Full wwPDB X-ray Structure Validation Report ⓘ

Oct 16, 2023 – 01:20 AM EDT

PDB ID	:	2E9F
Title	:	Crystal Structure of T.th.HB8 Argininosuccinate lyase complexed with L-Arginine
Authors	:	Goto, M.
Deposited on	:	2007-01-25
Resolution	:	2.80 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
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

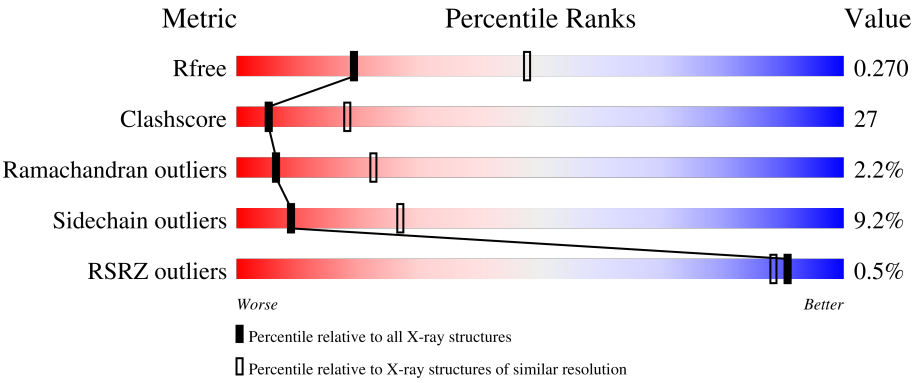
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.80 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}	130704	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)

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 of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. 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	462	55% 36% 6%
1	B	462	% 53% 38% 6%
1	C	462	52% 38% 6%
1	D	462	% 52% 40% 6%

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
2	ARG	B	491	-	-	X	-
2	ARG	B	492	-	-	X	-

2 Entry composition

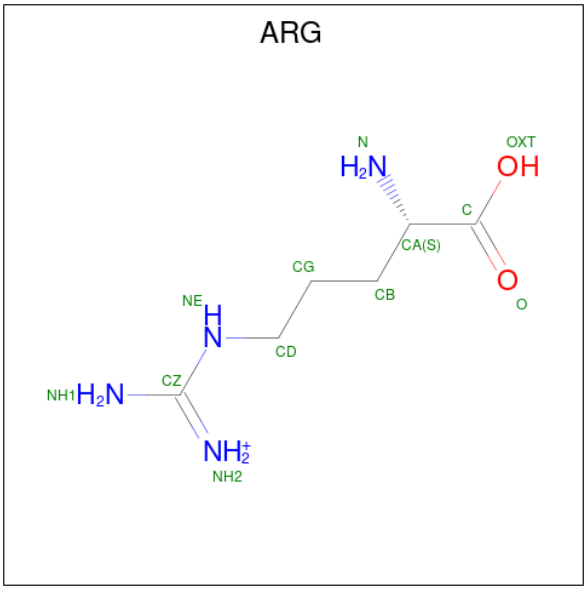
There are 3 unique types of molecules in this entry. The entry contains 14218 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Argininosuccinate lyase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	449	Total	C	N	O	S	0	0	0
			3530	2243	636	644	7			
1	B	450	Total	C	N	O	S	0	0	0
			3528	2241	637	643	7			
1	C	448	Total	C	N	O	S	0	0	0
			3498	2227	626	638	7			
1	D	449	Total	C	N	O	S	0	0	0
			3479	2216	625	631	7			

- Molecule 2 is ARGININE (three-letter code: ARG) (formula: $C_6H_{15}N_4O_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	B	1	Total	C	N	O	0	0
			12	6	4	2		
2	B	1	Total	C	N	O	0	0
			12	6	4	2		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	B	1	Total C N O 12 6 4 2	0	0
2	B	1	Total C N O 12 6 4 2	0	0

- Molecule 3 is water.

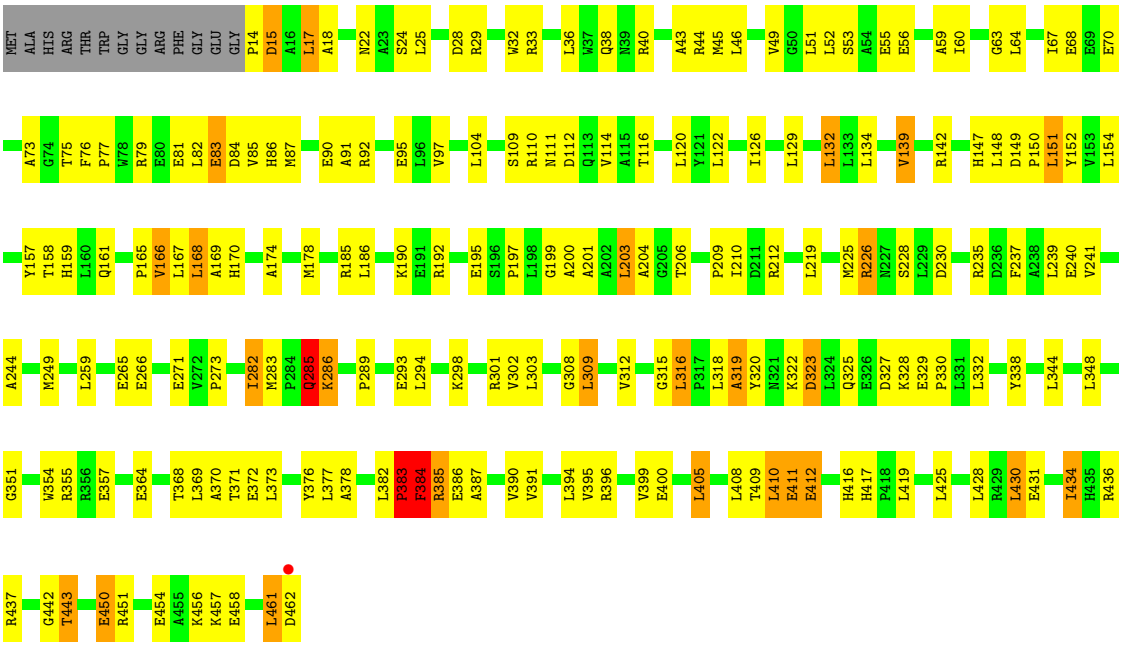
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	34	Total O 34 34	0	0
3	B	41	Total O 41 41	0	0
3	C	30	Total O 30 30	0	0
3	D	30	Total O 30 30	0	0

3 Residue-property plots (i)

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

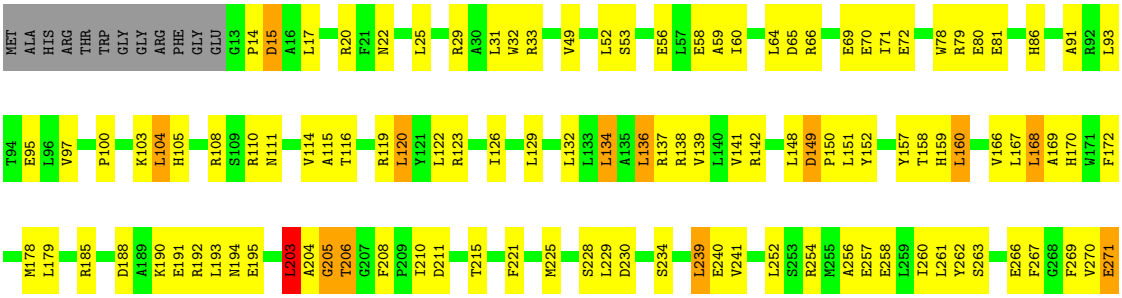
• Molecule 1: Argininosuccinate lyase

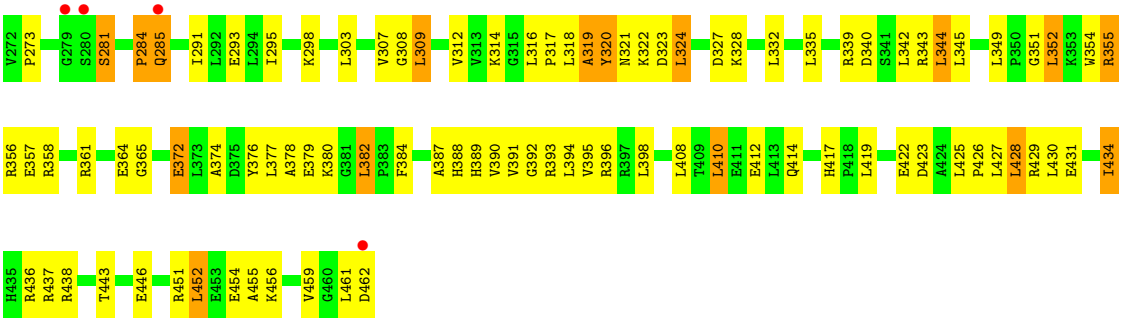
Chain A:



• Molecule 1: Argininosuccinate lyase

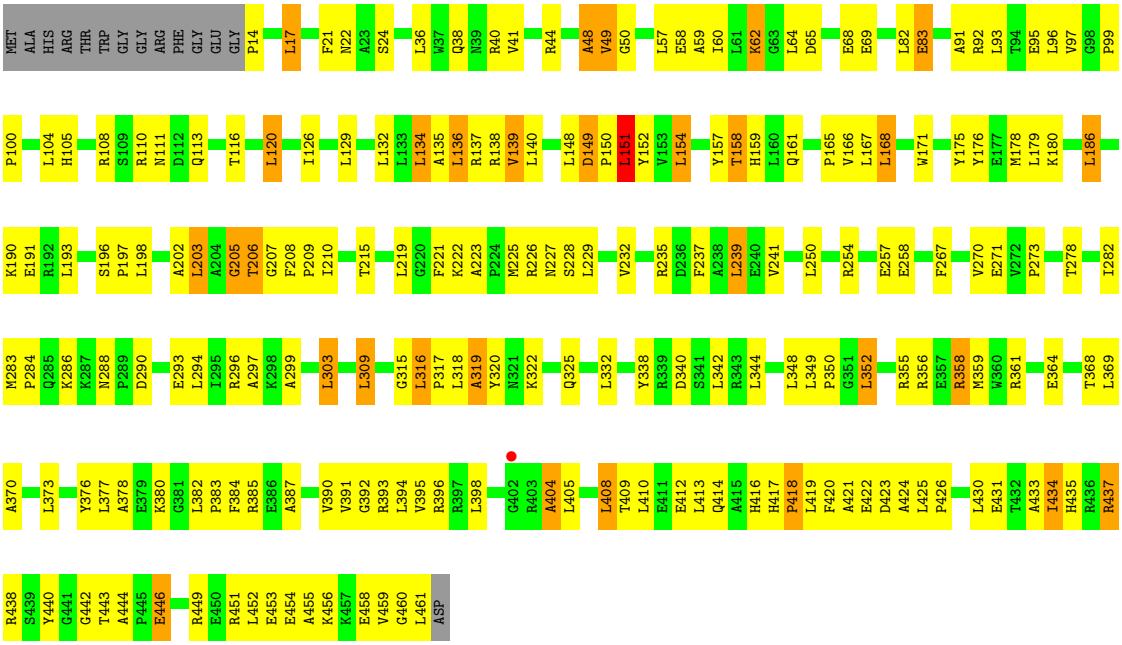
Chain B:





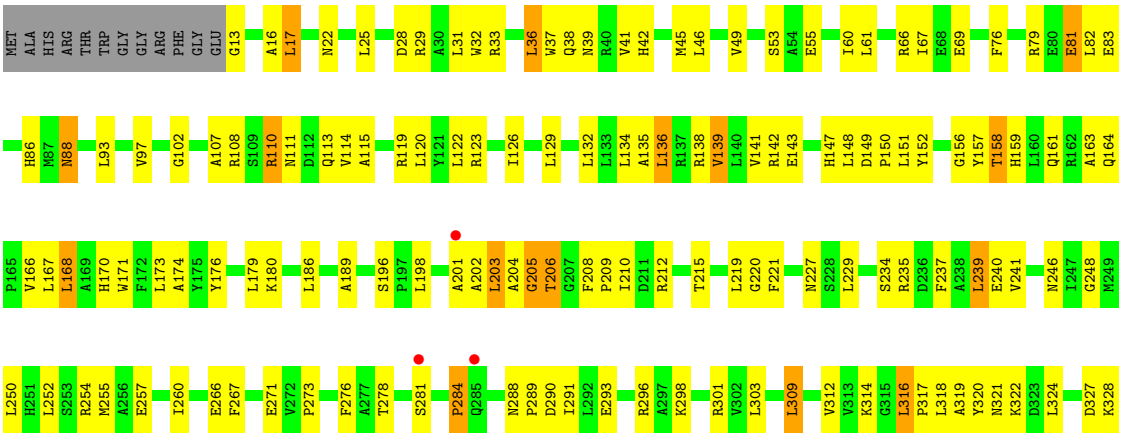
• Molecule 1: Argininosuccinate lyase

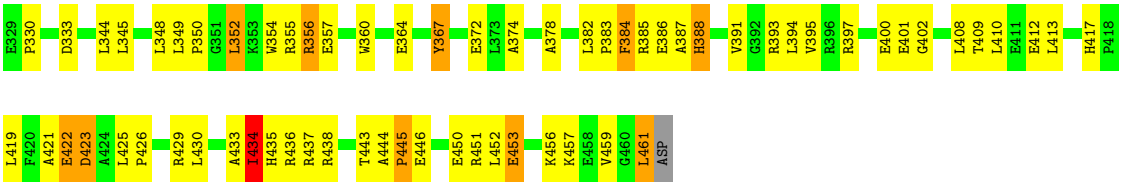
Chain C:



• Molecule 1: Argininosuccinate lyase

Chain D:




E329
P330
D333
L344
L345
L348
L349
P350
G351
L352
K353
W354
R355
R356
E357
W360
E364
Y367
E372
L373
A374
A378
L382
P383
F384
R385
E386
A387
H388
V391
G392
R393
L394
V395
R396
R397
E400
E401
G402
L408
T409
L410
E411
E412
L413
H417
P418
L419
F420
A421
E422
D423
A424
L425
P426
R429
L430
A433
T434
H435
R436
R437
R438
T443
A444
P445
E446
E450
R451
L452
E453
K456
K457
E458
V459
G460
L461
ASP

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	78.34Å 119.79Å 257.84Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	34.29 – 2.80 34.97 – 2.80	Depositor EDS
% Data completeness (in resolution range)	85.6 (34.29-2.80) 85.7 (34.97-2.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.95 (at 2.81Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.205 , 0.271 0.206 , 0.270	Depositor DCC
R_{free} test set	5234 reflections (10.08%)	wwPDB-VP
Wilson B-factor (Å^2)	50.7	Xtriage
Anisotropy	0.404	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 43.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	14218	wwPDB-VP
Average B, all atoms (Å^2)	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.08% 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

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	0.40	0/3600	0.65	0/4877
1	B	0.40	0/3597	0.65	2/4873 (0.0%)
1	C	0.38	0/3568	0.64	0/4839
1	D	0.38	0/3548	0.64	3/4814 (0.1%)
All	All	0.39	0/14313	0.64	5/19403 (0.0%)

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	B	0	1

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	284	PRO	N-CA-CB	5.68	110.11	103.30
1	D	156	GLY	N-CA-C	-5.52	99.29	113.10
1	B	104	LEU	CA-CB-CG	5.46	127.85	115.30
1	D	348	LEU	CA-CB-CG	5.35	127.61	115.30
1	B	284	PRO	N-CA-CB	5.25	109.60	103.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	320	TYR	Sidechain

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	3530	0	3538	217	0
1	B	3528	0	3530	214	0
1	C	3498	0	3495	196	0
1	D	3479	0	3456	197	0
2	B	48	0	48	22	0
3	A	34	0	0	1	0
3	B	41	0	0	2	0
3	C	30	0	0	1	0
3	D	30	0	0	3	0
All	All	14218	0	14067	747	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 27.

All (747) 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:B:59:ALA:HB1	1:B:97:VAL:HG21	1.32	1.11
1:A:456:LYS:HB3	1:A:461:LEU:HB3	1.28	1.05
1:B:167:LEU:HD13	1:B:443:THR:HG22	1.42	1.02
1:A:167:LEU:H	1:A:443:THR:HG21	1.26	0.99
1:C:99:PRO:HG2	1:C:100:PRO:HD3	1.43	0.98
1:B:372:GLU:HG3	1:B:436:ARG:HD3	1.47	0.96
1:D:167:LEU:HD13	1:D:443:THR:HG22	1.44	0.96
1:D:349:LEU:O	1:D:352:LEU:HD22	1.67	0.95
1:C:459:VAL:HG23	1:C:460:GLY:H	1.28	0.94
1:D:410:LEU:HD23	1:D:425:LEU:HD21	1.49	0.93
1:A:364:GLU:HB2	1:A:430:LEU:HD12	1.51	0.91
1:A:461:LEU:HD13	1:A:462:ASP:H	1.34	0.91
1:D:60:ILE:HG23	1:D:93:LEU:HD21	1.51	0.90
1:A:383:PRO:O	1:A:384:PHE:HB3	1.71	0.88
1:D:111:ASN:HD22	1:D:202:ALA:HA	1.39	0.88
1:D:459:VAL:HG23	1:D:461:LEU:HD22	1.58	0.86
1:B:166:VAL:HA	1:B:443:THR:HG21	1.57	0.85
1:D:372:GLU:HG2	1:D:436:ARG:HG3	1.60	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:62:LYS:HE2	1:C:62:LYS:HA	1.59	0.83
1:B:158:THR:HG22	1:B:159:HIS:ND1	1.93	0.83
1:C:409:THR:OG1	1:C:412:GLU:HG3	1.79	0.83
1:D:25:LEU:O	1:D:29:ARG:HG3	1.79	0.83
1:C:390:VAL:HA	1:C:393:ARG:NH1	1.93	0.82
1:C:361:ARG:HH11	1:C:361:ARG:HG2	1.45	0.82
1:D:38:GLN:HE22	1:D:113:GLN:HG3	1.42	0.81
1:B:105:HIS:HD2	1:B:108:ARG:HE	1.25	0.81
1:C:315:GLY:O	1:D:257:GLU:HG2	1.82	0.80
1:A:45:MET:HE1	1:A:210:ILE:HG13	1.63	0.80
1:A:167:LEU:H	1:A:443:THR:CG2	1.93	0.80
1:B:97:VAL:O	1:B:97:VAL:HG22	1.81	0.80
1:A:240:GLU:HG3	1:B:185:ARG:HD3	1.64	0.80
1:D:81:GLU:CD	1:D:81:GLU:H	1.85	0.79
1:B:97:VAL:O	1:B:100:PRO:HD2	1.82	0.78
1:A:185:ARG:HD3	1:B:240:GLU:HG3	1.66	0.78
1:D:429:ARG:HD3	3:D:1048:HOH:O	1.83	0.78
1:C:438:ARG:HH22	1:C:446:GLU:HG3	1.47	0.77
1:A:461:LEU:CD1	1:A:462:ASP:H	1.97	0.77
1:B:410:LEU:HD22	1:B:414:GLN:HG3	1.66	0.77
1:B:372:GLU:CG	1:B:436:ARG:HD3	2.15	0.76
1:A:325:GLN:HE21	2:B:492:ARG:HA	1.51	0.76
1:D:196:SER:HB2	1:D:221:PHE:CD2	2.20	0.76
1:A:40:ARG:O	1:A:44:ARG:HG3	1.85	0.75
1:B:417:HIS:HD2	1:B:419:LEU:H	1.35	0.75
1:C:454:GLU:O	1:C:458:GLU:HG3	1.87	0.75
1:B:372:GLU:HG3	1:B:436:ARG:HH11	1.52	0.74
1:B:293:GLU:OE2	1:D:159:HIS:HD2	1.70	0.74
1:B:392:GLY:O	1:B:396:ARG:HG3	1.87	0.73
1:B:398:LEU:HD21	1:B:408:LEU:HD21	1.71	0.73
1:B:308:GLY:O	1:B:312:VAL:HG23	1.89	0.73
1:A:149:ASP:HB3	1:A:150:PRO:HD3	1.70	0.73
1:C:134:LEU:HD11	1:C:138:ARG:NH2	2.04	0.72
1:B:115:ALA:O	1:B:119:ARG:HG3	1.88	0.72
1:D:82:LEU:HB2	1:D:88:ASN:ND2	2.05	0.72
1:C:299:ALA:HB3	1:D:314:LYS:NZ	2.04	0.71
1:D:372:GLU:CG	1:D:436:ARG:HG3	2.21	0.71
1:A:139:VAL:HA	1:A:142:ARG:HG2	1.71	0.71
1:D:111:ASN:ND2	1:D:202:ALA:HA	2.06	0.71
1:A:157:TYR:O	1:B:319:ALA:HB3	1.90	0.71
1:B:110:ARG:HB2	2:B:491:ARG:HD2	1.72	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:429:ARG:HG3	1:D:429:ARG:HH11	1.56	0.71
1:A:357:GLU:CD	1:A:357:GLU:H	1.94	0.71
1:A:24:SER:HB3	1:A:325:GLN:NE2	2.06	0.70
1:A:167:LEU:HD22	1:A:169:ALA:HB3	1.73	0.70
1:C:136:LEU:HD13	1:C:179:LEU:HD21	1.74	0.70
1:A:411:GLU:H	1:A:411:GLU:CD	1.95	0.70
1:C:116:THR:HG22	1:C:120:LEU:CD2	2.21	0.70
1:A:383:PRO:HA	1:B:103:LYS:HE2	1.74	0.69
1:B:167:LEU:H	1:B:443:THR:CG2	2.05	0.69
1:B:398:LEU:HD11	1:B:408:LEU:HD21	1.73	0.69
1:B:438:ARG:HH12	1:B:446:GLU:HB2	1.58	0.69
1:A:461:LEU:HD12	1:A:461:LEU:H	1.56	0.69
1:D:387:ALA:O	1:D:391:VAL:HG12	1.92	0.69
1:A:199:GLY:O	1:A:212:ARG:HD2	1.92	0.69
1:A:385:ARG:HG3	1:A:385:ARG:HH11	1.58	0.69
1:D:22:ASN:HD21	1:D:322:LYS:HE2	1.58	0.69
1:B:364:GLU:HB2	1:B:430:LEU:HB2	1.74	0.68
1:C:196:SER:HB2	1:C:221:PHE:CD2	2.29	0.68
1:A:70:GLU:CG	1:A:75:THR:HG23	2.23	0.68
1:C:390:VAL:HA	1:C:393:ARG:HH11	1.56	0.68
1:B:136:LEU:O	1:B:139:VAL:HG22	1.93	0.68
1:B:285:GLN:HE21	1:B:285:GLN:HA	1.59	0.68
1:A:249:MET:HG3	1:A:302:VAL:HG21	1.75	0.67
1:D:93:LEU:O	1:D:97:VAL:HG22	1.93	0.67
1:A:282:ILE:HG22	1:A:283:MET:N	2.09	0.67
1:B:59:ALA:HB1	1:B:97:VAL:CG2	2.16	0.67
1:B:149:ASP:CB	1:B:150:PRO:HD3	2.25	0.67
1:C:41:VAL:HG21	1:C:219:LEU:HG	1.76	0.67
1:C:126:ILE:HG23	1:C:186:LEU:HG	1.76	0.67
1:C:99:PRO:CG	1:C:100:PRO:HD3	2.22	0.67
1:C:116:THR:HG22	1:C:120:LEU:HD21	1.75	0.67
1:C:459:VAL:HG23	1:C:460:GLY:N	2.07	0.67
1:B:195:GLU:HB3	1:B:225:MET:HG3	1.75	0.67
1:D:22:ASN:ND2	1:D:322:LYS:HE2	2.10	0.67
1:C:110:ARG:HH11	1:C:113:GLN:HE22	1.40	0.66
1:D:408:LEU:HB3	1:D:413:LEU:HD11	1.78	0.66
1:C:382:LEU:HD22	1:C:383:PRO:HD2	1.75	0.66
1:D:198:LEU:HD23	1:D:215:THR:HB	1.78	0.66
1:A:46:LEU:HB2	1:A:52:LEU:HD12	1.78	0.66
1:B:52:LEU:HD21	1:B:60:ILE:HD12	1.77	0.66
1:D:166:VAL:HA	1:D:443:THR:HG21	1.77	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:320:TYR:OH	2:B:491:ARG:HB3	1.95	0.65
1:A:25:LEU:O	1:A:29:ARG:HG3	1.97	0.65
1:A:319:ALA:CB	1:B:157:TYR:O	2.45	0.65
1:D:252:LEU:HD22	1:D:345:LEU:HD12	1.78	0.65
1:A:239:LEU:HD11	1:A:309:LEU:HD22	1.78	0.65
1:A:372:GLU:OE2	1:A:436:ARG:HG2	1.96	0.65
1:B:53:SER:OG	1:B:56:GLU:HG3	1.96	0.65
1:A:64:LEU:HA	1:A:67:ILE:HD12	1.78	0.64
1:C:378:ALA:HA	1:C:382:LEU:O	1.97	0.64
1:D:374:ALA:HB2	1:D:391:VAL:HG11	1.79	0.64
1:A:308:GLY:O	1:A:312:VAL:HG23	1.98	0.64
1:A:158:THR:HG22	1:A:159:HIS:ND1	2.11	0.64
1:D:203:LEU:O	1:D:204:ALA:HB3	1.97	0.64
1:A:18:ALA:HB1	1:D:291:ILE:HD11	1.79	0.64
1:C:282:ILE:O	1:C:284:PRO:HD3	1.97	0.64
1:D:167:LEU:HD21	1:D:445:PRO:HG3	1.79	0.64
1:C:239:LEU:HD13	1:C:309:LEU:HD13	1.79	0.64
1:D:459:VAL:CG2	1:D:461:LEU:HD22	2.26	0.64
1:A:70:GLU:HG3	1:A:75:THR:HG23	1.80	0.63
1:B:204:ALA:O	1:B:205:GLY:O	2.16	0.63
1:C:369:LEU:HD12	1:C:369:LEU:H	1.62	0.63
1:C:369:LEU:HD12	1:C:369:LEU:N	2.13	0.63
1:A:391:VAL:O	1:A:395:VAL:HG23	1.99	0.63
1:B:239:LEU:HD13	1:B:309:LEU:HD13	1.81	0.63
1:D:364:GLU:CB	1:D:430:LEU:HD22	2.28	0.63
1:D:422:GLU:O	1:D:425:LEU:HD23	1.99	0.63
1:C:271:GLU:HB2	1:C:355:ARG:HH22	1.63	0.63
1:A:199:GLY:HA3	1:A:212:ARG:HG2	1.81	0.63
1:D:141:VAL:HG11	1:D:461:LEU:HD21	1.80	0.62
1:A:197:PRO:HB3	1:A:225:MET:CE	2.29	0.62
2:B:493:ARG:HB3	1:D:320:TYR:OH	1.98	0.62
1:A:82:LEU:O	1:A:83:GLU:HG2	2.00	0.62
1:A:59:ALA:HB1	1:A:97:VAL:HG13	1.81	0.62
1:A:22:ASN:OD1	1:A:322:LYS:HE2	2.00	0.62
1:C:456:LYS:HB3	1:C:461:LEU:HA	1.82	0.62
1:B:270:VAL:HG21	1:B:352:LEU:HG	1.82	0.62
1:B:364:GLU:HB2	1:B:430:LEU:HD22	1.81	0.62
1:C:65:ASP:O	1:C:69:GLU:HG3	1.99	0.62
1:D:49:VAL:HG21	1:D:209:PRO:O	2.00	0.62
1:D:136:LEU:HD13	1:D:179:LEU:HD21	1.82	0.62
1:D:417:HIS:HD2	1:D:419:LEU:H	1.47	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:369:LEU:H	1:A:369:LEU:HD22	1.65	0.61
1:C:398:LEU:HD13	1:C:404:ALA:O	2.00	0.61
1:A:111:ASN:OD1	2:B:492:ARG:NH1	2.32	0.61
1:B:110:ARG:O	1:B:114:VAL:HG23	2.01	0.61
1:B:152:TYR:CE2	1:B:356:ARG:HB2	2.35	0.61
1:B:271:GLU:HG3	1:B:355:ARG:NH1	2.15	0.61
1:B:20:ARG:HG2	1:B:20:ARG:HH11	1.66	0.61
1:B:149:ASP:CB	1:B:150:PRO:CD	2.79	0.61
1:C:197:PRO:HB3	1:C:225:MET:SD	2.39	0.61
1:D:410:LEU:HD23	1:D:425:LEU:CD2	2.27	0.61
1:C:434:ILE:HD13	1:C:434:ILE:O	2.01	0.61
1:C:273:PRO:HD3	1:C:352:LEU:HD12	1.83	0.60
1:D:168:LEU:HD11	1:D:354:TRP:CD2	2.36	0.60
1:B:378:ALA:HA	1:B:382:LEU:O	2.00	0.60
1:B:79:ARG:HB3	1:B:81:GLU:HG2	1.83	0.60
1:B:136:LEU:HD13	1:B:179:LEU:HD21	1.83	0.60
1:B:256:ALA:O	1:B:260:ILE:HG13	2.01	0.60
1:D:289:PRO:O	1:D:293:GLU:HG3	2.01	0.60
1:C:175:TYR:O	1:C:179:LEU:HD13	2.02	0.60
1:C:157:TYR:O	1:D:319:ALA:CB	2.49	0.60
1:A:159:HIS:HD2	1:C:293:GLU:OE2	1.83	0.60
1:A:369:LEU:HD22	1:A:369:LEU:N	2.17	0.60
1:B:429:ARG:HD2	1:B:431:GLU:OE1	2.02	0.60
1:D:122:LEU:O	1:D:126:ILE:HG13	2.02	0.60
1:D:434:ILE:O	1:D:444:ALA:HA	2.02	0.60
1:A:417:HIS:HD2	1:A:419:LEU:H	1.49	0.60
1:A:17:LEU:HD22	1:D:344:LEU:HD21	1.83	0.59
1:A:167:LEU:N	1:A:443:THR:HG21	2.08	0.59
1:B:105:HIS:CD2	1:B:108:ARG:HE	2.12	0.59
1:A:195:GLU:HB3	1:A:225:MET:CG	2.32	0.59
1:D:67:ILE:HG23	1:D:76:PHE:CE2	2.37	0.59
1:C:158:THR:O	1:C:159:HIS:HB2	2.02	0.59
1:D:152:TYR:CZ	1:D:356:ARG:HG2	2.37	0.59
1:A:86:HIS:HE1	1:A:114:VAL:HG23	1.67	0.59
2:B:493:ARG:HD2	1:D:110:ARG:HB3	1.85	0.59
1:B:376:TYR:OH	1:B:380:LYS:HE3	2.02	0.59
1:A:116:THR:O	1:A:120:LEU:HB2	2.02	0.59
1:B:122:LEU:HD13	1:B:241:VAL:HG21	1.85	0.59
1:C:105:HIS:HB3	1:D:384:PHE:CE1	2.38	0.59
1:D:158:THR:HB	1:D:163:ALA:HB2	1.84	0.59
1:C:451:ARG:HH11	1:C:451:ARG:HG2	1.68	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:197:PRO:HB3	1:A:225:MET:HE1	1.84	0.58
1:B:203:LEU:N	1:B:203:LEU:HD12	2.19	0.58
2:B:494:ARG:HD2	1:C:110:ARG:HB2	1.86	0.58
1:C:193:LEU:C	1:C:193:LEU:HD12	2.24	0.58
1:C:440:TYR:HB3	1:D:212:ARG:HD3	1.85	0.58
1:D:364:GLU:HB2	1:D:430:LEU:HB2	1.84	0.58
2:B:493:ARG:NH1	1:D:111:ASN:OD1	2.37	0.58
1:C:82:LEU:O	1:C:83:GLU:HB2	2.04	0.58
1:C:116:THR:O	1:C:120:LEU:HD22	2.04	0.58
1:A:195:GLU:HB3	1:A:225:MET:HG3	1.85	0.58
1:D:53:SER:OG	1:D:55:GLU:HG2	2.04	0.57
1:D:364:GLU:HB2	1:D:430:LEU:HD22	1.87	0.57
1:A:126:ILE:HG21	1:A:190:LYS:HB2	1.87	0.57
1:A:228:SER:OG	1:B:170:HIS:HE1	1.85	0.57
1:B:262:TYR:HB3	1:B:269:PHE:HB2	1.85	0.57
1:D:327:ASP:O	1:D:330:PRO:HG2	2.04	0.57
1:B:149:ASP:O	1:B:151:LEU:N	2.36	0.57
1:C:22:ASN:HD21	1:C:322:LYS:NZ	2.02	0.57
1:C:152:TYR:CE2	1:C:356:ARG:HB2	2.39	0.57
1:D:45:MET:CE	1:D:210:ILE:HD12	2.34	0.57
1:A:328:LYS:NZ	2:B:492:ARG:O	2.32	0.57
1:C:299:ALA:HB3	1:D:314:LYS:HZ2	1.68	0.57
1:D:360:TRP:NE1	1:D:430:LEU:HD23	2.19	0.57
1:A:373:LEU:O	1:A:376:TYR:HB3	2.04	0.57
1:C:206:THR:CG2	1:C:208:PHE:HD1	2.17	0.57
1:D:67:ILE:HG23	1:D:76:PHE:HE2	1.70	0.57
1:D:38:GLN:NE2	1:D:113:GLN:HG3	2.17	0.57
1:A:86:HIS:CE1	1:A:114:VAL:HG23	2.40	0.57
1:A:17:LEU:HD13	1:D:344:LEU:HD22	1.87	0.56
1:A:320:TYR:OH	2:B:492:ARG:HB3	2.04	0.56
1:A:289:PRO:O	1:A:293:GLU:HG3	2.05	0.56
1:A:457:LYS:HA	1:A:461:LEU:HG	1.88	0.56
1:B:376:TYR:CZ	1:B:380:LYS:HE3	2.40	0.56
1:B:438:ARG:HH12	1:B:446:GLU:CB	2.19	0.56
1:C:92:ARG:HG3	1:C:96:LEU:HD11	1.86	0.56
1:D:148:LEU:HD12	1:D:452:LEU:HD22	1.88	0.56
1:D:425:LEU:N	1:D:426:PRO:HD2	2.20	0.56
1:A:384:PHE:C	1:A:384:PHE:CD2	2.79	0.56
1:C:271:GLU:HB2	1:C:355:ARG:NH2	2.20	0.56
1:A:49:VAL:HG23	1:A:51:LEU:HG	1.87	0.56
1:A:286:LYS:HA	1:C:161:GLN:NE2	2.21	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:25:LEU:HA	1:D:28:ASP:OD1	2.06	0.56
1:A:129:LEU:HD21	1:A:338:TYR:HD2	1.70	0.56
1:A:431:GLU:O	1:A:434:ILE:HD11	2.06	0.56
1:B:120:LEU:HD13	1:B:221:PHE:CZ	2.40	0.56
1:B:357:GLU:HG2	1:B:361:ARG:HH12	1.71	0.56
1:D:250:LEU:O	1:D:254:ARG:HG3	2.06	0.56
1:C:149:ASP:HB3	1:C:150:PRO:CD	2.36	0.55
1:C:318:LEU:O	1:C:319:ALA:HB3	2.06	0.55
1:A:149:ASP:O	1:A:150:PRO:C	2.43	0.55
1:B:314:LYS:NZ	1:D:312:VAL:HA	2.21	0.55
1:D:31:LEU:N	1:D:31:LEU:HD12	2.22	0.55
1:A:45:MET:HE1	1:A:210:ILE:CG1	2.35	0.55
1:A:450:GLU:O	1:A:450:GLU:OE2	2.25	0.55
1:B:291:ILE:O	1:B:295:ILE:HG13	2.07	0.55
1:B:344:LEU:HD13	1:C:17:LEU:HD13	1.87	0.55
1:B:193:LEU:HD12	1:B:193:LEU:C	2.27	0.55
1:B:410:LEU:HD22	1:B:410:LEU:O	2.07	0.55
1:D:136:LEU:O	1:D:139:VAL:HG13	2.06	0.55
1:D:417:HIS:CD2	1:D:419:LEU:HB2	2.42	0.55
1:A:396:ARG:O	1:A:399:VAL:HG22	2.07	0.55
1:D:408:LEU:HB3	1:D:413:LEU:CD1	2.36	0.55
1:A:25:LEU:HA	1:A:28:ASP:OD1	2.06	0.55
1:A:209:PRO:HD3	1:B:379:GLU:OE2	2.07	0.55
1:D:235:ARG:NH1	1:D:324:LEU:HB3	2.21	0.55
1:A:382:LEU:HD23	1:A:383:PRO:HD2	1.89	0.55
1:C:348:LEU:HD23	1:C:348:LEU:C	2.27	0.55
1:D:316:LEU:HD23	1:D:317:PRO:HD2	1.89	0.55
1:A:64:LEU:HD23	1:A:67:ILE:HD12	1.89	0.55
1:A:170:HIS:HE1	1:B:228:SER:OG	1.89	0.55
1:B:410:LEU:O	1:B:414:GLN:HG3	2.06	0.55
2:B:494:ARG:NH1	1:C:111:ASN:OD1	2.40	0.55
1:D:252:LEU:HD22	1:D:345:LEU:CD1	2.37	0.55
1:A:70:GLU:HG2	1:A:75:THR:HG23	1.89	0.54
1:A:79:ARG:NH1	1:A:81:GLU:OE2	2.40	0.54
1:D:429:ARG:HG3	1:D:429:ARG:NH1	2.20	0.54
1:A:157:TYR:O	1:B:319:ALA:CB	2.53	0.54
1:A:167:LEU:HB2	1:A:443:THR:HG22	1.88	0.54
1:B:351:GLY:HA3	3:B:1053:HOH:O	2.06	0.54
1:C:206:THR:HG22	1:C:208:PHE:HD1	1.72	0.54
1:A:294:LEU:O	1:A:298:LYS:HG3	2.07	0.54
1:A:318:LEU:O	1:A:319:ALA:HB3	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:168:LEU:HD11	1:B:354:TRP:CD2	2.42	0.54
1:A:18:ALA:CB	1:D:291:ILE:HD11	2.38	0.54
1:A:79:ARG:NH2	1:A:91:ALA:HB1	2.23	0.54
1:A:394:LEU:HB2	1:A:416:HIS:CD2	2.42	0.54
1:C:36:LEU:HD21	1:C:68:GLU:HB2	1.90	0.54
1:C:134:LEU:O	1:C:138:ARG:HB2	2.06	0.54
1:A:56:GLU:O	1:A:60:ILE:HG13	2.07	0.54
1:B:141:VAL:CG2	1:B:455:ALA:HB1	2.37	0.54
1:A:149:ASP:HB3	1:A:150:PRO:CD	2.37	0.54
1:C:299:ALA:HB3	1:D:314:LYS:HZ1	1.71	0.54
1:B:328:LYS:O	1:B:332:LEU:HD23	2.08	0.54
1:C:422:GLU:O	1:C:425:LEU:HD23	2.08	0.54
1:C:316:LEU:HD23	1:C:317:PRO:HD2	1.90	0.54
1:D:167:LEU:CD1	1:D:443:THR:HG22	2.29	0.54
1:D:417:HIS:HD2	1:D:419:LEU:HB2	1.71	0.54
1:B:22:ASN:OD1	1:B:322:LYS:HE2	2.08	0.53
1:B:159:HIS:CD2	1:D:288:ASN:HB3	2.43	0.53
1:B:191:GLU:HG3	1:B:192:ARG:N	2.23	0.53
1:A:36:LEU:HD21	1:A:68:GLU:HB2	1.90	0.53
1:A:301:ARG:HG3	3:A:1057:HOH:O	2.07	0.53
1:B:114:VAL:HG21	2:B:491:ARG:HB2	1.90	0.53
1:D:158:THR:O	1:D:161:GLN:HB2	2.08	0.53
1:D:397:ARG:O	1:D:400:GLU:HG2	2.08	0.53
1:C:451:ARG:HG2	1:C:451:ARG:NH1	2.23	0.53
1:B:158:THR:HG22	1:B:159:HIS:CE1	2.44	0.53
1:A:394:LEU:HD21	1:A:408:LEU:HD11	1.89	0.53
1:C:319:ALA:CB	1:D:157:TYR:O	2.56	0.53
1:D:120:LEU:CD1	1:D:123:ARG:NH2	2.72	0.53
1:B:392:GLY:O	1:B:395:VAL:HG22	2.09	0.53
1:A:348:LEU:HD23	1:A:348:LEU:C	2.29	0.53
1:D:189:ALA:HA	1:D:240:GLU:OE2	2.08	0.53
1:A:165:PRO:HD3	1:A:368:THR:HG21	1.91	0.53
1:A:79:ARG:HH21	1:A:91:ALA:HB1	1.75	0.52
1:A:239:LEU:HD12	1:A:309:LEU:HD13	1.90	0.52
1:B:65:ASP:O	1:B:69:GLU:HG3	2.09	0.52
1:B:320:TYR:CZ	2:B:491:ARG:HB3	2.44	0.52
1:C:92:ARG:HG3	1:C:96:LEU:CD1	2.39	0.52
1:C:405:LEU:HD23	1:C:405:LEU:O	2.10	0.52
1:C:443:THR:HG22	1:D:204:ALA:HB1	1.91	0.52
1:C:456:LYS:CB	1:C:461:LEU:HD23	2.39	0.52
1:B:195:GLU:HB3	1:B:225:MET:CG	2.38	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:45:MET:CE	1:A:210:ILE:HG13	2.36	0.52
1:B:159:HIS:CD2	1:D:293:GLU:OE2	2.63	0.52
1:D:202:ALA:O	1:D:203:LEU:HB3	2.09	0.52
2:B:494:ARG:HB3	1:C:320:TYR:OH	2.10	0.52
1:D:60:ILE:HG23	1:D:93:LEU:CD2	2.33	0.52
1:A:266:GLU:HG2	1:C:267:PHE:CG	2.45	0.52
1:B:307:VAL:HG12	1:C:303:LEU:HD13	1.91	0.52
1:B:357:GLU:N	1:B:357:GLU:OE2	2.43	0.52
1:B:384:PHE:O	1:B:388:HIS:ND1	2.43	0.52
1:B:427:LEU:N	1:B:427:LEU:HD12	2.25	0.52
1:C:442:GLY:HA2	1:D:205:GLY:H	1.74	0.52
1:D:394:LEU:HD23	1:D:395:VAL:N	2.25	0.52
1:C:154:LEU:HB3	1:C:359:MET:HE3	1.92	0.52
1:C:394:LEU:O	1:C:398:LEU:HG	2.10	0.52
1:C:456:LYS:HB3	1:C:461:LEU:HD23	1.92	0.52
1:D:421:ALA:O	1:D:423:ASP:N	2.43	0.52
1:B:382:LEU:HD12	1:B:387:ALA:HB2	1.91	0.52
1:C:14:PRO:HA	3:C:1014:HOH:O	2.09	0.52
1:D:450:GLU:HG2	1:D:451:ARG:NH2	2.25	0.52
1:B:167:LEU:H	1:B:443:THR:HG23	1.73	0.52
1:C:338:TYR:CE2	1:C:342:LEU:HD11	2.45	0.52
1:D:45:MET:HE1	1:D:210:ILE:HD12	1.92	0.52
1:A:114:VAL:HG21	2:B:492:ARG:O	2.10	0.52
1:B:93:LEU:O	1:B:97:VAL:HG12	2.09	0.52
1:B:270:VAL:CG2	1:B:352:LEU:HG	2.39	0.52
1:A:273:PRO:HG3	1:A:351:GLY:O	2.10	0.51
1:C:228:SER:OG	1:D:170:HIS:HE1	1.93	0.51
1:D:39:ASN:HD22	1:D:108:ARG:HH12	1.58	0.51
1:C:62:LYS:HE2	1:C:62:LYS:CA	2.37	0.51
1:C:410:LEU:HA	1:C:413:LEU:HD12	1.91	0.51
1:D:134:LEU:HD11	1:D:138:ARG:CZ	2.40	0.51
1:C:459:VAL:CG2	1:C:460:GLY:H	2.13	0.51
1:D:417:HIS:CD2	1:D:419:LEU:H	2.26	0.51
1:A:87:MET:HE3	1:A:90:GLU:HB3	1.93	0.51
1:D:352:LEU:HD21	1:D:354:TRP:HE1	1.76	0.51
1:A:167:LEU:CB	1:A:443:THR:HG22	2.41	0.51
1:A:192:ARG:NH2	1:B:188:ASP:OD1	2.44	0.51
1:B:430:LEU:O	1:B:434:ILE:HG12	2.10	0.51
1:D:276:PHE:HD1	1:D:291:ILE:HD12	1.76	0.51
1:B:298:LYS:HD2	1:C:21:PHE:CZ	2.46	0.51
1:A:44:ARG:HB3	1:A:44:ARG:CZ	2.41	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:437:ARG:NH1	1:B:206:THR:HA	2.26	0.51
1:A:122:LEU:O	1:A:126:ILE:HG13	2.10	0.51
1:B:211:ASP:O	1:B:215:THR:HG23	2.11	0.51
1:C:57:LEU:C	1:C:59:ALA:H	2.15	0.51
1:A:235:ARG:O	1:A:239:LEU:HD13	2.11	0.51
1:A:286:LYS:HA	1:C:161:GLN:HE21	1.76	0.51
1:D:433:ALA:C	1:D:435:HIS:H	2.14	0.51
1:A:82:LEU:C	1:A:83:GLU:HG2	2.32	0.50
1:A:91:ALA:O	1:A:95:GLU:HG3	2.11	0.50
1:A:265:GLU:OE2	1:A:285:GLN:HG2	2.12	0.50
1:A:285:GLN:O	1:A:286:LYS:C	2.49	0.50
1:A:315:GLY:O	1:B:257:GLU:HG2	2.11	0.50
1:B:203:LEU:HD13	1:B:204:ALA:N	2.26	0.50
1:C:91:ALA:O	1:C:95:GLU:HG3	2.10	0.50
1:B:141:VAL:HG22	1:B:455:ALA:HB1	1.93	0.50
1:C:151:LEU:HD11	1:C:167:LEU:HD11	1.92	0.50
1:B:344:LEU:CD1	1:C:17:LEU:HD13	2.40	0.50
1:C:373:LEU:O	1:C:376:TYR:HB3	2.11	0.50
1:A:385:ARG:HG3	1:A:385:ARG:NH1	2.23	0.50
1:B:321:ASN:O	1:B:324:LEU:HB2	2.12	0.50
1:B:357:GLU:CD	1:B:358:ARG:H	2.15	0.50
1:B:394:LEU:C	1:B:394:LEU:HD23	2.32	0.50
1:B:427:LEU:HG	1:B:436:ARG:HD2	1.93	0.50
1:C:250:LEU:O	1:C:254:ARG:HG3	2.11	0.50
1:A:79:ARG:HD2	1:A:81:GLU:OE2	2.11	0.50
1:A:344:LEU:CD2	1:D:17:LEU:HD13	2.42	0.50
1:C:349:LEU:HB2	1:C:350:PRO:HD3	1.94	0.50
1:C:207:GLY:HA3	1:D:436:ARG:CZ	2.41	0.50
1:C:437:ARG:HD3	1:D:206:THR:HA	1.92	0.50
1:D:123:ARG:HH12	1:D:220:GLY:C	2.14	0.50
1:A:195:GLU:CD	1:A:225:MET:HG2	2.32	0.50
1:C:257:GLU:OE1	1:C:296:ARG:NH1	2.37	0.50
1:C:273:PRO:HD3	1:C:352:LEU:CD1	2.42	0.50
1:C:318:LEU:HG	1:C:319:ALA:H	1.76	0.50
1:D:143:GLU:O	1:D:147:HIS:HD2	1.94	0.50
1:A:394:LEU:HB2	1:A:416:HIS:NE2	2.25	0.50
1:D:360:TRP:CE2	1:D:430:LEU:HD23	2.47	0.50
1:D:409:THR:OG1	1:D:412:GLU:HG3	2.12	0.50
1:A:38:GLN:HA	1:A:219:LEU:HD21	1.94	0.49
1:A:32:TRP:CE2	1:A:33:ARG:HG3	2.48	0.49
1:B:188:ASP:O	1:B:191:GLU:HG2	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:93:LEU:O	1:C:97:VAL:HG12	2.12	0.49
1:D:239:LEU:CD1	1:D:309:LEU:HB3	2.42	0.49
1:A:170:HIS:CG	1:A:443:THR:HG23	2.48	0.49
1:A:226:ARG:HB2	1:B:451:ARG:HD3	1.95	0.49
1:A:454:GLU:O	1:A:458:GLU:HG3	2.11	0.49
1:B:357:GLU:CG	1:B:361:ARG:HH12	2.25	0.49
1:B:417:HIS:CD2	1:B:419:LEU:H	2.22	0.49
1:C:376:TYR:HE2	1:C:420:PHE:HA	1.77	0.49
1:A:63:GLY:O	1:A:67:ILE:HG13	2.12	0.49
1:B:91:ALA:O	1:B:95:GLU:HG3	2.12	0.49
1:A:167:LEU:HD22	1:A:169:ALA:CB	2.40	0.49
1:B:66:ARG:O	1:B:70:GLU:HG3	2.13	0.49
1:D:42:HIS:O	1:D:46:LEU:HG	2.12	0.49
1:B:316:LEU:HD21	1:B:324:LEU:HD13	1.95	0.49
1:A:87:MET:HE3	1:A:87:MET:O	2.12	0.49
1:A:77:PRO:CG	1:A:92:ARG:HD3	2.43	0.49
1:A:161:GLN:HB3	1:C:286:LYS:HG3	1.93	0.49
1:B:393:ARG:HG3	1:B:396:ARG:HH21	1.77	0.49
1:C:44:ARG:HG2	1:C:44:ARG:HH11	1.76	0.49
1:C:149:ASP:OD2	1:C:150:PRO:HD3	2.13	0.49
1:A:158:THR:O	1:A:159:HIS:HB2	2.13	0.49
1:C:361:ARG:HG2	1:C:361:ARG:NH1	2.20	0.49
1:D:235:ARG:HG3	1:D:324:LEU:HD12	1.94	0.49
1:A:386:GLU:O	1:A:390:VAL:HG23	2.12	0.49
1:B:349:LEU:O	1:B:352:LEU:HB2	2.13	0.49
1:C:278:THR:OG1	1:C:288:ASN:HB2	2.11	0.49
1:A:159:HIS:CD2	1:C:288:ASN:HB3	2.48	0.48
1:B:438:ARG:NH1	1:B:438:ARG:HB2	2.28	0.48
1:D:391:VAL:O	1:D:395:VAL:HG23	2.13	0.48
1:B:410:LEU:HB2	1:B:425:LEU:HD11	1.94	0.48
1:A:456:LYS:HE2	1:A:461:LEU:CB	2.44	0.48
1:B:167:LEU:H	1:B:443:THR:HG21	1.77	0.48
1:C:364:GLU:HB2	1:C:430:LEU:HD22	1.93	0.48
1:D:271:GLU:OE2	1:D:355:ARG:NH2	2.46	0.48
1:A:59:ALA:HB1	1:A:97:VAL:CG1	2.44	0.48
1:A:437:ARG:HH11	1:B:206:THR:HA	1.79	0.48
1:A:168:LEU:HD11	1:A:354:TRP:CD2	2.47	0.48
1:B:188:ASP:HA	1:B:191:GLU:HG2	1.96	0.48
1:B:318:LEU:O	1:B:319:ALA:HB3	2.13	0.48
1:D:372:GLU:HG3	1:D:436:ARG:HE	1.77	0.48
1:A:237:PHE:O	1:A:241:VAL:HG23	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:120:LEU:HD21	1:D:219:LEU:HD22	1.95	0.48
1:D:239:LEU:HD13	1:D:309:LEU:CD1	2.44	0.48
1:A:147:HIS:HB3	1:A:152:TYR:HB2	1.96	0.48
1:C:376:TYR:CZ	1:C:424:ALA:HB2	2.49	0.48
1:D:138:ARG:HB3	1:D:142:ARG:NH1	2.29	0.48
1:A:289:PRO:HD2	1:C:159:HIS:HB3	1.96	0.48
1:C:382:LEU:HD12	1:C:387:ALA:HB2	1.96	0.48
1:A:319:ALA:HB1	1:B:157:TYR:O	2.13	0.47
1:D:120:LEU:HD11	1:D:123:ARG:NH2	2.29	0.47
1:A:70:GLU:HB3	1:A:76:PHE:HB2	1.96	0.47
1:A:165:PRO:HD3	1:A:368:THR:CG2	2.43	0.47
1:B:20:ARG:HG2	1:B:20:ARG:NH1	2.28	0.47
1:B:335:LEU:O	1:B:339:ARG:HB2	2.14	0.47
1:C:149:ASP:CB	1:C:150:PRO:CD	2.93	0.47
1:C:431:GLU:CD	1:C:431:GLU:H	2.17	0.47
1:B:123:ARG:HD3	1:B:194:ASN:OD1	2.14	0.47
1:C:60:ILE:HG23	1:C:93:LEU:HD21	1.96	0.47
1:D:318:LEU:O	1:D:319:ALA:HB3	2.14	0.47
1:A:109:SER:HB3	1:A:201:ALA:O	2.15	0.47
1:B:273:PRO:HD3	1:B:352:LEU:HD12	1.96	0.47
1:B:398:LEU:HD21	1:B:408:LEU:CD2	2.43	0.47
1:B:446:GLU:OE1	1:B:446:GLU:HA	2.14	0.47
1:D:167:LEU:H	1:D:443:THR:CG2	2.28	0.47
1:A:271:GLU:OE1	1:A:355:ARG:NH2	2.48	0.47
1:A:316:LEU:HB3	1:B:254:ARG:NH1	2.30	0.47
1:A:318:LEU:H	1:B:258:GLU:CD	2.17	0.47
1:B:167:LEU:N	1:B:443:THR:CG2	2.77	0.47
1:C:425:LEU:N	1:C:426:PRO:CD	2.78	0.47
1:A:167:LEU:CD2	1:A:169:ALA:H	2.28	0.47
1:B:134:LEU:HD22	1:B:138:ARG:NE	2.30	0.47
1:B:267:PHE:CD1	1:D:266:GLU:HG2	2.49	0.47
1:B:396:ARG:HB3	1:B:396:ARG:NH1	2.30	0.47
1:C:409:THR:N	1:C:412:GLU:OE1	2.46	0.47
1:D:410:LEU:HD13	1:D:410:LEU:O	2.14	0.47
1:B:327:ASP:OD1	1:B:328:LYS:HG3	2.15	0.47
1:C:226:ARG:NH2	1:D:180:LYS:HE2	2.30	0.47
1:A:110:ARG:HB3	2:B:492:ARG:HD2	1.97	0.47
1:B:374:ALA:HA	1:B:391:VAL:HG21	1.97	0.47
1:D:173:LEU:O	1:D:176:TYR:HB3	2.15	0.47
1:B:148:LEU:HD23	1:B:169:ALA:CB	2.45	0.46
1:C:349:LEU:O	1:C:352:LEU:HB2	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:31:LEU:N	1:B:31:LEU:HD12	2.29	0.46
1:C:410:LEU:O	1:C:414:GLN:HG3	2.14	0.46
1:A:325:GLN:NE2	2:B:492:ARG:HA	2.24	0.46
1:B:166:VAL:CA	1:B:443:THR:HG21	2.38	0.46
1:B:408:LEU:HD13	1:B:412:GLU:OE1	2.15	0.46
1:D:13:GLY:N	3:D:1007:HOH:O	2.47	0.46
1:D:393:ARG:HH11	1:D:393:ARG:HB3	1.81	0.46
1:A:322:LYS:HB3	1:D:293:GLU:HB2	1.97	0.46
1:B:97:VAL:O	1:B:97:VAL:CG2	2.54	0.46
1:B:281:SER:OG	1:D:388:HIS:ND1	2.46	0.46
1:D:164:GLN:HG2	1:D:437:ARG:HH21	1.80	0.46
1:D:278:THR:OG1	1:D:288:ASN:HB2	2.15	0.46
1:A:329:GLU:N	1:A:330:PRO:HD2	2.31	0.46
1:C:453:GLU:OE2	1:C:456:LYS:HD3	2.16	0.46
1:D:79:ARG:HB3	1:D:81:GLU:OE1	2.14	0.46
1:A:174:ALA:O	1:A:178:MET:HG3	2.16	0.46
1:B:167:LEU:N	1:B:443:THR:HG21	2.30	0.46
1:B:345:LEU:O	1:B:349:LEU:HG	2.15	0.46
1:C:455:ALA:O	1:C:459:VAL:HG22	2.15	0.46
1:A:70:GLU:OE1	1:A:92:ARG:NH2	2.49	0.46
1:A:230:ASP:OD2	1:B:178:MET:HG3	2.13	0.46
1:C:24:SER:HB3	1:C:325:GLN:NE2	2.30	0.46
1:C:196:SER:HB2	1:C:221:PHE:CG	2.51	0.46
1:D:120:LEU:HD12	1:D:123:ARG:NH2	2.31	0.46
1:D:143:GLU:O	1:D:147:HIS:CD2	2.69	0.46
1:A:325:GLN:C	1:A:327:ASP:H	2.19	0.46
1:A:417:HIS:NE2	1:A:419:LEU:HD12	2.31	0.46
1:B:252:LEU:HD22	1:B:345:LEU:HD12	1.98	0.46
1:B:307:VAL:CG1	1:C:303:LEU:HD13	2.46	0.46
1:C:349:LEU:HA	1:C:352:LEU:HD22	1.96	0.46
1:B:111:ASN:OD1	2:B:491:ARG:NH1	2.40	0.46
1:B:151:LEU:HD21	1:B:434:ILE:HD12	1.98	0.46
1:B:344:LEU:HD22	1:C:17:LEU:HD13	1.97	0.46
1:C:157:TYR:O	1:D:319:ALA:HB3	2.16	0.46
1:A:372:GLU:CD	1:A:436:ARG:HG2	2.37	0.46
1:B:364:GLU:CB	1:B:430:LEU:HD22	2.45	0.46
2:B:494:ARG:HA	1:C:325:GLN:HE21	1.81	0.46
1:D:13:GLY:O	1:D:16:ALA:HB3	2.15	0.46
1:D:66:ARG:O	1:D:69:GLU:HB2	2.16	0.46
1:A:70:GLU:HG2	1:A:76:PHE:HA	1.98	0.45
1:B:271:GLU:HG3	1:B:355:ARG:HH12	1.80	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:425:LEU:N	1:B:426:PRO:HD2	2.31	0.45
1:C:202:ALA:O	1:C:203:LEU:HB3	2.16	0.45
1:C:395:VAL:CG2	1:C:396:ARG:N	2.79	0.45
1:A:43:ALA:HA	1:A:46:LEU:HD12	1.98	0.45
1:A:405:LEU:HD23	1:A:408:LEU:HD12	1.98	0.45
1:B:343:ARG:HB3	1:C:17:LEU:HD11	1.98	0.45
1:C:40:ARG:HG3	1:C:64:LEU:HD13	1.97	0.45
1:A:14:PRO:O	1:A:15:ASP:HB2	2.16	0.45
1:A:206:THR:HA	1:B:437:ARG:NH1	2.32	0.45
1:A:316:LEU:HB3	1:B:254:ARG:HH11	1.80	0.45
1:B:239:LEU:HD11	1:B:309:LEU:HB3	1.97	0.45
1:C:175:TYR:HA	1:C:178:MET:HE3	1.98	0.45
1:D:135:ALA:O	1:D:139:VAL:HG12	2.16	0.45
1:A:170:HIS:CB	1:A:443:THR:HG23	2.47	0.45
1:A:197:PRO:CD	1:A:225:MET:HE3	2.46	0.45
1:A:206:THR:HA	1:B:437:ARG:HH11	1.81	0.45
1:B:425:LEU:O	1:B:428:LEU:HD22	2.16	0.45
1:D:248:GLY:O	1:D:252:LEU:HG	2.17	0.45
1:A:378:ALA:HA	1:A:382:LEU:O	2.16	0.45
1:B:136:LEU:HD13	1:B:179:LEU:CD2	2.46	0.45
1:B:261:LEU:C	1:B:263:SER:H	2.18	0.45
1:B:266:GLU:HG2	1:D:267:PHE:CG	2.51	0.45
1:B:398:LEU:CD1	1:B:408:LEU:HD21	2.44	0.45
1:C:190:LYS:O	1:C:193:LEU:HG	2.16	0.45
1:D:394:LEU:HD23	1:D:394:LEU:C	2.37	0.45
1:A:456:LYS:HE2	1:A:461:LEU:HB3	1.98	0.45
1:D:171:TRP:O	1:D:174:ALA:HB3	2.16	0.45
1:D:278:THR:HG23	1:D:290:ASP:OD1	2.16	0.45
1:D:393:ARG:HB3	1:D:393:ARG:NH1	2.32	0.45
1:A:186:LEU:HD12	1:A:244:ALA:HB1	1.99	0.45
1:C:340:ASP:O	1:C:344:LEU:HD23	2.16	0.45
1:C:392:GLY:O	1:C:395:VAL:HG22	2.16	0.45
1:D:425:LEU:N	1:D:425:LEU:HD22	2.32	0.45
1:B:126:ILE:HG21	1:B:190:LYS:HB2	1.98	0.45
1:B:398:LEU:CD2	1:B:408:LEU:HD21	2.42	0.45
1:C:92:ARG:O	1:C:96:LEU:HG	2.17	0.45
1:C:165:PRO:HD3	1:C:368:THR:CG2	2.47	0.45
1:C:410:LEU:C	1:C:410:LEU:HD23	2.37	0.45
1:D:158:THR:O	1:D:159:HIS:HB2	2.17	0.45
1:D:37:TRP:CE2	1:D:219:LEU:HD23	2.52	0.44
1:D:120:LEU:HD13	1:D:221:PHE:CZ	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:166:VAL:CG1	1:D:167:LEU:N	2.80	0.44
1:B:86:HIS:CE1	1:B:114:VAL:HG22	2.53	0.44
1:C:38:GLN:HE21	1:C:108:ARG:HH11	1.65	0.44
1:C:267:PHE:O	1:C:358:ARG:HD2	2.17	0.44
1:D:255:MET:CE	1:D:345:LEU:HD13	2.48	0.44
1:A:437:ARG:HH12	1:B:206:THR:HG22	1.82	0.44
1:B:459:VAL:HG23	1:B:461:LEU:HG	2.00	0.44
1:C:134:LEU:HD11	1:C:138:ARG:CZ	2.47	0.44
1:C:318:LEU:HD12	1:C:318:LEU:HA	1.76	0.44
1:C:433:ALA:C	1:C:435:HIS:H	2.21	0.44
1:A:239:LEU:HD12	1:A:239:LEU:N	2.32	0.44
1:A:451:ARG:HA	1:A:451:ARG:NE	2.32	0.44
1:B:167:LEU:CD1	1:B:443:THR:HG22	2.30	0.44
1:B:261:LEU:C	1:B:263:SER:N	2.71	0.44
1:C:382:LEU:HD13	1:C:383:PRO:N	2.32	0.44
1:A:461:LEU:HD12	1:A:461:LEU:N	2.30	0.44
1:C:176:TYR:O	1:C:180:LYS:HB2	2.18	0.44
1:C:380:LYS:NZ	1:C:419:LEU:O	2.50	0.44
1:C:382:LEU:HD13	1:C:383:PRO:CD	2.48	0.44
1:A:32:TRP:CZ2	1:A:33:ARG:CZ	3.01	0.44
1:A:159:HIS:HE1	2:B:491:ARG:NH2	2.15	0.44
1:B:387:ALA:HA	1:B:390:VAL:HG12	1.99	0.44
1:C:270:VAL:HG22	1:C:271:GLU:N	2.33	0.44
1:D:149:ASP:HA	1:D:150:PRO:C	2.38	0.44
1:D:430:LEU:O	1:D:434:ILE:HG13	2.18	0.44
1:A:87:MET:CE	1:A:90:GLU:HB3	2.48	0.44
1:A:323:ASP:OD1	1:D:296:ARG:HD3	2.18	0.44
1:B:393:ARG:HG3	1:B:396:ARG:NH2	2.32	0.44
1:C:38:GLN:HE22	1:C:113:GLN:HG3	1.82	0.44
1:C:369:LEU:H	1:C:369:LEU:CD1	2.29	0.44
1:A:85:VAL:HG13	1:A:86:HIS:N	2.33	0.43
1:B:33:ARG:NH2	1:B:72:GLU:OE2	2.51	0.43
1:B:166:VAL:HG12	1:B:167:LEU:N	2.32	0.43
1:D:400:GLU:C	1:D:402:GLY:H	2.21	0.43
1:B:25:LEU:O	1:B:29:ARG:HD2	2.18	0.43
1:B:168:LEU:HD22	1:B:172:PHE:CE1	2.53	0.43
1:C:395:VAL:HG23	1:C:396:ARG:N	2.33	0.43
1:D:301:ARG:NH2	1:D:333:ASP:OD1	2.48	0.43
1:B:137:ARG:HG3	1:B:137:ARG:HH11	1.83	0.43
1:C:322:LYS:HA	1:C:322:LYS:HD2	1.70	0.43
1:C:408:LEU:HA	1:C:412:GLU:OE1	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:203:LEU:HD23	1:A:203:LEU:N	2.32	0.43
1:A:461:LEU:CD1	1:A:462:ASP:N	2.74	0.43
1:D:273:PRO:HG2	1:D:276:PHE:HD2	1.84	0.43
1:A:109:SER:O	1:A:112:ASP:OD2	2.36	0.43
1:A:235:ARG:HA	1:A:237:PHE:CE1	2.54	0.43
1:B:451:ARG:NE	1:B:451:ARG:HA	2.33	0.43
1:D:298:LYS:O	1:D:301:ARG:HG2	2.19	0.43
1:D:309:LEU:HD23	1:D:309:LEU:HA	1.82	0.43
1:A:318:LEU:O	1:A:319:ALA:CB	2.66	0.43
1:B:25:LEU:HD11	1:B:78:TRP:CE3	2.53	0.43
1:B:408:LEU:HD13	1:B:412:GLU:CD	2.39	0.43
1:C:116:THR:HG22	1:C:120:LEU:HD22	1.97	0.43
1:C:137:ARG:HA	1:C:140:LEU:HD12	1.99	0.43
1:C:168:LEU:O	1:C:171:TRP:HB3	2.19	0.43
1:C:377:LEU:HB2	1:C:387:ALA:HB1	2.00	0.43
1:D:136:LEU:HD13	1:D:179:LEU:CD2	2.47	0.43
1:D:237:PHE:O	1:D:241:VAL:HG23	2.19	0.43
1:D:367:TYR:CD1	1:D:367:TYR:N	2.86	0.43
1:D:385:ARG:O	1:D:386:GLU:C	2.57	0.43
1:C:340:ASP:O	1:C:344:LEU:CD2	2.67	0.43
1:C:384:PHE:CG	1:C:385:ARG:N	2.86	0.43
1:D:61:LEU:HD23	1:D:61:LEU:HA	1.88	0.43
1:B:273:PRO:HG3	1:B:351:GLY:O	2.19	0.43
1:C:134:LEU:O	1:C:134:LEU:HD22	2.19	0.43
1:C:368:THR:HB	1:C:369:LEU:HD12	2.01	0.43
1:C:398:LEU:HD21	1:C:408:LEU:HD21	2.00	0.43
1:D:32:TRP:O	1:D:36:LEU:HB2	2.17	0.43
1:A:325:GLN:HE21	2:B:492:ARG:CA	2.27	0.43
1:C:297:ALA:C	1:C:299:ALA:H	2.22	0.43
1:C:318:LEU:O	1:C:319:ALA:CB	2.67	0.43
1:C:443:THR:CG2	1:D:204:ALA:HB1	2.49	0.43
1:D:115:ALA:O	1:D:119:ARG:HG3	2.18	0.43
1:A:382:LEU:HD13	1:A:387:ALA:HA	2.00	0.42
1:B:25:LEU:HD23	1:B:80:GLU:HA	2.01	0.42
1:B:456:LYS:HD2	1:B:462:ASP:N	2.34	0.42
1:D:82:LEU:HB2	1:D:88:ASN:HD21	1.83	0.42
1:D:321:ASN:H	1:D:324:LEU:HD23	1.84	0.42
1:A:24:SER:HB3	1:A:325:GLN:CD	2.40	0.42
1:A:200:ALA:O	1:A:204:ALA:O	2.37	0.42
1:D:382:LEU:O	1:D:383:PRO:C	2.57	0.42
1:B:423:ASP:O	1:B:426:PRO:HD2	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:227:ASN:OD1	1:C:229:LEU:HB2	2.19	0.42
1:B:388:HIS:HB3	1:D:281:SER:CB	2.49	0.42
1:D:107:ALA:HB2	1:D:208:PHE:CG	2.54	0.42
1:D:246:ASN:O	1:D:250:LEU:HG	2.19	0.42
1:D:446:GLU:HB2	3:D:1125:HOH:O	2.20	0.42
1:A:203:LEU:O	1:A:228:SER:CB	2.68	0.42
1:B:454:GLU:HB2	3:B:1130:HOH:O	2.19	0.42
1:C:318:LEU:HG	1:C:319:ALA:N	2.33	0.42
1:D:82:LEU:O	1:D:83:GLU:HB2	2.19	0.42
1:D:324:LEU:H	1:D:324:LEU:HD22	1.84	0.42
1:B:160:LEU:HD23	1:B:160:LEU:HA	1.73	0.42
1:B:230:ASP:OD2	1:B:234:SER:HB3	2.19	0.42
1:B:239:LEU:CD1	1:B:309:LEU:HB3	2.50	0.42
1:C:135:ALA:O	1:C:139:VAL:HG13	2.20	0.42
1:D:41:VAL:HG21	1:D:219:LEU:HG	2.02	0.42
1:A:84:ASP:OD1	1:A:84:ASP:C	2.58	0.42
1:B:49:VAL:O	1:B:49:VAL:CG1	2.68	0.42
1:C:222:LYS:O	1:C:223:ALA:HB2	2.19	0.42
1:C:258:GLU:OE2	1:D:318:LEU:HB2	2.19	0.42
1:D:86:HIS:CE1	1:D:114:VAL:HG23	2.54	0.42
1:D:196:SER:HB2	1:D:221:PHE:CG	2.54	0.42
1:B:141:VAL:HG13	1:B:452:LEU:CD2	2.50	0.42
1:B:377:LEU:CD2	1:B:419:LEU:HB2	2.49	0.42
1:C:294:LEU:HD23	1:C:294:LEU:HA	1.92	0.42
1:C:421:ALA:HB3	1:C:423:ASP:OD2	2.20	0.42
1:D:203:LEU:O	1:D:204:ALA:CB	2.62	0.42
1:A:399:VAL:HG23	1:A:400:GLU:N	2.35	0.41
1:A:442:GLY:HA2	1:B:205:GLY:H	1.83	0.41
1:C:369:LEU:HD23	1:C:433:ALA:CB	2.50	0.41
1:A:29:ARG:O	1:A:32:TRP:HB3	2.19	0.41
1:B:60:ILE:O	1:B:64:LEU:HG	2.20	0.41
1:B:285:GLN:HA	1:B:285:GLN:NE2	2.31	0.41
1:B:372:GLU:HG3	1:B:436:ARG:CD	2.33	0.41
2:B:494:ARG:HD2	1:C:110:ARG:CB	2.48	0.41
1:D:364:GLU:HB3	1:D:430:LEU:HD22	1.99	0.41
1:A:116:THR:OG1	1:A:197:PRO:HG2	2.20	0.41
1:A:409:THR:O	1:A:410:LEU:C	2.58	0.41
1:B:344:LEU:CD2	1:C:17:LEU:HD13	2.49	0.41
1:D:260:ILE:HD11	1:D:293:GLU:HA	2.01	0.41
1:D:456:LYS:HA	1:D:461:LEU:CD2	2.50	0.41
1:A:149:ASP:C	1:A:151:LEU:N	2.72	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:370:ALA:HB3	1:C:282:ILE:HG23	2.03	0.41
1:B:364:GLU:OE2	1:B:429:ARG:HA	2.20	0.41
1:C:205:GLY:O	1:D:437:ARG:HD3	2.21	0.41
1:A:73:ALA:HB3	1:A:75:THR:HG22	2.02	0.41
1:A:166:VAL:HG21	1:B:229:LEU:HD11	2.03	0.41
1:B:340:ASP:O	1:B:344:LEU:HD22	2.21	0.41
1:D:425:LEU:N	1:D:426:PRO:CD	2.83	0.41
1:A:87:MET:HE3	1:A:91:ALA:N	2.36	0.41
1:A:197:PRO:HD3	1:A:225:MET:HE3	2.02	0.41
1:B:116:THR:O	1:B:120:LEU:HB2	2.20	0.41
1:B:345:LEU:HD23	1:B:345:LEU:HA	1.88	0.41
1:C:237:PHE:O	1:C:241:VAL:HG23	2.21	0.41
1:C:459:VAL:CG2	1:C:460:GLY:N	2.79	0.41
1:D:378:ALA:HA	1:D:382:LEU:O	2.21	0.41
1:D:382:LEU:HD23	1:D:382:LEU:HA	1.83	0.41
1:A:159:HIS:CD2	1:C:293:GLU:OE2	2.70	0.41
1:A:197:PRO:N	1:A:225:MET:HE3	2.36	0.41
1:A:203:LEU:O	1:A:228:SER:HB2	2.20	0.41
1:B:136:LEU:HD12	1:B:342:LEU:HD22	2.02	0.41
1:C:410:LEU:O	1:C:410:LEU:HD23	2.20	0.41
1:C:417:HIS:HA	1:C:418:PRO:HD2	1.70	0.41
1:D:433:ALA:C	1:D:435:HIS:N	2.74	0.41
1:B:141:VAL:HG21	1:B:455:ALA:HB1	2.02	0.41
1:D:32:TRP:CE2	1:D:33:ARG:HG3	2.56	0.41
1:A:79:ARG:HB3	1:A:81:GLU:HG3	2.03	0.41
1:A:132:LEU:HD12	1:A:132:LEU:HA	1.90	0.41
1:A:167:LEU:HD22	1:A:169:ALA:H	1.86	0.41
1:A:197:PRO:HD3	1:A:225:MET:CE	2.51	0.41
1:A:282:ILE:CG2	1:C:370:ALA:HB3	2.51	0.41
1:A:318:LEU:HB2	1:B:258:GLU:OE1	2.20	0.41
1:A:377:LEU:HD13	1:A:382:LEU:HD12	2.03	0.41
1:B:86:HIS:HE1	1:B:114:VAL:HG22	1.85	0.41
1:B:142:ARG:HG3	1:B:461:LEU:HD11	2.03	0.41
1:B:261:LEU:O	1:B:263:SER:N	2.54	0.41
1:B:396:ARG:HB3	1:B:396:ARG:HH11	1.86	0.41
1:C:48:ALA:O	1:C:50:GLY:N	2.54	0.41
1:C:148:LEU:HD23	1:C:148:LEU:HA	1.80	0.41
1:D:239:LEU:HD11	1:D:309:LEU:HB3	2.02	0.41
1:D:349:LEU:N	1:D:350:PRO:HD2	2.36	0.41
1:C:49:VAL:HG13	1:C:209:PRO:O	2.21	0.41
1:D:110:ARG:HA	1:D:110:ARG:HD3	1.80	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:411:GLU:O	1:A:412:GLU:HB2	2.21	0.40
1:A:417:HIS:CD2	1:A:419:LEU:HB2	2.56	0.40
1:B:136:LEU:CD1	1:B:179:LEU:HD21	2.51	0.40
1:B:206:THR:HB	1:B:208:PHE:H	1.85	0.40
1:C:60:ILE:O	1:C:64:LEU:HG	2.20	0.40
1:C:391:VAL:O	1:C:395:VAL:HG13	2.20	0.40
1:D:453:GLU:O	1:D:457:LYS:HG2	2.21	0.40
1:A:139:VAL:HA	1:A:142:ARG:CG	2.45	0.40
1:B:15:ASP:N	1:B:15:ASP:OD1	2.54	0.40
1:B:364:GLU:CD	1:B:430:LEU:H	2.24	0.40
1:A:371:THR:HA	1:C:282:ILE:HD13	2.03	0.40
1:B:285:GLN:HE21	1:B:285:GLN:CA	2.31	0.40
1:C:154:LEU:HD23	1:C:359:MET:HE3	2.03	0.40
1:C:198:LEU:HD23	1:C:215:THR:HB	2.02	0.40
1:C:348:LEU:HD23	1:C:349:LEU:N	2.36	0.40
1:C:361:ARG:NH1	1:C:361:ARG:CG	2.81	0.40
1:C:437:ARG:C	1:C:444:ALA:HB2	2.42	0.40
1:D:136:LEU:HA	1:D:139:VAL:HG13	2.02	0.40
1:A:259:LEU:HD23	1:A:259:LEU:HA	1.82	0.40
1:A:430:LEU:O	1:A:434:ILE:HG13	2.21	0.40
1:B:60:ILE:HG23	1:B:93:LEU:HD21	2.02	0.40
1:C:116:THR:C	1:C:120:LEU:HD22	2.42	0.40
1:C:393:ARG:HB2	1:C:416:HIS:CE1	2.57	0.40
1:C:422:GLU:C	1:C:424:ALA:H	2.25	0.40
1:D:409:THR:O	1:D:410:LEU:C	2.60	0.40
1:A:77:PRO:HG3	1:A:92:ARG:HD3	2.04	0.40
1:A:192:ARG:HH11	1:A:240:GLU:CD	2.23	0.40
1:A:417:HIS:CD2	1:A:419:LEU:H	2.36	0.40
1:B:32:TRP:CD2	1:B:71:ILE:HG21	2.56	0.40
1:C:417:HIS:CE1	1:C:419:LEU:HD12	2.57	0.40
1:D:151:LEU:HD11	1:D:167:LEU:HD21	2.02	0.40
1:D:227:ASN:OD1	1:D:229:LEU:HB2	2.22	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	447/462 (97%)	401 (90%)	34 (8%)	12 (3%)	5	17
1	B	448/462 (97%)	410 (92%)	30 (7%)	8 (2%)	8	28
1	C	446/462 (96%)	400 (90%)	34 (8%)	12 (3%)	5	17
1	D	447/462 (97%)	395 (88%)	44 (10%)	8 (2%)	8	28
All	All	1788/1848 (97%)	1606 (90%)	142 (8%)	40 (2%)	6	22

All (40) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	282	ILE
1	A	319	ALA
1	B	149	ASP
1	B	205	GLY
1	C	203	LEU
1	D	203	LEU
1	D	284	PRO
1	D	422	GLU
1	A	286	LYS
1	A	384	PHE
1	A	412	GLU
1	B	203	LEU
1	B	284	PRO
1	B	319	ALA
1	C	205	GLY
1	C	319	ALA
1	D	201	ALA
1	D	205	GLY
1	A	15	ASP
1	A	203	LEU
1	A	410	LEU
1	C	49	VAL
1	A	151	LEU
1	C	48	ALA
1	C	58	GLU
1	C	83	GLU
1	C	149	ASP
1	C	404	ALA

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Mol	Chain	Res	Type
1	D	423	ASP
1	A	83	GLU
1	A	285	GLN
1	C	151	LEU
1	C	437	ARG
1	D	102	GLY
1	A	383	PRO
1	B	281	SER
1	B	365	GLY
1	C	418	PRO
1	B	317	PRO
1	D	434	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	353/369 (96%)	323 (92%)	30 (8%)	10 31
1	B	351/369 (95%)	318 (91%)	33 (9%)	8 26
1	C	348/369 (94%)	314 (90%)	34 (10%)	8 24
1	D	340/369 (92%)	309 (91%)	31 (9%)	9 27
All	All	1392/1476 (94%)	1264 (91%)	128 (9%)	9 27

All (128) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	17	LEU
1	A	53	SER
1	A	55	GLU
1	A	104	LEU
1	A	132	LEU
1	A	134	LEU
1	A	139	VAL
1	A	148	LEU
1	A	154	LEU

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Mol	Chain	Res	Type
1	A	166	VAL
1	A	168	LEU
1	A	226	ARG
1	A	285	GLN
1	A	303	LEU
1	A	309	LEU
1	A	316	LEU
1	A	323	ASP
1	A	332	LEU
1	A	383	PRO
1	A	384	PHE
1	A	385	ARG
1	A	405	LEU
1	A	411	GLU
1	A	425	LEU
1	A	428	LEU
1	A	430	LEU
1	A	434	ILE
1	A	443	THR
1	A	450	GLU
1	A	461	LEU
1	B	14	PRO
1	B	15	ASP
1	B	17	LEU
1	B	58	GLU
1	B	104	LEU
1	B	120	LEU
1	B	129	LEU
1	B	132	LEU
1	B	134	LEU
1	B	136	LEU
1	B	160	LEU
1	B	168	LEU
1	B	203	LEU
1	B	206	THR
1	B	210	ILE
1	B	239	LEU
1	B	271	GLU
1	B	285	GLN
1	B	303	LEU
1	B	309	LEU
1	B	323	ASP

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Mol	Chain	Res	Type
1	B	324	LEU
1	B	344	LEU
1	B	352	LEU
1	B	355	ARG
1	B	372	GLU
1	B	382	LEU
1	B	389	HIS
1	B	410	LEU
1	B	422	GLU
1	B	428	LEU
1	B	434	ILE
1	B	452	LEU
1	C	17	LEU
1	C	62	LYS
1	C	104	LEU
1	C	120	LEU
1	C	129	LEU
1	C	132	LEU
1	C	134	LEU
1	C	136	LEU
1	C	139	VAL
1	C	151	LEU
1	C	154	LEU
1	C	158	THR
1	C	166	VAL
1	C	168	LEU
1	C	186	LEU
1	C	191	GLU
1	C	206	THR
1	C	210	ILE
1	C	232	VAL
1	C	235	ARG
1	C	239	LEU
1	C	283	MET
1	C	290	ASP
1	C	303	LEU
1	C	309	LEU
1	C	316	LEU
1	C	332	LEU
1	C	352	LEU
1	C	358	ARG
1	C	408	LEU

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Mol	Chain	Res	Type
1	C	434	ILE
1	C	446	GLU
1	C	449	ARG
1	C	452	LEU
1	D	17	LEU
1	D	36	LEU
1	D	81	GLU
1	D	88	ASN
1	D	110	ARG
1	D	129	LEU
1	D	132	LEU
1	D	136	LEU
1	D	139	VAL
1	D	158	THR
1	D	168	LEU
1	D	186	LEU
1	D	206	THR
1	D	234	SER
1	D	239	LEU
1	D	303	LEU
1	D	309	LEU
1	D	316	LEU
1	D	328	LYS
1	D	352	LEU
1	D	356	ARG
1	D	357	GLU
1	D	367	TYR
1	D	384	PHE
1	D	388	HIS
1	D	401	GLU
1	D	434	ILE
1	D	438	ARG
1	D	445	PRO
1	D	453	GLU
1	D	461	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (33) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	86	HIS
1	A	159	HIS
1	A	161	GLN

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Mol	Chain	Res	Type
1	A	170	HIS
1	A	246	ASN
1	A	325	GLN
1	A	414	GLN
1	A	417	HIS
1	B	86	HIS
1	B	105	HIS
1	B	170	HIS
1	B	213	HIS
1	B	246	ASN
1	B	285	GLN
1	B	325	GLN
1	B	417	HIS
1	C	22	ASN
1	C	38	GLN
1	C	42	HIS
1	C	113	GLN
1	C	161	GLN
1	C	170	HIS
1	C	285	GLN
1	C	325	GLN
1	C	388	HIS
1	D	38	GLN
1	D	39	ASN
1	D	86	HIS
1	D	147	HIS
1	D	159	HIS
1	D	170	HIS
1	D	416	HIS
1	D	417	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

4 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	ARG	B	492	-	10,11,11	0.57	0	11,13,13	1.05	0
2	ARG	B	493	-	10,11,11	0.63	0	11,13,13	0.99	0
2	ARG	B	491	-	10,11,11	0.67	0	11,13,13	0.89	0
2	ARG	B	494	-	10,11,11	0.64	0	11,13,13	0.84	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	ARG	B	492	-	-	1/11/11/11	-
2	ARG	B	493	-	-	1/11/11/11	-
2	ARG	B	491	-	-	1/11/11/11	-
2	ARG	B	494	-	-	1/11/11/11	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	494	ARG	NE-CD-CG-CB
2	B	491	ARG	NE-CD-CG-CB
2	B	493	ARG	NE-CD-CG-CB

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Mol	Chain	Res	Type	Atoms
2	B	492	ARG	NE-CD-CG-CB

There are no ring outliers.

4 monomers are involved in 22 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	492	ARG	8	0
2	B	493	ARG	3	0
2	B	491	ARG	6	0
2	B	494	ARG	5	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	449/462 (97%)	-0.51	1 (0%)	95	94	25, 42, 58, 81	0
1	B	450/462 (97%)	-0.52	4 (0%)	84	80	22, 38, 57, 79	0
1	C	448/462 (96%)	-0.51	1 (0%)	95	94	25, 42, 64, 72	0
1	D	449/462 (97%)	-0.39	3 (0%)	87	84	28, 45, 61, 77	0
All	All	1796/1848 (97%)	-0.48	9 (0%)	91	88	22, 42, 62, 81	0

All (9) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	279	GLY	3.1
1	A	462	ASP	2.7
1	D	285	GLN	2.6
1	B	285	GLN	2.4
1	B	280	SER	2.4
1	B	462	ASP	2.4
1	C	402	GLY	2.2
1	D	281	SER	2.2
1	D	201	ALA	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

There are no monosaccharides in this entry.

6.4 Ligands

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. 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	B-factors(Å^2)	Q<0.9
2	ARG	B	491	12/12	0.89	0.23	33,35,38,40	0
2	ARG	B	492	12/12	0.90	0.23	45,49,50,51	0
2	ARG	B	494	12/12	0.92	0.18	42,46,48,49	0
2	ARG	B	493	12/12	0.93	0.22	33,43,50,51	0

6.5 Other polymers

There are no such residues in this entry.