



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 05:05 AM UTC

PDB ID : 3VB9 / pdb_00003vb9
Title : Crystal structure of VPA0735 from *Vibrio parahaemolyticus* in monoclinic form, NorthEast Structural Genomics target VpR109
Authors : Seetharaman, J.; Neely, H.; Cunningham, K.; Ciccocanti, C.; Bjelic, S.; Acton, T.B.; Xiao, R.; Everett, J.K.; Montelione, G.T.; Tong, L.; Hunt, J.F.; Northeast Structural Genomics Consortium (NESG)
Deposited on : 2011-12-31
Resolution : 2.10 Å (reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<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 : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

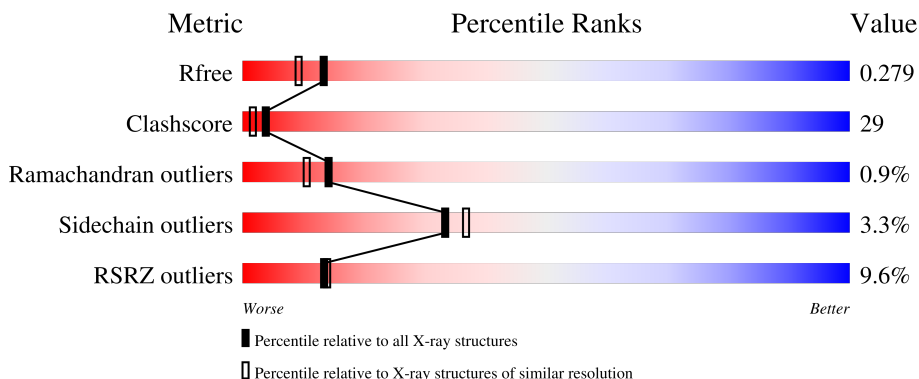
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	6658 (2.10-2.10)
Clashscore	190562	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)
RSRZ outliers	180081	6662 (2.10-2.10)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	483	 7% 49% 42% • 5%
1	B	483	 15% 48% 42% 5% •
1	C	483	 8% 55% 37% • 5%
1	D	483	 5% 59% 33% • 5%

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 15733 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 Uncharacterized protein VPA0735.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	Se			
1	A	460	3717	2382	623	698	14	0	0	0
1	B	462	3736	2393	627	702	14	0	0	0
1	C	460	3717	2382	623	698	14	0	0	0
1	D	460	3717	2382	623	698	14	0	0	0

- Molecule 2 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	2	Total 2	Mg 2	0	0
2	B	2	Total 2	Mg 2	0	0
2	C	1	Total 1	Mg 1	0	0
2	D	2	Total 2	Mg 2	0	0

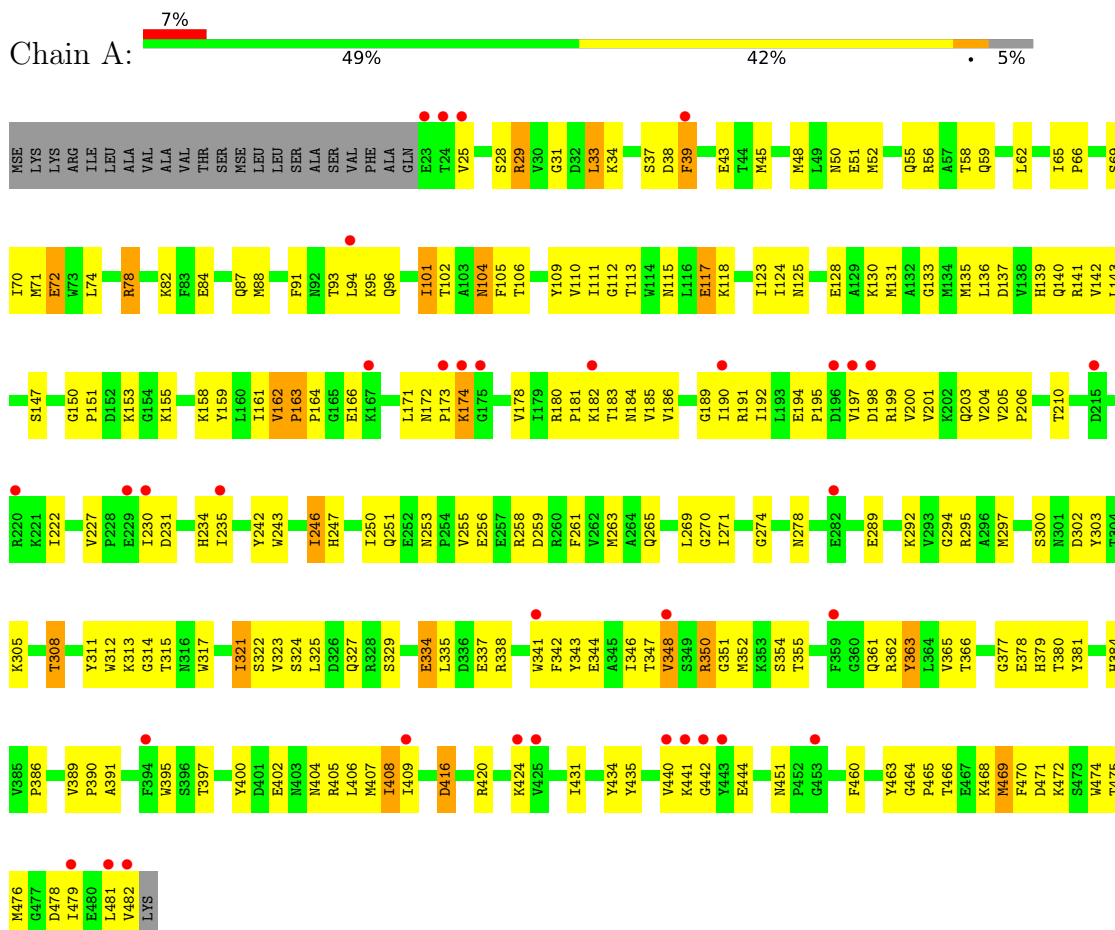
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	197	Total 197	O 197	0	0
3	B	217	Total 217	O 217	0	0
3	C	190	Total 190	O 190	0	0
3	D	235	Total 235	O 235	0	0

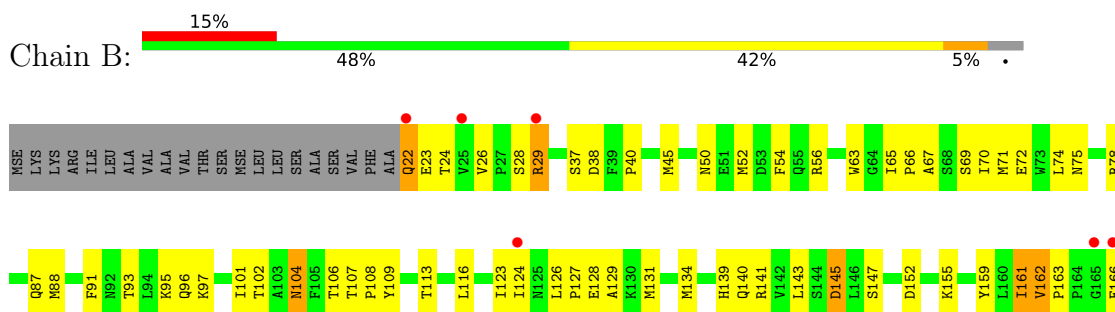
3 Residue-property plots

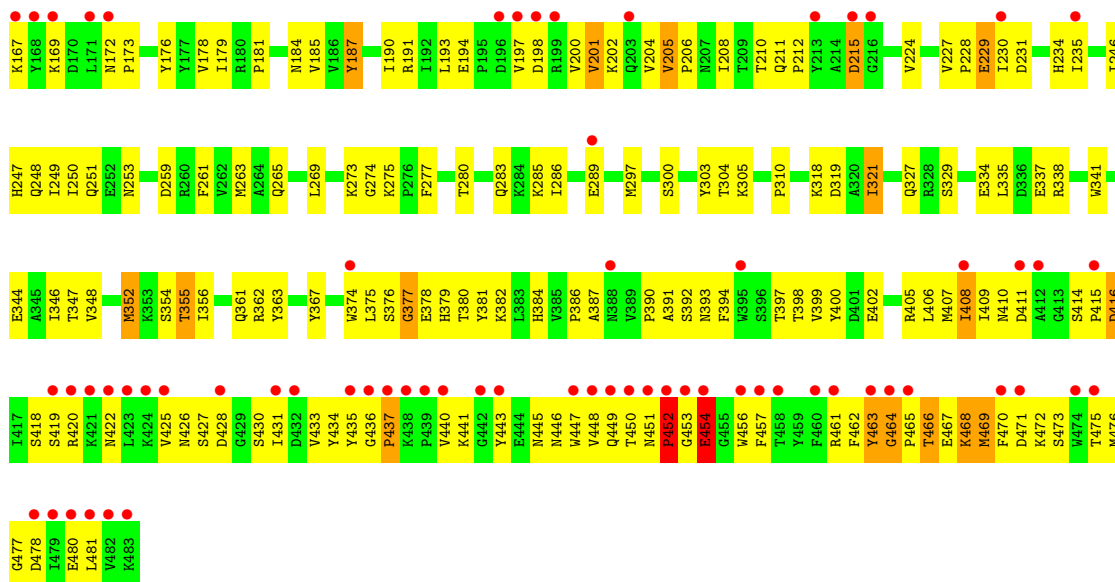
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Uncharacterized protein VPA0735

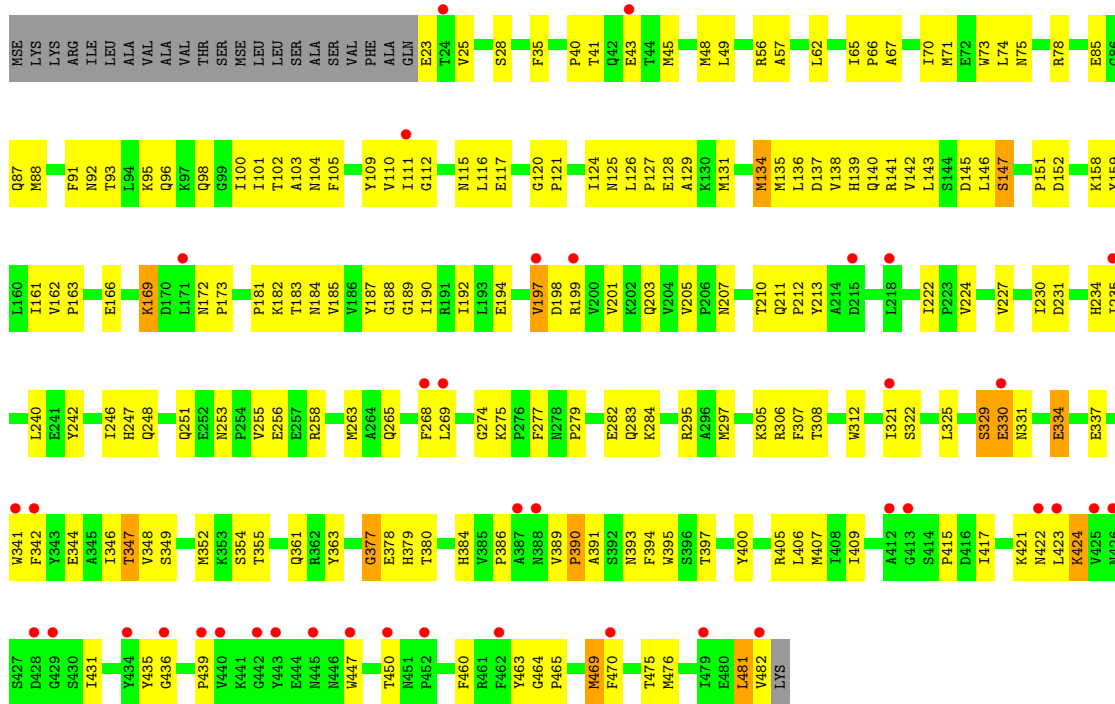


- Molecule 1: Uncharacterized protein VPA0735



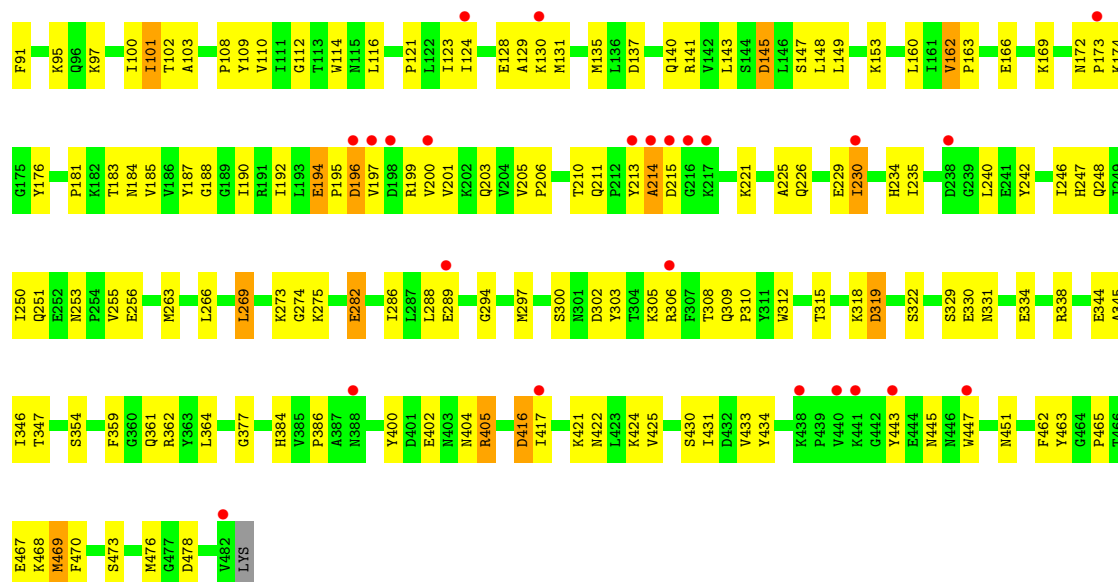


• Molecule 1: Uncharacterized protein VPA0735



• Molecule 1: Uncharacterized protein VPA0735





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	63.27Å 106.93Å 157.18Å 90.00° 94.80° 90.00°	Depositor
Resolution (Å)	39.99 – 2.10 39.99 – 2.10	Depositor EDS
% Data completeness (in resolution range)	89.9 (39.99-2.10) 92.1 (39.99-2.10)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.63 (at 2.08Å)	Xtrriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.224 , 0.274 0.224 , 0.279	Depositor DCC
R_{free} test set	19578 reflections (8.24%)	wwPDB-VP
Wilson B-factor (Å ²)	19.2	Xtrriage
Anisotropy	0.831	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 54.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	15733	wwPDB-VP
Average B, all atoms (Å ²)	25.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 72.02 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 2.3721e-06. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ 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

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	0.41	0/3803	0.98	19/5137 (0.4%)
1	B	0.41	0/3822	0.96	18/5160 (0.3%)
1	C	0.40	0/3803	0.91	7/5137 (0.1%)
1	D	0.41	0/3803	0.94	11/5137 (0.2%)
All	All	0.41	0/15231	0.95	55/20571 (0.3%)

There are no bond length outliers.

All (55) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	351	GLY	N-CA-C	13.96	132.62	115.31
1	A	352	MSE	N-CA-C	-12.76	96.21	113.30
1	A	352	MSE	N-CA-CB	-10.89	94.17	110.61
1	A	204	VAL	N-CA-C	10.12	119.95	110.74
1	B	414	SER	CA-C-N	7.74	127.38	119.56
1	B	414	SER	C-N-CA	7.74	127.38	119.56
1	D	269	LEU	N-CA-C	-7.52	104.10	113.28
1	A	416	ASP	N-CA-C	7.33	117.69	108.45
1	B	464	GLY	CA-C-N	7.19	128.82	119.84
1	B	464	GLY	C-N-CA	7.19	128.82	119.84
1	D	162	VAL	N-CA-C	7.15	116.49	108.05
1	D	467	GLU	N-CA-C	7.03	119.84	111.33
1	B	416	ASP	N-CA-C	6.53	116.68	108.45
1	D	354	SER	N-CA-C	6.38	119.23	110.24
1	B	246	ILE	N-CA-C	-6.32	104.35	110.42
1	D	141	ARG	N-CA-C	-6.32	100.27	110.32
1	D	329	SER	N-CA-C	-6.23	101.24	110.46
1	A	278	ASN	CA-C-N	6.20	126.23	119.90
1	A	278	ASN	C-N-CA	6.20	126.23	119.90
1	B	319	ASP	N-CA-C	-6.19	100.88	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	377	GLY	N-CA-C	6.18	121.27	114.40
1	A	350	ARG	N-CA-C	-6.13	104.59	111.28
1	B	329	SER	N-CA-C	-6.12	100.93	110.17
1	A	377	GLY	N-CA-C	6.05	121.74	113.99
1	C	377	GLY	N-CA-C	5.97	122.72	115.31
1	B	466	THR	N-CA-C	5.97	117.46	111.07
1	B	145	ASP	N-CA-C	-5.95	101.96	110.59
1	D	416	ASP	N-CA-C	5.84	115.99	108.34
1	B	354	SER	N-CA-C	5.79	118.41	110.24
1	D	145	ASP	N-CA-C	-5.73	102.04	110.52
1	B	162	VAL	N-CA-C	5.68	114.75	108.05
1	A	355	THR	N-CA-C	-5.65	105.14	113.61
1	C	355	THR	N-CA-C	-5.63	105.00	113.89
1	B	141	ARG	N-CA-C	-5.55	101.49	110.32
1	A	162	VAL	N-CA-C	5.53	114.57	108.05
1	D	319	ASP	N-CA-C	-5.49	101.52	109.59
1	C	354	SER	N-CA-C	5.45	117.92	110.24
1	A	329	SER	N-CA-C	-5.41	102.00	110.17
1	C	145	ASP	N-CA-C	-5.41	102.51	110.52
1	B	355	THR	N-CA-C	-5.40	104.97	113.02
1	C	329	SER	N-CA-C	-5.33	102.13	110.17
1	A	163	PRO	CA-C-N	5.30	124.92	119.56
1	A	163	PRO	C-N-CA	5.30	124.92	119.56
1	D	194	GLU	CA-C-N	5.29	125.11	119.28
1	D	194	GLU	C-N-CA	5.29	125.11	119.28
1	A	150	GLY	CA-C-N	5.29	124.92	119.05
1	A	150	GLY	C-N-CA	5.29	124.92	119.05
1	A	78	ARG	N-CA-C	5.27	116.84	111.14
1	B	321	ILE	N-CA-C	5.25	114.86	106.88
1	C	205	VAL	CB-CA-C	-5.24	108.72	113.70
1	A	343	TYR	N-CA-C	-5.16	105.72	112.23
1	C	120	GLY	N-CA-C	-5.14	101.86	112.34
1	B	205	VAL	CB-CA-C	-5.08	108.88	113.70
1	B	204	VAL	N-CA-C	5.07	116.48	111.67
1	A	354	SER	N-CA-C	5.00	117.49	110.23

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	3717	0	3643	250	0
1	B	3736	0	3664	284	0
1	C	3717	0	3643	209	0
1	D	3717	0	3643	153	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
2	C	1	0	0	0	0
2	D	2	0	0	0	0
3	A	197	0	0	12	0
3	B	217	0	0	18	0
3	C	190	0	0	11	0
3	D	235	0	0	9	0
All	All	15733	0	14593	844	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 29.

All (844) 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:300:SER:HA	1:B:45:MSE:HE2	1.18	1.14
1:C:105:PHE:HB2	1:C:407:MSE:HE1	1.32	1.11
1:C:135:MSE:HE3	1:C:146:LEU:HD11	1.32	1.10
1:A:303:TYR:HB2	1:B:45:MSE:HE1	1.30	1.09
1:C:45:MSE:HE1	1:D:303:TYR:HB2	1.24	1.09
1:A:105:PHE:HB2	1:A:407:MSE:HE1	1.33	1.07
1:A:297:MSE:HB3	1:B:52:MSE:HE3	1.36	1.07
1:B:378:GLU:HB3	1:B:452:PRO:HD3	1.34	1.07
1:C:45:MSE:HE2	1:D:300:SER:HA	1.34	1.06
1:C:66:PRO:HA	1:C:342:PHE:CD2	1.92	1.02
1:B:392:SER:HB3	1:B:463:TYR:HB3	1.38	1.01
1:C:66:PRO:HA	1:C:342:PHE:HD2	1.26	1.01
1:D:88:MSE:HE3	1:D:210:THR:HG21	1.48	0.95
1:D:140:GLN:HE22	1:D:347:THR:H	1.17	0.92
1:B:251:GLN:HE22	1:B:274:GLY:H	1.13	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:251:GLN:HE22	1:A:274:GLY:H	1.18	0.91
1:C:330:GLU:HB3	3:C:603:HOH:O	1.68	0.91
1:B:415:PRO:HA	1:B:447:TRP:HZ3	1.36	0.91
1:A:70:ILE:HD11	1:A:140:GLN:HG2	1.52	0.90
1:C:397:THR:HG21	1:C:435:TYR:OH	1.72	0.90
1:C:49:LEU:HD13	1:D:306:ARG:HD2	1.50	0.90
1:D:57:ALA:HB2	1:D:269:LEU:HD21	1.53	0.89
1:D:308:THR:HG22	1:D:309:GLN:H	1.39	0.88
1:C:141:ARG:HD2	1:C:182:LYS:NZ	1.89	0.88
1:A:297:MSE:HB3	1:B:52:MSE:CE	2.05	0.87
1:C:197:VAL:HG13	1:C:198:ASP:H	1.39	0.86
1:C:140:GLN:HG2	1:C:140:GLN:O	1.75	0.86
1:C:62:LEU:HD11	1:C:297:MSE:CE	2.06	0.85
1:D:62:LEU:HD11	1:D:297:MSE:HE3	1.56	0.85
1:A:52:MSE:HE2	1:B:297:MSE:HB3	1.58	0.84
1:C:92:ASN:H	1:C:96:GLN:NE2	1.74	0.84
1:C:344:GLU:HA	1:C:405:ARG:HD2	1.60	0.84
1:A:62:LEU:HD11	1:B:52:MSE:HE2	1.60	0.83
1:A:294:GLY:HA2	1:A:297:MSE:HE2	1.58	0.83
1:A:45:MSE:HE1	1:B:303:TYR:HB2	1.61	0.83
1:A:397:THR:HG21	1:A:435:TYR:OH	1.77	0.83
1:B:390:PRO:C	1:B:465:PRO:HD2	2.04	0.83
1:A:104:ASN:C	1:A:104:ASN:HD22	1.87	0.83
1:B:134:MSE:CE	1:B:352:MSE:HE1	2.09	0.82
1:A:62:LEU:CD1	1:B:52:MSE:HE2	2.09	0.82
1:A:62:LEU:HD11	1:A:297:MSE:HE3	1.62	0.81
1:D:101:ILE:H	1:D:234:HIS:HE1	1.27	0.81
1:B:375:LEU:O	1:B:454:GLU:HG2	1.78	0.81
1:A:66:PRO:HG2	1:A:338:ARG:HG2	1.61	0.81
1:A:325:LEU:HD12	1:A:350:ARG:HH21	1.45	0.80
1:D:184:ASN:H	1:D:253:ASN:HD22	1.27	0.80
1:B:29:ARG:HH11	1:B:29:ARG:HB3	1.44	0.80
1:D:282:GLU:HG3	3:D:811:HOH:O	1.81	0.79
1:B:71:MSE:HB2	1:B:249:ILE:HD11	1.63	0.79
1:C:307:PHE:HD1	1:C:308:THR:HG23	1.46	0.79
1:D:251:GLN:HE22	1:D:274:GLY:H	1.29	0.79
1:C:263:MSE:HE1	3:C:679:HOH:O	1.83	0.79
1:A:88:MSE:HE3	1:A:210:THR:HG21	1.64	0.79
1:B:215:ASP:CG	1:D:289:GLU:HG2	2.08	0.79
1:B:191:ARG:HH22	1:B:352:MSE:CE	1.96	0.78
1:B:402:GLU:HB2	1:B:454:GLU:OE2	1.84	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:143:LEU:HD13	1:C:181:PRO:HG3	1.66	0.78
1:A:184:ASN:H	1:A:253:ASN:HD22	1.32	0.77
1:B:430:SER:HB3	3:B:796:HOH:O	1.84	0.77
1:D:140:GLN:NE2	1:D:347:THR:H	1.82	0.77
1:B:397:THR:HG21	1:B:434:TYR:OH	1.85	0.76
1:B:74:LEU:O	1:B:78:ARG:HG2	1.85	0.76
1:C:251:GLN:HE22	1:C:274:GLY:H	1.33	0.76
1:A:395:TRP:HZ2	1:A:431:ILE:HD12	1.48	0.76
1:B:435:TYR:CE2	1:B:437:PRO:HD2	2.21	0.76
1:A:300:SER:CA	1:B:45:MSE:HE2	2.08	0.76
1:B:476:MSE:SE	1:B:477:GLY:H	2.18	0.76
1:D:101:ILE:H	1:D:234:HIS:CE1	2.04	0.75
1:C:139:HIS:CD2	1:C:258:ARG:HH22	2.04	0.75
1:C:134:MSE:HE2	1:C:134:MSE:O	1.84	0.75
1:C:469:MSE:HE2	1:C:470:PHE:CD1	2.22	0.75
1:A:37:SER:HB3	1:B:454:GLU:HB3	1.68	0.75
1:B:104:ASN:HD22	1:B:104:ASN:C	1.95	0.75
1:A:481:LEU:HD22	1:A:482:VAL:HG23	1.67	0.74
1:C:342:PHE:HE1	1:C:347:THR:H	1.35	0.74
1:B:88:MSE:HE3	1:B:210:THR:HG21	1.69	0.74
1:A:37:SER:HB3	1:B:454:GLU:CB	2.18	0.74
1:D:294:GLY:HA2	1:D:297:MSE:HE2	1.69	0.74
1:B:95:LYS:HG2	1:B:229:GLU:HG3	1.68	0.74
1:B:134:MSE:HE2	1:B:352:MSE:HE1	1.70	0.73
1:C:62:LEU:HD11	1:C:297:MSE:HE3	1.70	0.73
1:D:108:PRO:HG2	1:D:197:VAL:HG13	1.69	0.73
1:B:184:ASN:H	1:B:253:ASN:HD22	1.36	0.73
1:C:65:ILE:HB	1:C:66:PRO:HD3	1.70	0.73
1:B:390:PRO:O	1:B:465:PRO:HD2	1.87	0.73
1:B:462:PHE:O	1:B:463:TYR:HB2	1.89	0.73
1:B:415:PRO:HA	1:B:447:TRP:CZ3	2.21	0.73
1:A:45:MSE:CE	1:B:303:TYR:HB2	2.19	0.72
1:B:411:ASP:OD2	1:B:448:VAL:HG21	1.89	0.72
1:A:182:LYS:HE3	1:A:258:ARG:HH21	1.53	0.72
1:A:65:ILE:HB	1:A:66:PRO:HD3	1.72	0.72
1:C:141:ARG:CD	1:C:182:LYS:HZ3	2.03	0.72
1:C:141:ARG:CD	1:C:182:LYS:NZ	2.53	0.72
1:A:469:MSE:HE2	1:A:470:PHE:HD1	1.54	0.72
1:A:110:VAL:C	1:A:111:ILE:HD12	2.14	0.71
1:A:481:LEU:HD23	1:A:482:VAL:H	1.54	0.71
1:A:321:ILE:N	1:A:321:ILE:HD12	2.05	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:37:SER:O	1:B:454:GLU:HB3	1.90	0.71
1:C:137:ASP:OD2	1:C:182:LYS:HE2	1.90	0.71
1:D:308:THR:HG22	1:D:309:GLN:N	2.05	0.71
1:B:376:SER:HA	1:B:454:GLU:HA	1.72	0.71
1:A:481:LEU:HD23	1:A:482:VAL:N	2.05	0.71
1:A:45:MSE:CE	1:B:300:SER:HA	2.21	0.70
1:B:71:MSE:HB2	1:B:249:ILE:CD1	2.20	0.70
1:B:104:ASN:ND2	1:B:106:THR:H	1.89	0.70
1:A:109:TYR:HB3	1:A:111:ILE:CD1	2.21	0.70
1:B:338:ARG:CZ	3:B:601:HOH:O	2.40	0.70
1:C:199:ARG:HH11	1:C:199:ARG:HB2	1.56	0.70
1:B:104:ASN:HD22	1:B:106:THR:H	1.39	0.70
1:B:185:VAL:H	1:B:253:ASN:HD21	1.39	0.70
1:C:247:HIS:O	1:C:251:GLN:HG2	1.90	0.70
1:A:124:ILE:HD13	1:A:210:THR:HG22	1.74	0.69
1:C:45:MSE:HE1	1:D:303:TYR:CB	2.13	0.69
1:B:161:ILE:HD12	1:B:161:ILE:N	2.07	0.69
1:B:468:LYS:HZ3	1:B:468:LYS:HB2	1.57	0.69
1:B:380:THR:HG23	1:B:435:TYR:HB2	1.75	0.69
1:C:92:ASN:H	1:C:96:GLN:HE21	1.40	0.69
1:C:307:PHE:CD1	1:C:308:THR:HG23	2.28	0.69
1:C:105:PHE:HB2	1:C:407:MSE:CE	2.18	0.69
1:B:197:VAL:O	1:B:201:VAL:HG12	1.93	0.68
1:C:101:ILE:H	1:C:234:HIS:HE1	1.39	0.68
1:B:247:HIS:O	1:B:251:GLN:HG2	1.93	0.68
1:B:286:ILE:HD12	3:B:729:HOH:O	1.93	0.68
1:B:420:ARG:HB2	3:B:707:HOH:O	1.93	0.68
1:A:45:MSE:HE2	1:B:300:SER:O	1.94	0.68
1:D:75:ASN:HD21	1:D:248:GLN:HE22	1.40	0.68
1:A:185:VAL:H	1:A:253:ASN:HD21	1.43	0.67
1:A:201:VAL:O	1:A:205:VAL:HG22	1.93	0.67
1:A:235:ILE:HD11	1:A:406:LEU:HD21	1.75	0.67
1:B:65:ILE:HB	1:B:66:PRO:HD3	1.75	0.67
1:C:62:LEU:HD11	1:C:297:MSE:HE2	1.74	0.67
1:C:469:MSE:HE2	1:C:470:PHE:HD1	1.58	0.67
1:A:182:LYS:HG2	3:A:718:HOH:O	1.94	0.67
1:B:382:LYS:HB2	1:B:481:LEU:HD11	1.77	0.67
1:D:101:ILE:HD11	1:D:405:ARG:HB2	1.77	0.67
1:A:109:TYR:HB3	1:A:111:ILE:HD13	1.76	0.67
1:B:40:PRO:CG	1:B:45:MSE:HE3	2.25	0.66
1:B:29:ARG:HB3	1:B:29:ARG:NH1	2.09	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:250:ILE:HD12	1:A:263:MSE:SE	2.45	0.66
1:A:71:MSE:HE1	1:A:74:LEU:HD23	1.77	0.66
1:A:205:VAL:CG2	1:A:206:PRO:HD3	2.25	0.66
1:C:184:ASN:H	1:C:253:ASN:HD22	1.42	0.66
1:A:93:THR:OG1	1:A:96:GLN:HG3	1.95	0.66
1:B:393:ASN:H	1:B:463:TYR:HB2	1.61	0.65
1:B:440:VAL:HA	1:B:443:TYR:HE1	1.61	0.65
1:D:282:GLU:O	1:D:286:ILE:HD13	1.96	0.65
1:A:303:TYR:CB	1:B:45:MSE:HE1	2.18	0.65
1:D:185:VAL:H	1:D:253:ASN:HD21	1.44	0.65
1:C:230:ILE:HD12	1:C:231:ASP:H	1.61	0.65
1:C:395:TRP:HZ2	1:C:431:ILE:HD12	1.61	0.65
1:D:130:LYS:HG3	1:D:148:LEU:HD11	1.78	0.65
1:D:66:PRO:HG2	3:D:610:HOH:O	1.96	0.65
1:B:451:ASN:HB3	1:B:452:PRO:HD2	1.77	0.65
1:A:270:GLY:C	1:A:271:ILE:HD12	2.22	0.64
1:C:141:ARG:HD2	1:C:182:LYS:HZ3	1.62	0.64
1:C:475:THR:HG22	1:C:476:MSE:N	2.12	0.64
1:B:191:ARG:HH22	1:B:352:MSE:HE2	1.61	0.64
1:B:470:PHE:CD2	1:B:472:LYS:HE3	2.33	0.64
1:D:87:GLN:C	1:D:88:MSE:HE2	2.22	0.64
1:B:344:GLU:HA	1:B:405:ARG:HD2	1.80	0.64
1:A:101:ILE:H	1:A:234:HIS:HE1	1.44	0.64
1:C:93:THR:H	1:C:96:GLN:HE21	1.44	0.64
1:A:153:LYS:HB2	1:A:155:LYS:HE2	1.80	0.64
1:B:87:GLN:C	1:B:88:MSE:HE2	2.23	0.64
1:C:349:SER:OG	1:C:352:MSE:HE3	1.98	0.64
1:B:440:VAL:HA	1:B:443:TYR:CE1	2.33	0.64
1:C:436:GLY:C	1:C:450:THR:HG22	2.22	0.64
1:A:45:MSE:HE3	1:B:300:SER:HA	1.80	0.64
1:B:335:LEU:HA	1:B:338:ARG:HH11	1.62	0.64
1:B:382:LYS:HE3	1:B:431:ILE:HD13	1.80	0.64
1:C:139:HIS:O	1:C:140:GLN:HB3	1.98	0.64
1:D:465:PRO:HB2	1:D:469:MSE:HG2	1.79	0.64
1:A:104:ASN:C	1:A:104:ASN:ND2	2.56	0.64
1:B:391:ALA:HA	1:B:465:PRO:HD3	1.80	0.64
1:B:397:THR:O	1:B:416:ASP:HB2	1.98	0.63
1:C:93:THR:H	1:C:96:GLN:NE2	1.97	0.63
1:C:101:ILE:HA	1:C:406:LEU:HD23	1.78	0.63
1:C:334:GLU:HB3	1:C:337:GLU:HB2	1.80	0.63
1:C:469:MSE:HE3	1:C:470:PHE:HA	1.81	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:250:ILE:HD12	1:D:263:MSE:SE	2.48	0.63
1:D:184:ASN:H	1:D:253:ASN:ND2	1.97	0.63
1:B:250:ILE:O	1:B:273:LYS:HD3	1.99	0.63
1:B:435:TYR:CD2	1:B:437:PRO:HD2	2.34	0.63
1:A:469:MSE:HE2	1:A:470:PHE:CD1	2.32	0.62
1:B:468:LYS:HG3	1:B:469:MSE:N	2.12	0.62
1:A:104:ASN:ND2	1:A:106:THR:H	1.97	0.62
1:B:215:ASP:OD1	1:D:289:GLU:HG2	1.99	0.62
1:C:116:LEU:HD21	1:C:161:ILE:HG22	1.81	0.62
1:D:253:ASN:O	1:D:273:LYS:HE3	2.00	0.62
1:A:131:MSE:SE	1:A:190:ILE:HG21	2.49	0.62
1:A:289:GLU:HG3	1:B:29:ARG:HG3	1.82	0.62
1:A:313:LYS:HZ2	1:A:314:GLY:HA3	1.63	0.62
1:B:193:LEU:HD13	1:B:463:TYR:HE1	1.65	0.62
1:A:258:ARG:NH1	3:A:601:HOH:O	2.32	0.61
1:A:39:PHE:HD1	1:B:374:TRP:HB3	1.65	0.61
1:B:29:ARG:HH11	1:B:29:ARG:CB	2.13	0.61
1:A:70:ILE:CD1	1:A:140:GLN:HG2	2.28	0.61
1:A:205:VAL:HG22	1:A:206:PRO:HD3	1.83	0.61
1:B:191:ARG:NH2	1:B:352:MSE:HE2	2.15	0.61
1:A:125:ASN:HD22	1:A:158:LYS:HG2	1.66	0.61
1:C:297:MSE:HE3	1:D:52:MSE:HG3	1.81	0.61
1:C:88:MSE:HB2	1:C:224:VAL:HG22	1.83	0.61
1:B:410:ASN:CG	1:B:448:VAL:HG13	2.26	0.61
1:D:81:PHE:HE1	1:D:230:ILE:HD11	1.66	0.61
1:B:399:VAL:HG12	1:B:408:ILE:HG21	1.83	0.60
1:C:135:MSE:HE2	1:C:188:GLY:HA2	1.83	0.60
1:C:377:GLY:O	1:C:450:THR:HG23	2.00	0.60
1:D:95:LYS:HG2	1:D:229:GLU:OE2	2.01	0.60
1:C:124:ILE:HD13	1:C:210:THR:HG22	1.84	0.60
1:C:341:TRP:CZ3	1:C:347:THR:O	2.54	0.60
1:B:172:ASN:HD22	1:B:178:VAL:HG21	1.66	0.60
1:C:242:TYR:CE2	1:C:246:ILE:HD11	2.35	0.60
1:D:183:THR:HG22	1:D:256:GLU:OE2	2.02	0.60
1:C:125:ASN:HD22	1:C:158:LYS:HG2	1.67	0.60
1:A:300:SER:HA	1:B:45:MSE:CE	2.12	0.60
1:A:71:MSE:CE	1:A:74:LEU:HD23	2.32	0.60
1:D:330:GLU:HB3	3:D:656:HOH:O	2.02	0.59
1:C:182:LYS:HG2	3:C:728:HOH:O	2.02	0.59
1:A:59:GLN:NE2	1:B:56:ARG:HE	2.00	0.59
1:A:341:TRP:CZ3	1:A:347:THR:O	2.55	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:108:PRO:HB2	1:D:192:ILE:HD13	1.84	0.59
1:B:387:ALA:CB	1:B:428:ASP:HB3	2.33	0.59
1:D:101:ILE:HD13	1:D:405:ARG:O	2.02	0.59
1:A:182:LYS:CE	1:A:258:ARG:HH21	2.15	0.59
1:D:81:PHE:CE1	1:D:230:ILE:HD11	2.36	0.59
1:A:141:ARG:CD	1:A:182:LYS:NZ	2.66	0.59
1:C:45:MSE:HE2	1:D:300:SER:CA	2.23	0.59
1:D:197:VAL:O	1:D:201:VAL:HG23	2.03	0.59
1:D:310:PRO:HA	1:D:318:LYS:HG2	1.84	0.59
1:B:338:ARG:NE	3:B:601:HOH:O	2.36	0.59
1:A:407:MSE:O	1:A:409:ILE:HD12	2.02	0.59
1:C:101:ILE:H	1:C:234:HIS:CE1	2.21	0.59
1:B:247:HIS:HE1	1:B:275:LYS:O	1.86	0.58
1:B:418:SER:O	1:B:420:ARG:N	2.36	0.58
1:D:377:GLY:HA3	1:D:451:ASN:O	2.03	0.58
1:C:185:VAL:H	1:C:253:ASN:HD21	1.51	0.58
1:D:88:MSE:SE	1:D:112:GLY:HA3	2.53	0.58
1:C:102:THR:HA	1:C:400:TYR:CE1	2.38	0.58
1:A:84:GLU:H	1:A:87:GLN:HE21	1.51	0.58
1:A:235:ILE:HD11	1:A:406:LEU:CD2	2.32	0.58
1:C:197:VAL:HG13	1:C:198:ASP:N	2.15	0.58
1:A:174:LYS:NZ	1:A:174:LYS:HB3	2.19	0.58
1:B:377:GLY:HA3	1:B:450:THR:O	2.03	0.58
1:A:113:THR:HG23	1:A:186:VAL:O	2.04	0.58
1:B:410:ASN:ND2	1:B:448:VAL:HG13	2.18	0.58
1:B:235:ILE:HD11	1:B:406:LEU:HG	1.86	0.58
1:D:101:ILE:HD11	1:D:405:ARG:HG3	1.85	0.58
1:C:78:ARG:NE	1:C:85:GLU:OE2	2.31	0.58
1:A:166:GLU:H	1:A:166:GLU:CD	2.12	0.58
1:A:271:ILE:HD12	1:A:271:ILE:N	2.19	0.58
1:C:199:ARG:HG3	1:C:203:GLN:HE22	1.68	0.58
1:C:124:ILE:HB	1:C:159:TYR:HB2	1.86	0.57
1:C:141:ARG:NH1	1:C:258:ARG:CZ	2.67	0.57
1:A:50:ASN:ND2	1:B:29:ARG:HH21	2.02	0.57
1:B:67:ALA:HB1	1:B:249:ILE:HD12	1.86	0.57
1:C:75:ASN:HD21	1:C:248:GLN:HE22	1.50	0.57
1:B:50:ASN:ND2	1:B:286:ILE:HD11	2.20	0.57
1:B:374:TRP:NE1	3:B:753:HOH:O	2.21	0.57
1:C:136:LEU:HD11	1:C:347:THR:OG1	2.04	0.57
1:A:246:ILE:O	1:A:250:ILE:HG12	2.04	0.57
1:D:110:VAL:HB	1:D:190:ILE:HB	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:172:ASN:HD22	1:A:178:VAL:HG21	1.70	0.57
1:C:325:LEU:HD12	1:C:325:LEU:H	1.70	0.57
1:A:29:ARG:HD2	1:B:54:PHE:CE2	2.40	0.57
1:A:87:GLN:C	1:A:88:MSE:HE2	2.29	0.57
1:B:128:GLU:HG3	1:B:155:LYS:HA	1.87	0.57
1:A:102:THR:HA	1:A:400:TYR:CE1	2.40	0.57
1:B:230:ILE:HG13	1:B:231:ASP:N	2.20	0.56
1:B:466:THR:HG23	1:B:470:PHE:CE1	2.38	0.56
1:C:424:LYS:HB2	1:C:424:LYS:NZ	2.20	0.56
1:A:39:PHE:CD2	1:B:402:GLU:HG3	2.40	0.56
1:A:58:THR:HG22	1:A:297:MSE:HE1	1.85	0.56
1:D:71:MSE:HE3	1:D:71:MSE:HA	1.87	0.56
1:D:121:PRO:HB2	1:D:213:TYR:HB3	1.86	0.56
1:A:222:ILE:HD11	3:A:777:HOH:O	2.05	0.56
1:B:187:TYR:CD1	1:B:187:TYR:C	2.83	0.56
1:C:91:PHE:CD2	1:C:227:VAL:HG21	2.41	0.56
1:D:417:ILE:CD1	1:D:433:VAL:HG13	2.36	0.56
1:A:56:ARG:HD3	1:A:265:GLN:HB3	1.88	0.56
1:C:222:ILE:HD11	3:C:659:HOH:O	2.06	0.56
1:A:424:LYS:HE3	1:A:442:GLY:O	2.06	0.56
1:B:101:ILE:HA	1:B:406:LEU:HD23	1.87	0.56
1:B:131:MSE:SE	1:B:190:ILE:HG21	2.55	0.56
1:D:58:THR:HG22	1:D:297:MSE:HE1	1.87	0.56
1:D:404:ASN:O	1:D:405:ARG:HG2	2.05	0.56
1:B:334:GLU:HB3	1:B:337:GLU:HB2	1.88	0.56
1:C:135:MSE:HE3	1:C:146:LEU:CD1	2.21	0.56
1:D:315:THR:HA	1:D:478:ASP:OD2	2.05	0.56
1:A:465:PRO:HB2	1:A:469:MSE:HG2	1.86	0.55
1:C:62:LEU:CD1	1:C:297:MSE:CE	2.82	0.55
1:A:172:ASN:N	1:A:173:PRO:HD3	2.19	0.55
1:B:155:LYS:HB2	1:B:155:LYS:NZ	2.21	0.55
1:B:102:THR:HA	1:B:400:TYR:CE1	2.41	0.55
1:B:425:VAL:HG12	1:B:426:ASN:N	2.21	0.55
1:C:140:GLN:CD	1:C:342:PHE:CD1	2.85	0.55
1:C:41:THR:OG1	1:C:43:GLU:HG2	2.06	0.55
1:A:101:ILE:HD12	1:A:344:GLU:O	2.07	0.55
1:A:141:ARG:HD2	1:A:182:LYS:NZ	2.22	0.55
1:A:341:TRP:CZ3	1:A:348:VAL:HG13	2.41	0.55
1:D:131:MSE:SE	1:D:190:ILE:HG21	2.57	0.55
1:A:479:ILE:HD12	1:A:479:ILE:N	2.22	0.55
1:B:104:ASN:HD21	1:B:107:THR:H	1.52	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:111:ILE:HD13	1:C:187:TYR:OH	2.07	0.55
1:C:161:ILE:HD12	1:C:161:ILE:N	2.22	0.55
1:C:282:GLU:HG3	1:C:283:GLN:N	2.22	0.55
1:C:450:THR:HG21	3:C:663:HOH:O	2.07	0.55
1:B:194:GLU:HB2	1:B:200:VAL:HG21	1.88	0.55
1:C:141:ARG:HD2	1:C:182:LYS:HZ1	1.71	0.55
1:A:475:THR:HG22	1:A:476:MSE:N	2.22	0.55
1:B:327:GLN:HA	1:B:334:GLU:OE1	2.07	0.55
1:C:169:LYS:HE2	3:C:788:HOH:O	2.07	0.55
1:A:194:GLU:HG2	3:A:768:HOH:O	2.07	0.54
1:C:199:ARG:HB2	1:C:199:ARG:NH1	2.22	0.54
1:D:78:ARG:O	1:D:82:LYS:HA	2.07	0.54
1:D:404:ASN:C	1:D:405:ARG:HG2	2.31	0.54
1:B:104:ASN:C	1:B:104:ASN:ND2	2.60	0.54
1:B:235:ILE:HD11	1:B:406:LEU:CG	2.37	0.54
1:B:398:THR:O	1:B:457:PHE:CB	2.55	0.54
1:B:440:VAL:O	1:B:441:LYS:HB3	2.08	0.54
1:C:105:PHE:CB	1:C:407:MSE:HE1	2.23	0.54
1:D:246:ILE:O	1:D:250:ILE:HG12	2.07	0.54
1:C:56:ARG:HD3	1:C:265:GLN:HB3	1.88	0.54
1:B:91:PHE:HB2	1:B:109:TYR:HB2	1.90	0.54
1:B:93:THR:OG1	1:B:96:GLN:HG3	2.06	0.54
1:A:28:SER:HB3	1:A:33:LEU:HD21	1.90	0.54
1:A:62:LEU:HD13	1:B:52:MSE:HE2	1.87	0.54
1:B:408:ILE:HG23	1:B:447:TRP:CH2	2.43	0.54
1:C:141:ARG:NH1	1:C:258:ARG:NH2	2.56	0.54
1:A:62:LEU:HD11	1:A:297:MSE:CE	2.35	0.54
1:A:295:ARG:NE	3:A:635:HOH:O	2.41	0.54
1:C:341:TRP:CH2	1:C:347:THR:O	2.60	0.54
1:D:58:THR:HG22	1:D:297:MSE:CE	2.37	0.54
1:A:78:ARG:NH2	1:A:118:LYS:HE2	2.23	0.54
1:D:30:VAL:HG11	1:D:51:GLU:HG2	1.88	0.54
1:B:97:LYS:HE2	1:B:109:TYR:CD2	2.43	0.54
1:B:102:THR:HG21	1:B:456:TRP:CH2	2.43	0.54
1:B:215:ASP:HB2	1:C:28:SER:C	2.33	0.54
1:C:135:MSE:CE	1:C:188:GLY:HA2	2.37	0.54
1:B:468:LYS:C	1:B:468:LYS:HZ2	2.15	0.53
1:A:128:GLU:HG3	1:A:155:LYS:HA	1.91	0.53
1:B:172:ASN:ND2	1:B:178:VAL:HG21	2.24	0.53
1:B:185:VAL:H	1:B:253:ASN:ND2	2.06	0.53
1:B:408:ILE:HG12	1:B:447:TRP:HZ2	1.72	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:308:THR:CG2	1:D:309:GLN:H	2.18	0.53
1:A:104:ASN:HD22	1:A:106:THR:H	1.55	0.53
1:B:78:ARG:HD2	3:B:728:HOH:O	2.08	0.53
1:D:247:HIS:HE1	1:D:275:LYS:O	1.91	0.53
1:A:444:GLU:CD	1:A:444:GLU:H	2.17	0.53
1:C:378:GLU:HG2	1:C:379:HIS:CD2	2.44	0.53
1:A:469:MSE:HG3	1:A:470:PHE:N	2.23	0.53
1:B:381:TYR:HD2	1:B:449:GLN:HE22	1.56	0.53
1:D:135:MSE:HE2	1:D:188:GLY:CA	2.38	0.53
1:D:425:VAL:HA	1:D:431:ILE:CD1	2.38	0.53
1:A:45:MSE:HE2	1:B:300:SER:HA	1.90	0.53
1:A:161:ILE:N	1:A:161:ILE:HD12	2.24	0.53
1:C:135:MSE:HE2	1:C:135:MSE:HA	1.91	0.53
1:A:242:TYR:CE1	1:A:246:ILE:HD11	2.43	0.53
1:A:315:THR:HA	1:A:478:ASP:OD2	2.09	0.53
1:B:191:ARG:HH22	1:B:352:MSE:HE1	1.72	0.53
1:B:382:LYS:HG3	1:B:431:ILE:HG23	1.89	0.53
1:B:468:LYS:HE2	3:B:677:HOH:O	2.08	0.53
1:C:361:GLN:HG2	1:C:463:TYR:CZ	2.44	0.53
1:D:131:MSE:SE	1:D:190:ILE:CG2	3.07	0.53
1:D:101:ILE:CD1	1:D:405:ARG:HB2	2.39	0.53
1:B:102:THR:HG21	1:B:456:TRP:HH2	1.74	0.52
1:B:285:LYS:HB2	3:B:729:HOH:O	2.10	0.52
1:A:334:GLU:O	1:A:338:ARG:HB2	2.08	0.52
1:D:101:ILE:HD12	1:D:344:GLU:O	2.10	0.52
1:A:378:GLU:HG2	1:A:379:HIS:ND1	2.24	0.52
1:B:101:ILE:H	1:B:234:HIS:CE1	2.28	0.52
1:A:137:ASP:OD2	1:A:182:LYS:HE2	2.09	0.52
1:D:417:ILE:HD13	1:D:433:VAL:HG13	1.92	0.52
1:C:331:ASN:HB3	1:D:255:VAL:HG21	1.90	0.52
1:D:172:ASN:N	1:D:173:PRO:HD3	2.25	0.52
1:A:39:PHE:CD1	1:B:374:TRP:HB3	2.45	0.52
1:C:347:THR:HG23	1:C:352:MSE:HE1	1.91	0.52
1:B:40:PRO:HG2	1:B:45:MSE:HE3	1.91	0.52
1:D:114:TRP:HE1	1:D:116:LEU:HD23	1.74	0.52
1:A:72:GLU:OE1	1:A:72:GLU:HA	2.09	0.52
1:C:475:THR:CG2	1:C:476:MSE:N	2.72	0.52
1:C:182:LYS:HE3	1:C:258:ARG:HH21	1.75	0.52
1:D:199:ARG:O	1:D:203:GLN:HG3	2.10	0.52
1:A:101:ILE:HD13	1:A:405:ARG:O	2.11	0.51
1:B:29:ARG:HD2	3:B:762:HOH:O	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:66:PRO:CG	1:A:338:ARG:HG2	2.36	0.51
1:C:131:MSE:HE2	1:C:190:ILE:HG22	1.91	0.51
1:D:108:PRO:CG	1:D:197:VAL:HG13	2.39	0.51
1:A:101:ILE:H	1:A:234:HIS:CE1	2.26	0.51
1:D:101:ILE:HG23	1:D:345:ALA:HA	1.92	0.51
1:A:111:ILE:HD12	1:A:111:ILE:N	2.25	0.51
1:A:468:LYS:HD3	3:A:693:HOH:O	2.09	0.51
1:B:387:ALA:HB1	1:B:428:ASP:HB3	1.93	0.51
1:B:451:ASN:O	1:B:453:GLY:N	2.42	0.51
1:D:361:GLN:HG2	1:D:463:TYR:CZ	2.45	0.51
1:A:441:LYS:HG3	1:A:441:LYS:O	2.11	0.51
1:B:129:ALA:HB3	1:B:131:MSE:HE2	1.93	0.51
1:B:321:ILE:HD12	1:B:321:ILE:N	2.25	0.51
1:B:341:TRP:HE1	1:B:348:VAL:CG1	2.24	0.51
1:C:295:ARG:HG3	1:C:295:ARG:HH11	1.76	0.51
1:D:57:ALA:HB2	1:D:269:LEU:CD2	2.35	0.51
1:B:101:ILE:H	1:B:234:HIS:HE1	1.59	0.51
1:C:116:LEU:HD21	1:C:161:ILE:CG2	2.39	0.51
1:B:172:ASN:N	1:B:173:PRO:HD3	2.25	0.51
1:B:335:LEU:HD12	1:B:338:ARG:NH1	2.26	0.51
1:D:30:VAL:HG12	1:D:30:VAL:O	2.09	0.51
1:B:147:SER:HA	1:B:152:ASP:OD1	2.11	0.51
1:C:126:LEU:HD21	1:C:190:ILE:CD1	2.40	0.51
1:D:101:ILE:HD11	1:D:405:ARG:CG	2.40	0.51
1:A:140:GLN:NE2	1:A:346:ILE:HD12	2.26	0.50
1:A:305:LYS:HE3	3:A:733:HOH:O	2.11	0.50
1:B:285:LYS:O	1:B:289:GLU:HG3	2.09	0.50
1:B:457:PHE:HZ	1:B:478:ASP:CG	2.19	0.50
1:B:467:GLU:HA	1:B:472:LYS:HD2	1.93	0.50
1:A:302:ASP:O	1:A:305:LYS:HG3	2.11	0.50
1:B:40:PRO:HG3	1:B:45:MSE:HE3	1.92	0.50
1:B:335:LEU:HA	1:B:338:ARG:NH1	2.26	0.50
1:C:45:MSE:CE	1:D:303:TYR:HB2	2.17	0.50
1:C:230:ILE:HD12	1:C:231:ASP:N	2.25	0.50
1:D:240:LEU:HG	1:D:288:LEU:HD21	1.92	0.50
1:A:29:ARG:NH1	1:A:29:ARG:HG3	2.26	0.50
1:B:454:GLU:C	1:B:454:GLU:CD	2.80	0.50
1:C:390:PRO:HB2	1:C:469:MSE:HB3	1.92	0.50
1:A:185:VAL:H	1:A:253:ASN:ND2	2.09	0.50
1:B:390:PRO:C	1:B:465:PRO:CD	2.81	0.50
1:B:408:ILE:HG12	1:B:447:TRP:CZ2	2.47	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:464:GLY:N	3:B:783:HOH:O	2.40	0.50
1:B:468:LYS:HB2	1:B:468:LYS:NZ	2.26	0.50
1:D:425:VAL:HG22	1:D:431:ILE:HD11	1.93	0.50
1:C:146:LEU:O	1:C:147:SER:HB3	2.12	0.50
1:C:73:TRP:CZ3	1:C:346:ILE:HD13	2.46	0.50
1:C:88:MSE:HE3	1:C:210:THR:HG21	1.93	0.50
1:A:28:SER:HB3	1:A:33:LEU:CD2	2.41	0.50
1:A:341:TRP:HZ3	1:A:348:VAL:HG13	1.77	0.50
1:B:230:ILE:HD12	1:B:231:ASP:H	1.75	0.50
1:B:467:GLU:HG3	3:B:724:HOH:O	2.11	0.50
1:D:192:ILE:N	1:D:192:ILE:HD12	2.27	0.50
1:A:91:PHE:CD2	1:A:227:VAL:HG21	2.47	0.49
1:A:139:HIS:CD2	1:A:258:ARG:HH22	2.30	0.49
1:C:182:LYS:HG3	1:C:183:THR:HG23	1.94	0.49
1:D:230:ILE:HD13	1:D:230:ILE:H	1.76	0.49
1:D:123:ILE:HD13	1:D:160:LEU:HD13	1.94	0.49
1:A:29:ARG:HG3	1:A:29:ARG:HH11	1.77	0.49
1:A:313:LYS:NZ	3:A:764:HOH:O	2.45	0.49
1:C:40:PRO:CG	1:C:45:MSE:HE3	2.43	0.49
1:C:71:MSE:HE1	1:C:74:LEU:HD23	1.95	0.49
1:A:235:ILE:HD11	1:A:406:LEU:CG	2.42	0.49
1:B:356:ILE:N	1:B:356:ILE:HD12	2.27	0.49
1:C:91:PHE:HB2	1:C:109:TYR:HB2	1.94	0.49
1:D:302:ASP:O	1:D:305:LYS:HG3	2.13	0.49
1:A:408:ILE:HD13	1:A:409:ILE:N	2.28	0.49
1:C:166:GLU:HA	1:C:166:GLU:OE1	2.11	0.49
1:A:37:SER:O	1:A:38:ASP:HB2	2.13	0.49
1:A:133:GLY:HA3	1:A:190:ILE:HD13	1.95	0.49
1:D:123:ILE:CD1	1:D:160:LEU:HD13	2.42	0.49
1:A:37:SER:HB3	1:B:454:GLU:HB2	1.91	0.49
1:C:141:ARG:HD2	1:C:182:LYS:CE	2.42	0.49
1:D:102:THR:HA	1:D:400:TYR:CE1	2.47	0.49
1:D:430:SER:O	1:D:431:ILE:HD13	2.13	0.49
1:A:174:LYS:HB3	1:A:174:LYS:HZ3	1.78	0.49
1:A:243:TRP:CZ3	1:A:246:ILE:HD12	2.48	0.49
1:B:230:ILE:CG1	1:B:231:ASP:N	2.76	0.49
1:A:346:ILE:C	1:A:347:THR:HG23	2.38	0.48
1:A:197:VAL:HG23	1:A:198:ASP:N	2.28	0.48
1:A:363:TYR:CD1	1:A:363:TYR:N	2.81	0.48
1:B:194:GLU:CB	1:B:200:VAL:HG21	2.43	0.48
1:B:398:THR:HA	1:B:416:ASP:HB3	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:476:MSE:CG	1:B:477:GLY:N	2.76	0.48
1:D:196:ASP:HB2	3:D:807:HOH:O	2.13	0.48
1:A:141:ARG:NH1	1:A:258:ARG:CZ	2.77	0.48
1:B:69:SER:OG	1:B:346:ILE:HD13	2.12	0.48
1:C:213:TYR:CD1	1:C:213:TYR:C	2.91	0.48
1:A:303:TYR:HB2	1:B:45:MSE:CE	2.23	0.48
1:A:380:THR:O	1:A:482:VAL:N	2.46	0.48
1:B:341:TRP:HE1	1:B:348:VAL:HG13	1.77	0.48
1:C:111:ILE:HG12	1:C:189:GLY:HA2	1.96	0.48
1:C:199:ARG:HG3	1:C:203:GLN:NE2	2.27	0.48
1:D:211:GLN:CD	1:D:221:LYS:HD3	2.39	0.48
1:A:341:TRP:HZ3	1:A:347:THR:O	1.97	0.48
1:A:381:TYR:HB3	1:A:479:ILE:CG2	2.44	0.48
1:B:63:TRP:HA	1:B:335:LEU:HD11	1.96	0.48
1:B:134:MSE:HE1	1:B:352:MSE:HE1	1.92	0.48
1:C:322:SER:HB2	3:C:660:HOH:O	2.13	0.48
1:A:43:GLU:HG2	3:A:790:HOH:O	2.13	0.48
1:A:52:MSE:O	1:A:56:ARG:HG3	2.14	0.48
1:C:87:GLN:C	1:C:88:MSE:HE2	2.38	0.48
1:A:141:ARG:CD	1:A:182:LYS:HZ3	2.26	0.48
1:B:251:GLN:O	1:B:273:LYS:HE3	2.13	0.48
1:C:405:ARG:NH1	3:C:680:HOH:O	2.46	0.48
1:C:255:VAL:HG21	1:D:331:ASN:HB3	1.95	0.48
1:D:123:ILE:HG22	1:D:124:ILE:N	2.28	0.48
1:D:205:VAL:HB	1:D:206:PRO:HD3	1.95	0.48
1:B:335:LEU:CD1	1:B:338:ARG:HH12	2.27	0.48
1:C:182:LYS:CE	1:C:258:ARG:HH21	2.27	0.48
1:D:266:LEU:HD23	1:D:269:LEU:HD22	1.94	0.48
1:A:141:ARG:CZ	1:A:182:LYS:HZ1	2.27	0.48
1:B:139:HIS:HD2	3:B:633:HOH:O	1.96	0.48
1:D:100:ILE:HB	1:D:103:ALA:HB2	1.95	0.48
1:C:121:PRO:HB2	1:C:213:TYR:O	2.14	0.47
1:A:130:LYS:HD2	1:A:194:GLU:CD	2.39	0.47
1:C:141:ARG:CZ	1:C:182:LYS:HZ1	2.27	0.47
1:C:235:ILE:HD11	1:C:406:LEU:HG	1.95	0.47
1:C:321:ILE:HD12	1:C:341:TRP:CZ2	2.49	0.47
1:D:143:LEU:HD11	1:D:181:PRO:HB3	1.96	0.47
1:B:390:PRO:HB2	1:B:468:LYS:HB3	1.96	0.47
1:A:115:ASN:OD1	1:A:117:GLU:HB3	2.14	0.47
1:D:87:GLN:NE2	1:D:225:ALA:HB2	2.29	0.47
1:D:101:ILE:HD11	1:D:405:ARG:CB	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:481:LEU:HD13	1:C:481:LEU:C	2.39	0.47
1:C:143:LEU:CD1	1:C:181:PRO:HG3	2.43	0.47
1:D:27:PRO:HB3	3:D:645:HOH:O	2.15	0.47
1:A:51:GLU:O	1:A:55:GLN:HG3	2.14	0.47
1:A:192:ILE:HD12	1:A:192:ILE:N	2.29	0.47
1:A:289:GLU:HG3	1:B:29:ARG:HD2	1.96	0.47
1:A:395:TRP:CZ2	1:A:431:ILE:HD12	2.39	0.47
1:B:140:GLN:NE2	1:B:346:ILE:HD12	2.30	0.47
1:C:70:ILE:HD13	1:C:346:ILE:HD11	1.97	0.47
1:D:226:GLN:HG2	3:D:718:HOH:O	2.14	0.47
1:D:247:HIS:O	1:D:251:GLN:HG2	2.14	0.47
1:A:420:ARG:HG2	1:A:420:ARG:HH11	1.80	0.47
1:B:37:SER:O	1:B:38:ASP:HB2	2.14	0.47
1:C:100:ILE:HB	1:C:103:ALA:HB2	1.96	0.47
1:B:72:GLU:OE1	1:B:72:GLU:HA	2.15	0.47
1:B:392:SER:HB3	1:B:463:TYR:CB	2.27	0.47
1:A:78:ARG:O	1:A:82:LYS:HA	2.14	0.47
1:B:435:TYR:O	1:B:448:VAL:HA	2.14	0.47
1:B:461:ARG:CG	1:B:461:ARG:HH11	2.28	0.47
1:D:62:LEU:CD1	1:D:297:MSE:HE3	2.35	0.47
1:A:182:LYS:HD2	1:A:256:GLU:OE1	2.13	0.46
1:C:389:VAL:C	1:C:391:ALA:H	2.23	0.46
1:D:75:ASN:HD21	1:D:248:GLN:NE2	2.11	0.46
1:A:460:PHE:CD2	1:A:476:MSE:HE1	2.51	0.46
1:B:310:PRO:HA	1:B:318:LYS:HG2	1.96	0.46
1:C:197:VAL:O	1:C:201:VAL:HG23	2.15	0.46
1:A:184:ASN:H	1:A:253:ASN:ND2	2.07	0.46
1:C:66:PRO:CA	1:C:342:PHE:CD2	2.83	0.46
1:B:108:PRO:CG	1:B:197:VAL:HG13	2.45	0.46
1:B:184:ASN:H	1:B:253:ASN:ND2	2.07	0.46
1:D:50:ASN:ND2	1:D:286:ILE:HD11	2.30	0.46
1:A:469:MSE:HE3	1:A:470:PHE:HA	1.97	0.46
1:B:22:GLN:HE21	1:B:22:GLN:HB2	1.59	0.46
1:B:434:TYR:HB3	1:B:447:TRP:HD1	1.81	0.46
1:A:135:MSE:HE2	1:A:161:ILE:HG12	1.97	0.46
1:B:201:VAL:HG23	1:B:205:VAL:HG21	1.96	0.46
1:C:111:ILE:CG2	1:C:112:GLY:N	2.79	0.46
1:D:124:ILE:CD1	1:D:210:THR:HG22	2.45	0.46
1:C:67:ALA:HA	1:C:138:VAL:O	2.15	0.46
1:C:363:TYR:CD1	1:C:363:TYR:N	2.83	0.46
1:D:424:LYS:HD3	1:D:443:TYR:CE1	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:70:ILE:CD1	1:B:346:ILE:HD11	2.46	0.46
1:B:215:ASP:OD2	1:D:289:GLU:HG2	2.14	0.46
1:B:387:ALA:HB2	1:B:428:ASP:HB3	1.96	0.46
1:B:435:TYR:N	1:B:449:GLN:HG3	2.30	0.46
1:D:72:GLU:OE1	1:D:72:GLU:HA	2.15	0.46
1:A:235:ILE:HD13	1:A:404:ASN:O	2.16	0.46
1:A:335:LEU:HD21	3:A:657:HOH:O	2.16	0.46
1:A:365:VAL:HG22	1:A:366:THR:N	2.30	0.46
1:B:355:THR:H	1:B:356:ILE:HD12	1.81	0.46
1:B:377:GLY:HA2	1:B:449:GLN:HB3	1.96	0.46
1:A:101:ILE:HD12	1:A:344:GLU:C	2.40	0.46
1:A:312:TRP:CZ3	1:A:476:MSE:HB3	2.51	0.46
1:A:366:THR:HG21	1:A:479:ILE:CD1	2.46	0.46
1:B:75:ASN:HD21	1:B:248:GLN:HE22	1.63	0.46
1:B:251:GLN:HE22	1:B:274:GLY:N	1.96	0.46
1:D:322:SER:HB2	3:D:626:HOH:O	2.14	0.46
1:A:84:GLU:H	1:A:87:GLN:NE2	2.13	0.45
1:A:182:LYS:CD	1:A:256:GLU:OE1	2.64	0.45
1:B:229:GLU:HG2	3:B:770:HOH:O	2.15	0.45
1:B:384:HIS:O	1:B:386:PRO:HD3	2.16	0.45
1:C:235:ILE:HD11	1:C:406:LEU:CG	2.46	0.45
1:C:417:ILE:HG23	1:C:423:LEU:HD21	1.99	0.45
1:A:101:ILE:HD13	1:A:102:THR:N	2.32	0.45
1:A:183:THR:CG2	1:A:256:GLU:OE2	2.64	0.45
1:A:199:ARG:O	1:A:203:GLN:HG3	2.15	0.45
1:C:128:GLU:O	1:C:129:ALA:HB2	2.17	0.45
1:C:279:PRO:HB2	1:C:284:LYS:CG	2.46	0.45
1:B:434:TYR:HB3	1:B:449:GLN:HE21	1.82	0.45
1:D:71:MSE:HE1	1:D:74:LEU:HD23	1.98	0.45
1:A:91:PHE:HB2	1:A:109:TYR:HB2	1.99	0.45
1:A:313:LYS:HZ2	1:A:314:GLY:CA	2.30	0.45
1:C:342:PHE:CZ	1:C:346:ILE:HG13	2.51	0.45
1:A:171:LEU:O	1:A:180:ARG:NH2	2.49	0.45
1:D:137:ASP:OD1	1:D:137:ASP:C	2.60	0.45
1:D:149:LEU:HD21	1:D:359:PHE:HB3	1.98	0.45
1:D:201:VAL:HG13	1:D:205:VAL:HG21	1.98	0.45
1:D:468:LYS:HG2	1:D:473:SER:OG	2.16	0.45
1:A:261:PHE:O	1:A:265:GLN:HG3	2.17	0.45
1:C:48:MSE:HE2	1:C:48:MSE:HA	1.99	0.45
1:C:308:THR:HG21	1:C:322:SER:OG	2.16	0.45
1:A:194:GLU:CB	1:A:200:VAL:HG21	2.47	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:108:PRO:HG2	1:B:197:VAL:HG13	1.98	0.45
1:B:198:ASP:OD1	1:B:202:LYS:HE3	2.16	0.45
1:B:352:MSE:HG2	1:B:363:TYR:CE1	2.51	0.45
1:C:279:PRO:HB2	1:C:284:LYS:HG3	1.98	0.45
1:A:136:LEU:HD11	1:A:347:THR:HA	1.99	0.45
1:A:142:VAL:HG21	1:A:325:LEU:HD22	1.99	0.45
1:A:164:PRO:HD2	3:A:627:HOH:O	2.16	0.45
1:B:104:ASN:HB2	3:B:808:HOH:O	2.16	0.45
1:B:470:PHE:O	1:B:471:ASP:HB2	2.17	0.45
1:C:131:MSE:SE	1:C:190:ILE:HG21	2.67	0.45
1:C:115:ASN:OD1	1:C:117:GLU:HB3	2.17	0.45
1:A:308:THR:HG21	1:A:322:SER:OG	2.16	0.44
1:B:261:PHE:O	1:B:265:GLN:HG3	2.16	0.44
1:B:361:GLN:HA	1:B:461:ARG:O	2.17	0.44
1:D:416:ASP:O	1:D:417:ILE:HG13	2.17	0.44
1:A:255:VAL:HG22	1:A:263:MSE:HE3	1.99	0.44
1:C:305:LYS:HG2	1:C:307:PHE:CE1	2.53	0.44
1:D:184:ASN:N	1:D:253:ASN:HD22	2.04	0.44
1:D:421:LYS:HE2	1:D:445:ASN:HB3	1.99	0.44
1:A:39:PHE:CD1	1:B:454:GLU:HG3	2.53	0.44
1:A:111:ILE:HG13	1:A:189:GLY:HA2	1.99	0.44
1:A:361:GLN:HG2	1:A:463:TYR:CE1	2.53	0.44
1:B:427:SER:O	1:B:428:ASP:CB	2.66	0.44
1:B:457:PHE:HZ	1:B:478:ASP:OD2	2.00	0.44
1:A:194:GLU:HB2	1:A:200:VAL:HG21	1.99	0.44
1:A:361:GLN:HG2	1:A:463:TYR:CZ	2.51	0.44
1:B:126:LEU:HA	1:B:127:PRO:HD3	1.86	0.44
1:B:390:PRO:HG2	1:B:473:SER:HB3	1.99	0.44
1:C:393:ASN:O	1:C:394:PHE:HB3	2.16	0.44
1:A:292:LYS:HD3	1:B:26:VAL:HG12	2.00	0.44
1:B:159:TYR:HD2	1:B:179:ILE:HD11	1.81	0.44
1:B:362:ARG:HD2	1:B:362:ARG:HA	1.85	0.44
1:B:475:THR:HG22	1:B:476:MSE:N	2.32	0.44
1:C:151:PRO:HG2	1:C:159:TYR:OH	2.18	0.44
1:D:187:TYR:CD1	1:D:187:TYR:C	2.96	0.44
1:A:366:THR:HG21	1:A:479:ILE:HD13	2.00	0.44
1:A:481:LEU:CD2	1:A:482:VAL:HG23	2.41	0.44
1:B:280:THR:OG1	1:B:283:GLN:HG3	2.17	0.44
1:C:104:ASN:OD1	1:C:104:ASN:C	2.61	0.44
1:C:136:LEU:HD11	1:C:347:THR:HA	1.99	0.44
1:C:183:THR:CG2	1:C:256:GLU:OE2	2.66	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:277:PHE:CE1	1:C:279:PRO:HG3	2.52	0.44
1:C:347:THR:HG23	1:C:352:MSE:SE	2.67	0.44
1:D:319:ASP:HA	1:D:364:LEU:HD23	2.00	0.44
1:A:163:PRO:HA	1:A:164:PRO:HD3	1.86	0.44
1:B:215:ASP:HB2	1:C:28:SER:HA	1.99	0.44
1:B:341:TRP:NE1	1:B:348:VAL:CG1	2.80	0.44
1:B:457:PHE:CZ	1:B:478:ASP:OD2	2.71	0.44
1:D:73:TRP:CZ3	1:D:346:ILE:HD13	2.53	0.44
1:D:27:PRO:HB2	3:D:835:HOH:O	2.18	0.44
1:A:111:ILE:CG2	1:A:112:GLY:N	2.81	0.44
1:B:378:GLU:CB	1:B:452:PRO:HD3	2.24	0.44
1:B:399:VAL:HA	1:B:457:PHE:HB3	2.00	0.44
1:B:476:MSE:HG3	1:B:477:GLY:N	2.33	0.44
1:C:71:MSE:CE	1:C:74:LEU:HD23	2.47	0.44
1:C:389:VAL:HA	1:C:390:PRO:HD3	1.87	0.44
1:C:464:GLY:N	1:C:465:PRO:CD	2.81	0.44
1:A:140:GLN:CD	1:A:346:ILE:HD12	2.43	0.43
1:C:235:ILE:HD11	1:C:406:LEU:HD21	1.99	0.43
1:C:312:TRP:CG	1:C:475:THR:HG23	2.53	0.43
1:B:230:ILE:CD1	1:B:231:ASP:H	2.30	0.43
1:B:425:VAL:HG12	1:B:426:ASN:H	1.82	0.43
1:C:141:ARG:HH12	1:C:258:ARG:CZ	2.31	0.43
1:A:25:VAL:HG22	1:A:34:LYS:HG2	2.00	0.43
1:B:50:ASN:HD21	1:B:286:ILE:HD11	1.83	0.43
1:C:341:TRP:HZ3	1:C:348:VAL:HB	1.83	0.43
1:C:436:GLY:CA	1:C:450:THR:HG22	2.48	0.43
1:A:235:ILE:HD11	1:A:406:LEU:HG	1.99	0.43
1:A:342:PHE:HZ	1:A:348:VAL:CG2	2.31	0.43
1:B:375:LEU:HD13	1:B:457:PHE:CE1	2.53	0.43
1:C:182:LYS:HD2	1:C:256:GLU:OE1	2.19	0.43
1:C:203:GLN:O	1:C:207:ASN:ND2	2.51	0.43
1:C:255:VAL:HG22	1:C:263:MSE:HE3	2.00	0.43
1:C:380:THR:HA	1:C:435:TYR:O	2.18	0.43
1:D:362:ARG:HD2	1:D:362:ARG:HA	1.76	0.43
1:A:321:ILE:HG13	1:A:341:TRP:CE2	2.53	0.43
1:A:380:THR:HA	1:A:435:TYR:O	2.18	0.43
1:B:379:HIS:HB3	1:B:480:GLU:OE2	2.19	0.43
1:D:91:PHE:HB2	1:D:109:TYR:HB2	2.00	0.43
1:D:425:VAL:HA	1:D:431:ILE:HD13	1.99	0.43
1:A:251:GLN:HE22	1:A:274:GLY:N	2.00	0.43
1:A:312:TRP:CG	1:A:475:THR:HG23	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:408:ILE:HD11	1:A:451:ASN:OD1	2.18	0.43
1:B:95:LYS:CG	1:B:229:GLU:HG3	2.44	0.43
1:B:104:ASN:ND2	1:B:107:THR:H	2.15	0.43
1:B:162:VAL:HA	1:B:163:PRO:HD3	1.86	0.43
1:B:410:ASN:CB	1:B:448:VAL:HG13	2.49	0.43
1:D:469:MSE:HG3	1:D:470:PHE:N	2.33	0.43
1:A:390:PRO:HD3	1:A:474:TRP:CD2	2.54	0.43
1:B:123:ILE:HD13	1:B:176:TYR:HE2	1.83	0.43
1:B:143:LEU:CD1	1:B:181:PRO:HB3	2.49	0.43
1:B:161:ILE:N	1:B:161:ILE:CD1	2.76	0.43
1:B:382:LYS:HE3	1:B:431:ILE:HG21	2.01	0.43
1:B:408:ILE:HD12	1:B:409:ILE:N	2.34	0.43
1:C:40:PRO:HG2	1:C:45:MSE:HE3	2.01	0.43
1:C:384:HIS:O	1:C:386:PRO:HD3	2.18	0.43
1:D:97:LYS:HE2	1:D:109:TYR:CD2	2.54	0.43
1:D:194:GLU:HA	1:D:195:PRO:HD3	1.83	0.43
1:B:124:ILE:CD1	1:B:210:THR:HG22	2.49	0.43
1:B:193:LEU:HD13	1:B:463:TYR:CE1	2.51	0.43
1:C:147:SER:HA	1:C:152:ASP:OD2	2.19	0.43
1:C:194:GLU:HG3	3:C:686:HOH:O	2.18	0.43
1:A:39:PHE:CD1	1:B:454:GLU:CD	2.96	0.43
1:A:475:THR:CG2	1:A:476:MSE:N	2.81	0.43
1:C:73:TRP:HZ3	1:C:346:ILE:HD13	1.83	0.43
1:C:421:LYS:HG2	1:C:422:ASN:N	2.34	0.43
1:C:439:PRO:HG3	1:C:447:TRP:CZ3	2.54	0.42
1:D:148:LEU:O	1:D:153:LYS:HA	2.19	0.42
1:D:174:LYS:HG3	3:D:780:HOH:O	2.19	0.42
1:B:426:ASN:C	1:B:428:ASP:H	2.27	0.42
1:B:467:GLU:HG2	1:B:472:LYS:HD2	2.00	0.42
1:C:172:ASN:N	1:C:173:PRO:HD3	2.34	0.42
1:A:195:PRO:HD2	3:A:741:HOH:O	2.19	0.42
1:A:247:HIS:O	1:A:251:GLN:HG2	2.19	0.42
1:A:391:ALA:HA	1:A:464:GLY:O	2.19	0.42
1:B:205:VAL:HB	1:B:206:PRO:HD3	2.00	0.42
1:B:382:LYS:HE3	1:B:431:ILE:CG2	2.49	0.42
1:B:461:ARG:CG	1:B:461:ARG:NH1	2.83	0.42
1:C:56:ARG:HB3	1:C:265:GLN:HB3	2.01	0.42
1:C:91:PHE:CE2	1:C:227:VAL:HG21	2.54	0.42
1:D:135:MSE:HE2	1:D:188:GLY:HA3	2.00	0.42
1:A:342:PHE:CZ	1:A:348:VAL:HG22	2.55	0.42
1:B:211:GLN:HA	1:B:212:PRO:HD3	1.93	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:57:ALA:HB2	1:C:269:LEU:CD1	2.50	0.42
1:C:211:GLN:HA	1:C:212:PRO:HD3	1.83	0.42
1:C:475:THR:CG2	1:C:476:MSE:H	2.33	0.42
1:D:166:GLU:OE2	1:D:169:LYS:HD2	2.19	0.42
1:D:230:ILE:HD13	1:D:230:ILE:N	2.34	0.42
1:D:462:PHE:CE2	1:D:469:MSE:HE3	2.54	0.42
1:A:45:MSE:HE1	1:B:304:THR:N	2.34	0.42
1:A:48:MSE:HE2	1:A:48:MSE:HA	2.02	0.42
1:A:143:LEU:HD11	1:A:181:PRO:HB3	2.02	0.42
1:B:70:ILE:HD13	1:B:346:ILE:HD11	2.00	0.42
1:A:205:VAL:HG23	1:A:206:PRO:HD3	1.98	0.42
1:A:402:GLU:C	1:A:402:GLU:CD	2.88	0.42
1:D:384:HIS:O	1:D:386:PRO:HD3	2.20	0.42
1:A:69:SER:OG	1:A:346:ILE:HD13	2.19	0.42
1:A:197:VAL:O	1:A:201:VAL:HG23	2.20	0.42
1:C:110:VAL:HB	1:C:190:ILE:HB	2.02	0.42
1:C:247:HIS:HE1	1:C:275:LYS:O	2.03	0.42
1:C:268:PHE:HE2	1:D:306:ARG:HD3	1.85	0.42
1:A:88:MSE:HE2	1:A:88:MSE:N	2.34	0.42
1:A:317:TRP:CZ2	1:A:479:ILE:HD11	2.55	0.42
1:A:342:PHE:HZ	1:A:348:VAL:HG22	1.84	0.42
1:B:71:MSE:CB	1:B:249:ILE:HD11	2.44	0.42
1:B:361:GLN:HG2	1:B:462:PHE:CZ	2.55	0.42
1:C:131:MSE:HE3	1:C:192:ILE:HG12	2.02	0.42
1:C:349:SER:CB	1:C:352:MSE:HE3	2.50	0.42
1:D:162:VAL:HA	1:D:163:PRO:HD3	1.96	0.42
1:D:421:LYS:HG2	1:D:422:ASN:N	2.34	0.42
1:B:88:MSE:HG2	3:B:688:HOH:O	2.19	0.41
1:C:139:HIS:O	1:C:140:GLN:CB	2.66	0.41
1:D:196:ASP:O	1:D:200:VAL:HG22	2.20	0.41
1:A:141:ARG:NE	1:A:182:LYS:HZ1	2.18	0.41
1:A:183:THR:HG22	1:A:256:GLU:OE2	2.19	0.41
1:C:23:GLU:HA	1:C:35:PHE:O	2.20	0.41
1:D:101:ILE:HD12	1:D:344:GLU:C	2.45	0.41
1:D:101:ILE:HG12	1:D:235:ILE:HG22	2.00	0.41
1:D:214:ALA:O	1:D:215:ASP:C	2.63	0.41
1:A:141:ARG:NH1	1:A:258:ARG:NH2	2.68	0.41
1:A:258:ARG:NH1	1:A:259:ASP:OD2	2.54	0.41
1:A:327:GLN:CD	1:A:338:ARG:HD2	2.45	0.41
1:B:375:LEU:O	1:B:454:GLU:CG	2.59	0.41
1:D:462:PHE:CD2	1:D:469:MSE:HE3	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:323:VAL:HG22	1:A:324:SER:O	2.20	0.41
1:B:408:ILE:HD13	3:B:756:HOH:O	2.19	0.41
1:C:162:VAL:O	1:C:181:PRO:HD2	2.19	0.41
1:C:247:HIS:CE1	1:C:275:LYS:O	2.74	0.41
1:C:407:MSE:HE2	1:C:415:PRO:HG2	2.01	0.41
1:C:460:PHE:CZ	1:C:476:MSE:HE1	2.56	0.41
1:D:128:GLU:O	1:D:129:ALA:HB2	2.20	0.41
1:A:251:GLN:NE2	1:A:274:GLY:H	2.01	0.41
1:C:162:VAL:HA	1:C:163:PRO:HD3	1.89	0.41
1:D:286:ILE:HD12	1:D:286:ILE:N	2.36	0.41
1:D:402:GLU:C	1:D:402:GLU:CD	2.88	0.41
1:B:227:VAL:HA	1:B:228:PRO:HD3	1.87	0.41
1:C:182:LYS:CD	1:C:256:GLU:OE1	2.69	0.41
1:D:66:PRO:HG3	1:D:338:ARG:HG2	2.01	0.41
1:A:190:ILE:HG22	1:A:191:ARG:N	2.35	0.41
1:A:230:ILE:HG12	1:A:231:ASP:N	2.34	0.41
1:B:167:LYS:HE3	1:C:25:VAL:O	2.19	0.41
1:B:378:GLU:O	1:B:435:TYR:HE1	2.04	0.41
1:B:402:GLU:CD	1:B:402:GLU:C	2.88	0.41
1:C:98:GLN:OE1	1:C:409:ILE:HD11	2.21	0.41
1:A:123:ILE:O	1:A:210:THR:HA	2.21	0.41
1:B:445:ASN:OD1	1:B:445:ASN:N	2.53	0.41
1:B:468:LYS:NZ	1:B:468:LYS:CB	2.83	0.41
1:C:240:LEU:HD11	1:C:284:LYS:HD2	2.03	0.41
1:D:312:TRP:CZ3	1:D:476:MSE:HB3	2.56	0.41
1:A:56:ARG:HD3	1:A:265:GLN:CB	2.50	0.41
1:A:384:HIS:O	1:A:386:PRO:HD3	2.21	0.41
1:A:390:PRO:HB3	1:A:466:THR:OG1	2.21	0.41
1:B:335:LEU:HD12	1:B:338:ARG:HH12	1.86	0.41
1:B:382:LYS:CB	1:B:481:LEU:HD11	2.49	0.41
1:B:394:PHE:CD1	1:B:394:PHE:C	2.98	0.41
1:B:407:MSE:HB3	1:B:415:PRO:HB3	2.02	0.41
1:B:422:ASN:HB2	1:B:445:ASN:OD1	2.21	0.41
1:B:451:ASN:N	1:B:451:ASN:HD22	2.18	0.41
1:C:312:TRP:CZ3	1:C:476:MSE:HB3	2.56	0.41
1:D:242:TYR:O	1:D:246:ILE:HG12	2.21	0.41
1:D:434:TYR:O	1:D:447:TRP:HA	2.21	0.41
1:A:72:GLU:HB3	1:A:234:HIS:O	2.21	0.41
1:A:162:VAL:HA	1:A:163:PRO:HD3	1.93	0.41
1:A:362:ARG:NH1	1:A:469:MSE:HE2	2.35	0.41
1:A:397:THR:O	1:A:416:ASP:HB2	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:471:ASP:O	1:A:472:LYS:HB2	2.21	0.41
1:B:116:LEU:HD11	1:B:161:ILE:HG22	2.02	0.41
1:B:166:GLU:HG2	1:B:169:LYS:HD3	2.03	0.41
1:B:259:ASP:O	1:B:263:MSE:HG2	2.20	0.41
1:C:88:MSE:HG2	3:C:614:HOH:O	2.20	0.41
1:C:140:GLN:O	1:C:140:GLN:CG	2.56	0.41
1:C:422:ASN:HA	3:C:771:HOH:O	2.20	0.41
1:A:111:ILE:HG22	1:A:112:GLY:N	2.36	0.40
1:A:174:LYS:NZ	1:A:174:LYS:CB	2.84	0.40
1:A:205:VAL:HG23	1:A:206:PRO:CD	2.52	0.40
1:A:292:LYS:HD2	1:B:28:SER:HB3	2.02	0.40
1:A:434:TYR:CD1	1:A:440:VAL:HG21	2.56	0.40
1:B:346:ILE:C	1:B:347:THR:HG23	2.46	0.40
1:B:398:THR:O	1:B:457:PHE:HB2	2.21	0.40
1:C:282:GLU:HG3	1:C:283:GLN:H	1.85	0.40
1:A:28:SER:OG	1:A:31:GLY:O	2.34	0.40
1:A:151:PRO:HD2	1:A:159:TYR:OH	2.20	0.40
1:B:208:ILE:O	1:B:224:VAL:HG23	2.20	0.40
1:B:399:VAL:HB	1:B:447:TRP:CZ2	2.56	0.40
1:D:88:MSE:HE1	1:D:114:TRP:CZ3	2.57	0.40
1:D:89:GLY:HA2	1:D:225:ALA:O	2.21	0.40
1:D:135:MSE:HE2	1:D:188:GLY:HA2	2.03	0.40
1:D:185:VAL:H	1:D:253:ASN:ND2	2.16	0.40
1:A:39:PHE:CZ	1:B:367:TYR:HB3	2.57	0.40
1:A:66:PRO:HG2	1:A:338:ARG:CG	2.40	0.40
1:A:334:GLU:HB3	1:A:337:GLU:HB2	2.04	0.40
1:B:23:GLU:O	1:B:24:THR:HG23	2.21	0.40
1:B:74:LEU:HB2	1:B:113:THR:HG21	2.03	0.40
1:B:140:GLN:HE22	1:B:346:ILE:HD12	1.86	0.40
1:B:247:HIS:CG	1:B:277:PHE:HB2	2.57	0.40
1:B:433:VAL:HG23	1:B:446:ASN:HA	2.02	0.40
1:A:141:ARG:CZ	1:A:327:GLN:OE1	2.70	0.40
1:A:194:GLU:HA	1:A:195:PRO:HD3	1.84	0.40
1:B:435:TYR:CZ	1:B:437:PRO:HD2	2.55	0.40
1:B:436:GLY:O	1:B:448:VAL:HG23	2.20	0.40
1:C:62:LEU:CD1	1:C:297:MSE:HE2	2.45	0.40
1:C:66:PRO:O	1:C:342:PHE:CE2	2.74	0.40
1:C:126:LEU:HA	1:C:127:PRO:HD3	1.85	0.40
1:C:481:LEU:HD22	1:C:482:VAL:N	2.35	0.40
1:A:311:TYR:OH	1:A:469:MSE:HE3	2.21	0.40
1:A:389:VAL:HA	1:A:390:PRO:HD3	1.88	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:363:TYR:N	1:B:363:TYR:CD1	2.89	0.40
1:B:378:GLU:OE1	1:B:379:HIS:CE1	2.74	0.40
1:B:470:PHE:CG	1:B:472:LYS:HE3	2.57	0.40
1:B:477:GLY:HA3	3:B:635:HOH:O	2.20	0.40
1:C:140:GLN:OE1	1:C:342:PHE:CD1	2.75	0.40
1:C:141:ARG:CD	1:C:182:LYS:HZ1	2.31	0.40
1:C:142:VAL:CG2	1:C:348:VAL:HG13	2.52	0.40
1:D:37:SER:O	1:D:38:ASP:HB2	2.22	0.40
1:D:116:LEU:HD11	1:D:181:PRO:HG3	2.04	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	458/483 (95%)	436 (95%)	20 (4%)	2 (0%)	30	28
1	B	460/483 (95%)	428 (93%)	26 (6%)	6 (1%)	9	6
1	C	458/483 (95%)	435 (95%)	18 (4%)	5 (1%)	11	8
1	D	458/483 (95%)	432 (94%)	23 (5%)	3 (1%)	18	15
All	All	1834/1932 (95%)	1731 (94%)	87 (5%)	16 (1%)	14	10

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	419	SER
1	B	452	PRO
1	C	334	GLU
1	A	334	GLU
1	B	437	PRO
1	C	147	SER

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Mol	Chain	Res	Type
1	C	197	VAL
1	B	454	GLU
1	B	463	TYR
1	D	334	GLU
1	B	215	ASP
1	D	214	ALA
1	A	147	SER
1	C	390	PRO
1	D	147	SER
1	C	330	GLU

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	405/408 (99%)	387 (96%)	18 (4%)	25	26
1	B	407/408 (100%)	391 (96%)	16 (4%)	28	31
1	C	405/408 (99%)	396 (98%)	9 (2%)	45	53
1	D	405/408 (99%)	395 (98%)	10 (2%)	42	48
All	All	1622/1632 (99%)	1569 (97%)	53 (3%)	33	37

All (53) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	29	ARG
1	A	33	LEU
1	A	39	PHE
1	A	72	GLU
1	A	94	LEU
1	A	95	LYS
1	A	101	ILE
1	A	104	ASN
1	A	117	GLU
1	A	174	LYS
1	A	246	ILE

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Mol	Chain	Res	Type
1	A	269	LEU
1	A	308	THR
1	A	321	ILE
1	A	348	VAL
1	A	363	TYR
1	A	408	ILE
1	A	469	MSE
1	B	22	GLN
1	B	29	ARG
1	B	104	ASN
1	B	145	ASP
1	B	161	ILE
1	B	187	TYR
1	B	201	VAL
1	B	229	GLU
1	B	269	LEU
1	B	305	LYS
1	B	352	MSE
1	B	408	ILE
1	B	452	PRO
1	B	454	GLU
1	B	468	LYS
1	B	469	MSE
1	C	95	LYS
1	C	134	MSE
1	C	169	LYS
1	C	306	ARG
1	C	329	SER
1	C	347	THR
1	C	424	LYS
1	C	469	MSE
1	C	481	LEU
1	D	33	LEU
1	D	70	ILE
1	D	101	ILE
1	D	145	ASP
1	D	176	TYR
1	D	196	ASP
1	D	230	ILE
1	D	282	GLU
1	D	405	ARG
1	D	469	MSE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (64) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	50	ASN
1	A	59	GLN
1	A	87	GLN
1	A	104	ASN
1	A	125	ASN
1	A	172	ASN
1	A	207	ASN
1	A	234	HIS
1	A	248	GLN
1	A	251	GLN
1	A	253	ASN
1	A	301	ASN
1	A	384	HIS
1	A	403	ASN
1	A	426	ASN
1	A	445	ASN
1	A	449	GLN
1	B	22	GLN
1	B	59	GLN
1	B	98	GLN
1	B	104	ASN
1	B	139	HIS
1	B	172	ASN
1	B	203	GLN
1	B	234	HIS
1	B	247	HIS
1	B	248	GLN
1	B	251	GLN
1	B	253	ASN
1	B	301	ASN
1	B	379	HIS
1	B	449	GLN
1	B	451	ASN
1	C	79	ASN
1	C	87	GLN
1	C	92	ASN
1	C	96	GLN
1	C	125	ASN
1	C	140	GLN
1	C	203	GLN
1	C	211	GLN

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Mol	Chain	Res	Type
1	C	234	HIS
1	C	247	HIS
1	C	248	GLN
1	C	251	GLN
1	C	253	ASN
1	C	301	ASN
1	C	361	GLN
1	C	368	GLN
1	C	379	HIS
1	C	403	ASN
1	C	404	ASN
1	C	422	ASN
1	D	75	ASN
1	D	87	GLN
1	D	98	GLN
1	D	125	ASN
1	D	140	GLN
1	D	234	HIS
1	D	247	HIS
1	D	251	GLN
1	D	253	ASN
1	D	373	ASN
1	D	404	ASN

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 7 ligands modelled in this entry, 7 are monoatomic - leaving 0 for Mogul analysis.

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.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	446/483 (92%)	0.51	35 (7%) 19 20	10, 24, 45, 55	0
1	B	448/483 (92%)	0.97	73 (16%) 4 4	8, 24, 51, 68	0
1	C	446/483 (92%)	0.58	39 (8%) 16 16	8, 24, 45, 64	0
1	D	446/483 (92%)	0.41	25 (5%) 30 32	10, 21, 40, 59	0
All	All	1786/1932 (92%)	0.62	172 (9%) 13 14	8, 23, 45, 68	0

All (172) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	447	TRP	14.4
1	B	463	TYR	7.7
1	B	437	PRO	7.2
1	B	474	TRP	7.1
1	B	215	ASP	7.0
1	B	451	ASN	6.9
1	B	454	GLU	6.8
1	B	457	PHE	6.6
1	B	456	TRP	6.3
1	B	435	TYR	6.1
1	B	452	PRO	6.0
1	B	420	ARG	5.8
1	B	453	GLY	5.7
1	B	481	LEU	5.6
1	D	215	ASP	5.4
1	C	342	PHE	5.0
1	B	198	ASP	5.0
1	B	374	TRP	4.9
1	B	428	ASP	4.7
1	B	443	TYR	4.7
1	B	470	PHE	4.6

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Mol	Chain	Res	Type	RSRZ
1	A	482	VAL	4.5
1	D	482	VAL	4.3
1	D	447	TRP	4.3
1	A	230	ILE	4.3
1	B	415	PRO	4.2
1	B	432	ASP	4.2
1	B	421	LYS	4.2
1	B	482	VAL	4.2
1	C	482	VAL	4.2
1	B	450	THR	4.2
1	B	436	GLY	4.1
1	B	478	ASP	4.0
1	C	268	PHE	4.0
1	B	442	GLY	4.0
1	D	440	VAL	3.9
1	B	408	ILE	3.9
1	C	428	ASP	3.7
1	B	230	ILE	3.7
1	B	411	ASP	3.6
1	D	217	LYS	3.6
1	B	448	VAL	3.5
1	B	479	ILE	3.5
1	C	341	TRP	3.4
1	B	465	PRO	3.4
1	B	449	GLN	3.4
1	B	483	LYS	3.2
1	A	39	PHE	3.2
1	B	197	VAL	3.2
1	B	431	ILE	3.1
1	B	439	PRO	3.1
1	D	214	ALA	3.1
1	A	341	TRP	3.1
1	B	458	THR	3.1
1	B	235	ILE	3.1
1	C	479	ILE	3.1
1	B	216	GLY	3.0
1	D	388	ASN	3.0
1	A	25	VAL	3.0
1	C	423	LEU	3.0
1	A	441	LYS	2.9
1	C	443	TYR	2.9
1	B	388	ASN	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	479	ILE	2.9
1	B	419	SER	2.9
1	D	130	LYS	2.9
1	D	306	ARG	2.8
1	B	424	LYS	2.8
1	C	422	ASN	2.8
1	C	439	PRO	2.8
1	B	169	LYS	2.8
1	B	438	LYS	2.8
1	C	450	THR	2.8
1	B	172	ASN	2.8
1	C	426	ASN	2.8
1	B	461	ARG	2.8
1	D	196	ASP	2.8
1	D	216	GLY	2.8
1	B	168	TYR	2.7
1	D	213	TYR	2.7
1	B	29	ARG	2.7
1	B	422	ASN	2.6
1	C	470	PHE	2.6
1	A	197	VAL	2.6
1	A	23	GLU	2.6
1	B	167	LYS	2.6
1	A	235	ILE	2.6
1	A	440	VAL	2.6
1	C	436	GLY	2.6
1	C	445	ASN	2.6
1	B	124	ILE	2.5
1	C	235	ILE	2.5
1	A	190	ILE	2.5
1	B	440	VAL	2.5
1	D	124	ILE	2.5
1	A	481	LEU	2.5
1	D	200	VAL	2.5
1	D	289	GLU	2.5
1	D	27	PRO	2.5
1	A	424	LYS	2.5
1	C	440	VAL	2.4
1	C	330	GLU	2.4
1	A	24	THR	2.4
1	B	460	PHE	2.4
1	C	462	PHE	2.4

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Mol	Chain	Res	Type	RSRZ
1	C	111	ILE	2.4
1	C	425	VAL	2.4
1	A	443	TYR	2.4
1	C	388	ASN	2.4
1	B	425	VAL	2.4
1	B	199	ARG	2.4
1	D	441	LYS	2.4
1	A	196	ASP	2.4
1	A	215	ASP	2.4
1	B	289	GLU	2.3
1	B	165	GLY	2.3
1	B	471	ASP	2.3
1	D	230	ILE	2.3
1	B	475	THR	2.3
1	B	22	GLN	2.3
1	B	171	LEU	2.3
1	C	215	ASP	2.3
1	D	198	ASP	2.3
1	A	425	VAL	2.3
1	D	197	VAL	2.3
1	C	412	ALA	2.3
1	B	213	TYR	2.3
1	C	429	GLY	2.3
1	D	238	ASP	2.3
1	A	220	ARG	2.3
1	B	412	ALA	2.3
1	C	269	LEU	2.3
1	D	417	ILE	2.2
1	C	197	VAL	2.2
1	A	174	LYS	2.2
1	A	229	GLU	2.2
1	B	203	GLN	2.2
1	B	395	TRP	2.2
1	A	394	PHE	2.2
1	C	321	ILE	2.2
1	A	175	GLY	2.2
1	A	453	GLY	2.2
1	C	447	TRP	2.2
1	B	423	LEU	2.1
1	A	282	GLU	2.1
1	B	196	ASP	2.1
1	D	173	PRO	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	464	GLY	2.1
1	C	442	GLY	2.1
1	C	387	ALA	2.1
1	A	167	LYS	2.1
1	A	182	LYS	2.1
1	C	434	TYR	2.1
1	D	443	TYR	2.1
1	A	173	PRO	2.1
1	A	94	LEU	2.1
1	C	43	GLU	2.1
1	C	24	THR	2.1
1	C	199	ARG	2.1
1	A	442	GLY	2.1
1	C	413	GLY	2.1
1	A	409	ILE	2.1
1	A	359	PHE	2.1
1	B	25	VAL	2.1
1	B	480	GLU	2.0
1	A	198	ASP	2.0
1	C	452	PRO	2.0
1	D	438	LYS	2.0
1	A	348	VAL	2.0
1	B	166	GLU	2.0
1	C	171	LEU	2.0
1	C	218	LEU	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides 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. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q < 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	MG	D	502	1/1	0.95	0.25	20,20,20,20	0
2	MG	B	502	1/1	0.97	0.26	21,21,21,21	0
2	MG	A	502	1/1	0.98	0.25	16,16,16,16	0
2	MG	B	501	1/1	0.98	0.12	18,18,18,18	0
2	MG	C	501	1/1	0.99	0.02	13,13,13,13	0
2	MG	D	501	1/1	0.99	0.05	14,14,14,14	0
2	MG	A	501	1/1	0.99	0.05	16,16,16,16	0

6.5 Other polymers [i](#)

There are no such residues in this entry.