



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 07:35 PM GMT

PDB ID : 1G8X
Title : STRUCTURE OF A GENETICALLY ENGINEERED MOLECULAR MOTOR
Authors : Kliche, W.; Fujita-Becker, S.; Kollmar, M.; Manstein, D.J.; Kull, F.J.
Deposited on : 2000-11-21
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
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

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

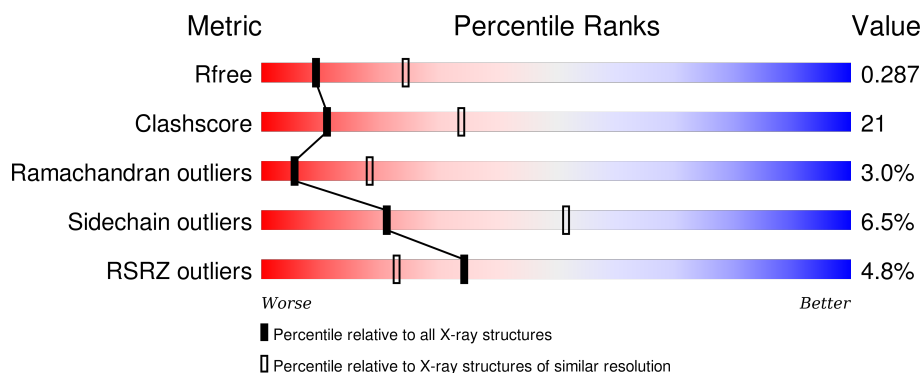
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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}	91344	2393 (2.80-2.80)
Clashscore	102246	2827 (2.80-2.80)
Ramachandran outliers	100387	2782 (2.80-2.80)
Sidechain outliers	100360	2784 (2.80-2.80)
RSRZ outliers	91569	2404 (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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	1010	 6% 61% 33% 6%
1	B	1010	 4% 62% 34% •

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 16292 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called MYOSIN II HEAVY CHAIN FUSED TO ALPHA-ACTININ 3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1009	Total	C	N	O	S	0	0	0
			8111	5131	1406	1556	18			
1	B	1009	Total	C	N	O	S	0	0	0
			8111	5131	1406	1556	18			

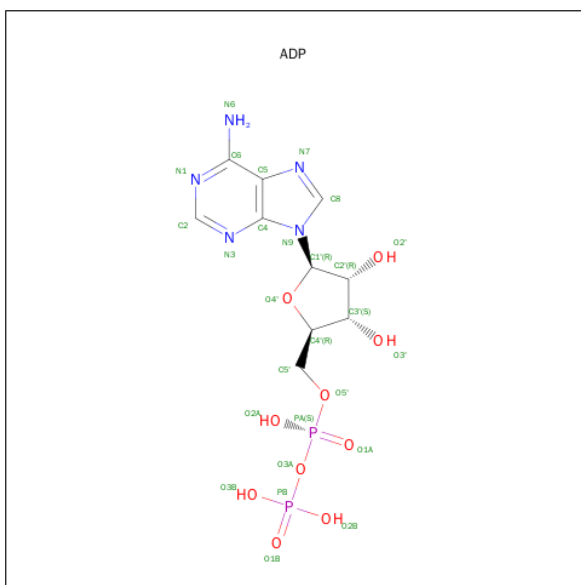
There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	238	GLU	ARG	engineered	UNP P08799
A	312	CYS	TYR	engineered	UNP P08799
A	321	GLU	SER	engineered	UNP P08799
A	443	SER	GLN	engineered	UNP P08799
A	489	VAL	LEU	engineered	UNP P08799
B	238	GLU	ARG	engineered	UNP P08799
B	312	CYS	TYR	engineered	UNP P08799
B	321	GLU	SER	engineered	UNP P08799
B	443	SER	GLN	engineered	UNP P08799
B	489	VAL	LEU	engineered	UNP P08799

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 3 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: C₁₀H₁₅N₅O₁₀P₂).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total 27	C 10	N 5	O 10	P 2	0	0
3	B	1	Total 27	C 10	N 5	O 10	P 2	0	0

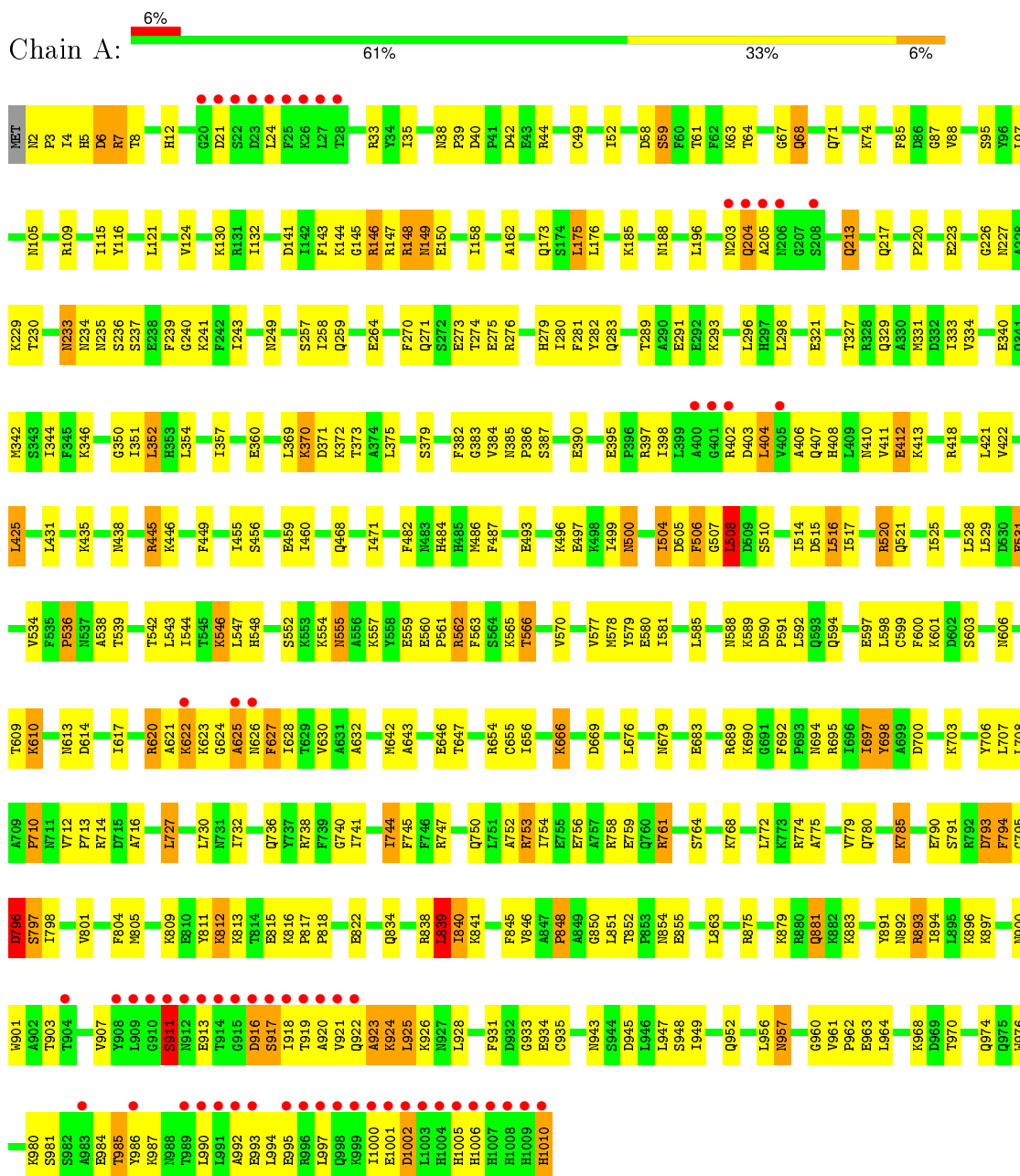
- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	7	Total O 7 7	0	0
4	B	7	Total O 7 7	0	0

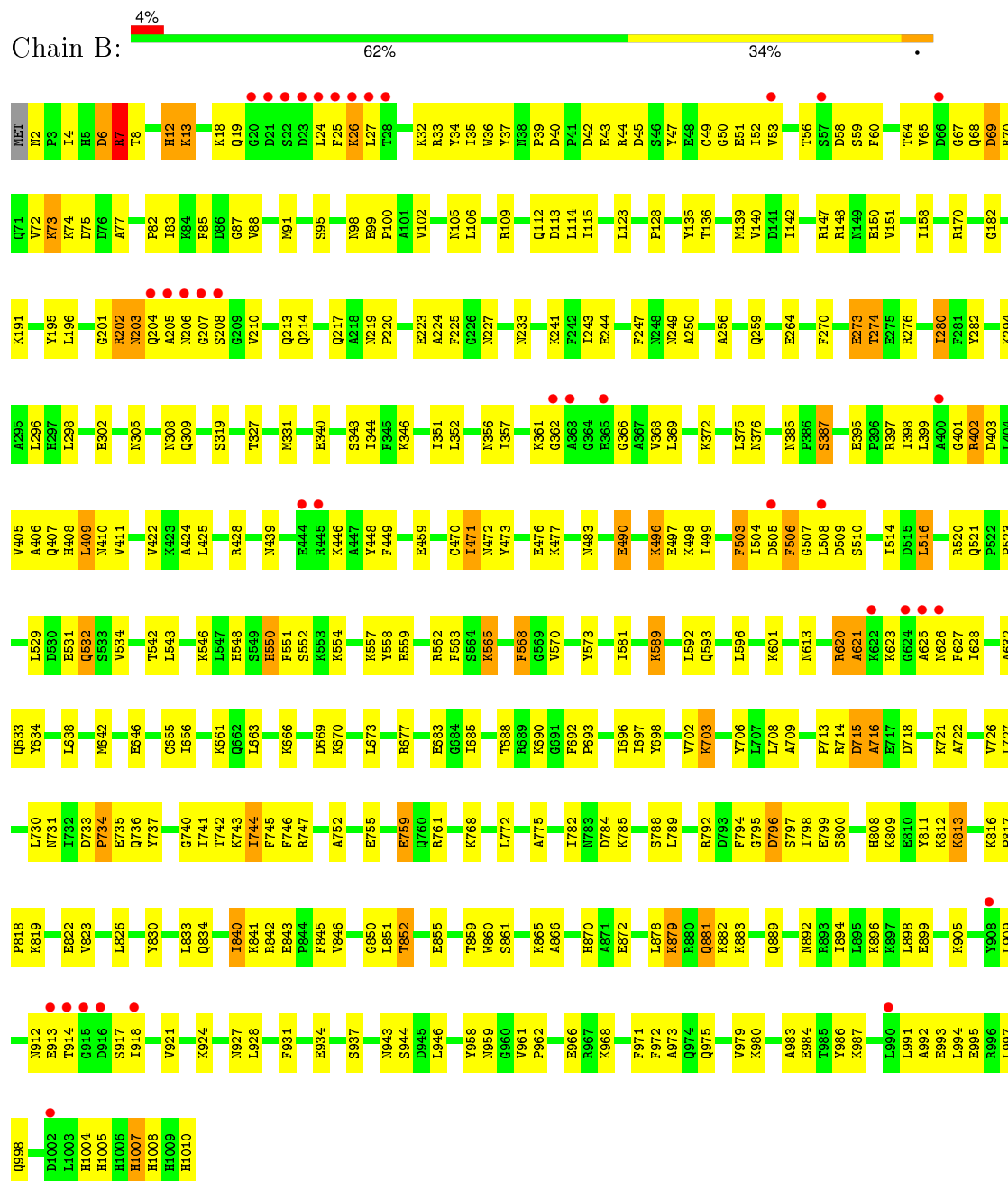
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: MYOSIN II HEAVY CHAIN FUSED TO ALPHA-ACTININ 3



● Molecule 1: MYOSIN II HEAVY CHAIN FUSED TO ALPHA-ACTININ 3



4 Data and refinement statistics

Property	Value	Source
Space group	P 2 ₁ 2 ₁ 2	Depositor
Cell constants a, b, c, α , β , γ	135.42Å 155.42Å 143.19Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	41.15 – 2.80 41.15 – 2.80	Depositor EDS
% Data completeness (in resolution range)	97.7 (41.15-2.80) 97.5 (41.15-2.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.82 (at 2.81Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.232 , 0.290 0.231 , 0.287	Depositor DCC
R_{free} test set	5989 reflections (8.17%)	DCC
Wilson B-factor (Å ²)	49.5	Xtriage
Anisotropy	0.593	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 55.6	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 73342 reflections	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	16292	wwPDB-VP
Average B, all atoms (Å ²)	52.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.24% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	0.44	2/8267 (0.0%)	0.63	6/11157 (0.1%)
1	B	0.41	1/8267 (0.0%)	0.61	3/11157 (0.0%)
All	All	0.43	3/16534 (0.0%)	0.62	9/22314 (0.0%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	446	LYS	C-N	-8.43	1.14	1.34
1	A	759	GLU	CD-OE2	7.89	1.34	1.25
1	B	759	GLU	CD-OE2	6.98	1.33	1.25

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	796	ASP	CB-CA-C	-7.93	94.54	110.40
1	A	911	SER	N-CA-C	-7.33	91.20	111.00
1	B	796	ASP	N-CA-C	6.19	127.72	111.00
1	B	796	ASP	CB-CA-C	-5.97	98.46	110.40
1	A	508	LEU	CA-CB-CG	5.90	128.86	115.30
1	B	496	LYS	N-CA-C	-5.61	95.87	111.00
1	A	796	ASP	N-CA-C	5.30	125.31	111.00
1	A	445	ARG	O-C-N	-5.17	114.43	122.70
1	A	506	PHE	N-CA-C	5.03	124.57	111.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	8111	0	8037	348	0
1	B	8111	0	8038	326	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	27	0	12	0	0
3	B	27	0	12	2	0
4	A	7	0	0	1	0
4	B	7	0	0	1	0
All	All	16292	0	16099	673	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 21.

All (673) 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:834:GLN:HE22	1:B:845:PHE:HB3	1.17	1.05
1:A:697:ILE:HD13	1:A:697:ILE:H	1.19	1.04
1:B:532:GLN:OE1	1:B:542:THR:HG22	1.66	0.95
1:A:623:LYS:HE3	1:A:626:ASN:H	1.31	0.95
1:B:543:LEU:HD23	1:B:581:ILE:HD11	1.48	0.94
1:A:848:PRO:HB2	1:A:851:LEU:HD23	1.50	0.92
1:A:2:ASN:HD21	1:A:5:HIS:HD2	1.14	0.90
1:B:918:ILE:HG13	1:B:997:LEU:HD22	1.55	0.89
1:B:509:ASP:HB2	1:B:557:LYS:HZ3	1.38	0.88
1:A:233:ASN:ND2	1:A:235:ASN:H	1.70	0.88
1:B:797:SER:OG	1:B:799:GLU:OE1	1.93	0.86
1:B:796:ASP:O	1:B:881:GLN:OE1	1.93	0.86
1:A:273:GLU:O	1:A:274:THR:HB	1.73	0.86
1:A:817:PRO:HB2	1:A:818:PRO:HD3	1.58	0.85
1:A:931:PHE:O	1:A:934:GLU:HG2	1.76	0.85
1:B:35:ILE:HD11	1:B:77:ALA:HB1	1.59	0.84
1:A:2:ASN:HD21	1:A:5:HIS:CD2	1.95	0.84
1:A:925:LEU:HD21	1:A:990:LEU:HB3	1.60	0.84
1:B:703:LYS:O	1:B:703:LYS:HE2	1.79	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:986:TYR:O	1:A:990:LEU:HB2	1.79	0.83
1:A:520:ARG:HG3	1:A:521:GLN:HG2	1.61	0.83
1:A:543:LEU:HD23	1:A:581:ILE:HD11	1.60	0.83
1:A:68:GLN:H	1:A:68:GLN:HE21	1.26	0.83
1:B:509:ASP:HB2	1:B:557:LYS:NZ	1.93	0.82
1:B:601:LYS:HG2	1:B:613:ASN:ND2	1.94	0.82
1:B:809:LYS:O	1:B:813:LYS:HD3	1.80	0.81
1:B:225:PHE:HA	1:B:280:ILE:HD11	1.62	0.81
1:A:622:LYS:HE2	1:A:624:GLY:H	1.43	0.80
1:A:697:ILE:H	1:A:697:ILE:CD1	1.94	0.79
1:A:907:VAL:O	1:A:911:SER:HB3	1.82	0.79
1:B:302:GLU:HA	1:B:308:ASN:HB3	1.63	0.78
1:A:455:ILE:HD12	1:A:456:SER:H	1.49	0.78
1:A:539:THR:O	1:A:542:THR:HG22	1.83	0.78
1:B:834:GLN:NE2	1:B:845:PHE:HB3	1.96	0.77
1:A:555:ASN:ND2	1:A:557:LYS:H	1.81	0.76
1:A:697:ILE:HD13	1:A:697:ILE:N	2.00	0.76
1:B:139:MET:HE2	1:B:142:ILE:HD12	1.67	0.76
1:A:654:ARG:HD2	1:A:679:ASN:HB2	1.66	0.76
1:A:68:GLN:H	1:A:68:GLN:NE2	1.83	0.76
1:A:666:LYS:HE2	1:A:666:LYS:HA	1.66	0.75
1:B:68:GLN:NE2	1:B:70:ARG:HH21	1.85	0.75
1:A:516:LEU:HD22	1:A:516:LEU:O	1.87	0.74
1:A:839:LEU:O	1:A:841:LYS:N	2.21	0.73
1:A:233:ASN:HD22	1:A:234:ASN:N	1.87	0.73
1:A:351:ILE:HG23	1:A:422:VAL:HG13	1.70	0.73
1:B:655:CYS:C	1:B:656:ILE:HD12	2.09	0.72
1:A:628:ILE:HG13	1:A:632:ALA:HB3	1.70	0.72
1:B:499:ILE:HD11	1:B:740:GLY:HA2	1.70	0.72
1:A:493:GLU:HG2	1:A:695:ARG:HH12	1.52	0.72
1:A:555:ASN:HD22	1:A:557:LYS:H	1.37	0.72
1:A:147:ARG:HD3	1:A:150:GLU:OE1	1.90	0.72
1:A:839:LEU:C	1:A:841:LYS:H	1.94	0.71
1:A:753:ARG:HH11	1:A:753:ARG:HG2	1.53	0.71
1:A:274:THR:CG2	1:A:274:THR:O	2.38	0.71
1:B:508:LEU:O	1:B:508:LEU:HD13	1.91	0.71
1:A:371:ASP:C	1:A:372:LYS:HD2	2.11	0.71
1:A:520:ARG:HH11	1:A:520:ARG:HA	1.54	0.70
1:A:398:ILE:HD13	1:A:407:GLN:HG3	1.73	0.70
1:A:589:LYS:HD3	1:A:589:LYS:O	1.91	0.70
1:B:13:LYS:HE3	1:B:13:LYS:HA	1.74	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:809:LYS:O	1:A:813:LYS:HD3	1.92	0.69
1:A:141:ASP:HA	1:A:144:LYS:HE2	1.72	0.69
1:A:925:LEU:HD11	1:A:990:LEU:HD13	1.74	0.69
1:B:224:ALA:O	1:B:280:ILE:HG13	1.92	0.69
1:B:532:GLN:HE21	1:B:532:GLN:HA	1.56	0.69
1:B:782:ILE:HG21	1:B:859:THR:HG22	1.75	0.69
1:B:1007:HIS:HA	1:B:1010:HIS:CD2	2.28	0.69
1:B:918:ILE:HD11	1:B:998:GLN:HA	1.74	0.68
1:A:58:ASP:HA	1:A:74:LYS:HD2	1.74	0.68
1:A:706:TYR:HB2	1:A:712:VAL:HG23	1.76	0.68
1:A:342:MET:HG3	1:A:346:LYS:HZ3	1.58	0.68
1:B:817:PRO:HB2	1:B:818:PRO:HD3	1.75	0.68
1:B:241:LYS:HD2	1:B:243:ILE:HD11	1.76	0.68
1:A:848:PRO:HB2	1:A:851:LEU:CD2	2.24	0.68
1:A:811:TYR:O	1:A:811:TYR:CD2	2.46	0.68
1:B:273:GLU:O	1:B:274:THR:HB	1.93	0.67
1:A:340:GLU:O	1:A:344:ILE:HG13	1.93	0.67
1:B:795:GLY:HA3	1:B:800:SER:OG	1.95	0.67
1:B:621:ALA:O	1:B:628:ILE:HD13	1.93	0.67
1:A:708:LEU:HD13	1:A:730:LEU:HD11	1.77	0.67
1:A:922:GLN:HB2	1:A:994:LEU:HD11	1.77	0.66
1:B:25:PHE:O	1:B:26:LYS:HG3	1.96	0.66
1:B:385:ASN:HB3	1:B:387:SER:OG	1.95	0.66
1:B:497:GLU:OE1	1:B:742:THR:HG22	1.95	0.66
1:A:918:ILE:HG23	1:A:922:GLN:HE21	1.59	0.66
1:A:921:VAL:HG12	1:A:994:LEU:HD21	1.77	0.66
1:B:797:SER:OG	1:B:799:GLU:CD	2.34	0.66
1:A:628:ILE:HD11	1:A:632:ALA:HB1	1.78	0.66
1:A:620:ARG:HB3	1:A:628:ILE:HG22	1.77	0.66
1:A:342:MET:HG3	1:A:346:LYS:NZ	2.10	0.66
1:A:121:LEU:HD11	1:A:486:MET:HA	1.78	0.66
1:B:768:LYS:O	1:B:772:LEU:HD13	1.95	0.66
1:B:399:LEU:HD12	1:B:403:ASP:O	1.97	0.65
1:B:361:LYS:HA	1:B:361:LYS:HE3	1.78	0.65
1:B:623:LYS:NZ	1:B:625:ALA:HB3	2.12	0.65
1:B:516:LEU:HD12	1:B:557:LYS:HB2	1.78	0.65
1:A:925:LEU:HD21	1:A:990:LEU:CB	2.25	0.65
1:B:601:LYS:HG2	1:B:613:ASN:HD21	1.61	0.65
1:B:822:GLU:O	1:B:826:LEU:HG	1.97	0.65
1:B:914:THR:O	1:B:914:THR:HG22	1.97	0.65
1:A:797:SER:O	1:A:881:GLN:HG2	1.96	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:85:PHE:O	1:B:88:VAL:HG13	1.97	0.65
1:A:774:ARG:HH21	1:A:822:GLU:CD	2.00	0.65
1:A:276:ARG:HG2	1:A:282:TYR:CZ	2.31	0.65
1:B:851:LEU:N	1:B:851:LEU:HD12	2.12	0.65
1:B:565:LYS:NZ	1:B:565:LYS:HB3	2.12	0.64
1:A:775:ALA:O	1:A:779:VAL:HG23	1.97	0.64
1:A:296:LEU:HB2	1:A:298:LEU:HG	1.79	0.64
1:B:496:LYS:C	1:B:498:LYS:H	2.00	0.64
1:A:948:SER:O	1:A:952:GLN:HG3	1.97	0.64
1:B:510:SER:O	1:B:514:ILE:HG13	1.96	0.64
1:B:401:GLY:C	1:B:402:ARG:HD3	2.18	0.64
1:B:2:ASN:ND2	1:B:4:ILE:HB	2.12	0.64
1:A:552:SER:O	1:A:554:LYS:HG3	1.97	0.64
1:B:139:MET:HE2	1:B:139:MET:HA	1.80	0.64
1:B:709:ALA:HB2	1:B:726:VAL:HA	1.80	0.64
1:A:852:THR:CG2	1:A:855:GLU:H	2.10	0.64
1:B:958:TYR:O	1:B:961:VAL:HG23	1.98	0.64
1:A:706:TYR:CE1	1:A:707:LEU:HG	2.33	0.63
1:B:692:PHE:CE1	1:B:747:ARG:HG2	2.32	0.63
1:B:59:SER:HB2	1:B:72:VAL:O	1.98	0.63
1:B:504:ILE:HD11	1:B:690:LYS:NZ	2.13	0.63
1:A:543:LEU:CD2	1:A:581:ILE:HD11	2.29	0.63
1:B:628:ILE:HG23	1:B:632:ALA:HB3	1.79	0.63
1:A:622:LYS:HA	1:A:622:LYS:HE3	1.79	0.63
1:B:718:ASP:OD1	1:B:721:LYS:HG3	1.99	0.63
1:B:123:LEU:HD22	1:B:158:ILE:HG13	1.81	0.63
1:B:18:LYS:HD2	1:B:18:LYS:N	2.14	0.63
1:B:562:ARG:HH22	1:B:563:PHE:HE1	1.46	0.63
1:B:924:LYS:HA	1:B:927:ASN:ND2	2.14	0.62
1:A:893:ARG:NH1	1:A:897:LYS:HE3	2.14	0.62
1:B:623:LYS:HZ3	1:B:625:ALA:HB3	1.63	0.62
1:A:497:GLU:HB2	1:A:499:ILE:HD13	1.81	0.62
1:A:241:LYS:HD2	1:A:243:ILE:HD11	1.80	0.62
1:B:991:LEU:O	1:B:995:GLU:HG3	2.00	0.62
1:A:793:ASP:CG	1:A:794:PHE:N	2.52	0.62
1:B:351:ILE:HG23	1:B:422:VAL:HG13	1.82	0.62
1:A:597:GLU:O	1:A:601:LYS:HB2	1.99	0.62
1:A:601:LYS:HG2	1:A:613:ASN:HD21	1.65	0.62
1:B:280:ILE:HD12	1:B:280:ILE:H	1.64	0.62
1:A:493:GLU:HG2	1:A:695:ARG:NH1	2.15	0.61
1:B:59:SER:HA	1:B:74:LYS:H	1.64	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:899:GLU:HG3	1:B:975:GLN:HE22	1.65	0.61
1:B:715:ASP:O	1:B:716:ALA:HB2	2.00	0.61
1:B:91:MET:CE	1:B:106:LEU:HD13	2.30	0.61
1:B:534:VAL:O	1:B:534:VAL:HG22	2.00	0.61
1:A:538:ALA:HB1	1:A:542:THR:HG21	1.81	0.61
1:B:808:HIS:NE2	1:B:812:LYS:HE3	2.16	0.61
1:B:202:ARG:O	1:B:203:ASN:C	2.39	0.61
1:B:840:ILE:CG2	1:B:842:ARG:HG2	2.30	0.61
1:A:431:LEU:HD22	1:A:617:ILE:HG12	1.82	0.61
1:A:772:LEU:HD11	1:A:845:PHE:HZ	1.66	0.61
1:B:943:ASN:HD22	1:B:972:PHE:HE1	1.49	0.61
1:A:68:GLN:N	1:A:68:GLN:NE2	2.49	0.61
1:B:961:VAL:HB	1:B:962:PRO:HD3	1.82	0.60
1:B:928:LEU:HD13	1:B:928:LEU:O	2.01	0.60
1:A:158:ILE:HG23	1:A:175:LEU:HD21	1.83	0.60
1:A:594:GLN:O	1:A:598:LEU:HG	2.02	0.60
1:B:6:ASP:O	1:B:8:THR:N	2.34	0.60
1:A:148:ARG:HG3	1:A:148:ARG:HH11	1.66	0.60
1:B:99:GLU:N	1:B:100:PRO:HD2	2.15	0.60
1:B:830:TYR:O	1:B:834:GLN:HG2	2.01	0.60
1:A:274:THR:HG22	1:A:274:THR:O	2.00	0.60
1:A:528:LEU:HD12	1:A:547:LEU:HD23	1.83	0.60
1:B:744:ILE:HD12	1:B:746:PHE:CZ	2.37	0.60
1:A:606:ASN:O	1:A:609:THR:HG22	2.01	0.60
1:B:789:LEU:O	1:B:870:HIS:HD2	1.85	0.59
1:A:697:ILE:HD11	1:A:700:ASP:OD1	2.02	0.59
1:A:459:GLU:OE1	1:A:471:ILE:HD12	2.02	0.59
1:B:217:GLN:O	1:B:220:PRO:HD2	2.02	0.59
1:A:623:LYS:NZ	1:A:625:ALA:HB3	2.17	0.59
1:B:369:LEU:CD2	1:B:375:LEU:HD12	2.33	0.59
1:B:846:VAL:HG13	1:B:846:VAL:O	2.02	0.59
1:B:775:ALA:HB3	1:B:851:LEU:HD23	1.83	0.59
1:A:496:LYS:O	1:A:741:ILE:HD12	2.03	0.59
1:B:98:ASN:O	1:B:102:VAL:HG23	2.03	0.59
1:A:566:THR:HB	1:A:580:GLU:OE1	2.03	0.59
1:A:516:LEU:O	1:A:525:ILE:HG13	2.03	0.59
1:A:398:ILE:HD13	1:A:407:GLN:CG	2.33	0.59
1:A:487:PHE:CZ	1:A:506:PHE:HA	2.37	0.59
1:B:593:GLN:HB2	1:B:596:LEU:HD12	1.84	0.59
1:A:505:ASP:O	1:A:506:PHE:HB2	2.04	0.58
1:B:879:LYS:O	1:B:883:LYS:HB2	2.02	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:793:ASP:C	1:A:795:GLY:H	2.06	0.58
1:B:273:GLU:CD	1:B:273:GLU:H	2.06	0.58
1:A:291:GLU:CD	1:A:291:GLU:H	2.07	0.58
1:B:73:LYS:HB2	1:B:73:LYS:NZ	2.19	0.58
1:A:994:LEU:HA	1:A:997:LEU:HB2	1.85	0.58
1:A:913:GLU:HG3	1:A:920:ALA:O	2.04	0.58
1:A:928:LEU:HD13	1:A:928:LEU:O	2.04	0.58
1:A:507:GLY:O	1:A:508:LEU:HD13	2.04	0.58
1:B:68:GLN:HE22	1:B:70:ARG:HH21	1.52	0.58
1:B:45:ASP:HB3	1:B:673:LEU:HD12	1.85	0.57
1:B:459:GLU:HG3	1:B:471:ILE:HG21	1.85	0.57
1:A:2:ASN:N	1:A:3:PRO:HD3	2.19	0.57
1:B:213:GLN:HA	1:B:213:GLN:NE2	2.19	0.57
1:A:879:LYS:O	1:A:883:LYS:HG3	2.04	0.57
1:B:543:LEU:CD2	1:B:581:ILE:HD11	2.29	0.57
1:A:555:ASN:HD22	1:A:557:LYS:N	2.02	0.57
1:B:620:ARG:O	1:B:621:ALA:HB2	2.05	0.57
1:B:718:ASP:CG	1:B:721:LYS:HG3	2.25	0.57
1:B:562:ARG:HB3	1:B:562:ARG:HH11	1.70	0.57
1:B:819:LYS:O	1:B:823:VAL:HG23	2.03	0.57
1:A:753:ARG:NH1	1:A:753:ARG:HG2	2.20	0.57
1:B:73:LYS:HG3	1:B:75:ASP:H	1.69	0.57
1:A:529:LEU:HD23	1:A:529:LEU:O	2.04	0.57
1:B:270:PHE:HA	1:B:309:GLN:NE2	2.19	0.57
1:B:498:LYS:HB2	1:B:741:ILE:HD11	1.85	0.57
1:B:943:ASN:ND2	1:B:968:LYS:HE2	2.20	0.56
1:A:548:HIS:CE1	1:A:560:GLU:HG3	2.40	0.56
1:A:984:GLU:C	1:A:986:TYR:H	2.08	0.56
1:A:497:GLU:CB	1:A:499:ILE:HD13	2.36	0.56
1:B:223:GLU:HG3	4:B:2206:HOH:O	2.04	0.56
1:A:213:GLN:HE21	1:A:213:GLN:HA	1.70	0.56
1:B:994:LEU:HD23	1:B:995:GLU:N	2.20	0.56
1:A:507:GLY:O	1:A:508:LEU:O	2.23	0.56
1:A:410:ASN:HD22	1:A:411:VAL:H	1.52	0.56
1:B:878:LEU:HG	1:B:882:LYS:NZ	2.20	0.56
1:A:233:ASN:HD22	1:A:233:ASN:C	2.09	0.56
1:A:410:ASN:ND2	1:A:411:VAL:H	2.03	0.56
1:A:404:LEU:H	1:A:404:LEU:HD23	1.69	0.56
1:B:68:GLN:O	1:B:70:ARG:HG3	2.05	0.56
1:B:123:LEU:HD22	1:B:158:ILE:CG1	2.36	0.56
1:A:327:THR:HG22	1:A:331:MET:HE2	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:905:LYS:CG	1:B:931:PHE:HE1	2.19	0.56
1:A:455:ILE:CD1	1:A:456:SER:H	2.19	0.56
1:A:990:LEU:HD23	1:A:993:GLU:OE2	2.06	0.55
1:A:520:ARG:HG3	1:A:521:GLN:N	2.21	0.55
1:B:280:ILE:N	1:B:280:ILE:HD12	2.21	0.55
1:B:562:ARG:CB	1:B:562:ARG:NH1	2.69	0.55
1:A:7:ARG:CD	1:A:21:ASP:HB3	2.35	0.55
1:A:891:TYR:CE2	1:A:964:LEU:HD22	2.41	0.55
1:A:240:GLY:HA2	1:A:455:ILE:HD13	1.87	0.55
1:B:713:PRO:HG2	1:B:715:ASP:O	2.06	0.55
1:A:531:GLU:O	1:A:534:VAL:HG12	2.05	0.55
1:A:4:ILE:HD12	1:A:146:ARG:NH1	2.22	0.55
1:A:385:ASN:OD1	1:A:387:SER:HB2	2.07	0.55
1:A:130:LYS:HD2	1:B:302:GLU:HG3	1.89	0.55
1:A:431:LEU:HD23	1:A:431:LEU:O	2.07	0.54
1:A:421:LEU:O	1:A:425:LEU:HB2	2.08	0.54
1:B:496:LYS:O	1:B:497:GLU:HB3	2.07	0.54
1:B:402:ARG:N	1:B:402:ARG:HD3	2.22	0.54
1:A:561:PRO:HB3	1:A:578:MET:CE	2.37	0.54
1:B:669:ASP:OD2	1:B:670:LYS:N	2.40	0.54
1:A:816:LYS:HB3	1:A:817:PRO:HD3	1.89	0.54
1:A:508:LEU:HD22	1:A:508:LEU:O	2.07	0.54
1:B:980:LYS:O	1:B:983:ALA:HB3	2.08	0.54
1:A:280:ILE:HD12	1:A:281:PHE:H	1.72	0.54
1:A:811:TYR:O	1:A:811:TYR:CG	2.60	0.54
1:B:59:SER:HA	1:B:74:LYS:CB	2.37	0.54
1:B:744:ILE:C	1:B:744:ILE:HD13	2.28	0.54
1:B:35:ILE:O	1:B:49:CYS:HA	2.07	0.54
1:B:497:GLU:CD	1:B:742:THR:HG22	2.28	0.54
1:B:60:PHE:CE1	1:B:74:LYS:HE2	2.43	0.54
1:A:213:GLN:HG3	1:A:333:ILE:HG21	1.90	0.54
1:B:785:LYS:O	1:B:788:SER:HB3	2.08	0.54
1:B:37:TYR:HE1	1:B:39:PRO:HA	1.72	0.54
1:A:1006:HIS:O	1:A:1010:HIS:HB2	2.08	0.54
1:B:305:ASN:ND2	1:B:356:ASN:HA	2.23	0.54
1:A:566:THR:O	1:A:581:ILE:HG22	2.07	0.54
1:A:379:SER:HB3	1:A:384:VAL:O	2.07	0.54
1:A:40:ASP:C	1:A:42:ASP:H	2.11	0.54
1:A:916:ASP:O	1:A:917:SER:HB3	2.08	0.54
1:B:59:SER:HA	1:B:74:LYS:HB2	1.89	0.54
1:B:223:GLU:HG2	1:B:227:ASN:ND2	2.23	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:327:THR:O	1:B:331:MET:HG3	2.08	0.54
1:B:499:ILE:HD11	1:B:740:GLY:CA	2.36	0.53
1:A:289:THR:O	1:A:293:LYS:HG3	2.08	0.53
1:B:943:ASN:HD21	1:B:968:LYS:HE2	1.74	0.53
1:B:706:TYR:CE2	1:B:714:ARG:HG3	2.43	0.53
1:B:398:ILE:HG22	1:B:405:VAL:O	2.09	0.53
1:B:213:GLN:HE21	1:B:213:GLN:HA	1.72	0.53
1:A:903:THR:O	1:A:907:VAL:HG23	2.09	0.53
1:B:744:ILE:HD13	1:B:745:PHE:N	2.23	0.53
1:B:56:THR:C	1:B:58:ASP:H	2.11	0.53
1:A:402:ARG:HH11	1:A:402:ARG:HG2	1.73	0.53
1:A:893:ARG:HH12	1:A:897:LYS:HE3	1.74	0.53
1:B:357:ILE:HD11	1:B:375:LEU:HA	1.89	0.53
1:A:410:ASN:ND2	1:A:411:VAL:N	2.57	0.53
1:B:109:ARG:O	1:B:114:LEU:HB2	2.09	0.53
1:A:798:ILE:N	1:A:798:ILE:HD12	2.24	0.53
1:B:33:ARG:O	1:B:52:ILE:HG12	2.09	0.53
1:A:793:ASP:O	1:A:795:GLY:N	2.42	0.53
1:A:592:LEU:HD23	1:A:597:GLU:OE2	2.09	0.53
1:A:354:LEU:O	1:A:418:ARG:NH1	2.41	0.53
1:A:217:GLN:O	1:A:220:PRO:HD2	2.09	0.53
1:B:210:VAL:O	1:B:214:GLN:HG3	2.08	0.53
1:A:997:LEU:C	1:A:1001:GLU:HB2	2.29	0.52
1:A:217:GLN:C	1:A:220:PRO:HD2	2.29	0.52
1:B:558:TYR:CD2	1:B:559:GLU:N	2.77	0.52
1:A:797:SER:OG	1:A:798:ILE:N	2.42	0.52
1:A:744:ILE:HD13	1:A:745:PHE:N	2.24	0.52
1:A:622:LYS:CE	1:A:624:GLY:H	2.17	0.52
1:A:520:ARG:NH1	1:A:520:ARG:HA	2.23	0.52
1:A:924:LYS:C	1:A:926:LYS:H	2.13	0.52
1:A:926:LYS:O	1:A:926:LYS:HD3	2.09	0.52
1:A:544:ILE:HG12	1:A:548:HIS:NE2	2.25	0.52
1:A:327:THR:HG22	1:A:331:MET:CE	2.40	0.52
1:B:296:LEU:HB2	1:B:298:LEU:HG	1.90	0.52
1:A:796:ASP:O	1:A:796:ASP:OD2	2.28	0.52
1:B:872:GLU:OE1	1:B:872:GLU:HA	2.10	0.52
1:B:696:ILE:O	1:B:743:LYS:HB2	2.10	0.52
1:B:798:ILE:N	1:B:798:ILE:HD12	2.24	0.52
1:A:917:SER:O	1:A:997:LEU:HD13	2.09	0.52
1:B:918:ILE:CG1	1:B:997:LEU:HD22	2.36	0.52
1:A:59:SER:N	1:A:74:LYS:HG3	2.25	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:899:GLU:HA	1:B:971:PHE:HZ	1.75	0.52
1:B:201:GLY:O	1:B:203:ASN:N	2.43	0.52
1:A:280:ILE:HD12	1:A:281:PHE:N	2.24	0.52
1:A:402:ARG:HG2	1:A:402:ARG:NH1	2.24	0.52
1:A:500:ASN:HD22	1:A:500:ASN:C	2.13	0.52
1:A:555:ASN:C	1:A:555:ASN:HD22	2.14	0.51
1:B:531:GLU:O	1:B:534:VAL:HG12	2.09	0.51
1:A:561:PRO:HB3	1:A:578:MET:HE1	1.91	0.51
1:A:892:ASN:HB3	1:A:896:LYS:HZ2	1.75	0.51
1:A:987:LYS:HD3	1:A:987:LYS:O	2.09	0.51
1:A:839:LEU:C	1:A:841:LYS:N	2.56	0.51
1:B:994:LEU:HD23	1:B:994:LEU:C	2.30	0.51
1:B:909:LEU:HD22	1:B:983:ALA:HA	1.92	0.51
1:B:115:ILE:HG21	1:B:128:PRO:HB3	1.91	0.51
1:B:565:LYS:HZ2	1:B:565:LYS:HB3	1.74	0.51
1:B:562:ARG:HB2	1:B:562:ARG:CZ	2.40	0.51
1:B:375:LEU:O	1:B:375:LEU:HD23	2.10	0.51
1:B:573:TYR:OH	1:B:683:GLU:OE2	2.29	0.51
1:A:357:ILE:HG23	1:A:369:LEU:HD11	1.92	0.51
1:A:589:LYS:HD2	1:A:591:PRO:HB3	1.93	0.51
1:B:497:GLU:OE2	1:B:742:THR:HG22	2.10	0.51
1:A:404:LEU:H	1:A:404:LEU:CD2	2.24	0.51
1:A:896:LYS:O	1:A:900:ASN:ND2	2.44	0.51
1:A:115:ILE:HD13	1:A:132:ILE:HD11	1.92	0.51
1:B:95:SER:HB3	1:B:752:ALA:HB2	1.93	0.51
1:A:666:LYS:CA	1:A:666:LYS:HE2	2.38	0.51
1:B:223:GLU:HG2	1:B:227:ASN:CG	2.30	0.51
1:A:736:GLN:HB3	1:A:750:GLN:HG2	1.92	0.51
1:B:918:ILE:CD1	1:B:998:GLN:HA	2.41	0.51
1:A:922:GLN:C	1:A:924:LYS:H	2.13	0.51
1:A:372:LYS:N	1:A:372:LYS:HD2	2.25	0.51
1:A:793:ASP:CG	1:A:794:PHE:H	2.12	0.51
1:A:162:ALA:O	1:A:173:GLN:HG3	2.10	0.51
1:B:244:GLU:O	1:B:256:ALA:HA	2.11	0.51
1:B:270:PHE:HA	1:B:309:GLN:HE22	1.76	0.51
1:A:850:GLY:O	1:A:851:LEU:HD13	2.11	0.51
1:B:477:LYS:HD3	1:B:514:ILE:HD13	1.92	0.51
1:A:95:SER:HB3	1:A:752:ALA:HB2	1.93	0.51
1:A:622:LYS:HE3	1:A:623:LYS:H	1.76	0.50
1:B:840:ILE:HD13	1:B:840:ILE:O	2.11	0.50
1:B:99:GLU:H	1:B:100:PRO:HD2	1.74	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:449:PHE:C	1:B:449:PHE:CD2	2.85	0.50
1:B:993:GLU:O	1:B:997:LEU:HB2	2.10	0.50
1:B:909:LEU:HD13	1:B:983:ALA:HA	1.93	0.50
1:A:901:TRP:NE1	1:A:935:CYS:SG	2.84	0.50
1:A:911:SER:O	1:A:911:SER:OG	2.25	0.50
1:A:61:THR:HG23	1:A:71:GLN:HG2	1.93	0.50
1:B:744:ILE:HD12	1:B:746:PHE:CE2	2.47	0.50
1:B:520:ARG:HH11	1:B:520:ARG:HG2	1.77	0.50
1:A:143:PHE:HA	1:A:146:ARG:HG3	1.94	0.50
1:A:204:GLN:O	1:A:205:ALA:HB3	2.12	0.50
1:A:817:PRO:HB2	1:A:818:PRO:CD	2.37	0.49
1:A:918:ILE:HG22	1:A:918:ILE:O	2.11	0.49
1:A:398:ILE:HD13	1:A:407:GLN:HB2	1.94	0.49
1:A:510:SER:O	1:A:514:ILE:HG13	2.12	0.49
1:A:520:ARG:HG3	1:A:521:GLN:CG	2.39	0.49
1:A:852:THR:HG22	1:A:855:GLU:H	1.75	0.49
1:A:499:ILE:HD11	1:A:740:GLY:CA	2.43	0.49
1:A:925:LEU:CD1	1:A:990:LEU:HD13	2.41	0.49
1:A:68:GLN:N	1:A:68:GLN:HE21	2.03	0.49
1:B:496:LYS:O	1:B:497:GLU:CB	2.61	0.49
1:B:735:GLU:O	1:B:747:ARG:HD2	2.12	0.49
1:B:135:TYR:CD1	1:B:191:LYS:HD2	2.47	0.49
1:A:588:ASN:HA	1:A:630:VAL:HB	1.93	0.49
1:A:962:PRO:HB2	1:A:963:GLU:OE2	2.13	0.49
1:B:688:THR:O	1:B:693:PRO:HG3	2.12	0.49
1:B:696:ILE:HG22	1:B:697:ILE:O	2.12	0.49
1:A:7:ARG:NE	1:A:21:ASP:HB3	2.27	0.49
1:A:697:ILE:HG12	1:A:697:ILE:O	2.13	0.49
1:B:620:ARG:HG3	1:B:633:GLN:OE1	2.13	0.49
1:B:136:THR:O	1:B:140:VAL:HG23	2.12	0.49
1:B:273:GLU:O	1:B:274:THR:CB	2.61	0.49
1:A:410:ASN:HD21	1:A:412:GLU:HG3	1.78	0.49
1:A:692:PHE:CE1	1:A:747:ARG:HG3	2.47	0.49
1:A:622:LYS:HE3	1:A:623:LYS:N	2.28	0.49
1:A:109:ARG:HG2	1:A:109:ARG:HH11	1.78	0.49
1:A:622:LYS:HE2	1:A:624:GLY:N	2.22	0.48
1:A:811:TYR:HD1	1:A:815:GLU:HB2	1.78	0.48
1:A:398:ILE:HD12	1:A:398:ILE:N	2.28	0.48
1:A:124:VAL:HG13	1:A:656:ILE:HD13	1.94	0.48
1:A:931:PHE:C	1:A:933:GLY:H	2.16	0.48
1:A:993:GLU:HG3	1:A:994:LEU:HD22	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:656:ILE:HD12	1:B:656:ILE:N	2.29	0.48
1:B:2:ASN:HD21	1:B:4:ILE:HB	1.76	0.48
1:B:47:TYR:CD2	1:B:100:PRO:HB3	2.49	0.48
1:B:505:ASP:O	1:B:507:GLY:N	2.43	0.48
1:B:532:GLN:HG2	1:B:543:LEU:HB2	1.94	0.48
1:A:793:ASP:C	1:A:795:GLY:N	2.67	0.48
1:A:354:LEU:HD11	1:A:382:PHE:HE1	1.78	0.48
1:B:840:ILE:O	1:B:841:LYS:HB2	2.14	0.48
1:B:223:GLU:O	1:B:227:ASN:HB2	2.13	0.48
1:B:1005:HIS:O	1:B:1005:HIS:ND1	2.46	0.48
1:A:981:SER:O	1:A:984:GLU:HB2	2.14	0.48
1:A:852:THR:HG23	1:A:854:ASN:H	1.78	0.48
1:B:562:ARG:HB2	1:B:562:ARG:NH1	2.27	0.48
1:A:761:ARG:O	1:A:764:SER:HB3	2.13	0.48
1:A:894:ILE:O	1:A:897:LYS:HB2	2.14	0.48
1:B:95:SER:CB	1:B:752:ALA:HB2	2.43	0.48
1:B:505:ASP:O	1:B:506:PHE:CD1	2.67	0.48
1:A:919:THR:HA	1:A:923:ALA:HB3	1.96	0.48
1:A:468:GLN:OE1	1:A:468:GLN:N	2.47	0.48
1:A:520:ARG:NH1	1:A:520:ARG:HB2	2.29	0.48
1:B:742:THR:CG2	1:B:743:LYS:HE3	2.44	0.48
1:B:140:VAL:HG13	1:B:195:TYR:CD1	2.49	0.48
1:A:985:THR:O	1:A:985:THR:HG22	2.14	0.48
1:A:626:ASN:O	1:A:627:PHE:O	2.31	0.48
1:B:546:LYS:HE2	1:B:550:HIS:CE1	2.48	0.48
1:A:610:LYS:HZ3	1:A:610:LYS:HB2	1.79	0.48
1:B:249:ASN:OD1	1:B:250:ALA:N	2.47	0.48
1:A:223:GLU:O	1:A:227:ASN:HB2	2.14	0.48
1:A:943:ASN:HD21	1:A:968:LYS:NZ	2.12	0.48
1:A:921:VAL:CG1	1:A:994:LEU:HD21	2.43	0.47
1:B:243:ILE:N	1:B:243:ILE:HD13	2.27	0.47
1:B:852:THR:CG2	1:B:855:GLU:HB2	2.44	0.47
1:B:139:MET:CE	1:B:142:ILE:HD12	2.43	0.47
1:B:361:LYS:HA	1:B:361:LYS:CE	2.44	0.47
1:A:943:ASN:O	1:A:947:LEU:HG	2.14	0.47
1:A:176:LEU:HD12	1:A:176:LEU:N	2.30	0.47
1:A:515:ASP:C	1:A:517:ILE:N	2.66	0.47
1:B:296:LEU:CD2	1:B:346:LYS:HG2	2.45	0.47
1:B:626:ASN:CG	1:B:627:PHE:H	2.18	0.47
1:B:472:ASN:O	1:B:476:GLU:HG2	2.15	0.47
1:A:846:VAL:HG12	1:A:846:VAL:O	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:34:TYR:HA	1:B:50:GLY:O	2.14	0.47
1:A:990:LEU:O	1:A:994:LEU:HD23	2.13	0.47
1:A:375:LEU:HD11	1:A:390:GLU:HB2	1.96	0.47
1:A:1000:ILE:O	1:A:1000:ILE:HG22	2.14	0.47
1:A:520:ARG:CA	1:A:520:ARG:HH11	2.26	0.47
1:B:620:ARG:HG2	1:B:620:ARG:HH11	1.80	0.47
1:B:6:ASP:C	1:B:8:THR:H	2.17	0.47
1:B:833:LEU:O	1:B:833:LEU:HD12	2.14	0.47
1:B:850:GLY:N	1:B:855:GLU:OE1	2.44	0.47
1:B:733:ASP:HA	1:B:734:PRO:HD2	1.83	0.47
1:B:45:ASP:CG	1:B:677:ARG:HH22	2.17	0.47
1:B:207:GLY:O	1:B:210:VAL:HB	2.14	0.47
1:B:18:LYS:HD3	1:B:112:GLN:OE1	2.14	0.47
1:B:516:LEU:HD12	1:B:557:LYS:CB	2.45	0.47
1:B:816:LYS:HB3	1:B:817:PRO:HD3	1.96	0.47
1:A:727:LEU:HD12	1:A:732:ILE:HD12	1.95	0.47
1:A:628:ILE:HG13	1:A:632:ALA:CB	2.42	0.46
1:B:785:LYS:HE2	1:B:811:TYR:CE1	2.50	0.46
1:A:6:ASP:O	1:A:8:THR:N	2.48	0.46
1:B:398:ILE:HG12	1:B:399:LEU:N	2.30	0.46
1:A:149:ASN:C	1:A:149:ASN:ND2	2.69	0.46
1:A:369:LEU:CD2	1:A:375:LEU:HD12	2.45	0.46
1:B:241:LYS:HA	1:B:259:GLN:O	2.16	0.46
1:B:924:LYS:HA	1:B:927:ASN:HD22	1.81	0.46
1:A:507:GLY:C	1:A:508:LEU:HD13	2.35	0.46
1:B:139:MET:HA	1:B:139:MET:CE	2.44	0.46
1:A:695:ARG:N	1:A:695:ARG:HD2	2.31	0.46
1:B:698:TYR:CE2	1:B:744:ILE:HB	2.51	0.46
1:A:87:GLY:H	1:A:105:ASN:ND2	2.12	0.46
1:A:945:ASP:O	1:A:949:ILE:HG13	2.14	0.46
1:B:894:ILE:CG2	1:B:946:LEU:HD21	2.45	0.46
1:B:4:ILE:HD11	1:B:151:VAL:HG12	1.98	0.46
1:A:892:ASN:O	1:A:896:LYS:HG3	2.16	0.46
1:A:655:CYS:C	1:A:656:ILE:HD12	2.36	0.46
1:B:504:ILE:HD11	1:B:690:LYS:HZ3	1.78	0.46
1:A:499:ILE:HD11	1:A:740:GLY:HA2	1.96	0.46
1:B:483:ASN:HB3	1:B:506:PHE:HE1	1.81	0.46
1:B:395:GLU:HG2	1:B:407:GLN:O	2.16	0.46
1:A:798:ILE:N	1:A:798:ILE:CD1	2.79	0.46
1:B:98:ASN:N	1:B:98:ASN:ND2	2.61	0.46
1:B:878:LEU:O	1:B:882:LYS:HG2	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:979:VAL:HG23	1:B:980:LYS:N	2.31	0.46
1:A:851:LEU:HD22	1:A:851:LEU:N	2.31	0.46
1:B:504:ILE:HD11	1:B:690:LYS:HZ2	1.78	0.46
1:B:562:ARG:CB	1:B:562:ARG:HH11	2.28	0.46
1:A:7:ARG:HB2	1:A:7:ARG:NH1	2.31	0.46
1:A:992:ALA:HA	1:A:995:GLU:HG3	1.98	0.46
1:B:233:ASN:HD21	3:B:2100:ADP:H5'2	1.80	0.46
1:B:755:GLU:O	1:B:759:GLU:HG3	2.16	0.46
1:A:811:TYR:O	1:A:812:LYS:HG3	2.15	0.45
1:A:852:THR:HG23	1:A:855:GLU:H	1.82	0.45
1:A:40:ASP:C	1:A:42:ASP:N	2.70	0.45
1:A:85:PHE:O	1:A:88:VAL:HG13	2.16	0.45
1:B:205:ALA:HB3	1:B:208:SER:OG	2.16	0.45
1:B:409:LEU:HD23	1:B:409:LEU:N	2.32	0.45
1:A:334:VAL:O	1:A:334:VAL:HG12	2.15	0.45
1:A:976:TRP:O	1:A:980:LYS:HB2	2.16	0.45
1:B:147:ARG:HD2	1:B:150:GLU:OE1	2.16	0.45
1:A:497:GLU:HB3	1:A:499:ILE:CD1	2.46	0.45
1:A:421:LEU:HD21	1:A:600:PHE:CE1	2.52	0.45
1:B:785:LYS:HE2	1:B:811:TYR:CD1	2.51	0.45
1:A:520:ARG:CZ	1:A:520:ARG:HB2	2.46	0.45
1:B:852:THR:HG23	1:B:855:GLU:HB2	1.97	0.45
1:B:692:PHE:CD1	1:B:747:ARG:HG2	2.51	0.45
1:A:500:ASN:ND2	1:A:500:ASN:C	2.70	0.45
1:B:490:GLU:OE1	1:B:490:GLU:HA	2.16	0.45
1:B:294:LYS:O	1:B:294:LYS:HG3	2.15	0.45
1:B:397:ARG:HA	1:B:406:ALA:HA	1.99	0.45
1:B:715:ASP:O	1:B:716:ALA:CB	2.64	0.45
1:B:362:GLY:HA2	1:B:368:VAL:HG22	1.98	0.45
1:B:928:LEU:HD23	1:B:986:TYR:HD1	1.82	0.45
1:B:99:GLU:N	1:B:100:PRO:CD	2.79	0.45
1:B:979:VAL:O	1:B:983:ALA:N	2.49	0.45
1:A:752:ALA:O	1:A:756:GLU:HG3	2.16	0.45
1:B:366:GLY:HA3	1:B:408:HIS:CE1	2.51	0.45
1:B:733:ASP:O	1:B:735:GLU:N	2.50	0.45
1:B:968:LYS:HB3	1:B:968:LYS:NZ	2.32	0.44
1:B:548:HIS:O	1:B:552:SER:HB3	2.17	0.44
1:B:1007:HIS:ND1	1:B:1007:HIS:C	2.69	0.44
1:A:449:PHE:CD2	1:A:449:PHE:C	2.90	0.44
1:A:539:THR:N	1:A:542:THR:HG22	2.32	0.44
1:A:589:LYS:HD3	1:A:589:LYS:C	2.36	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:149:ASN:HD22	1:A:149:ASN:C	2.20	0.44
1:A:562:ARG:HD2	1:A:563:PHE:CE1	2.52	0.44
1:B:638:LEU:HD12	1:B:638:LEU:O	2.17	0.44
1:B:568:PHE:C	1:B:568:PHE:CD1	2.91	0.44
1:B:918:ILE:HD11	1:B:998:GLN:CA	2.43	0.44
1:A:922:GLN:HB2	1:A:994:LEU:CD1	2.46	0.44
1:B:851:LEU:CD1	1:B:851:LEU:N	2.77	0.44
1:B:369:LEU:HD23	1:B:375:LEU:HD12	1.99	0.44
1:A:548:HIS:ND1	1:A:560:GLU:HG3	2.33	0.44
1:A:146:ARG:HB3	1:A:146:ARG:HE	1.53	0.44
1:A:785:LYS:NZ	1:A:785:LYS:HB2	2.32	0.44
1:A:383:GLY:O	1:A:603:SER:HA	2.18	0.44
1:A:230:THR:HB	1:A:275:GLU:OE2	2.17	0.44
1:A:395:GLU:HG2	1:A:408:HIS:ND1	2.32	0.44
1:A:397:ARG:HA	1:A:406:ALA:HA	2.00	0.44
1:B:934:GLU:HA	1:B:937:SER:OG	2.17	0.44
1:A:229:LYS:HG3	1:A:234:ASN:HA	2.00	0.44
1:B:696:ILE:N	1:B:696:ILE:HD12	2.32	0.44
1:A:243:ILE:HD12	1:A:258:ILE:HG12	1.99	0.44
1:A:738:ARG:HD3	1:A:738:ARG:HA	1.77	0.44
1:B:1004:HIS:O	1:B:1004:HIS:CD2	2.71	0.44
1:B:661:LYS:HE3	1:B:663:LEU:HD12	1.99	0.44
1:A:768:LYS:O	1:A:772:LEU:HD13	2.17	0.44
1:A:40:ASP:O	1:A:42:ASP:N	2.51	0.44
1:B:170:ARG:HG3	1:B:448:TYR:OH	2.18	0.44
1:B:736:GLN:HA	1:B:747:ARG:HG3	2.00	0.43
1:B:112:GLN:O	1:B:113:ASP:HB2	2.18	0.43
1:B:921:VAL:HG11	1:B:994:LEU:HB2	2.01	0.43
1:B:761:ARG:CZ	1:B:842:ARG:HH11	2.31	0.43
1:A:840:ILE:O	1:A:840:ILE:HG22	2.17	0.43
1:B:398:ILE:HG12	1:B:399:LEU:H	1.83	0.43
1:B:898:LEU:HB3	1:B:971:PHE:CE2	2.53	0.43
1:A:697:ILE:O	1:A:698:TYR:C	2.57	0.43
1:A:703:LYS:HG3	1:A:714:ARG:NH2	2.33	0.43
1:A:713:PRO:HD2	1:A:716:ALA:HB2	2.00	0.43
1:A:622:LYS:HE3	1:A:622:LYS:CA	2.47	0.43
1:B:68:GLN:HE22	1:B:70:ARG:NH2	2.16	0.43
1:B:620:ARG:O	1:B:621:ALA:CB	2.66	0.43
1:A:148:ARG:HG3	1:A:148:ARG:NH1	2.31	0.43
1:A:834:GLN:HA	1:A:834:GLN:OE1	2.19	0.43
1:A:431:LEU:HD23	1:A:431:LEU:C	2.38	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:905:LYS:HB3	1:B:931:PHE:HE1	1.84	0.43
1:B:43:GLU:OE1	1:B:670:LYS:HD2	2.19	0.43
1:A:158:ILE:CG2	1:A:175:LEU:HD21	2.49	0.43
1:A:95:SER:HA	1:A:694:ASN:HD21	1.83	0.43
1:A:961:VAL:N	1:A:962:PRO:CD	2.81	0.43
1:A:732:ILE:HD11	1:A:754:ILE:HG12	1.99	0.43
1:A:539:THR:H	1:A:542:THR:HG22	1.83	0.43
1:B:405:VAL:HG23	1:B:405:VAL:O	2.18	0.43
1:B:878:LEU:HG	1:B:882:LYS:HZ2	1.84	0.43
1:A:116:TYR:HE2	1:A:188:ASN:HD21	1.66	0.43
1:B:503:PHE:HE1	1:B:690:LYS:HB2	1.84	0.43
1:A:279:HIS:O	1:A:283:GLN:HG3	2.19	0.43
1:B:737:TYR:HB2	1:B:744:ILE:HD11	2.01	0.43
1:A:610:LYS:HA	1:A:610:LYS:HZ2	1.84	0.43
1:A:515:ASP:C	1:A:517:ILE:H	2.20	0.43
1:A:507:GLY:O	1:A:508:LEU:C	2.56	0.43
1:A:350:GLY:HA3	1:A:382:PHE:CE2	2.53	0.43
1:A:610:LYS:NZ	1:A:610:LYS:HB2	2.34	0.43
1:B:702:VAL:HG21	1:B:722:ALA:HB3	2.00	0.43
1:A:360:GLU:OE2	1:A:370:LYS:HD2	2.19	0.43
1:A:185:LYS:HE2	1:A:185:LYS:HB2	1.82	0.43
1:B:529:LEU:HD13	1:B:543:LEU:HD21	2.01	0.42
1:B:372:LYS:O	1:B:376:ASN:ND2	2.52	0.42
1:B:823:VAL:HG21	1:B:860:TRP:CE3	2.53	0.42
1:B:87:GLY:H	1:B:105:ASN:ND2	2.17	0.42
1:A:901:TRP:CZ2	1:A:935:CYS:SG	3.13	0.42
1:A:7:ARG:HH11	1:A:7:ARG:CB	2.32	0.42
1:B:473:TYR:O	1:B:476:GLU:HB2	2.19	0.42
1:A:970:THR:O	1:A:974:GLN:HB2	2.19	0.42
1:A:233:ASN:HB3	1:A:236:SER:HB2	2.01	0.42
1:A:918:ILE:HG23	1:A:922:GLN:NE2	2.29	0.42
1:A:924:LYS:HB3	1:A:924:LYS:HE3	1.94	0.42
1:A:351:ILE:CG2	1:A:422:VAL:HG13	2.46	0.42
1:A:88:VAL:N	1:A:105:ASN:HD21	2.17	0.42
1:A:270:PHE:C	1:A:271:GLN:NE2	2.73	0.42
1:A:570:VAL:HG22	1:A:579:TYR:HE2	1.83	0.42
1:A:233:ASN:ND2	1:A:233:ASN:C	2.73	0.42
1:A:893:ARG:HH11	1:A:893:ARG:HG2	1.83	0.42
1:A:412:GLU:OE2	1:A:413:LYS:HG3	2.20	0.42
1:B:424:ALA:O	1:B:428:ARG:HG3	2.19	0.42
1:A:1002:ASP:HA	1:A:1005:HIS:HB3	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:372:LYS:O	1:A:373:THR:C	2.57	0.42
1:B:620:ARG:HG2	1:B:620:ARG:NH1	2.35	0.42
1:A:610:LYS:HD3	1:A:614:ASP:HB2	2.02	0.42
1:A:482:PHE:C	1:A:482:PHE:CD1	2.93	0.42
1:B:812:LYS:C	1:B:813:LYS:HD2	2.39	0.42
1:B:1007:HIS:HA	1:B:1010:HIS:NE2	2.34	0.42
1:B:866:ALA:O	1:B:870:HIS:HB2	2.20	0.42
1:B:102:VAL:HG21	1:B:685:ILE:HD13	2.02	0.42
1:B:340:GLU:O	1:B:343:SER:HB2	2.20	0.42
1:B:557:LYS:HD3	1:B:557:LYS:HA	1.83	0.42
1:B:496:LYS:C	1:B:498:LYS:N	2.68	0.42
1:B:733:ASP:C	1:B:735:GLU:H	2.24	0.42
1:A:158:ILE:HA	1:A:158:ILE:HD12	1.94	0.42
1:B:375:LEU:HD23	1:B:375:LEU:C	2.40	0.42
1:A:801:VAL:O	1:A:805:MET:HG3	2.19	0.42
1:B:642:MET:O	1:B:646:GLU:HG3	2.20	0.42
1:A:504:ILE:HG13	1:A:504:ILE:O	2.20	0.42
1:A:455:ILE:HD12	1:A:456:SER:N	2.25	0.41
1:A:676:LEU:HD23	1:A:679:ASN:HD21	1.85	0.41
1:B:851:LEU:C	1:B:852:THR:HG22	2.41	0.41
1:A:879:LYS:HE2	1:A:879:LYS:HB3	1.94	0.41
1:A:956:LEU:O	1:A:957:ASN:C	2.57	0.41
1:B:984:GLU:O	1:B:987:LYS:N	2.53	0.41
1:A:460:ILE:HG12	1:A:577:VAL:HG22	2.02	0.41
1:A:237:SER:HB2	4:A:1203:HOH:O	2.18	0.41
1:B:36:TRP:CZ3	1:B:49:CYS:HB3	2.56	0.41
1:B:592:LEU:O	1:B:593:GLN:C	2.59	0.41
1:B:785:LYS:HD2	1:B:785:LYS:HA	1.91	0.41
1:B:892:ASN:O	1:B:896:LYS:HG3	2.20	0.41
1:B:470:CYS:HB3	1:B:634:TYR:CE1	2.55	0.41
1:A:369:LEU:C	1:A:371:ASP:H	2.23	0.41
1:B:962:PRO:O	1:B:966:GLU:HG3	2.21	0.41
1:B:792:ARG:HA	1:B:794:PHE:CZ	2.55	0.41
1:B:708:LEU:HD13	1:B:730:LEU:HD11	2.03	0.41
1:B:852:THR:HG21	1:B:855:GLU:OE2	2.20	0.41
1:A:546:LYS:HB2	1:A:546:LYS:NZ	2.34	0.41
1:B:106:LEU:HD12	1:B:106:LEU:HA	1.92	0.41
1:A:63:LYS:O	1:A:64:THR:C	2.59	0.41
1:A:33:ARG:O	1:A:52:ILE:HG13	2.20	0.41
1:B:666:LYS:HE3	1:B:666:LYS:HB3	1.95	0.41
1:A:97:LEU:O	1:A:689:ARG:NH1	2.52	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:375:LEU:CD2	1:B:375:LEU:C	2.89	0.41
1:A:35:ILE:O	1:A:49:CYS:HA	2.21	0.41
1:B:32:LYS:HD3	1:B:51:GLU:CD	2.41	0.41
1:A:385:ASN:HA	1:A:386:PRO:HD2	1.81	0.41
1:B:233:ASN:ND2	3:B:2100:ADP:H5'2	2.36	0.41
1:B:340:GLU:O	1:B:344:ILE:HG13	2.21	0.41
1:B:7:ARG:HD2	1:B:12:HIS:CE1	2.56	0.41
1:B:589:LYS:HB2	1:B:589:LYS:HE3	1.86	0.41
1:A:538:ALA:CB	1:A:542:THR:HG21	2.49	0.41
1:B:928:LEU:CD2	1:B:986:TYR:HD1	2.35	0.41
1:B:45:ASP:OD2	1:B:677:ARG:NH2	2.47	0.41
1:B:523:PRO:O	1:B:551:PHE:HZ	2.03	0.41
1:A:321:GLU:H	1:A:321:GLU:HG3	1.57	0.41
1:A:589:LYS:O	1:A:590:ASP:C	2.60	0.40
1:B:82:PRO:HD2	1:B:85:PHE:CD1	2.56	0.40
1:A:852:THR:HG23	1:A:854:ASN:N	2.36	0.40
1:B:123:LEU:CD2	1:B:158:ILE:HG13	2.48	0.40
1:B:182:GLY:HA2	1:B:233:ASN:HD22	1.86	0.40
1:A:848:PRO:CB	1:A:851:LEU:HD23	2.36	0.40
1:A:812:LYS:HG2	1:A:816:LYS:HD2	2.04	0.40
1:B:302:GLU:CD	1:B:302:GLU:H	2.24	0.40
1:B:851:LEU:O	1:B:852:THR:CB	2.70	0.40
1:A:257:SER:HA	1:A:438:ASN:OD1	2.21	0.40
1:B:40:ASP:C	1:B:42:ASP:H	2.25	0.40
1:B:65:VAL:O	1:B:65:VAL:HG12	2.20	0.40
1:B:446:LYS:O	1:B:446:LYS:HG3	2.20	0.40
1:B:736:GLN:O	1:B:747:ARG:HG3	2.21	0.40
1:B:276:ARG:HB3	1:B:282:TYR:CE2	2.56	0.40
1:A:565:LYS:HA	1:A:565:LYS:HD3	1.85	0.40
1:B:772:LEU:HD11	1:B:845:PHE:HZ	1.86	0.40
1:A:901:TRP:C	1:A:903:THR:H	2.24	0.40
1:B:52:ILE:HD12	1:B:60:PHE:CD2	2.56	0.40
1:B:992:ALA:HA	1:B:995:GLU:OE1	2.21	0.40
1:B:217:GLN:C	1:B:220:PRO:HD2	2.42	0.40
1:A:352:LEU:HD12	1:A:352:LEU:HA	1.83	0.40
1:A:226:GLY:HA3	1:A:239:PHE:CE2	2.57	0.40
1:A:785:LYS:HG3	1:A:863:LEU:HD11	2.04	0.40
1:A:642:MET:O	1:A:646:GLU:HG3	2.22	0.40
1:A:643:ALA:O	1:A:647:THR:HG23	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	1007/1010 (100%)	887 (88%)	88 (9%)	32 (3%)	5	17
1	B	1007/1010 (100%)	875 (87%)	104 (10%)	28 (3%)	6	21
All	All	2014/2020 (100%)	1762 (88%)	192 (10%)	60 (3%)	5	18

All (60) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	24	LEU
1	A	203	ASN
1	A	204	GLN
1	A	508	LEU
1	A	536	PRO
1	A	621	ALA
1	A	627	PHE
1	A	812	LYS
1	A	840	ILE
1	A	917	SER
1	B	7	ARG
1	B	24	LEU
1	B	64	THR
1	B	203	ASN
1	B	206	ASN
1	B	506	PHE
1	B	621	ALA
1	B	716	ALA
1	B	852	THR
1	A	7	ARG
1	A	370	LYS
1	A	698	TYR
1	A	794	PHE
1	A	796	ASP
1	A	911	SER

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Mol	Chain	Res	Type
1	B	26	LYS
1	B	27	LEU
1	B	202	ARG
1	B	973	ALA
1	A	6	ASP
1	A	67	GLY
1	A	145	GLY
1	B	19	GLN
1	B	67	GLY
1	B	204	GLN
1	B	734	PRO
1	B	917	SER
1	A	504	ILE
1	A	599	CYS
1	A	925	LEU
1	A	957	ASN
1	A	960	GLY
1	B	69	ASP
1	B	959	ASN
1	A	39	PRO
1	A	59	SER
1	A	625	ALA
1	A	839	LEU
1	A	923	ALA
1	A	985	THR
1	B	6	ASP
1	B	731	ASN
1	B	83	ILE
1	B	264	GLU
1	B	274	THR
1	B	554	LYS
1	A	710	PRO
1	B	411	VAL
1	B	53	VAL
1	A	848	PRO

5.3.2 Protein sidechains ⓘ

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

The Analysed column shows the number of residues for which the sidechain conformation was

analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	884/885 (100%)	819 (93%)	65 (7%)	17	43
1	B	884/885 (100%)	834 (94%)	50 (6%)	25	58
All	All	1768/1770 (100%)	1653 (94%)	115 (6%)	21	52

All (115) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	12	HIS
1	A	38	ASN
1	A	44	ARG
1	A	68	GLN
1	A	146	ARG
1	A	148	ARG
1	A	149	ASN
1	A	175	LEU
1	A	196	LEU
1	A	213	GLN
1	A	233	ASN
1	A	249	ASN
1	A	259	GLN
1	A	264	GLU
1	A	329	GLN
1	A	352	LEU
1	A	403	ASP
1	A	404	LEU
1	A	412	GLU
1	A	425	LEU
1	A	435	LYS
1	A	445	ARG
1	A	484	HIS
1	A	500	ASN
1	A	508	LEU
1	A	516	LEU
1	A	520	ARG
1	A	531	GLU
1	A	536	PRO
1	A	546	LYS
1	A	555	ASN
1	A	559	GLU
1	A	562	ARG
1	A	566	THR

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Mol	Chain	Res	Type
1	A	585	LEU
1	A	610	LYS
1	A	620	ARG
1	A	622	LYS
1	A	666	LYS
1	A	669	ASP
1	A	683	GLU
1	A	690	LYS
1	A	697	ILE
1	A	710	PRO
1	A	727	LEU
1	A	744	ILE
1	A	753	ARG
1	A	758	ARG
1	A	761	ARG
1	A	780	GLN
1	A	785	LYS
1	A	790	GLU
1	A	791	SER
1	A	793	ASP
1	A	797	SER
1	A	804	PHE
1	A	838	ARG
1	A	839	LEU
1	A	875	ARG
1	A	881	GLN
1	A	893	ARG
1	A	916	ASP
1	A	924	LYS
1	A	1002	ASP
1	A	1010	HIS
1	B	7	ARG
1	B	12	HIS
1	B	13	LYS
1	B	44	ARG
1	B	69	ASP
1	B	73	LYS
1	B	148	ARG
1	B	196	LEU
1	B	219	ASN
1	B	247	PHE
1	B	273	GLU

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Mol	Chain	Res	Type
1	B	280	ILE
1	B	319	SER
1	B	352	LEU
1	B	387	SER
1	B	402	ARG
1	B	409	LEU
1	B	410	ASN
1	B	425	LEU
1	B	439	ASN
1	B	471	ILE
1	B	490	GLU
1	B	503	PHE
1	B	516	LEU
1	B	521	GLN
1	B	532	GLN
1	B	550	HIS
1	B	565	LYS
1	B	568	PHE
1	B	570	VAL
1	B	589	LYS
1	B	620	ARG
1	B	703	LYS
1	B	715	ASP
1	B	727	LEU
1	B	744	ILE
1	B	784	ASP
1	B	813	LYS
1	B	840	ILE
1	B	843	GLU
1	B	861	SER
1	B	865	LYS
1	B	879	LYS
1	B	881	GLN
1	B	889	GLN
1	B	912	ASN
1	B	913	GLU
1	B	944	SER
1	B	1007	HIS
1	B	1008	HIS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (63) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	5	HIS
1	A	68	GLN
1	A	105	ASN
1	A	149	ASN
1	A	188	ASN
1	A	204	GLN
1	A	213	GLN
1	A	233	ASN
1	A	234	ASN
1	A	271	GLN
1	A	376	ASN
1	A	407	GLN
1	A	410	ASN
1	A	491	GLN
1	A	500	ASN
1	A	555	ASN
1	A	613	ASN
1	A	616	ASN
1	A	633	GLN
1	A	637	GLN
1	A	694	ASN
1	A	720	GLN
1	A	729	HIS
1	A	731	ASN
1	A	780	GLN
1	A	870	HIS
1	A	889	GLN
1	A	892	ASN
1	A	900	ASN
1	A	922	GLN
1	A	936	GLN
1	A	943	ASN
1	A	952	GLN
1	A	1009	HIS
1	B	2	ASN
1	B	68	GLN
1	B	71	GLN
1	B	98	ASN
1	B	105	ASN
1	B	188	ASN
1	B	213	GLN
1	B	219	ASN
1	B	234	ASN

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Mol	Chain	Res	Type
1	B	259	GLN
1	B	283	GLN
1	B	309	GLN
1	B	439	ASN
1	B	479	GLN
1	B	485	HIS
1	B	511	GLN
1	B	550	HIS
1	B	576	GLN
1	B	594	GLN
1	B	613	ASN
1	B	637	GLN
1	B	834	GLN
1	B	870	HIS
1	B	881	GLN
1	B	912	ASN
1	B	927	ASN
1	B	943	ASN
1	B	975	GLN
1	B	1004	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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length

(or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	ADP	A	1100	2	22,29,29	1.81	5 (22%)	27,45,45	1.43	6 (22%)
3	ADP	B	2100	2	22,29,29	1.70	6 (27%)	27,45,45	1.37	4 (14%)

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
3	ADP	A	1100	2	-	0/12/32/32	0/3/3/3
3	ADP	B	2100	2	-	0/12/32/32	0/3/3/3

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1100	ADP	C8-N7	-3.35	1.28	1.34
3	B	2100	ADP	C8-N7	-2.80	1.29	1.34
3	B	2100	ADP	PB-O2B	-2.36	1.46	1.54
3	A	1100	ADP	PB-O2B	-2.17	1.46	1.54
3	B	2100	ADP	O4'-C4'	-2.14	1.40	1.45
3	A	1100	ADP	O4'-C1'	2.42	1.44	1.41
3	B	2100	ADP	O4'-C1'	2.55	1.44	1.41
3	B	2100	ADP	C4-N3	2.98	1.40	1.35
3	B	2100	ADP	C2-N1	3.85	1.41	1.33
3	A	1100	ADP	C4-N3	3.85	1.41	1.35
3	A	1100	ADP	C2-N1	3.86	1.41	1.33

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1100	ADP	N3-C2-N1	-3.88	125.92	128.89
3	B	2100	ADP	N3-C2-N1	-3.16	126.47	128.89
3	A	1100	ADP	O3B-PB-O1B	-2.00	104.13	110.58
3	A	1100	ADP	C4-C5-N7	2.03	111.35	109.48
3	A	1100	ADP	O2B-PB-O1B	2.06	117.20	110.58
3	B	2100	ADP	O2B-PB-O1B	2.07	117.24	110.58
3	A	1100	ADP	O3'-C3'-C2'	2.14	118.77	111.83
3	B	2100	ADP	O3'-C3'-C2'	2.41	119.65	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	2100	ADP	O3'-C3'-C4'	2.41	118.29	111.05
3	A	1100	ADP	O3'-C3'-C4'	2.63	118.93	111.05

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	2100	ADP	2	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å ²)	Q<0.9
1	A	1009/1010 (99%)	0.15	60 (5%)	26 16	17, 47, 100, 122	0
1	B	1009/1010 (99%)	0.08	37 (3%)	45 33	18, 50, 91, 118	0
All	All	2018/2020 (99%)	0.12	97 (4%)	34 23	17, 49, 96, 122	0

All (97) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	25	PHE	9.5
1	A	22	SER	8.8
1	B	22	SER	8.5
1	A	24	LEU	8.0
1	A	1007	HIS	8.0
1	A	25	PHE	7.8
1	A	1004	HIS	7.5
1	B	20	GLY	7.5
1	A	23	ASP	6.8
1	A	1010	HIS	6.7
1	A	206	ASN	6.6
1	B	625	ALA	6.3
1	B	28	THR	6.2
1	A	993	GLU	6.1
1	A	1000	ILE	6.0
1	B	23	ASP	6.0
1	A	28	THR	6.0
1	A	919	THR	5.9
1	A	915	GLY	5.9
1	A	1008	HIS	5.7
1	B	207	GLY	5.6
1	B	21	ASP	5.5
1	B	26	LYS	5.4
1	A	995	GLU	5.1

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Mol	Chain	Res	Type	RSRZ
1	A	921	VAL	4.9
1	A	27	LEU	4.7
1	B	24	LEU	4.7
1	B	27	LEU	4.7
1	A	1006	HIS	4.7
1	A	1003	LEU	4.6
1	A	21	ASP	4.4
1	A	917	SER	4.3
1	B	915	GLY	4.3
1	A	914	THR	4.2
1	A	916	ASP	4.1
1	A	918	ILE	4.0
1	B	914	THR	3.9
1	B	57	SER	3.9
1	A	1009	HIS	3.6
1	A	1005	HIS	3.5
1	A	992	ALA	3.5
1	A	26	LYS	3.4
1	A	996	ARG	3.4
1	A	912	ASN	3.4
1	A	920	ALA	3.3
1	B	205	ALA	3.3
1	B	1002	ASP	3.3
1	A	999	LYS	3.3
1	A	625	ALA	3.3
1	B	208	SER	3.1
1	A	909	LEU	3.1
1	A	1002	ASP	3.0
1	A	908	TYR	3.0
1	B	444	GLU	3.0
1	A	911	SER	3.0
1	B	206	ASN	3.0
1	B	913	GLU	2.9
1	A	402	ARG	2.9
1	B	445	ARG	2.9
1	A	913	GLU	2.8
1	B	990	LEU	2.7
1	A	401	GLY	2.7
1	B	622	LYS	2.7
1	A	910	GLY	2.7
1	B	362	GLY	2.6
1	B	916	ASP	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	205	ALA	2.6
1	B	505	ASP	2.5
1	B	365	GLU	2.5
1	A	626	ASN	2.5
1	A	922	GLN	2.4
1	A	20	GLY	2.4
1	B	624	GLY	2.4
1	B	363	ALA	2.4
1	B	908	TYR	2.4
1	A	405	VAL	2.4
1	B	918	ILE	2.4
1	A	991	LEU	2.3
1	A	904	THR	2.3
1	B	53	VAL	2.3
1	A	203	ASN	2.3
1	A	986	TYR	2.3
1	B	204	GLN	2.2
1	A	990	LEU	2.2
1	A	208	SER	2.2
1	A	989	THR	2.2
1	B	400	ALA	2.1
1	A	997	LEU	2.1
1	A	998	GLN	2.1
1	B	66	ASP	2.1
1	A	1001	GLU	2.1
1	B	508	LEU	2.0
1	B	626	ASN	2.0
1	A	400	ALA	2.0
1	A	983	ALA	2.0
1	A	204	GLN	2.0
1	A	622	LYS	2.0

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 carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
3	ADP	B	2100	27/27	0.98	0.19	0.18	22,32,37,38	0
3	ADP	A	1100	27/27	0.99	0.20	-0.24	17,27,34,36	0
2	MG	A	1101	1/1	0.98	0.25	-	21,21,21,21	0
2	MG	B	2101	1/1	0.96	0.26	-	23,23,23,23	0

6.5 Other polymers [i](#)

There are no such residues in this entry.