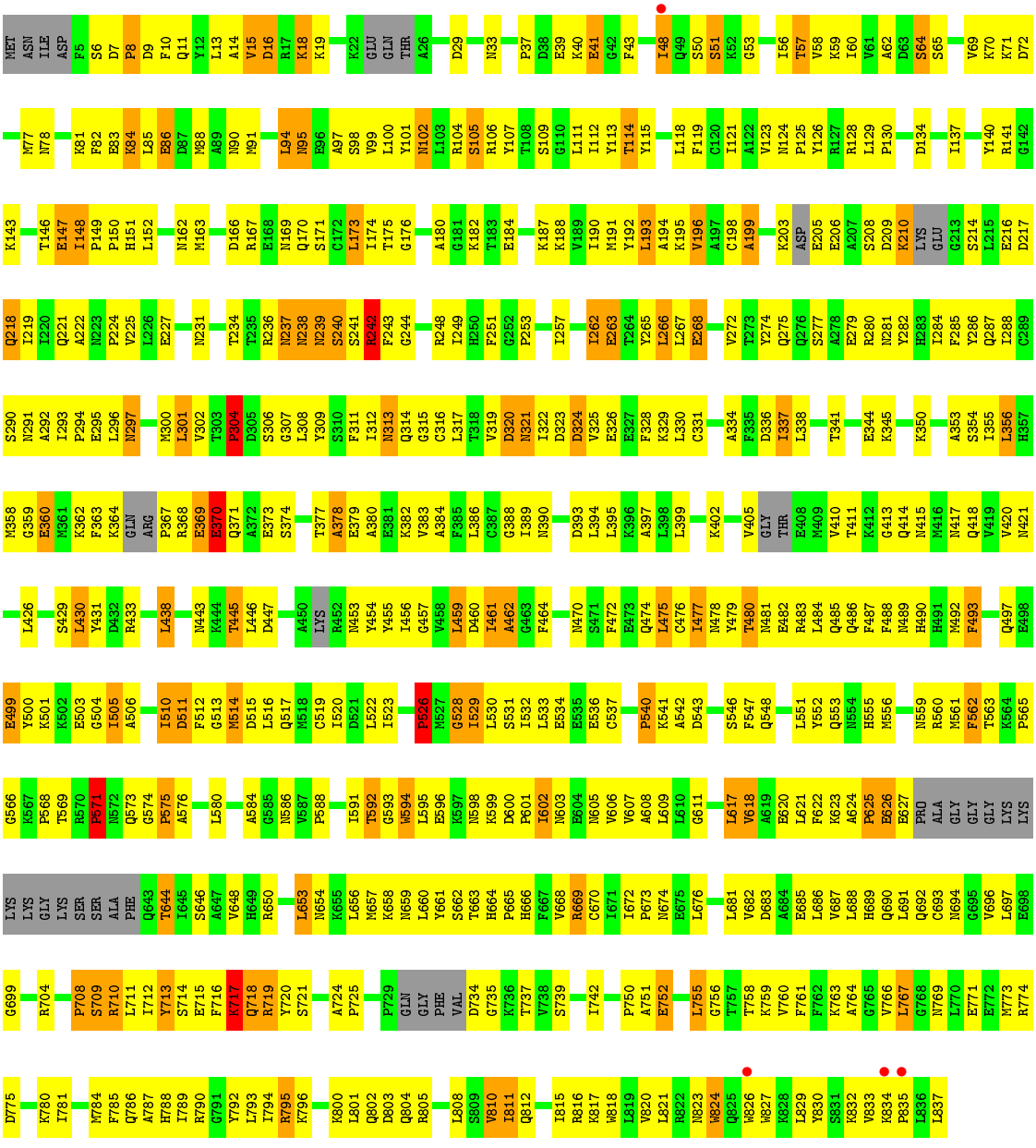
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	7	Total O 7 7	0	0
7	Y	1	Total O 1 1	0	0
7	Z	2	Total O 2 2	0	0

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.

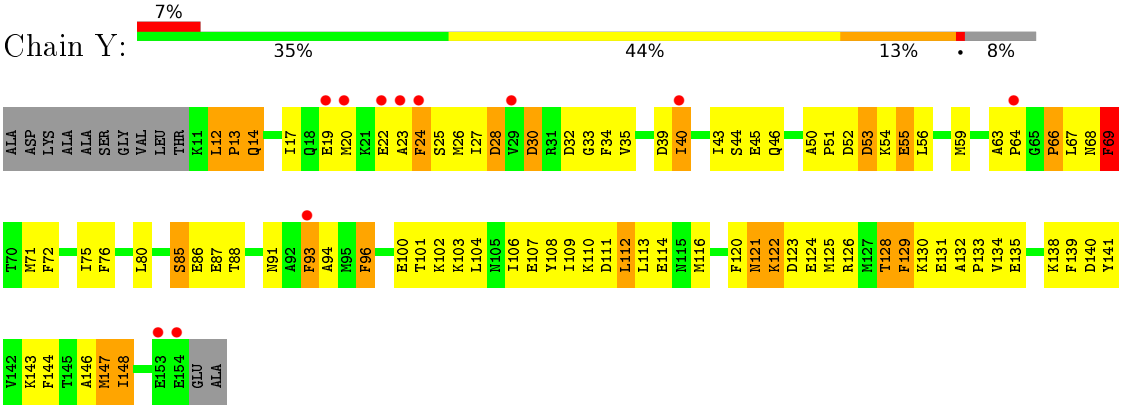
- Molecule 1: MYOSIN HEAVY CHAIN, STRIATED MUSCLE

Chain A:



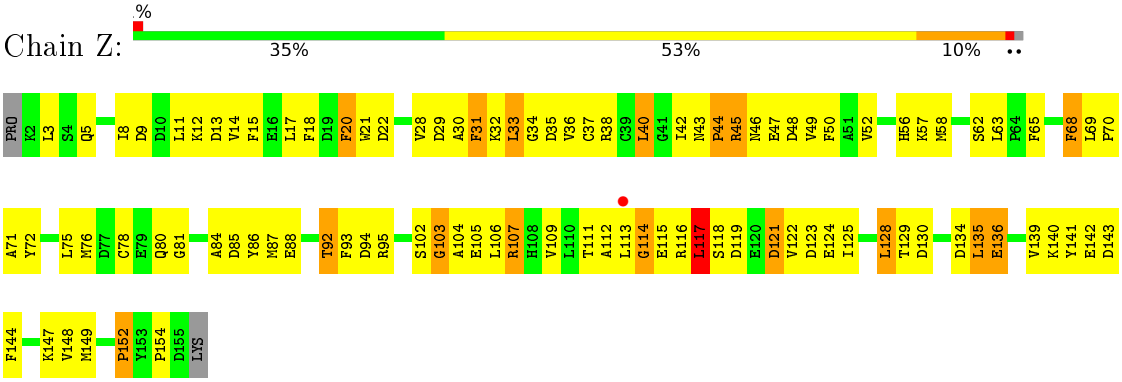
• Molecule 2: MYOSIN REGULATORY LIGHT CHAIN, STRIATED ADDUCTOR MUSCLE

Chain Y:



• Molecule 3: MYOSIN ESSENTIAL LIGHT CHAIN, STRIATED ADDUCTOR MUSCLE

Chain Z:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	159.85Å 51.23Å 84.07Å 90.00° 99.48° 90.00°	Depositor
Resolution (Å)	48.72 – 3.20 48.72 – 3.18	Depositor EDS
% Data completeness (in resolution range)	84.1 (48.72-3.20) 83.2 (48.72-3.18)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.11	Depositor
$< I/\sigma(I) >$ [1]	3.65 (at 3.19Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.259 , 0.313 0.256 , 0.291	Depositor DCC
R_{free} test set	1401 reflections (7.34%)	DCC
Wilson B-factor (Å^2)	79.2	Xtriage
Anisotropy	0.567	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.28 , 120.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.89	EDS
Total number of atoms	8147	wwPDB-VP
Average B, all atoms (Å^2)	84.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.84% 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, 0.333 respectively for untwinned datasets, and 0.375, 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: MG, CA, SO4

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	A	0.45	6/6101 (0.1%)	0.68	3/8285 (0.0%)
2	Y	0.39	0/1027	0.71	2/1392 (0.1%)
3	Z	0.42	0/1156	0.75	2/1569 (0.1%)
All	All	0.44	6/8284 (0.1%)	0.70	7/11246 (0.1%)

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	369	GLU	C-N	-7.86	1.16	1.34
1	A	370	GLU	CD-OE2	6.83	1.33	1.25
1	A	370	GLU	C-N	5.92	1.47	1.34
1	A	704	ARG	CZ-NH1	5.70	1.40	1.33
1	A	370	GLU	CD-OE1	5.34	1.31	1.25
1	A	704	ARG	CZ-NH2	5.02	1.39	1.33

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	Z	114	GLY	N-CA-C	-8.69	91.37	113.10
1	A	238	ASN	N-CA-C	-6.20	94.25	111.00
1	A	666	HIS	N-CA-C	-5.88	95.14	111.00
3	Z	117	LEU	N-CA-C	-5.80	95.34	111.00
2	Y	14	GLN	N-CA-C	5.73	126.47	111.00
2	Y	64	PRO	N-CA-CB	5.54	109.95	103.30
1	A	239	ASN	N-CA-C	-5.24	96.85	111.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5985	0	5526	574	0
2	Y	1011	0	860	144	0
3	Z	1133	0	995	113	0
4	A	5	0	0	1	0
5	A	1	0	0	0	0
5	Y	1	0	0	0	0
6	Z	1	0	0	0	0
7	A	7	0	0	0	0
7	Y	1	0	0	0	0
7	Z	2	0	0	0	0
All	All	8147	0	7381	793	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 51.

All (793) 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:833:VAL:HG11	2:Y:23:ALA:HA	1.12	1.11
1:A:321:ASN:HD22	1:A:321:ASN:N	1.48	1.06
1:A:321:ASN:H	1:A:321:ASN:ND2	1.44	1.03
1:A:459:LEU:HD12	1:A:460:ASP:H	1.24	1.01
1:A:56:ILE:HG22	1:A:57:THR:H	1.26	1.00
2:Y:126:ARG:HB3	2:Y:126:ARG:HH11	1.24	0.98
1:A:818:TRP:HB2	2:Y:148:ILE:HG23	1.43	0.97
1:A:833:VAL:HG11	2:Y:23:ALA:CA	1.97	0.95
2:Y:35:VAL:HB	2:Y:67:LEU:O	1.67	0.94
1:A:175:THR:HG22	1:A:176:GLY:H	1.33	0.94
1:A:672:ILE:HG23	1:A:686:LEU:HD21	1.49	0.94
1:A:755:LEU:H	1:A:755:LEU:HD23	1.31	0.94
2:Y:14:GLN:HE22	2:Y:17:ILE:HG21	1.33	0.94
2:Y:13:PRO:O	2:Y:17:ILE:HG12	1.68	0.93
1:A:510:ILE:HG23	1:A:511:ASP:H	1.32	0.92
3:Z:52:VAL:HG21	3:Z:75:LEU:HD11	1.50	0.91
2:Y:63:ALA:HB3	2:Y:67:LEU:HD22	1.51	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:833:VAL:CG1	2:Y:23:ALA:HA	1.99	0.90
1:A:721:SER:HA	1:A:742:ILE:HD11	1.53	0.90
1:A:128:ARG:O	1:A:129:LEU:HD23	1.72	0.89
2:Y:44:SER:HB3	2:Y:50:ALA:HA	1.52	0.89
1:A:362:LYS:HD3	1:A:363:PHE:H	1.38	0.89
1:A:694:ASN:HD22	1:A:696:VAL:HG22	1.37	0.88
2:Y:27:ILE:HA	2:Y:43:ILE:HG12	1.54	0.88
1:A:459:LEU:HD12	1:A:460:ASP:N	1.88	0.88
1:A:493:PHE:CD2	1:A:512:PHE:HB3	2.10	0.86
1:A:297:ASN:HD22	1:A:297:ASN:H	1.23	0.86
3:Z:109:VAL:HG13	3:Z:113:LEU:HD12	1.58	0.85
3:Z:69:LEU:HB3	3:Z:70:PRO:HD3	1.58	0.85
1:A:497:GLN:O	1:A:501:LYS:HD3	1.78	0.84
1:A:86:GLU:OE1	1:A:150:PRO:HD3	1.78	0.83
1:A:48:ILE:HA	1:A:58:VAL:HG12	1.59	0.83
1:A:826:TRP:HB3	2:Y:76:PHE:HE2	1.43	0.83
1:A:834:LYS:HA	1:A:837:LEU:HD12	1.58	0.83
3:Z:124:GLU:O	3:Z:128:LEU:HB2	1.78	0.82
1:A:443:ASN:O	1:A:447:ASP:HB2	1.79	0.82
1:A:371:GLN:NE2	1:A:414:GLN:H	1.77	0.82
3:Z:40:LEU:HD13	3:Z:72:TYR:CE1	2.17	0.80
1:A:107:TYR:HA	1:A:111:LEU:O	1.82	0.80
1:A:566:GLY:O	1:A:568:PRO:HD3	1.82	0.80
2:Y:126:ARG:HB3	2:Y:126:ARG:NH1	1.97	0.80
1:A:692:GLN:HA	1:A:697:LEU:HD12	1.64	0.79
2:Y:14:GLN:NE2	2:Y:17:ILE:HG21	1.97	0.79
1:A:173:LEU:HD12	1:A:173:LEU:H	1.48	0.79
1:A:360:GLU:HB2	1:A:379:GLU:HG2	1.63	0.79
1:A:514:MET:O	1:A:516:LEU:N	2.16	0.78
3:Z:31:PHE:CD2	3:Z:58:MET:HG2	2.17	0.78
1:A:111:LEU:HD12	1:A:111:LEU:H	1.48	0.78
1:A:721:SER:HA	1:A:742:ILE:CD1	2.12	0.78
1:A:603:ASN:O	1:A:607:VAL:HG23	1.84	0.78
2:Y:52:ASP:O	2:Y:55:GLU:HG2	1.83	0.78
1:A:371:GLN:HE22	1:A:414:GLN:H	1.30	0.77
1:A:459:LEU:HD21	1:A:656:LEU:HD21	1.65	0.77
1:A:475:LEU:HD12	1:A:594:TRP:CH2	2.20	0.77
1:A:686:LEU:O	1:A:690:GLN:HG3	1.85	0.77
1:A:594:TRP:HD1	1:A:594:TRP:H	1.33	0.77
1:A:290:SER:HB2	1:A:325:VAL:HG22	1.68	0.76
1:A:780:LYS:O	1:A:784:MET:HG2	1.85	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:175:THR:HG22	1:A:176:GLY:N	2.01	0.75
1:A:297:ASN:HD22	1:A:297:ASN:N	1.77	0.75
1:A:56:ILE:HG22	1:A:57:THR:N	2.00	0.75
2:Y:106:ILE:O	2:Y:109:ILE:HG22	1.85	0.75
3:Z:31:PHE:HD2	3:Z:58:MET:HG2	1.49	0.75
1:A:826:TRP:HB3	2:Y:76:PHE:CE2	2.21	0.74
1:A:274:TYR:C	1:A:275:GLN:HG3	2.07	0.74
1:A:682:VAL:HG12	1:A:683:ASP:N	2.01	0.74
1:A:512:PHE:CD1	1:A:513:GLY:N	2.55	0.74
1:A:379:GLU:O	1:A:383:VAL:HG23	1.88	0.74
1:A:112:ILE:HD13	1:A:125:PRO:HG3	1.70	0.73
1:A:174:ILE:HG12	1:A:668:VAL:HB	1.71	0.73
1:A:368:ARG:O	1:A:370:GLU:N	2.22	0.73
1:A:691:LEU:HD23	1:A:696:VAL:HG21	1.71	0.73
1:A:86:GLU:OE1	1:A:149:PRO:HA	1.89	0.72
1:A:816:ARG:HG3	1:A:816:ARG:HH11	1.55	0.72
3:Z:8:ILE:HD11	3:Z:69:LEU:HD11	1.72	0.72
1:A:687:VAL:HA	1:A:690:GLN:HE21	1.54	0.71
1:A:603:ASN:HB3	1:A:606:VAL:H	1.55	0.71
1:A:113:TYR:O	1:A:150:PRO:HB2	1.91	0.71
2:Y:106:ILE:HG23	2:Y:107:GLU:H	1.55	0.71
1:A:121:ILE:HD11	1:A:696:VAL:HG11	1.71	0.71
2:Y:51:PRO:HB2	2:Y:56:LEU:HD23	1.72	0.71
2:Y:112:LEU:HD22	2:Y:116:MET:HE1	1.73	0.70
3:Z:11:LEU:HD11	3:Z:68:PHE:HE2	1.56	0.70
1:A:284:ILE:HG23	1:A:285:PHE:N	2.05	0.70
1:A:805:ARG:HG3	3:Z:20:PHE:CE1	2.27	0.70
1:A:274:TYR:HA	1:A:314:GLN:OE1	1.91	0.70
1:A:464:PHE:CE2	1:A:584:ALA:HB3	2.26	0.70
1:A:724:ALA:N	1:A:725:PRO:HD3	2.06	0.70
1:A:112:ILE:HG21	1:A:125:PRO:HG3	1.73	0.70
1:A:510:ILE:HG23	1:A:511:ASP:N	2.06	0.69
1:A:286:TYR:OH	1:A:312:ILE:HB	1.91	0.69
1:A:711:LEU:HD12	1:A:716:PHE:HD1	1.57	0.69
1:A:685:GLU:O	1:A:689:HIS:HB2	1.93	0.69
1:A:288:ILE:HG23	1:A:300:MET:CE	2.23	0.69
1:A:56:ILE:CG2	1:A:57:THR:H	2.04	0.69
1:A:787:ALA:HB1	3:Z:44:PRO:O	1.93	0.68
2:Y:68:ASN:O	2:Y:69:PHE:HB2	1.93	0.68
1:A:7:ASP:O	1:A:9:ASP:N	2.23	0.68
1:A:786:GLN:OE1	3:Z:114:GLY:HA3	1.93	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:618:VAL:HA	1:A:621:LEU:HD12	1.75	0.68
1:A:493:PHE:CG	1:A:512:PHE:HB3	2.28	0.67
1:A:309:TYR:CD2	1:A:356:LEU:HB3	2.29	0.67
2:Y:126:ARG:CB	2:Y:126:ARG:HH11	2.06	0.67
1:A:719:ARG:HD2	1:A:720:TYR:CZ	2.29	0.67
1:A:95:ASN:OD1	1:A:98:SER:HB2	1.95	0.67
1:A:445:THR:HG22	1:A:446:LEU:N	2.09	0.67
1:A:514:MET:C	1:A:516:LEU:H	1.97	0.67
2:Y:53:ASP:HA	2:Y:56:LEU:HD12	1.77	0.67
1:A:272:VAL:HA	1:A:281:ASN:HD21	1.59	0.66
1:A:480:THR:HG22	1:A:653:LEU:HD11	1.77	0.66
1:A:561:MET:O	1:A:580:LEU:HD12	1.94	0.66
1:A:827:TRP:CZ3	2:Y:80:LEU:HD21	2.29	0.66
1:A:603:ASN:C	1:A:605:ASN:H	1.96	0.66
3:Z:17:LEU:O	3:Z:17:LEU:HD23	1.95	0.66
3:Z:45:ARG:HD2	3:Z:46:ASN:H	1.61	0.66
1:A:115:TYR:CZ	1:A:150:PRO:HA	2.31	0.66
1:A:262:ILE:HG23	1:A:263:GLU:N	2.09	0.66
1:A:682:VAL:CG1	1:A:683:ASP:N	2.58	0.66
1:A:624:ALA:O	1:A:626:GLU:N	2.29	0.66
1:A:821:LEU:HD11	1:A:827:TRP:CD2	2.31	0.66
1:A:837:LEU:HD13	2:Y:19:GLU:CB	2.26	0.66
1:A:487:PHE:CE2	1:A:665:PRO:HG3	2.31	0.65
3:Z:37:CYS:O	3:Z:40:LEU:HD12	1.95	0.65
1:A:59:LYS:NZ	1:A:59:LYS:HB3	2.11	0.65
1:A:111:LEU:N	1:A:111:LEU:HD12	2.11	0.65
1:A:694:ASN:HD22	1:A:696:VAL:CG2	2.08	0.65
3:Z:45:ARG:HD2	3:Z:46:ASN:N	2.12	0.65
1:A:84:LYS:CA	1:A:102:ASN:HD21	2.09	0.65
2:Y:12:LEU:H	2:Y:12:LEU:HD12	1.61	0.65
1:A:84:LYS:NZ	1:A:106:ARG:HA	2.12	0.65
1:A:389:ILE:HD11	1:A:394:LEU:HD22	1.77	0.65
1:A:163:MET:CE	1:A:456:ILE:HG13	2.27	0.64
1:A:40:LYS:O	1:A:41:GLU:HG2	1.96	0.64
1:A:288:ILE:HG23	1:A:300:MET:HE1	1.78	0.64
1:A:808:LEU:HD13	2:Y:112:LEU:HD12	1.79	0.64
1:A:820:VAL:HG13	1:A:821:LEU:N	2.12	0.64
1:A:275:GLN:NE2	1:A:314:GLN:HB2	2.12	0.64
2:Y:112:LEU:HA	2:Y:116:MET:HE3	1.78	0.64
1:A:113:TYR:CG	1:A:151:HIS:HA	2.32	0.64
1:A:294:PRO:HA	1:A:297:ASN:ND2	2.13	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:580:LEU:O	1:A:586:ASN:HA	1.96	0.64
2:Y:120:PHE:HA	2:Y:124:GLU:OE2	1.97	0.64
1:A:691:LEU:CD2	1:A:696:VAL:HG21	2.28	0.64
1:A:85:LEU:HD23	1:A:91:MET:HG2	1.78	0.64
1:A:292:ALA:HB2	1:A:325:VAL:HG13	1.80	0.63
1:A:362:LYS:HD3	1:A:363:PHE:N	2.09	0.63
2:Y:106:ILE:HG23	2:Y:107:GLU:N	2.13	0.63
1:A:674:ASN:CG	1:A:681:LEU:HD23	2.19	0.63
1:A:528:GLY:O	1:A:532:ILE:HG13	1.98	0.63
3:Z:52:VAL:HG21	3:Z:75:LEU:CD1	2.25	0.63
1:A:173:LEU:N	1:A:173:LEU:HD12	2.12	0.63
1:A:13:LEU:HD21	1:A:151:HIS:HD2	1.63	0.63
1:A:833:VAL:O	1:A:837:LEU:HG	1.98	0.63
2:Y:91:ASN:O	2:Y:94:ALA:N	2.32	0.63
1:A:242:ARG:NE	1:A:268:GLU:OE2	2.31	0.63
1:A:319:VAL:HG11	1:A:322:ILE:HD12	1.81	0.63
1:A:331:CYS:O	1:A:334:ALA:HB3	1.98	0.62
1:A:173:LEU:CD1	1:A:173:LEU:H	2.06	0.62
1:A:84:LYS:HA	1:A:102:ASN:HD21	1.62	0.62
2:Y:14:GLN:HA	2:Y:17:ILE:HB	1.82	0.62
1:A:817:LYS:O	1:A:820:VAL:HG12	1.99	0.62
2:Y:67:LEU:HA	2:Y:71:MET:HB3	1.81	0.62
1:A:192:TYR:CE1	1:A:196:VAL:HG21	2.35	0.61
1:A:603:ASN:C	1:A:605:ASN:N	2.52	0.61
3:Z:32:LYS:O	3:Z:36:VAL:HG23	2.00	0.61
1:A:286:TYR:O	1:A:324:ASP:HB3	2.00	0.61
3:Z:40:LEU:HD13	3:Z:72:TYR:HE1	1.63	0.61
1:A:140:TYR:CD1	1:A:148:ILE:HD11	2.35	0.61
1:A:415:ASN:H	1:A:418:GLN:HB2	1.66	0.61
3:Z:34:GLY:O	3:Z:38:ARG:HG3	2.01	0.61
1:A:487:PHE:CZ	1:A:665:PRO:HG3	2.35	0.61
1:A:692:GLN:CA	1:A:697:LEU:HD12	2.29	0.61
2:Y:120:PHE:HB3	2:Y:125:MET:HG2	1.81	0.61
1:A:218:GLN:HG2	1:A:338:LEU:HD13	1.83	0.61
1:A:140:TYR:CE1	1:A:148:ILE:HD11	2.35	0.61
1:A:187:LYS:O	1:A:190:ILE:N	2.34	0.61
1:A:214:SER:HB2	1:A:217:ASP:CG	2.21	0.61
1:A:710:ARG:HG2	1:A:710:ARG:O	2.01	0.61
1:A:789:ILE:O	1:A:792:TYR:HB3	2.01	0.61
2:Y:109:ILE:HD11	2:Y:113:LEU:HD21	1.81	0.61
2:Y:40:ILE:HD13	2:Y:59:MET:SD	2.41	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:15:VAL:HG23	1:A:111:LEU:HD21	1.83	0.60
1:A:429:SER:O	1:A:433:ARG:HG3	2.00	0.60
1:A:752:GLU:HG3	1:A:766:VAL:HG21	1.83	0.60
2:Y:24:PHE:HB3	2:Y:69:PHE:HE2	1.66	0.60
3:Z:148:VAL:O	3:Z:148:VAL:HG12	2.00	0.60
3:Z:20:PHE:C	3:Z:20:PHE:HD2	2.05	0.60
1:A:234:THR:O	1:A:237:ASN:CB	2.50	0.60
1:A:371:GLN:HE22	1:A:414:GLN:N	1.97	0.60
1:A:591:ILE:HD12	1:A:591:ILE:C	2.21	0.60
1:A:84:LYS:HB3	1:A:84:LYS:NZ	2.16	0.60
3:Z:43:ASN:N	3:Z:44:PRO:HD3	2.16	0.60
1:A:313:ASN:HD22	1:A:313:ASN:C	2.04	0.60
3:Z:111:THR:HG22	3:Z:117:LEU:O	2.00	0.60
3:Z:122:VAL:O	3:Z:125:ILE:HG22	2.00	0.60
1:A:788:HIS:HA	3:Z:43:ASN:OD1	2.02	0.60
1:A:86:GLU:CD	1:A:150:PRO:HD3	2.21	0.59
1:A:657:MET:SD	1:A:660:LEU:HD12	2.42	0.59
1:A:690:GLN:O	1:A:694:ASN:HB2	2.02	0.59
1:A:70:LYS:C	1:A:72:ASP:H	2.06	0.59
1:A:734:ASP:N	1:A:737:THR:HG1	2.00	0.59
3:Z:31:PHE:O	3:Z:31:PHE:CG	2.55	0.59
1:A:297:ASN:ND2	1:A:297:ASN:H	1.97	0.59
3:Z:65:PHE:HA	3:Z:68:PHE:HB3	1.83	0.59
1:A:275:GLN:HE21	1:A:314:GLN:CD	2.06	0.59
1:A:84:LYS:HE3	1:A:109:SER:OG	2.03	0.59
1:A:205:GLU:CB	1:A:208:SER:HB2	2.31	0.59
1:A:752:GLU:CG	1:A:766:VAL:HG21	2.33	0.59
1:A:817:LYS:HA	1:A:820:VAL:HG12	1.85	0.59
3:Z:52:VAL:CG2	3:Z:75:LEU:HD11	2.27	0.59
1:A:106:ARG:HE	1:A:114:THR:HG23	1.68	0.59
1:A:175:THR:CG2	1:A:176:GLY:H	2.13	0.59
1:A:591:ILE:HD12	1:A:592:THR:N	2.18	0.59
1:A:716:PHE:O	1:A:718:GLN:N	2.36	0.59
3:Z:12:LYS:CG	3:Z:13:ASP:N	2.66	0.59
1:A:801:LEU:HB3	3:Z:17:LEU:HD21	1.85	0.59
2:Y:112:LEU:HD22	2:Y:116:MET:CE	2.32	0.58
3:Z:9:ASP:O	3:Z:12:LYS:HG2	2.03	0.58
2:Y:94:ALA:C	2:Y:96:PHE:H	2.06	0.58
1:A:112:ILE:HD13	1:A:125:PRO:CG	2.34	0.58
1:A:137:ILE:O	1:A:141:ARG:HG3	2.03	0.58
3:Z:20:PHE:C	3:Z:20:PHE:CD2	2.75	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:834:LYS:HA	1:A:837:LEU:CD1	2.30	0.58
2:Y:121:ASN:ND2	2:Y:121:ASN:H	2.01	0.58
2:Y:24:PHE:HZ	2:Y:33:GLY:HA2	1.69	0.58
1:A:826:TRP:CZ2	2:Y:67:LEU:HD21	2.38	0.58
1:A:529:ILE:O	1:A:532:ILE:N	2.37	0.58
2:Y:106:ILE:O	2:Y:110:LYS:HG3	2.04	0.58
2:Y:112:LEU:O	2:Y:112:LEU:HD13	2.03	0.58
2:Y:114:GLU:OE1	2:Y:125:MET:HG3	2.03	0.58
1:A:601:PRO:C	1:A:602:ILE:HG13	2.24	0.58
3:Z:75:LEU:HA	3:Z:78:CYS:SG	2.43	0.58
1:A:134:ASP:HA	1:A:137:ILE:HD12	1.86	0.58
1:A:275:GLN:OE1	1:A:312:ILE:HA	2.03	0.58
1:A:514:MET:C	1:A:516:LEU:N	2.57	0.58
1:A:682:VAL:CG1	1:A:683:ASP:H	2.17	0.58
1:A:243:PHE:HB3	1:A:267:LEU:HD13	1.86	0.57
1:A:300:MET:HB3	1:A:353:ALA:HB2	1.84	0.57
1:A:175:THR:H	1:A:669:ARG:HH12	1.50	0.57
1:A:210:LYS:H	1:A:210:LYS:HD3	1.69	0.57
1:A:475:LEU:HD12	1:A:594:TRP:CZ3	2.38	0.57
1:A:712:ILE:O	1:A:714:SER:N	2.38	0.57
1:A:821:LEU:HD11	1:A:827:TRP:CE3	2.39	0.57
1:A:402:LYS:H	1:A:605:ASN:HD22	1.52	0.57
1:A:594:TRP:CD1	1:A:594:TRP:N	2.67	0.57
1:A:147:GLU:O	1:A:148:ILE:HB	2.03	0.57
1:A:390:ASN:CB	1:A:393:ASP:HB2	2.35	0.57
1:A:182:LYS:HB2	1:A:460:ASP:OD1	2.05	0.57
1:A:804:GLN:O	1:A:805:ARG:C	2.42	0.57
1:A:84:LYS:HZ3	1:A:106:ARG:HA	1.70	0.57
2:Y:85:SER:OG	2:Y:87:GLU:N	2.34	0.57
1:A:300:MET:HB3	1:A:353:ALA:CB	2.35	0.57
2:Y:85:SER:HB3	2:Y:88:THR:H	1.68	0.57
1:A:143:LYS:HA	1:A:143:LYS:HE3	1.86	0.57
1:A:522:LEU:O	1:A:522:LEU:HD23	2.05	0.57
1:A:617:LEU:O	1:A:620:GLU:N	2.38	0.57
1:A:818:TRP:CD1	2:Y:148:ILE:HA	2.40	0.57
3:Z:68:PHE:C	3:Z:68:PHE:CD2	2.79	0.57
1:A:106:ARG:NE	1:A:114:THR:HG23	2.19	0.56
1:A:410:VAL:HG12	1:A:411:THR:H	1.70	0.56
1:A:163:MET:HE3	1:A:456:ILE:HG13	1.86	0.56
1:A:78:ASN:ND2	1:A:98:SER:OG	2.37	0.56
2:Y:63:ALA:CB	2:Y:67:LEU:HD22	2.28	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:84:LYS:HA	1:A:102:ASN:ND2	2.20	0.56
1:A:371:GLN:HE22	1:A:413:GLY:HA2	1.70	0.56
3:Z:118:SER:O	3:Z:121:ASP:N	2.39	0.56
2:Y:114:GLU:OE1	2:Y:125:MET:HE2	2.05	0.56
1:A:85:LEU:H	1:A:102:ASN:HD21	1.52	0.56
1:A:484:LEU:O	1:A:487:PHE:HB3	2.06	0.56
1:A:713:TYR:CE1	1:A:760:VAL:HB	2.40	0.56
1:A:167:ARG:NE	1:A:454:TYR:OH	2.39	0.56
1:A:599:LYS:HG3	1:A:599:LYS:O	2.04	0.56
3:Z:107:ARG:HH11	3:Z:107:ARG:HG2	1.70	0.56
1:A:170:GLN:O	1:A:456:ILE:HA	2.05	0.56
1:A:173:LEU:HA	1:A:459:LEU:HB3	1.88	0.56
1:A:222:ALA:O	1:A:225:VAL:HG22	2.06	0.56
1:A:231:ASN:O	1:A:282:TYR:HA	2.04	0.56
1:A:503:GLU:O	1:A:505:ILE:HG22	2.06	0.56
2:Y:67:LEU:HD11	2:Y:75:ILE:HD13	1.88	0.56
1:A:101:TYR:O	1:A:105:SER:HB2	2.06	0.56
1:A:644:THR:O	1:A:648:VAL:HG23	2.06	0.56
2:Y:24:PHE:CZ	2:Y:33:GLY:HA2	2.41	0.56
1:A:493:PHE:HB2	1:A:512:PHE:HB2	1.88	0.55
1:A:363:PHE:HB3	1:A:373:GLU:O	2.05	0.55
1:A:6:SER:O	1:A:8:PRO:HD3	2.05	0.55
1:A:763:LYS:C	1:A:763:LYS:HD3	2.27	0.55
1:A:724:ALA:N	1:A:725:PRO:CD	2.70	0.55
3:Z:14:VAL:HG12	3:Z:36:VAL:HG13	1.88	0.55
1:A:519:CYS:O	1:A:523:ILE:HG13	2.06	0.55
3:Z:37:CYS:HA	3:Z:40:LEU:CD1	2.36	0.55
1:A:169:ASN:O	1:A:663:THR:HA	2.07	0.55
1:A:241:SER:O	1:A:243:PHE:N	2.39	0.55
1:A:820:VAL:CG1	1:A:821:LEU:N	2.70	0.55
1:A:82:PHE:HD2	1:A:85:LEU:HD22	1.71	0.55
3:Z:45:ARG:O	3:Z:46:ASN:C	2.45	0.55
3:Z:62:SER:O	3:Z:63:LEU:HD23	2.06	0.55
1:A:241:SER:C	1:A:243:PHE:H	2.09	0.55
1:A:336:ASP:O	1:A:338:LEU:N	2.40	0.55
1:A:493:PHE:HB2	1:A:512:PHE:CB	2.37	0.55
2:Y:93:PHE:O	2:Y:104:LEU:HD21	2.06	0.55
1:A:313:ASN:ND2	1:A:313:ASN:C	2.60	0.55
1:A:325:VAL:O	1:A:325:VAL:HG12	2.07	0.55
1:A:287:GLN:HB3	1:A:328:PHE:HB2	1.89	0.54
1:A:503:GLU:O	1:A:505:ILE:N	2.40	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:505:ILE:HG12	1:A:505:ILE:O	2.05	0.54
2:Y:109:ILE:O	2:Y:113:LEU:HG	2.07	0.54
3:Z:49:VAL:HA	3:Z:75:LEU:HD21	1.89	0.54
1:A:167:ARG:HG2	1:A:454:TYR:CE2	2.42	0.54
1:A:384:ALA:HB1	1:A:389:ILE:O	2.08	0.54
1:A:487:PHE:CZ	1:A:665:PRO:CG	2.90	0.54
1:A:111:LEU:CD1	1:A:111:LEU:H	2.18	0.54
1:A:712:ILE:HG13	1:A:715:GLU:H	1.73	0.54
1:A:390:ASN:HB2	1:A:393:ASP:HB2	1.89	0.54
1:A:767:LEU:O	1:A:771:GLU:HG2	2.07	0.54
1:A:88:MET:C	1:A:90:ASN:H	2.11	0.54
2:Y:35:VAL:HG23	2:Y:68:ASN:HA	1.88	0.54
3:Z:42:ILE:HD11	3:Z:76:MET:HE2	1.88	0.54
1:A:300:MET:O	1:A:301:LEU:HB2	2.07	0.54
2:Y:128:THR:C	2:Y:130:LYS:H	2.11	0.54
1:A:284:ILE:CG2	1:A:285:PHE:N	2.71	0.54
1:A:95:ASN:O	1:A:99:VAL:HG23	2.07	0.54
3:Z:20:PHE:O	3:Z:22:ASP:N	2.41	0.54
1:A:109:SER:HB2	1:A:111:LEU:HD13	1.90	0.54
1:A:389:ILE:HD12	1:A:394:LEU:HB2	1.90	0.54
1:A:192:TYR:O	1:A:195:LYS:N	2.41	0.54
1:A:459:LEU:HD11	1:A:461:ILE:HG12	1.88	0.54
2:Y:86:GLU:OE2	2:Y:146:ALA:HA	2.08	0.54
2:Y:85:SER:HB3	2:Y:88:THR:HB	1.90	0.54
1:A:182:LYS:HG2	4:A:995:SO4:O2	2.08	0.53
1:A:717:LYS:HD2	1:A:717:LYS:O	2.07	0.53
2:Y:121:ASN:HD22	2:Y:121:ASN:H	1.55	0.53
1:A:377:THR:O	1:A:378:ALA:C	2.46	0.53
1:A:750:PRO:C	1:A:752:GLU:H	2.10	0.53
1:A:712:ILE:HA	1:A:759:LYS:HA	1.90	0.53
3:Z:15:PHE:CZ	3:Z:28:VAL:HG23	2.43	0.53
1:A:603:ASN:HB2	1:A:606:VAL:HB	1.90	0.53
1:A:60:ILE:O	1:A:64:SER:HA	2.08	0.53
1:A:70:LYS:O	1:A:72:ASP:N	2.42	0.53
3:Z:12:LYS:HG3	3:Z:13:ASP:N	2.24	0.53
2:Y:108:TYR:CE1	2:Y:112:LEU:HD23	2.43	0.53
1:A:231:ASN:HA	1:A:240:SER:O	2.08	0.53
1:A:311:PHE:HA	1:A:314:GLN:NE2	2.24	0.53
2:Y:121:ASN:O	2:Y:123:ASP:N	2.42	0.53
3:Z:33:LEU:HD13	3:Z:63:LEU:CD1	2.39	0.53
1:A:374:SER:OG	1:A:395:LEU:HD22	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:510:ILE:O	1:A:512:PHE:N	2.41	0.53
1:A:834:LYS:N	1:A:835:PRO:CD	2.72	0.53
1:A:124:ASN:HB3	1:A:673:PRO:HD3	1.91	0.52
1:A:249:ILE:O	1:A:455:TYR:HB2	2.08	0.52
3:Z:44:PRO:HB3	3:Z:49:VAL:HG23	1.91	0.52
1:A:18:LYS:HD2	1:A:19:LYS:N	2.25	0.52
1:A:755:LEU:H	1:A:755:LEU:CD2	2.10	0.52
2:Y:85:SER:CB	2:Y:88:THR:H	2.22	0.52
1:A:330:LEU:H	1:A:330:LEU:HD12	1.73	0.52
1:A:474:GLN:O	1:A:478:ASN:ND2	2.40	0.52
1:A:510:ILE:CG2	1:A:511:ASP:H	2.14	0.52
1:A:769:ASN:O	1:A:773:MET:HB2	2.09	0.52
1:A:84:LYS:HA	1:A:106:ARG:HG3	1.91	0.52
1:A:323:ASP:HB3	1:A:326:GLU:HB2	1.91	0.52
1:A:464:PHE:CD2	1:A:584:ALA:HB3	2.44	0.52
1:A:151:HIS:ND1	1:A:152:LEU:N	2.57	0.52
1:A:543:ASP:O	1:A:546:SER:HB3	2.08	0.52
1:A:595:LEU:O	1:A:599:LYS:HG2	2.09	0.52
2:Y:144:PHE:CZ	2:Y:148:ILE:HD11	2.44	0.52
3:Z:102:SER:O	3:Z:105:GLU:N	2.43	0.52
1:A:218:GLN:HB3	1:A:446:LEU:CD2	2.40	0.52
1:A:811:ILE:O	1:A:815:ILE:HG13	2.09	0.52
2:Y:100:GLU:C	2:Y:102:LYS:H	2.13	0.52
1:A:438:LEU:HD23	1:A:438:LEU:O	2.10	0.52
2:Y:68:ASN:O	2:Y:69:PHE:CB	2.57	0.52
1:A:300:MET:O	1:A:386:LEU:HD11	2.10	0.52
1:A:291:ASN:HB2	1:A:304:PRO:HB3	1.92	0.51
1:A:326:GLU:OE2	1:A:329:LYS:HD3	2.11	0.51
1:A:601:PRO:O	1:A:602:ILE:HG23	2.10	0.51
2:Y:30:ASP:OD2	2:Y:30:ASP:N	2.33	0.51
2:Y:129:PHE:HA	2:Y:132:ALA:HB2	1.91	0.51
1:A:100:LEU:O	1:A:104:ARG:HB2	2.10	0.51
1:A:336:ASP:C	1:A:338:LEU:H	2.14	0.51
1:A:106:ARG:HH11	1:A:106:ARG:HG2	1.75	0.51
1:A:626:GLU:O	1:A:627:GLU:C	2.49	0.51
2:Y:144:PHE:O	2:Y:147:MET:HB3	2.11	0.51
1:A:162:ASN:HB2	1:A:170:GLN:NE2	2.26	0.51
1:A:262:ILE:CG2	1:A:263:GLU:N	2.73	0.51
1:A:371:GLN:NE2	1:A:399:LEU:O	2.43	0.51
1:A:552:TYR:O	1:A:556:MET:N	2.44	0.51
1:A:297:ASN:ND2	1:A:297:ASN:N	2.51	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:480:THR:HG22	1:A:653:LEU:CD1	2.41	0.51
1:A:501:LYS:HD2	1:A:501:LYS:N	2.26	0.51
1:A:472:PHE:HB2	1:A:594:TRP:CD1	2.45	0.51
1:A:617:LEU:O	1:A:618:VAL:C	2.48	0.51
1:A:501:LYS:CD	1:A:501:LYS:N	2.74	0.51
2:Y:22:GLU:HA	2:Y:25:SER:HB2	1.92	0.51
1:A:118:LEU:HD12	1:A:488:PHE:CE2	2.46	0.51
1:A:337:ILE:HG22	1:A:337:ILE:O	2.11	0.51
1:A:363:PHE:N	1:A:363:PHE:CD1	2.78	0.51
1:A:194:ALA:HA	1:A:257:ILE:HD12	1.93	0.51
1:A:430:LEU:O	1:A:433:ARG:N	2.44	0.51
1:A:480:THR:O	1:A:483:ARG:N	2.44	0.51
2:Y:72:PHE:O	2:Y:75:ILE:HG12	2.10	0.51
1:A:472:PHE:CZ	1:A:598:ASN:OD1	2.64	0.50
1:A:618:VAL:O	1:A:621:LEU:HB2	2.10	0.50
1:A:88:MET:SD	1:A:99:VAL:HG13	2.50	0.50
1:A:353:ALA:HA	1:A:356:LEU:HD22	1.93	0.50
1:A:591:ILE:HA	1:A:594:TRP:CE2	2.45	0.50
1:A:719:ARG:HD2	1:A:720:TYR:CE1	2.45	0.50
3:Z:11:LEU:HD11	3:Z:68:PHE:CE2	2.41	0.50
1:A:384:ALA:HA	1:A:389:ILE:HG12	1.92	0.50
2:Y:128:THR:O	2:Y:130:LYS:N	2.45	0.50
1:A:500:TYR:HA	1:A:505:ILE:HG23	1.93	0.50
1:A:793:LEU:O	1:A:796:LYS:HB3	2.12	0.50
2:Y:24:PHE:HZ	2:Y:33:GLY:CA	2.23	0.50
1:A:240:SER:O	1:A:242:ARG:N	2.44	0.50
1:A:275:GLN:HE21	1:A:314:GLN:HB2	1.75	0.50
1:A:221:GLN:C	1:A:224:PRO:HD2	2.31	0.50
3:Z:33:LEU:HD13	3:Z:63:LEU:HD12	1.94	0.50
1:A:194:ALA:HA	1:A:257:ILE:CD1	2.41	0.50
1:A:505:ILE:CG1	1:A:505:ILE:O	2.59	0.50
1:A:33:ASN:HB3	1:A:77:MET:SD	2.52	0.49
1:A:358:MET:SD	1:A:426:LEU:HD23	2.52	0.49
1:A:750:PRO:O	1:A:752:GLU:N	2.43	0.49
1:A:291:ASN:HB2	1:A:304:PRO:CB	2.41	0.49
2:Y:23:ALA:O	2:Y:26:MET:N	2.44	0.49
1:A:281:ASN:O	1:A:282:TYR:C	2.49	0.49
1:A:286:TYR:CZ	1:A:312:ILE:HB	2.46	0.49
1:A:503:GLU:HB2	1:A:505:ILE:HG22	1.95	0.49
1:A:593:GLY:O	1:A:596:GLU:N	2.40	0.49
1:A:796:LYS:HB2	3:Z:152:PRO:CG	2.42	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:827:TRP:HZ3	2:Y:80:LEU:HD21	1.74	0.49
2:Y:85:SER:OG	2:Y:86:GLU:N	2.45	0.49
1:A:221:GLN:O	1:A:224:PRO:HD2	2.12	0.49
1:A:800:LYS:HG2	1:A:804:GLN:NE2	2.27	0.49
3:Z:104:ALA:O	3:Z:105:GLU:C	2.51	0.49
1:A:530:LEU:HA	1:A:533:LEU:HB3	1.95	0.49
2:Y:28:ASP:HA	2:Y:39:ASP:HB3	1.95	0.49
1:A:147:GLU:O	1:A:148:ILE:CB	2.61	0.49
3:Z:109:VAL:O	3:Z:113:LEU:HG	2.13	0.49
1:A:227:GLU:O	1:A:231:ASN:HB2	2.13	0.49
1:A:321:ASN:H	1:A:321:ASN:HD22	0.65	0.49
1:A:248:ARG:HA	1:A:457:GLY:HA2	1.93	0.49
1:A:569:THR:C	1:A:571:PRO:HD3	2.33	0.49
1:A:690:GLN:O	1:A:694:ASN:N	2.46	0.49
3:Z:14:VAL:HG21	3:Z:40:LEU:HG	1.95	0.49
1:A:175:THR:CG2	1:A:176:GLY:N	2.73	0.49
1:A:323:ASP:OD2	1:A:326:GLU:HB2	2.13	0.49
1:A:555:HIS:HB2	1:A:562:PHE:CD1	2.48	0.49
1:A:659:ASN:O	1:A:662:SER:N	2.39	0.49
1:A:716:PHE:HD2	1:A:739:SER:OG	1.96	0.49
2:Y:12:LEU:O	2:Y:13:PRO:O	2.30	0.49
1:A:205:GLU:O	1:A:208:SER:HB3	2.13	0.49
1:A:355:ILE:HA	1:A:358:MET:HG3	1.93	0.49
1:A:826:TRP:O	2:Y:76:PHE:HZ	1.95	0.49
1:A:360:GLU:CB	1:A:379:GLU:HG2	2.38	0.48
1:A:85:LEU:N	1:A:102:ASN:HD21	2.09	0.48
2:Y:63:ALA:HB1	2:Y:67:LEU:HD13	1.95	0.48
2:Y:34:PHE:HA	2:Y:68:ASN:CB	2.43	0.48
2:Y:85:SER:HB3	2:Y:88:THR:CB	2.43	0.48
1:A:143:LYS:N	1:A:143:LYS:HD2	2.27	0.48
1:A:336:ASP:C	1:A:338:LEU:N	2.66	0.48
2:Y:20:MET:C	2:Y:69:PHE:HZ	2.17	0.48
2:Y:51:PRO:O	2:Y:56:LEU:HD21	2.13	0.48
2:Y:24:PHE:HB3	2:Y:69:PHE:CE2	2.47	0.48
3:Z:107:ARG:HG3	3:Z:122:VAL:HG11	1.95	0.48
1:A:371:GLN:HE22	1:A:413:GLY:CA	2.27	0.48
1:A:808:LEU:HD22	2:Y:112:LEU:CD1	2.43	0.48
3:Z:68:PHE:O	3:Z:71:ALA:HB3	2.13	0.48
1:A:192:TYR:O	1:A:193:LEU:C	2.51	0.48
1:A:284:ILE:HG13	1:A:288:ILE:HD13	1.96	0.48
2:Y:121:ASN:HD21	2:Y:124:GLU:HG3	1.77	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Z:139:VAL:HG22	3:Z:140:LYS:N	2.29	0.48
3:Z:15:PHE:CE2	3:Z:28:VAL:HG23	2.48	0.48
2:Y:44:SER:C	2:Y:46:GLN:H	2.17	0.48
3:Z:71:ALA:O	3:Z:75:LEU:CD1	2.61	0.48
1:A:291:ASN:HB2	1:A:304:PRO:CG	2.43	0.48
1:A:602:ILE:HD12	1:A:602:ILE:O	2.13	0.48
1:A:818:TRP:CB	2:Y:148:ILE:HG23	2.30	0.48
2:Y:96:PHE:CD1	2:Y:96:PHE:N	2.80	0.48
1:A:433:ARG:NE	1:A:622:PHE:CE2	2.81	0.48
1:A:330:LEU:N	1:A:330:LEU:HD12	2.28	0.48
2:Y:44:SER:CB	2:Y:50:ALA:HA	2.35	0.48
1:A:584:ALA:HB1	1:A:693:CYS:SG	2.54	0.48
1:A:607:VAL:HG13	1:A:622:PHE:HD2	1.79	0.48
1:A:808:LEU:HD13	2:Y:112:LEU:CD1	2.42	0.48
1:A:192:TYR:O	1:A:194:ALA:N	2.47	0.47
3:Z:47:GLU:HA	3:Z:50:PHE:HB2	1.95	0.47
1:A:379:GLU:O	1:A:382:LYS:N	2.47	0.47
1:A:350:LYS:HA	1:A:386:LEU:HD22	1.95	0.47
1:A:493:PHE:CE2	1:A:510:ILE:O	2.67	0.47
1:A:708:PRO:O	1:A:709:SER:C	2.52	0.47
1:A:718:GLN:O	1:A:718:GLN:NE2	2.47	0.47
2:Y:140:ASP:OD1	2:Y:143:LYS:N	2.21	0.47
1:A:167:ARG:O	1:A:167:ARG:HD3	2.14	0.47
1:A:296:LEU:O	1:A:300:MET:HG3	2.14	0.47
1:A:85:LEU:O	1:A:86:GLU:C	2.53	0.47
3:Z:144:PHE:O	3:Z:147:LYS:HB2	2.14	0.47
1:A:802:GLN:HA	3:Z:17:LEU:HD11	1.96	0.47
1:A:169:ASN:O	1:A:663:THR:CA	2.62	0.47
1:A:824:TRP:CZ2	1:A:826:TRP:HD1	2.32	0.47
3:Z:32:LYS:O	3:Z:35:ASP:N	2.47	0.47
1:A:389:ILE:CD1	1:A:394:LEU:HB2	2.44	0.47
1:A:623:LYS:O	1:A:623:LYS:HG3	2.14	0.47
1:A:830:TYR:C	1:A:832:LYS:H	2.18	0.47
2:Y:67:LEU:HD13	2:Y:71:MET:HG3	1.95	0.47
3:Z:94:ASP:HB2	3:Z:141:TYR:OH	2.14	0.47
1:A:601:PRO:O	1:A:602:ILE:HG13	2.14	0.47
2:Y:51:PRO:HB2	2:Y:56:LEU:CD2	2.42	0.47
1:A:231:ASN:HD22	1:A:239:ASN:CB	2.26	0.47
1:A:470:ASN:HB2	1:A:588:PRO:O	2.14	0.47
1:A:712:ILE:O	1:A:712:ILE:HG13	2.15	0.47
1:A:790:ARG:NH2	3:Z:116:ARG:O	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Y:94:ALA:C	2:Y:96:PHE:N	2.68	0.47
1:A:292:ALA:CB	1:A:325:VAL:HG13	2.45	0.47
1:A:503:GLU:CB	1:A:505:ILE:HG22	2.45	0.47
1:A:244:GLY:O	1:A:265:TYR:N	2.40	0.47
3:Z:28:VAL:O	3:Z:29:ASP:C	2.52	0.46
2:Y:93:PHE:CG	2:Y:141:TYR:HB2	2.50	0.46
1:A:552:TYR:O	1:A:556:MET:HB3	2.15	0.46
1:A:84:LYS:HZ3	1:A:84:LYS:HB3	1.79	0.46
2:Y:96:PHE:HB2	2:Y:104:LEU:HD22	1.97	0.46
3:Z:105:GLU:O	3:Z:106:LEU:C	2.53	0.46
1:A:608:ALA:O	1:A:611:GLY:N	2.42	0.46
1:A:526:PRO:O	1:A:531:SER:HB3	2.16	0.46
1:A:562:PHE:HD2	1:A:563:THR:N	2.13	0.46
1:A:50:SER:O	1:A:56:ILE:HG23	2.14	0.46
1:A:785:PHE:N	3:Z:86:TYR:HE1	2.12	0.46
1:A:123:VAL:O	1:A:125:PRO:HD3	2.16	0.46
1:A:222:ALA:O	1:A:225:VAL:CG2	2.64	0.46
1:A:818:TRP:HB2	2:Y:148:ILE:CG2	2.30	0.46
1:A:18:LYS:HD2	1:A:18:LYS:C	2.36	0.46
1:A:459:LEU:CD2	1:A:656:LEU:HD21	2.39	0.46
1:A:781:ILE:HA	1:A:784:MET:HG3	1.97	0.46
1:A:94:LEU:HG	1:A:94:LEU:O	2.15	0.46
2:Y:102:LYS:O	2:Y:103:LYS:HG3	2.16	0.46
3:Z:129:THR:O	3:Z:130:ASP:HB3	2.15	0.46
3:Z:57:LYS:CG	3:Z:58:MET:N	2.78	0.46
3:Z:88:GLU:O	3:Z:92:THR:CG2	2.64	0.46
1:A:251:PHE:CD1	1:A:251:PHE:N	2.83	0.46
1:A:529:ILE:O	1:A:532:ILE:HB	2.15	0.46
1:A:573:GLN:CG	1:A:574:GLY:N	2.79	0.46
1:A:56:ILE:HG22	1:A:57:THR:O	2.16	0.46
1:A:760:VAL:HG13	1:A:760:VAL:O	2.16	0.46
3:Z:107:ARG:HH21	3:Z:123:ASP:CG	2.19	0.46
3:Z:15:PHE:CE2	3:Z:28:VAL:CG2	2.99	0.46
1:A:478:ASN:O	1:A:482:GLU:HB2	2.16	0.46
1:A:402:LYS:N	1:A:605:ASN:HD22	2.13	0.46
2:Y:72:PHE:CD1	2:Y:75:ILE:HD11	2.51	0.46
1:A:792:TYR:CD2	3:Z:152:PRO:HD3	2.50	0.46
1:A:59:LYS:HG2	1:A:65:SER:O	2.16	0.46
1:A:674:ASN:ND2	1:A:681:LEU:O	2.42	0.46
1:A:816:ARG:HG3	1:A:816:ARG:NH1	2.27	0.46
2:Y:108:TYR:HE1	2:Y:112:LEU:HD23	1.79	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:294:PRO:O	1:A:296:LEU:N	2.49	0.45
1:A:569:THR:O	1:A:571:PRO:HD3	2.16	0.45
1:A:306:SER:O	1:A:308:LEU:N	2.49	0.45
1:A:811:ILE:HD13	2:Y:93:PHE:CD1	2.51	0.45
1:A:815:ILE:HG12	2:Y:148:ILE:CD1	2.46	0.45
2:Y:114:GLU:HG3	2:Y:114:GLU:O	2.15	0.45
3:Z:42:ILE:HG22	3:Z:43:ASN:N	2.31	0.45
2:Y:103:LYS:HD3	2:Y:138:LYS:CB	2.46	0.45
2:Y:44:SER:HB2	2:Y:50:ALA:CB	2.46	0.45
1:A:417:ASN:O	1:A:420:VAL:HG22	2.17	0.45
1:A:603:ASN:O	1:A:605:ASN:N	2.50	0.45
1:A:121:ILE:HA	1:A:669:ARG:O	2.16	0.45
2:Y:28:ASP:HA	2:Y:39:ASP:CB	2.46	0.45
1:A:148:ILE:HG13	1:A:149:PRO:HD2	1.98	0.45
1:A:288:ILE:C	1:A:290:SER:H	2.20	0.45
1:A:710:ARG:HH21	1:A:761:PHE:HE2	1.63	0.45
2:Y:35:VAL:CG2	2:Y:68:ASN:HA	2.47	0.45
1:A:218:GLN:CG	1:A:338:LEU:HD13	2.46	0.45
1:A:285:PHE:CZ	1:A:431:TYR:CE2	3.05	0.45
1:A:59:LYS:HB3	1:A:59:LYS:HZ3	1.80	0.45
1:A:786:GLN:O	1:A:789:ILE:HB	2.16	0.45
1:A:218:GLN:NE2	1:A:337:ILE:O	2.45	0.45
1:A:487:PHE:CE2	1:A:665:PRO:CG	2.99	0.45
1:A:326:GLU:O	1:A:330:LEU:HD13	2.17	0.45
1:A:501:LYS:CD	1:A:501:LYS:H	2.30	0.45
2:Y:121:ASN:N	2:Y:121:ASN:HD22	2.10	0.45
3:Z:87:MET:HE2	3:Z:142:GLU:HG3	1.98	0.45
1:A:293:ILE:O	1:A:293:ILE:HG22	2.17	0.45
1:A:481:ASN:O	1:A:485:GLN:N	2.44	0.45
1:A:669:ARG:HA	1:A:669:ARG:HH11	1.81	0.45
1:A:808:LEU:CD1	1:A:812:GLN:HG3	2.47	0.45
2:Y:109:ILE:HG23	2:Y:110:LYS:N	2.32	0.45
3:Z:71:ALA:O	3:Z:75:LEU:HD12	2.17	0.45
1:A:13:LEU:HD21	1:A:151:HIS:CD2	2.50	0.44
1:A:716:PHE:C	1:A:718:GLN:H	2.20	0.44
2:Y:123:ASP:O	2:Y:124:GLU:C	2.55	0.44
1:A:107:TYR:OH	1:A:673:PRO:HG2	2.17	0.44
1:A:362:LYS:CD	1:A:363:PHE:H	2.20	0.44
1:A:169:ASN:O	1:A:664:HIS:N	2.49	0.44
2:Y:66:PRO:O	2:Y:71:MET:HB3	2.17	0.44
1:A:397:ALA:O	1:A:603:ASN:ND2	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:266:LEU:HD11	1:A:476:CYS:HB3	1.99	0.44
1:A:785:PHE:O	1:A:786:GLN:C	2.55	0.44
2:Y:103:LYS:HG2	2:Y:140:ASP:HA	2.00	0.44
1:A:354:SER:HB3	1:A:386:LEU:HB3	1.98	0.44
1:A:540:PRO:O	1:A:542:ALA:N	2.49	0.44
1:A:627:GLU:N	1:A:627:GLU:OE1	2.50	0.44
1:A:785:PHE:HA	3:Z:86:TYR:CE1	2.53	0.44
1:A:102:ASN:HA	1:A:102:ASN:HD22	1.63	0.44
1:A:109:SER:HB2	1:A:111:LEU:CD1	2.47	0.44
1:A:697:LEU:C	1:A:699:GLY:N	2.71	0.44
1:A:756:GLY:HA3	1:A:759:LYS:O	2.16	0.44
1:A:362:LYS:CD	1:A:363:PHE:N	2.80	0.44
1:A:464:PHE:CE1	1:A:478:ASN:HB3	2.52	0.44
1:A:43:PHE:CZ	1:A:97:ALA:HB2	2.53	0.44
3:Z:69:LEU:C	3:Z:69:LEU:HD23	2.38	0.44
1:A:364:LYS:N	1:A:373:GLU:O	2.50	0.44
1:A:503:GLU:HB2	1:A:505:ILE:CG2	2.47	0.44
3:Z:69:LEU:HB3	3:Z:70:PRO:CD	2.37	0.44
1:A:106:ARG:NH1	1:A:106:ARG:HG2	2.33	0.44
1:A:33:ASN:N	1:A:33:ASN:HD22	2.16	0.44
1:A:341:THR:HB	1:A:344:GLU:HG3	2.00	0.44
1:A:575:PRO:O	1:A:576:ALA:HB2	2.18	0.44
1:A:789:ILE:O	1:A:792:TYR:N	2.51	0.44
1:A:803:ASP:O	1:A:804:GLN:C	2.56	0.44
1:A:827:TRP:C	1:A:829:LEU:N	2.69	0.43
2:Y:67:LEU:HD11	2:Y:72:PHE:HA	2.00	0.43
3:Z:18:PHE:O	3:Z:22:ASP:OD2	2.35	0.43
3:Z:93:PHE:CE2	3:Z:109:VAL:HG22	2.53	0.43
1:A:288:ILE:HG23	1:A:300:MET:SD	2.58	0.43
1:A:486:GLN:HE22	1:A:517:GLN:HE21	1.67	0.43
1:A:810:VAL:O	1:A:811:ILE:C	2.55	0.43
1:A:810:VAL:HG12	1:A:811:ILE:N	2.33	0.43
2:Y:134:VAL:HG12	2:Y:135:GLU:N	2.33	0.43
2:Y:20:MET:HB3	2:Y:69:PHE:CZ	2.53	0.43
2:Y:28:ASP:HA	2:Y:39:ASP:OD1	2.18	0.43
1:A:166:ASP:O	1:A:167:ARG:HB3	2.19	0.43
1:A:274:TYR:C	1:A:275:GLN:CG	2.82	0.43
1:A:266:LEU:HD12	1:A:477:ILE:CD1	2.48	0.43
1:A:488:PHE:O	1:A:489:ASN:C	2.57	0.43
1:A:827:TRP:C	1:A:829:LEU:H	2.20	0.43
3:Z:3:LEU:HD21	3:Z:76:MET:SD	2.58	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:284:ILE:HG23	1:A:285:PHE:H	1.79	0.43
1:A:371:GLN:CD	1:A:414:GLN:H	2.22	0.43
1:A:537:CYS:O	1:A:599:LYS:HD3	2.19	0.43
1:A:119:PHE:HE2	1:A:669:ARG:HE	1.66	0.43
2:Y:123:ASP:O	2:Y:126:ARG:N	2.51	0.43
1:A:350:LYS:HA	1:A:386:LEU:CD2	2.48	0.43
1:A:516:LEU:O	1:A:520:ILE:HG13	2.19	0.43
1:A:559:ASN:OD1	1:A:560:ARG:N	2.51	0.43
1:A:657:MET:O	1:A:661:TYR:HD2	2.01	0.43
1:A:816:ARG:NE	2:Y:124:GLU:OE1	2.46	0.43
3:Z:112:ALA:C	3:Z:113:LEU:HD23	2.39	0.43
3:Z:84:ALA:O	3:Z:88:GLU:HG2	2.19	0.43
1:A:405:VAL:HG12	1:A:405:VAL:O	2.18	0.43
1:A:218:GLN:HB3	1:A:446:LEU:HD21	1.99	0.43
2:Y:13:PRO:C	2:Y:17:ILE:HG12	2.36	0.43
2:Y:52:ASP:H	2:Y:55:GLU:CG	2.32	0.43
3:Z:37:CYS:C	3:Z:40:LEU:HD12	2.37	0.43
1:A:277:SER:O	1:A:279:GLU:HG3	2.18	0.43
1:A:792:TYR:OH	3:Z:152:PRO:HA	2.19	0.43
2:Y:128:THR:C	2:Y:130:LYS:N	2.71	0.43
1:A:84:LYS:CE	1:A:109:SER:OG	2.66	0.43
1:A:534:GLU:HG2	1:A:646:SER:OG	2.19	0.43
1:A:713:TYR:OH	1:A:756:GLY:N	2.52	0.43
3:Z:105:GLU:O	3:Z:109:VAL:N	2.46	0.43
1:A:14:ALA:O	1:A:15:VAL:HG23	2.19	0.42
1:A:190:ILE:CD1	1:A:249:ILE:HD11	2.49	0.42
1:A:300:MET:HE3	1:A:302:VAL:HG22	2.00	0.42
1:A:33:ASN:ND2	1:A:33:ASN:N	2.67	0.42
1:A:359:GLY:C	1:A:360:GLU:OE1	2.57	0.42
1:A:676:LEU:HD12	1:A:681:LEU:CD2	2.49	0.42
1:A:69:VAL:HG23	1:A:69:VAL:O	2.19	0.42
1:A:719:ARG:O	1:A:719:ARG:HD3	2.19	0.42
1:A:10:PHE:O	1:A:11:GLN:C	2.57	0.42
1:A:18:LYS:HE3	1:A:18:LYS:HB3	1.84	0.42
1:A:190:ILE:HD12	1:A:249:ILE:HD11	2.01	0.42
1:A:249:ILE:HG22	1:A:251:PHE:CE1	2.54	0.42
1:A:354:SER:O	1:A:358:MET:HG3	2.18	0.42
1:A:175:THR:HB	1:A:669:ARG:NH1	2.35	0.42
1:A:834:LYS:CA	1:A:837:LEU:HD12	2.40	0.42
2:Y:93:PHE:HB3	2:Y:141:TYR:CD2	2.54	0.42
3:Z:134:ASP:O	3:Z:136:GLU:N	2.51	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:267:LEU:HD12	1:A:268:GLU:H	1.83	0.42
1:A:821:LEU:C	1:A:823:ASN:H	2.23	0.42
1:A:82:PHE:HD2	1:A:85:LEU:CD2	2.33	0.42
2:Y:104:LEU:CD1	2:Y:109:ILE:HD13	2.49	0.42
1:A:834:LYS:HA	1:A:837:LEU:CG	2.49	0.42
1:A:231:ASN:ND2	1:A:239:ASN:O	2.52	0.42
1:A:490:HIS:O	1:A:493:PHE:HB3	2.19	0.42
3:Z:45:ARG:CD	3:Z:46:ASN:N	2.82	0.42
1:A:10:PHE:O	1:A:13:LEU:N	2.38	0.42
1:A:284:ILE:HG13	1:A:288:ILE:CD1	2.49	0.42
1:A:290:SER:CB	1:A:325:VAL:HG22	2.43	0.42
2:Y:110:LYS:HB3	2:Y:110:LYS:HE2	1.85	0.42
1:A:147:GLU:C	1:A:148:ILE:HG22	2.40	0.42
1:A:350:LYS:CA	1:A:386:LEU:HD22	2.49	0.42
2:Y:143:LYS:O	2:Y:144:PHE:C	2.57	0.42
3:Z:117:LEU:HD23	3:Z:117:LEU:HA	1.58	0.42
1:A:123:VAL:CG1	1:A:673:PRO:HG3	2.49	0.42
1:A:492:MET:O	1:A:493:PHE:C	2.58	0.42
1:A:180:ALA:HB1	1:A:670:CYS:HB3	2.02	0.42
1:A:688:LEU:O	1:A:689:HIS:C	2.57	0.42
1:A:821:LEU:HD11	1:A:827:TRP:CG	2.55	0.42
3:Z:102:SER:O	3:Z:103:GLY:C	2.58	0.42
1:A:384:ALA:O	1:A:388:GLY:N	2.53	0.42
1:A:461:ILE:O	1:A:462:ALA:O	2.37	0.42
1:A:624:ALA:O	1:A:625:PRO:C	2.58	0.42
1:A:85:LEU:H	1:A:102:ASN:ND2	2.16	0.42
3:Z:29:ASP:OD1	3:Z:31:PHE:N	2.43	0.42
3:Z:42:ILE:C	3:Z:44:PRO:HD3	2.40	0.42
3:Z:85:ASP:O	3:Z:86:TYR:C	2.58	0.42
1:A:499:GLU:O	1:A:500:TYR:C	2.59	0.42
1:A:608:ALA:O	1:A:609:LEU:C	2.56	0.42
1:A:70:LYS:C	1:A:72:ASP:N	2.71	0.42
1:A:815:ILE:HD11	2:Y:144:PHE:HE1	1.85	0.42
2:Y:106:ILE:CG2	2:Y:107:GLU:N	2.82	0.42
3:Z:5:GLN:HA	3:Z:8:ILE:HG22	2.02	0.42
1:A:285:PHE:CZ	1:A:431:TYR:HE2	2.38	0.41
1:A:59:LYS:HA	1:A:65:SER:O	2.20	0.41
1:A:650:ARG:O	1:A:654:ASN:ND2	2.53	0.41
1:A:657:MET:O	1:A:658:LYS:C	2.57	0.41
1:A:724:ALA:HB3	1:A:742:ILE:HG12	2.01	0.41
1:A:84:LYS:CA	1:A:102:ASN:ND2	2.80	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:414:GLN:OE1	1:A:418:GLN:NE2	2.52	0.41
1:A:453:ASN:O	1:A:454:TYR:CG	2.73	0.41
1:A:479:TYR:O	1:A:482:GLU:HB3	2.20	0.41
1:A:184:GLU:O	1:A:187:LYS:HB2	2.20	0.41
1:A:238:ASN:C	1:A:240:SER:N	2.73	0.41
3:Z:46:ASN:O	3:Z:50:PHE:N	2.41	0.41
1:A:715:GLU:O	1:A:718:GLN:HG3	2.20	0.41
1:A:792:TYR:CE2	3:Z:152:PRO:N	2.88	0.41
2:Y:121:ASN:O	2:Y:122:LYS:C	2.59	0.41
2:Y:28:ASP:HA	2:Y:39:ASP:CG	2.40	0.41
1:A:16:ASP:N	1:A:16:ASP:OD1	2.51	0.41
1:A:477:ILE:HG22	1:A:478:ASN:N	2.35	0.41
1:A:51:SER:HB3	1:A:56:ILE:HD12	2.02	0.41
1:A:523:ILE:HG22	1:A:530:LEU:CD1	2.51	0.41
1:A:788:HIS:CE1	3:Z:149:MET:HG2	2.56	0.41
3:Z:42:ILE:HG22	3:Z:43:ASN:H	1.86	0.41
3:Z:42:ILE:HG22	3:Z:44:PRO:HD3	2.03	0.41
1:A:216:GLU:CD	1:A:216:GLU:N	2.74	0.41
1:A:344:GLU:O	1:A:345:LYS:C	2.59	0.41
1:A:485:GLN:C	1:A:487:PHE:N	2.72	0.41
1:A:600:ASP:HA	1:A:601:PRO:HD3	1.87	0.41
1:A:794:ILE:O	1:A:795:ARG:C	2.59	0.41
1:A:820:VAL:CG1	1:A:821:LEU:H	2.32	0.41
1:A:817:LYS:CA	1:A:820:VAL:HG12	2.49	0.41
2:Y:63:ALA:CB	2:Y:67:LEU:HD13	2.51	0.41
1:A:279:GLU:O	1:A:315:GLY:HA3	2.21	0.41
1:A:294:PRO:C	1:A:296:LEU:N	2.74	0.41
1:A:622:PHE:CD1	1:A:622:PHE:N	2.89	0.41
1:A:653:LEU:O	1:A:653:LEU:HD23	2.21	0.41
1:A:793:LEU:O	1:A:796:LYS:N	2.53	0.41
2:Y:132:ALA:HA	2:Y:133:PRO:HD3	1.78	0.41
2:Y:69:PHE:HA	2:Y:72:PHE:HB3	2.02	0.41
3:Z:118:SER:O	3:Z:119:ASP:C	2.59	0.41
3:Z:128:LEU:HA	3:Z:128:LEU:HD13	1.79	0.41
1:A:126:TYR:HE2	1:A:673:PRO:HD2	1.86	0.41
1:A:280:ARG:HD2	1:A:317:LEU:O	2.20	0.41
1:A:334:ALA:O	1:A:338:LEU:HD23	2.20	0.41
2:Y:106:ILE:CG2	2:Y:107:GLU:H	2.28	0.41
1:A:171:SER:HB3	1:A:663:THR:HG21	2.02	0.41
1:A:272:VAL:CA	1:A:281:ASN:HD21	2.31	0.41
1:A:694:ASN:ND2	1:A:696:VAL:HG13	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Y:131:GLU:HG2	2:Y:131:GLU:O	2.21	0.41
3:Z:45:ARG:H	3:Z:48:ASP:HB2	1.86	0.41
3:Z:50:PHE:CE2	3:Z:56:HIS:CE1	3.09	0.41
1:A:284:ILE:CG2	1:A:285:PHE:H	2.34	0.41
1:A:536:GLU:HA	1:A:536:GLU:OE1	2.21	0.41
1:A:826:TRP:HZ2	2:Y:67:LEU:HD21	1.81	0.41
3:Z:30:ALA:C	3:Z:32:LYS:H	2.23	0.41
1:A:198:CYS:SG	1:A:199:ALA:N	2.94	0.40
1:A:377:THR:O	1:A:380:ALA:N	2.54	0.40
2:Y:100:GLU:O	2:Y:102:LYS:N	2.54	0.40
2:Y:40:ILE:O	2:Y:56:LEU:HD22	2.20	0.40
2:Y:52:ASP:O	2:Y:54:LYS:N	2.54	0.40
3:Z:139:VAL:CG2	3:Z:140:LYS:N	2.84	0.40
1:A:106:ARG:O	1:A:107:TYR:C	2.59	0.40
1:A:503:GLU:C	1:A:505:ILE:N	2.74	0.40
1:A:529:ILE:HG21	1:A:529:ILE:HD13	1.89	0.40
1:A:562:PHE:CD2	1:A:562:PHE:C	2.94	0.40
1:A:750:PRO:C	1:A:752:GLU:N	2.74	0.40
1:A:83:GLU:O	1:A:84:LYS:C	2.59	0.40
3:Z:17:LEU:C	3:Z:17:LEU:HD23	2.42	0.40
3:Z:20:PHE:C	3:Z:22:ASP:H	2.24	0.40
1:A:414:GLN:HB3	1:A:418:GLN:HB3	2.03	0.40
1:A:816:ARG:HE	2:Y:124:GLU:CD	2.24	0.40
2:Y:102:LYS:C	2:Y:141:TYR:CE1	2.94	0.40
3:Z:45:ARG:O	3:Z:48:ASP:N	2.54	0.40
1:A:785:PHE:CA	3:Z:86:TYR:CE1	3.05	0.40
1:A:218:GLN:O	1:A:219:ILE:C	2.60	0.40
1:A:461:ILE:C	1:A:462:ALA:O	2.58	0.40
1:A:480:THR:O	1:A:481:ASN:C	2.58	0.40
1:A:573:GLN:CG	1:A:574:GLY:H	2.33	0.40
2:Y:112:LEU:CD2	2:Y:116:MET:HE1	2.48	0.40
3:Z:129:THR:O	3:Z:130:ASP:CB	2.69	0.40
1:A:129:LEU:HA	1:A:130:PRO:HD3	1.78	0.40
1:A:234:THR:HG23	1:A:236:ARG:H	1.86	0.40
1:A:341:THR:O	1:A:344:GLU:N	2.55	0.40
1:A:719:ARG:HD3	1:A:774:ARG:NE	2.36	0.40
2:Y:100:GLU:C	2:Y:102:LYS:N	2.74	0.40
2:Y:22:GLU:O	2:Y:26:MET:N	2.55	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	785/837 (94%)	568 (72%)	149 (19%)	68 (9%)	1 5
2	Y	142/156 (91%)	102 (72%)	26 (18%)	14 (10%)	1 4
3	Z	152/156 (97%)	107 (70%)	36 (24%)	9 (6%)	2 16
All	All	1079/1149 (94%)	777 (72%)	211 (20%)	91 (8%)	1 6

All (91) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	62	ALA
1	A	71	LYS
1	A	206	GLU
1	A	237	ASN
1	A	242	ARG
1	A	304	PRO
1	A	369	GLU
1	A	378	ALA
1	A	462	ALA
1	A	511	ASP
1	A	515	ASP
1	A	528	GLY
1	A	540	PRO
1	A	547	PHE
1	A	594	TRP
1	A	602	ILE
1	A	626	GLU
1	A	708	PRO
1	A	810	VAL
1	A	811	ILE
2	Y	13	PRO
2	Y	53	ASP
2	Y	85	SER
3	Z	21	TRP

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Mol	Chain	Res	Type
3	Z	154	PRO
1	A	41	GLU
1	A	53	GLY
1	A	148	ILE
1	A	266	LEU
1	A	504	GLY
1	A	526	PRO
1	A	529	ILE
1	A	541	LYS
1	A	548	GLN
1	A	571	PRO
1	A	575	PRO
1	A	618	VAL
1	A	713	TYR
1	A	717	LYS
2	Y	40	ILE
2	Y	122	LYS
2	Y	129	PHE
2	Y	147	MET
3	Z	31	PHE
3	Z	81	GLY
3	Z	135	LEU
1	A	8	PRO
1	A	64	SER
1	A	81	LYS
1	A	193	LEU
1	A	199	ALA
1	A	295	GLU
1	A	324	ASP
1	A	445	THR
1	A	553	GLN
1	A	592	THR
1	A	709	SER
1	A	751	ALA
2	Y	69	PHE
2	Y	128	THR
2	Y	148	ILE
3	Z	33	LEU
1	A	86	GLU
1	A	188	LYS
1	A	240	SER
1	A	301	LEU

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Mol	Chain	Res	Type
1	A	320	ASP
1	A	493	PHE
1	A	506	ALA
1	A	617	LEU
1	A	625	PRO
1	A	824	TRP
2	Y	101	THR
3	Z	44	PRO
1	A	147	GLU
1	A	268	GLU
1	A	307	GLY
1	A	316	CYS
1	A	337	ILE
1	A	499	GLU
2	Y	45	GLU
1	A	15	VAL
1	A	253	PRO
1	A	764	ALA
2	Y	66	PRO
1	A	735	GLY
3	Z	152	PRO
1	A	565	PRO
2	Y	12	LEU
3	Z	103	GLY
1	A	510	ILE

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	583/730 (80%)	522 (90%)	61 (10%)	8 35
2	Y	89/133 (67%)	77 (86%)	12 (14%)	5 22
3	Z	106/132 (80%)	91 (86%)	15 (14%)	4 19
All	All	778/995 (78%)	690 (89%)	88 (11%)	7 31

All (88) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	16	ASP
1	A	18	LYS
1	A	29	ASP
1	A	37	PRO
1	A	39	GLU
1	A	48	ILE
1	A	51	SER
1	A	57	THR
1	A	84	LYS
1	A	94	LEU
1	A	95	ASN
1	A	102	ASN
1	A	105	SER
1	A	114	THR
1	A	146	THR
1	A	173	LEU
1	A	191	MET
1	A	196	VAL
1	A	203	LYS
1	A	209	ASP
1	A	210	LYS
1	A	218	GLN
1	A	242	ARG
1	A	262	ILE
1	A	263	GLU
1	A	297	ASN
1	A	304	PRO
1	A	313	ASN
1	A	320	ASP
1	A	321	ASN
1	A	356	LEU
1	A	360	GLU
1	A	367	PRO
1	A	370	GLU
1	A	421	ASN
1	A	430	LEU
1	A	438	LEU
1	A	459	LEU
1	A	461	ILE
1	A	475	LEU
1	A	477	ILE
1	A	480	THR

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Mol	Chain	Res	Type
1	A	505	ILE
1	A	514	MET
1	A	526	PRO
1	A	551	LEU
1	A	562	PHE
1	A	571	PRO
1	A	644	THR
1	A	653	LEU
1	A	669	ARG
1	A	710	ARG
1	A	717	LYS
1	A	718	GLN
1	A	719	ARG
1	A	752	GLU
1	A	755	LEU
1	A	758	THR
1	A	767	LEU
1	A	775	ASP
1	A	795	ARG
2	Y	24	PHE
2	Y	28	ASP
2	Y	30	ASP
2	Y	32	ASP
2	Y	55	GLU
2	Y	69	PHE
2	Y	93	PHE
2	Y	96	PHE
2	Y	111	ASP
2	Y	112	LEU
2	Y	121	ASN
2	Y	139	PHE
3	Z	20	PHE
3	Z	40	LEU
3	Z	45	ARG
3	Z	68	PHE
3	Z	80	GLN
3	Z	92	THR
3	Z	95	ARG
3	Z	107	ARG
3	Z	115	GLU
3	Z	117	LEU
3	Z	121	ASP

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Mol	Chain	Res	Type
3	Z	128	LEU
3	Z	135	LEU
3	Z	136	GLU
3	Z	143	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (32) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	11	GLN
1	A	33	ASN
1	A	102	ASN
1	A	162	ASN
1	A	170	GLN
1	A	275	GLN
1	A	297	ASN
1	A	313	ASN
1	A	321	ASN
1	A	371	GLN
1	A	417	ASN
1	A	478	ASN
1	A	485	GLN
1	A	489	ASN
1	A	517	GLN
1	A	553	GLN
1	A	555	HIS
1	A	598	ASN
1	A	603	ASN
1	A	654	ASN
1	A	659	ASN
1	A	666	HIS
1	A	678	GLN
1	A	694	ASN
1	A	718	GLN
1	A	769	ASN
1	A	788	HIS
1	A	804	GLN
1	A	825	GLN
2	Y	14	GLN
2	Y	91	ASN
2	Y	121	ASN

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

Of 4 ligands modelled in this entry, 3 are monoatomic - leaving 1 for Mogul analysis.

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	$\#\|Z\| > 2$
4	SO4	A	995	5	4,4,4	0.13	0	6,6,6	0.16	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
4	SO4	A	995	5	-	0/0/0/0	0/0/0/0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	995	SO4	1	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	803/837 (95%)	-0.24	4 (0%) 91 87	23, 78, 140, 146	2 (0%)
2	Y	144/156 (92%)	0.04	11 (7%) 17 9	34, 117, 145, 147	0
3	Z	154/156 (98%)	-0.30	1 (0%) 90 84	32, 72, 133, 145	0
All	All	1101/1149 (95%)	-0.21	16 (1%) 76 63	23, 80, 144, 147	2 (0%)

All (16) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	Y	40	ILE	4.9
2	Y	23	ALA	4.8
1	A	835	PRO	3.9
2	Y	20	MET	3.8
2	Y	29	VAL	3.7
1	A	826	TRP	3.7
2	Y	19	GLU	3.3
2	Y	154	GLU	3.0
2	Y	22	GLU	2.5
3	Z	113	LEU	2.3
2	Y	153	GLU	2.3
2	Y	64	PRO	2.3
1	A	48	ILE	2.2
2	Y	24	PHE	2.2
2	Y	93	PHE	2.1
1	A	834	LYS	2.1

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

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

6.3 Carbohydrates (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
4	SO4	A	995	5/5	0.90	0.26	3.31	74,89,107,134	0
6	CA	Z	998	1/1	0.92	0.30	2.08	107,107,107,107	0
5	MG	Y	997	1/1	0.92	0.14	-1.08	118,118,118,118	0
5	MG	A	996	1/1	0.97	0.09	-	38,38,38,38	0

6.5 Other polymers (i)

There are no such residues in this entry.