



Full wwPDB X-ray Structure Validation Report ⓘ

May 28, 2020 – 08:45 pm BST

PDB ID : 1URJ
Title : Single stranded DNA-binding protein(ICP8) from Herpes simplex virus-1
Authors : Panjikar, S.; Mapelli, M.; Tucker, P.A.
Deposited on : 2003-10-30
Resolution : 3.00 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Xtriage (Phenix) : 1.13
EDS : 2.11
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

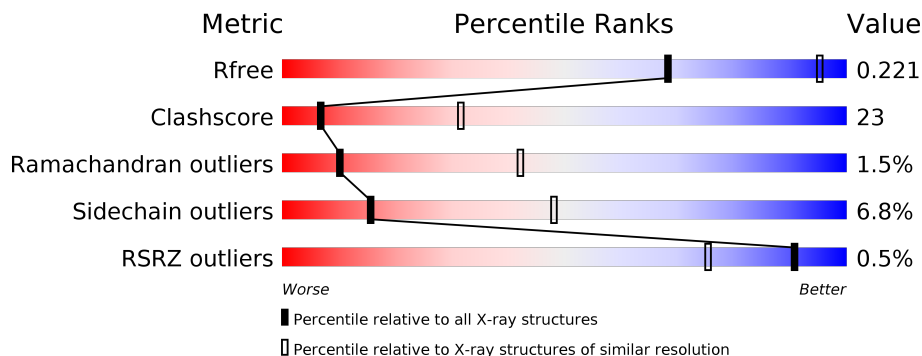
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (3.00-3.00)

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 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	1136	
1	B	1136	

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 15798 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 MAJOR DNA-BINDING PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	1029	7840	4968	1384	1444	44	0	0	1
1	B	1031	7853	4975	1386	1448	44	0	0	1

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	254	SER	CYS	engineered mutation	UNP P04296
A	455	SER	CYS	engineered mutation	UNP P04296
B	254	SER	CYS	engineered mutation	UNP P04296
B	455	SER	CYS	engineered mutation	UNP P04296

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 3 is MERCURY (II) ION (three-letter code: HG) (formula: Hg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	4	Total	Hg	0	0
			4	4		
3	A	4	Total	Hg	0	0
			4	4		

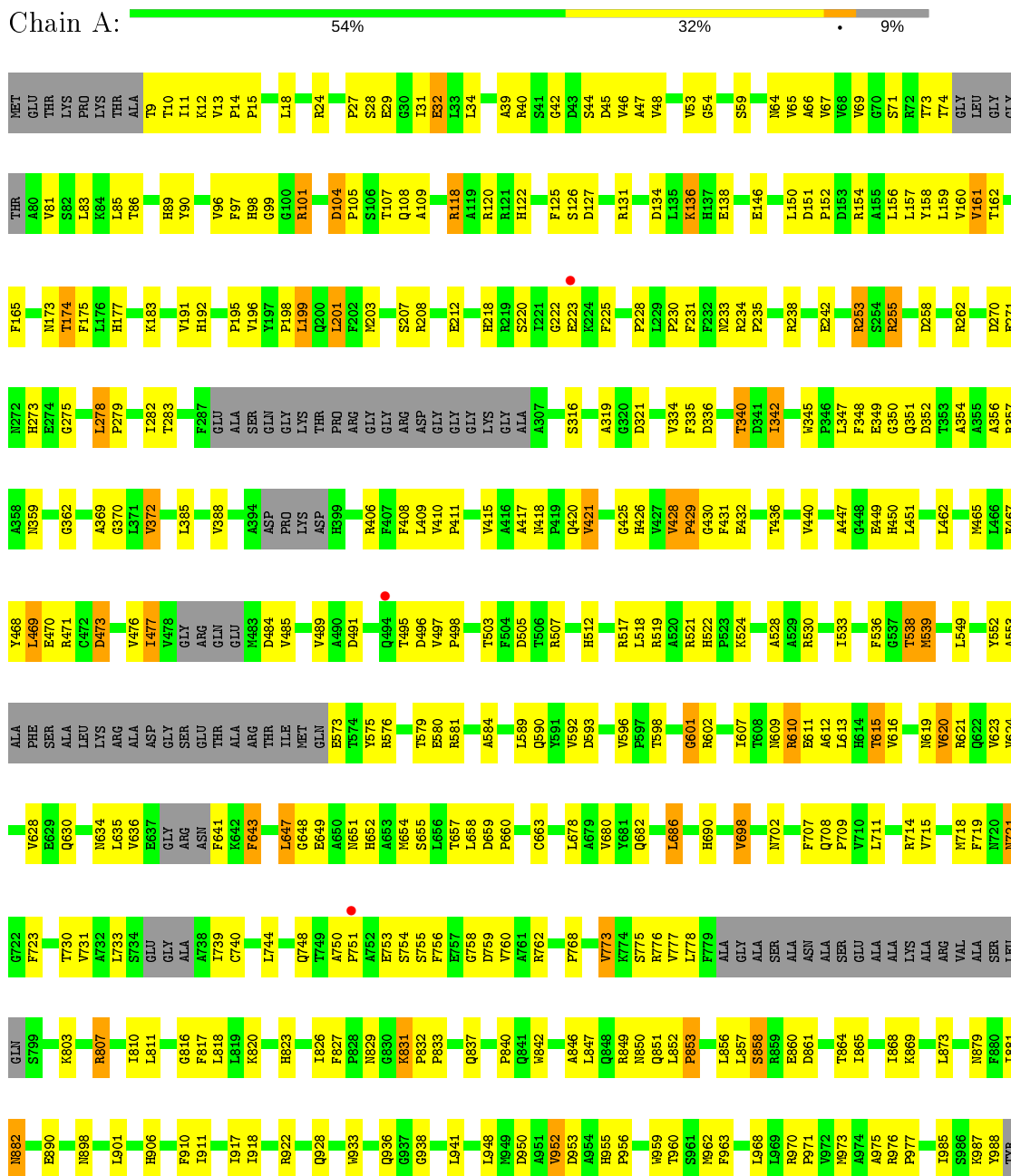
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	50	Total 50	O 50	0	0
4	B	45	Total 45	O 45	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 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: MAJOR DNA-BINDING PROTEIN





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	100.91Å 145.37Å 162.03Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 3.00 29.70 – 3.00	Depositor EDS
% Data completeness (in resolution range)	98.0 (20.00-3.00) 98.0 (29.70-3.00)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.44 (at 3.00Å)	Xtrriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.235 , 0.286 0.219 , 0.221	Depositor DCC
R_{free} test set	1211 reflections (2.56%)	wwPDB-VP
Wilson B-factor (Å ²)	50.5	Xtrriage
Anisotropy	0.403	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 42.7	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	0.90	EDS
Total number of atoms	15798	wwPDB-VP
Average B, all atoms (Å ²)	36.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.90% 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, 0.333 respectively for untwinned datasets, and 0.375, 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: ZN, HG

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	0.43	0/8009	0.65	0/10878
1	B	0.43	0/8023	0.65	0/10898
All	All	0.43	0/16032	0.65	0/21776

There are no bond length outliers.

There are no bond angle outliers.

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	7840	0	7742	370	0
1	B	7853	0	7752	362	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	4	0	0	0	0
3	B	4	0	0	0	0
4	A	50	0	0	6	0
4	B	45	0	0	4	0
All	All	15798	0	15494	724	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 23.

All (724) 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:494:GLN:HE21	1:B:494:GLN:HA	1.02	1.16
1:A:283:THR:HG23	1:A:420:GLN:HE21	1.21	1.04
1:A:1119:ASP:HB2	1:A:1122:LEU:HG	1.38	1.03
1:B:1119:ASP:HB2	1:B:1122:LEU:HG	1.39	1.01
1:B:1070:VAL:HG22	1:B:1122:LEU:HD22	1.40	1.00
1:A:1070:VAL:HG22	1:A:1122:LEU:HD22	1.39	1.00
1:A:107:THR:HG22	1:A:109:ALA:H	1.30	0.95
1:B:613:LEU:HD12	1:B:826:ILE:HD13	1.48	0.93
1:B:494:GLN:NE2	1:B:494:GLN:HA	1.83	0.92
1:B:107:THR:HG22	1:B:109:ALA:H	1.32	0.92
1:A:613:LEU:HD12	1:A:826:ILE:HD13	1.50	0.92
1:B:159:LEU:HG	1:B:161:VAL:HG22	1.51	0.90
1:B:428:VAL:HB	1:B:429:PRO:HD3	1.52	0.90
1:B:447:ALA:H	1:B:450:HIS:HD2	1.18	0.89
1:A:988:TYR:CE1	1:A:998:PHE:HB2	2.08	0.89
1:B:283:THR:HG23	1:B:420:GLN:HE21	1.39	0.88
1:A:159:LEU:HG	1:A:161:VAL:HG22	1.55	0.88
1:A:739:ILE:HD12	1:A:758:GLY:H	1.40	0.85
1:A:651:ASN:HB3	1:A:776:ARG:HA	1.58	0.85
1:A:428:VAL:HB	1:A:429:PRO:HD3	1.55	0.85
1:A:651:ASN:HA	1:A:777:VAL:HG23	1.60	0.84
1:A:447:ALA:H	1:A:450:HIS:HD2	1.21	0.84
1:A:1070:VAL:HG22	1:A:1122:LEU:CD2	2.07	0.83
1:B:1070:VAL:HG22	1:B:1122:LEU:CD2	2.08	0.83
1:A:283:THR:HG23	1:A:420:GLN:NE2	1.93	0.83
1:B:651:ASN:HB3	1:B:776:ARG:HA	1.60	0.83
1:A:857:LEU:HD22	1:A:857:LEU:H	1.44	0.82
1:B:316:SER:HB3	1:B:388:VAL:HG21	1.61	0.81
1:A:316:SER:HB3	1:A:388:VAL:HG21	1.62	0.81
1:A:429:PRO:HG2	1:A:430:GLY:H	1.45	0.81
1:A:11:ILE:HD12	1:A:12:LYS:H	1.47	0.80
1:A:340:THR:HG22	1:A:345:TRP:HE1	1.47	0.80
1:B:494:GLN:CA	1:B:494:GLN:HE21	1.87	0.80
1:A:1053:LEU:HD12	1:A:1091:LEU:HD22	1.66	0.78
1:B:428:VAL:CB	1:B:429:PRO:HD3	2.13	0.78
1:B:651:ASN:HA	1:B:777:VAL:HG23	1.66	0.78
1:A:428:VAL:CB	1:A:429:PRO:HD3	2.14	0.76
1:B:447:ALA:H	1:B:450:HIS:CD2	2.04	0.76
1:B:429:PRO:HG2	1:B:430:GLY:H	1.49	0.76
1:B:715:VAL:HA	1:B:718:MET:HE2	1.67	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1050:CYS:HB3	1:B:1054:ARG:HH21	1.49	0.76
1:B:596:VAL:HG12	1:B:598:THR:HG22	1.68	0.76
1:A:348:PHE:O	1:A:352:ASP:HB2	1.87	0.75
1:B:340:THR:HG22	1:B:345:TRP:HE1	1.51	0.75
1:B:428:VAL:HB	1:B:429:PRO:CD	2.15	0.75
1:A:1070:VAL:CG2	1:A:1122:LEU:HD22	2.16	0.74
1:B:352:ASP:OD1	1:B:357:ARG:NE	2.20	0.74
1:A:852:LEU:HD21	1:A:856:LEU:HD23	1.70	0.74
1:A:428:VAL:HB	1:A:429:PRO:CD	2.17	0.74
1:A:807:ARG:HH12	1:A:873:LEU:HD11	1.51	0.73
1:A:1050:CYS:HB3	1:A:1054:ARG:HH21	1.53	0.73
1:B:348:PHE:O	1:B:352:ASP:HB2	1.86	0.73
1:B:449:GLU:HG3	4:B:2006:HOH:O	1.87	0.73
1:B:1070:VAL:CG2	1:B:1122:LEU:HD22	2.17	0.73
1:B:225:PHE:CE2	1:B:744:LEU:HD13	2.23	0.73
1:B:1053:LEU:HD12	1:B:1091:LEU:HD22	1.69	0.73
1:A:18:LEU:HD23	1:A:198:PRO:HG3	1.71	0.73
1:A:473:ASP:HB3	1:A:517:ARG:HH12	1.53	0.72
1:A:136:LYS:HB3	1:A:136:LYS:HZ2	1.54	0.72
1:A:497:VAL:HG21	1:A:507:ARG:CZ	2.20	0.72
1:B:1053:LEU:HD22	1:B:1068:VAL:HG13	1.72	0.72
1:A:428:VAL:CG1	1:A:429:PRO:HD3	2.20	0.72
1:A:64:ASN:CG	1:A:334:VAL:HG13	2.10	0.72
1:B:715:VAL:HA	1:B:718:MET:CE	2.20	0.71
1:A:596:VAL:HG12	1:A:598:THR:HG22	1.72	0.71
1:A:1048:SER:N	1:B:477:ILE:HG21	2.05	0.71
1:A:678:LEU:O	1:A:682:GLN:HG3	1.91	0.71
1:B:18:LEU:HD23	1:B:198:PRO:HG3	1.72	0.71
1:B:283:THR:HG23	1:B:420:GLN:NE2	2.05	0.71
1:A:832:PRO:HB3	1:A:842:TRP:CD2	2.25	0.71
1:A:1053:LEU:HD22	1:A:1068:VAL:HG13	1.73	0.70
1:A:199:LEU:HD21	1:A:230:PRO:HG3	1.72	0.70
1:A:447:ALA:H	1:A:450:HIS:CD2	2.06	0.70
1:B:549:LEU:HB2	1:B:575:TYR:CE2	2.26	0.70
1:A:352:ASP:OD1	1:A:357:ARG:NE	2.20	0.70
1:B:497:VAL:HG21	1:B:507:ARG:CZ	2.21	0.70
1:A:573:GLU:CB	1:A:581:ARG:HH22	2.05	0.70
1:A:997:VAL:O	1:A:997:VAL:HG13	1.92	0.69
1:B:1127:GLU:O	1:B:1129:GLU:N	2.25	0.69
1:B:1066:SER:O	1:B:1070:VAL:HG23	1.93	0.69
1:A:340:THR:CG2	1:A:345:TRP:HE1	2.05	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1127:GLU:O	1:A:1129:GLU:N	2.25	0.68
1:B:428:VAL:CG1	1:B:429:PRO:HD3	2.22	0.68
1:A:852:LEU:HD13	1:A:857:LEU:HD21	1.76	0.68
1:B:120:ARG:HD3	1:B:126:SER:O	1.94	0.68
1:B:970:ARG:HB3	1:B:971:PRO:HD3	1.74	0.68
1:A:429:PRO:CG	1:A:430:GLY:H	2.06	0.68
1:B:199:LEU:HD21	1:B:230:PRO:HG3	1.74	0.68
1:B:678:LEU:O	1:B:682:GLN:HG3	1.92	0.68
1:A:621:ARG:HD3	4:A:2028:HOH:O	1.92	0.68
1:A:715:VAL:HA	1:A:718:MET:CE	2.24	0.68
1:A:275:GLY:HA2	1:A:708:GLN:HB3	1.74	0.68
1:A:613:LEU:HD12	1:A:826:ILE:CD1	2.24	0.68
1:B:107:THR:HG23	1:B:470:GLU:OE2	1.94	0.67
1:B:238:ARG:O	1:B:242:GLU:HG3	1.95	0.67
1:B:658:LEU:HD12	1:B:768:PRO:HB2	1.77	0.67
1:B:340:THR:CG2	1:B:345:TRP:HE1	2.08	0.67
1:B:1050:CYS:CB	1:B:1054:ARG:HH21	2.07	0.67
1:B:46:VAL:HG12	1:B:97:PHE:HA	1.74	0.67
1:A:89:HIS:CD2	1:A:660:PRO:HG3	2.30	0.67
1:A:970:ARG:HB3	1:A:971:PRO:HD3	1.77	0.66
1:A:406:ARG:HH11	1:A:690:HIS:HD2	1.42	0.66
1:B:632:MET:HE3	1:B:903:TYR:CD1	2.30	0.66
1:A:1097:LEU:O	1:A:1101:MET:HG2	1.96	0.66
1:B:370:GLY:HA3	1:B:963:PHE:CZ	2.31	0.66
1:A:120:ARG:HD3	1:A:126:SER:O	1.94	0.66
1:B:11:ILE:HD13	1:B:334:VAL:HG11	1.76	0.66
1:B:275:GLY:HA2	1:B:708:GLN:HB3	1.78	0.66
1:A:107:THR:HG23	1:A:470:GLU:OE2	1.95	0.66
1:A:778:LEU:HD23	1:A:911:ILE:HG22	1.78	0.66
1:B:370:GLY:HA3	1:B:963:PHE:HZ	1.60	0.65
1:A:1066:SER:O	1:A:1070:VAL:HG23	1.96	0.65
1:B:136:LYS:NZ	1:B:136:LYS:HB3	2.10	0.65
1:B:1125:ALA:C	1:B:1127:GLU:H	1.98	0.65
1:A:46:VAL:HG12	1:A:97:PHE:HA	1.79	0.65
1:A:576:ARG:O	1:A:580:GLU:HG3	1.97	0.65
1:A:1072:THR:HG21	1:A:1088:TRP:CH2	2.32	0.65
1:B:136:LYS:HB3	1:B:136:LYS:HZ2	1.60	0.65
1:A:1003:TRP:HZ2	1:A:1025:VAL:HG22	1.61	0.65
1:A:24:ARG:NH2	1:A:27:PRO:HB3	2.11	0.65
1:A:1050:CYS:CB	1:A:1054:ARG:HH21	2.10	0.64
1:B:24:ARG:NH2	1:B:27:PRO:HB3	2.12	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1125:ALA:C	1:A:1127:GLU:H	1.99	0.64
1:A:45:ASP:OD1	1:A:101:ARG:HD2	1.96	0.64
1:A:238:ARG:O	1:A:242:GLU:HG3	1.96	0.64
1:A:54:GLY:HA3	1:A:342:ILE:HD11	1.80	0.64
1:B:118:ARG:HD2	1:B:449:GLU:OE2	1.98	0.64
1:A:136:LYS:HB3	1:A:136:LYS:NZ	2.13	0.64
1:A:610:ARG:HD3	1:A:864:THR:OG1	1.98	0.64
1:B:988:TYR:CE1	1:B:998:PHE:HB2	2.33	0.64
1:B:283:THR:HG22	4:B:2020:HOH:O	1.98	0.63
1:B:476:VAL:O	1:B:477:ILE:HG13	1.98	0.63
1:A:473:ASP:HB2	1:A:518:LEU:CD2	2.28	0.63
1:B:1072:THR:HG21	1:B:1088:TRP:CH2	2.33	0.63
1:A:283:THR:OG1	1:A:420:GLN:HB3	1.98	0.63
1:A:9:THR:HG23	1:A:10:THR:H	1.63	0.63
1:A:592:VAL:HG12	1:A:593:ASP:N	2.12	0.63
1:A:10:THR:HA	1:A:730:THR:HG23	1.80	0.63
1:B:429:PRO:CG	1:B:430:GLY:H	2.10	0.63
1:A:636:VAL:HG23	1:A:643:PHE:HZ	1.64	0.62
1:A:177:HIS:HB3	1:A:195:PRO:HG2	1.80	0.62
1:B:1097:LEU:O	1:B:1101:MET:HG2	1.99	0.62
1:B:1119:ASP:CB	1:B:1122:LEU:HG	2.24	0.62
1:A:778:LEU:CD2	1:A:911:ILE:HG22	2.30	0.62
1:B:406:ARG:HH11	1:B:690:HIS:HD2	1.47	0.62
1:B:592:VAL:HG12	1:B:593:ASP:N	2.14	0.62
1:B:177:HIS:HB3	1:B:195:PRO:HG2	1.80	0.62
1:B:1003:TRP:HZ2	1:B:1025:VAL:HG22	1.65	0.62
1:B:807:ARG:HH12	1:B:873:LEU:HD11	1.65	0.62
1:A:90:TYR:CD2	1:A:160:VAL:HG12	2.35	0.61
1:B:420:GLN:HG2	1:B:431:PHE:CE2	2.35	0.61
1:B:647:LEU:HD23	1:B:648:GLY:N	2.14	0.61
1:B:861:ASP:O	1:B:865:ILE:HG12	2.01	0.61
1:A:1119:ASP:HB2	1:A:1122:LEU:CG	2.22	0.61
1:A:739:ILE:CD1	1:A:758:GLY:H	2.11	0.61
1:B:385:LEU:HD12	1:B:533:ILE:HG23	1.80	0.61
1:B:576:ARG:O	1:B:580:GLU:HG3	2.00	0.61
1:A:484:ASP:HA	1:A:928:GLN:NE2	2.16	0.61
1:A:810:ILE:HD11	1:A:869:LYS:HG2	1.82	0.61
1:A:420:GLN:HG2	1:A:431:PHE:CE2	2.36	0.61
1:B:1010:LYS:H	1:B:1010:LYS:HD2	1.65	0.61
1:B:90:TYR:CD2	1:B:160:VAL:HG12	2.36	0.61
1:A:385:LEU:HD12	1:A:533:ILE:HG23	1.83	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:45:ASP:OD1	1:B:101:ARG:HD2	2.00	0.61
1:B:613:LEU:HD12	1:B:826:ILE:CD1	2.27	0.61
1:A:807:ARG:NH1	1:A:873:LEU:HD11	2.16	0.60
1:A:832:PRO:HB3	1:A:842:TRP:CE2	2.36	0.60
1:A:610:ARG:HH11	1:A:610:ARG:HG2	1.66	0.60
1:B:1119:ASP:HB2	1:B:1122:LEU:CG	2.24	0.60
1:A:1083:LEU:HD22	1:A:1087:ASP:HB3	1.84	0.60
1:A:370:GLY:HA3	1:A:963:PHE:HZ	1.67	0.60
1:B:18:LEU:C	1:B:18:LEU:HD12	2.21	0.60
1:B:610:ARG:HG2	1:B:610:ARG:HH11	1.66	0.60
1:A:319:ALA:CB	1:A:686:LEU:HD13	2.32	0.60
1:B:253:ARG:NH2	1:B:682:GLN:OE1	2.35	0.60
1:A:1010:LYS:H	1:A:1010:LYS:HD2	1.67	0.60
1:B:104:ASP:N	1:B:104:ASP:OD2	2.35	0.60
1:B:54:GLY:HA3	1:B:342:ILE:HD11	1.83	0.60
1:A:484:ASP:HA	1:A:928:GLN:HE22	1.65	0.59
1:A:610:ARG:NH2	1:A:860:GLU:HB3	2.16	0.59
1:B:406:ARG:HH11	1:B:690:HIS:CD2	2.20	0.59
1:A:406:ARG:HH11	1:A:690:HIS:CD2	2.20	0.59
1:A:225:PHE:CE2	1:A:744:LEU:HD13	2.37	0.59
1:A:610:ARG:NH2	1:A:860:GLU:CB	2.65	0.59
1:B:203:MET:HE3	1:B:218:HIS:HD2	1.66	0.59
1:A:651:ASN:HB2	1:A:775:SER:O	2.03	0.59
1:A:861:ASP:O	1:A:865:ILE:HG12	2.02	0.59
1:B:817:PHE:CE2	1:B:818:LEU:HG	2.37	0.59
1:A:715:VAL:HA	1:A:718:MET:HE2	1.83	0.59
1:B:350:GLY:O	1:B:352:ASP:N	2.35	0.59
1:A:647:LEU:HD23	1:A:648:GLY:N	2.18	0.59
1:A:370:GLY:HA3	1:A:963:PHE:CZ	2.36	0.59
1:B:1083:LEU:HD22	1:B:1087:ASP:HB3	1.84	0.59
1:A:753:GLU:HG2	1:A:755:SER:OG	2.03	0.59
1:B:83:LEU:HD12	1:B:739:ILE:HG22	1.85	0.58
1:B:476:VAL:HG22	1:B:1014:PRO:HB2	1.85	0.58
1:B:71:SER:HB2	1:B:81:VAL:CG1	2.33	0.58
1:A:18:LEU:HD12	1:A:18:LEU:C	2.23	0.58
1:A:233:ASN:OD1	1:A:235:PRO:HD2	2.04	0.58
1:A:1070:VAL:HG22	1:A:1122:LEU:HD13	1.84	0.58
1:A:156:LEU:C	1:A:157:LEU:HD12	2.23	0.58
1:A:118:ARG:HD2	1:A:449:GLU:OE2	2.04	0.58
1:A:817:PHE:CE2	1:A:818:LEU:HG	2.38	0.58
1:A:827:PHE:CZ	1:A:865:ILE:HD13	2.39	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:278:LEU:HD22	1:A:321:ASP:OD1	2.04	0.57
1:A:847:LEU:HD23	1:A:852:LEU:HD12	1.84	0.57
1:B:616:VAL:O	1:B:620:VAL:HG13	2.05	0.57
1:A:1049:LEU:N	1:B:477:ILE:HG23	2.20	0.57
1:A:350:GLY:O	1:A:352:ASP:N	2.36	0.57
1:B:156:LEU:C	1:B:157:LEU:HD12	2.25	0.57
1:A:11:ILE:HD12	1:A:12:LYS:N	2.17	0.57
1:A:271:GLU:HB2	1:A:762:ARG:NH1	2.20	0.57
1:A:104:ASP:N	1:A:104:ASP:OD2	2.34	0.56
1:B:647:LEU:HD23	1:B:648:GLY:H	1.69	0.56
1:A:1053:LEU:CD1	1:A:1091:LEU:HD22	2.34	0.56
1:A:335:PHE:HB3	1:A:659:ASP:OD2	2.05	0.56
1:B:632:MET:HB3	1:B:903:TYR:CE2	2.40	0.56
1:A:731:VAL:HG11	1:A:760:VAL:HG21	1.88	0.56
1:B:266:HIS:CD2	4:B:2013:HOH:O	2.58	0.56
1:A:428:VAL:HG12	1:A:429:PRO:HD3	1.86	0.56
1:A:922:ARG:HD3	1:A:962:MET:SD	2.45	0.56
1:B:658:LEU:CD1	1:B:768:PRO:HB2	2.34	0.56
1:B:987:LYS:N	1:B:987:LYS:HD2	2.21	0.56
1:B:428:VAL:CB	1:B:429:PRO:CD	2.81	0.56
1:B:258:ASP:O	1:B:262:ARG:HG3	2.06	0.55
1:B:440:VAL:HG21	1:B:528:ALA:HB2	1.87	0.55
1:A:157:LEU:N	1:A:157:LEU:HD12	2.21	0.55
1:A:636:VAL:CG2	1:A:643:PHE:HZ	2.19	0.55
1:B:1069:PHE:HD2	1:B:1122:LEU:HD23	1.71	0.55
1:B:632:MET:HE2	1:B:903:TYR:HB3	1.87	0.55
1:A:519:ARG:HD2	1:A:519:ARG:O	2.06	0.55
1:A:987:LYS:N	1:A:987:LYS:HD2	2.21	0.55
1:A:1069:PHE:HD2	1:A:1122:LEU:HD23	1.71	0.55
1:A:203:MET:HE3	1:A:218:HIS:HD2	1.71	0.55
1:A:447:ALA:N	1:A:450:HIS:HD2	1.98	0.55
1:A:477:ILE:N	1:A:477:ILE:HD12	2.21	0.55
1:A:610:ARG:CZ	1:A:860:GLU:HB3	2.36	0.55
1:B:420:GLN:O	1:B:428:VAL:HG23	2.07	0.55
1:A:420:GLN:O	1:A:428:VAL:HG23	2.06	0.55
1:B:552:TYR:CE1	1:B:647:LEU:HB3	2.41	0.55
1:B:708:GLN:N	1:B:709:PRO:CD	2.69	0.55
1:A:616:VAL:O	1:A:620:VAL:HG13	2.07	0.55
1:A:652:HIS:CE1	1:A:777:VAL:HG22	2.41	0.55
1:A:613:LEU:CD1	1:A:826:ILE:HD13	2.31	0.55
1:B:447:ALA:N	1:B:450:HIS:HD2	1.96	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:40:ARG:HG3	1:B:47:ALA:HB2	1.88	0.55
1:A:552:TYR:CE1	1:A:647:LEU:HB3	2.42	0.55
1:A:715:VAL:HA	1:A:718:MET:HE3	1.90	0.54
1:A:1070:VAL:HG22	1:A:1122:LEU:CD1	2.37	0.54
1:B:647:LEU:HG	1:B:778:LEU:CD1	2.37	0.54
1:A:40:ARG:HG3	1:A:47:ALA:HB2	1.90	0.54
1:A:723:PHE:CB	1:A:999:GLN:HB2	2.37	0.54
1:B:1070:VAL:HG22	1:B:1122:LEU:HD13	1.88	0.54
1:A:429:PRO:CG	1:A:430:GLY:N	2.71	0.54
1:B:1069:PHE:O	1:B:1073:VAL:HG23	2.08	0.54
1:B:948:LEU:HD22	1:B:955:HIS:CE1	2.43	0.54
1:A:592:VAL:CG1	1:A:593:ASP:N	2.71	0.54
1:A:708:GLN:N	1:A:709:PRO:CD	2.70	0.54
1:B:28:SER:O	1:B:29:GLU:HG3	2.08	0.54
1:A:1119:ASP:CB	1:A:1122:LEU:HG	2.24	0.54
1:A:918:ILE:N	1:A:918:ILE:HD12	2.22	0.54
1:A:98:HIS:CD2	1:A:157:LEU:HD13	2.43	0.54
1:B:408:PHE:HA	1:B:686:LEU:HD23	1.90	0.54
1:A:476:VAL:H	1:A:477:ILE:HD12	1.73	0.54
1:B:421:VAL:HG22	1:B:426:HIS:C	2.29	0.54
1:B:864:THR:O	1:B:868:ILE:HG12	2.08	0.54
1:A:647:LEU:HG	1:A:778:LEU:CD1	2.38	0.53
1:B:203:MET:HE3	1:B:218:HIS:CD2	2.43	0.53
1:A:415:VAL:HG12	1:A:415:VAL:O	2.08	0.53
1:B:83:LEU:HD12	1:B:739:ILE:CG2	2.37	0.53
1:B:918:ILE:HD12	1:B:918:ILE:N	2.22	0.53
1:A:647:LEU:HD23	1:A:648:GLY:H	1.73	0.53
1:B:1053:LEU:CD1	1:B:1091:LEU:HD22	2.37	0.53
1:A:39:ALA:HB3	1:A:48:VAL:HG13	1.91	0.53
1:A:1053:LEU:C	1:A:1055:GLY:H	2.12	0.53
1:A:64:ASN:OD1	1:A:334:VAL:HG13	2.08	0.53
1:A:1092:LEU:C	1:A:1094:ASP:H	2.13	0.53
1:A:316:SER:HB3	1:A:388:VAL:CG2	2.37	0.53
1:A:744:LEU:HG	1:A:756:PHE:HZ	1.75	0.52
1:B:362:GLY:HA3	1:B:956:PRO:O	2.09	0.52
1:A:201:LEU:HD22	1:A:744:LEU:HD21	1.91	0.52
1:B:174:THR:HG23	1:B:175:PHE:N	2.23	0.52
1:B:174:THR:HG22	1:B:231:PHE:HB3	1.91	0.52
1:A:1049:LEU:CB	1:B:477:ILE:HG23	2.39	0.52
1:A:31:ILE:HG23	1:A:32:GLU:N	2.24	0.52
1:A:348:PHE:HB3	1:A:352:ASP:CG	2.30	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:519:ARG:HD2	1:B:519:ARG:O	2.10	0.52
1:A:1069:PHE:O	1:A:1073:VAL:HG23	2.09	0.52
1:A:711:LEU:O	1:A:715:VAL:HG23	2.10	0.52
1:B:1092:LEU:C	1:B:1094:ASP:H	2.12	0.52
1:B:922:ARG:HD3	1:B:962:MET:SD	2.49	0.52
1:A:28:SER:O	1:A:29:GLU:HG3	2.08	0.52
1:B:319:ALA:CB	1:B:686:LEU:HD13	2.39	0.52
1:B:98:HIS:CD2	1:B:157:LEU:HD13	2.44	0.52
1:B:131:ARG:HH12	1:B:212:GLU:CD	2.12	0.52
1:B:507:ARG:HG3	1:B:507:ARG:HH11	1.74	0.52
1:B:619:ASN:O	1:B:623:VAL:HG13	2.10	0.52
1:B:859:ARG:HG3	1:B:860:GLU:OE2	2.08	0.52
1:B:879:ASN:HD22	1:B:898:ASN:HD21	1.57	0.52
1:A:203:MET:CE	1:A:218:HIS:HD2	2.23	0.52
1:A:610:ARG:HH22	1:A:860:GLU:CB	2.23	0.52
1:A:635:LEU:HD13	1:A:641:PHE:CE2	2.45	0.52
1:B:1053:LEU:C	1:B:1055:GLY:H	2.12	0.52
1:A:359:ASN:OD1	1:A:956:PRO:HA	2.10	0.52
1:B:415:VAL:O	1:B:415:VAL:HG12	2.09	0.52
1:A:857:LEU:H	1:A:857:LEU:CD2	2.18	0.52
1:B:233:ASN:OD1	1:B:235:PRO:HD2	2.10	0.52
1:B:44:SER:OG	1:B:46:VAL:HG22	2.10	0.52
1:A:473:ASP:CB	1:A:517:ARG:HH12	2.21	0.52
1:B:90:TYR:HA	1:B:162:THR:HA	1.92	0.52
1:A:174:THR:HG23	1:A:175:PHE:N	2.25	0.51
1:A:258:ASP:O	1:A:262:ARG:HG3	2.09	0.51
1:B:1127:GLU:OE2	1:B:1128:ALA:HA	2.10	0.51
1:B:428:VAL:HG12	1:B:429:PRO:HD3	1.90	0.51
1:B:39:ALA:HB3	1:B:48:VAL:HG13	1.92	0.51
1:A:253:ARG:NH2	1:A:682:GLN:OE1	2.44	0.51
1:B:1070:VAL:HG13	1:B:1122:LEU:HD11	1.92	0.51
1:B:1123:GLU:HA	1:B:1126:HIS:HB3	1.93	0.51
1:B:99:GLY:HA3	1:B:156:LEU:HD23	1.92	0.51
1:A:203:MET:HE3	1:A:218:HIS:CD2	2.45	0.51
1:A:612:ALA:O	1:A:615:THR:HG23	2.10	0.51
1:B:462:LEU:O	1:B:465:MET:HB3	2.10	0.51
1:A:372:VAL:HG11	1:A:468:TYR:CG	2.46	0.51
1:B:157:LEU:HD12	1:B:157:LEU:N	2.25	0.51
1:B:484:ASP:HA	1:B:928:GLN:NE2	2.25	0.51
1:A:849:ARG:O	1:A:850:ASN:HB2	2.10	0.51
1:B:611:GLU:O	1:B:615:THR:HG22	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:711:LEU:O	1:B:715:VAL:HG23	2.10	0.51
1:A:44:SER:OG	1:A:46:VAL:HG22	2.11	0.51
1:A:837:GLN:HA	1:A:837:GLN:NE2	2.26	0.51
1:B:316:SER:HB3	1:B:388:VAL:CG2	2.37	0.51
1:B:592:VAL:CG1	1:B:593:ASP:N	2.73	0.51
1:A:90:TYR:HA	1:A:162:THR:HA	1.93	0.51
1:A:429:PRO:HD2	1:A:431:PHE:HD1	1.76	0.51
1:A:71:SER:HB2	1:A:81:VAL:CG1	2.41	0.51
1:A:1123:GLU:HA	1:A:1126:HIS:HB3	1.92	0.50
1:A:421:VAL:CG1	1:A:425:GLY:HA2	2.41	0.50
1:A:744:LEU:HG	1:A:756:PHE:CZ	2.45	0.50
1:B:138:GLU:OE2	1:B:234:ARG:HB2	2.11	0.50
1:B:372:VAL:HG11	1:B:468:TYR:CG	2.46	0.50
1:A:228:PRO:HB2	1:A:748:GLN:NE2	2.25	0.50
1:A:846:ALA:HB1	1:A:851:GLN:O	2.12	0.50
1:B:207:SER:HB2	1:B:208:ARG:CZ	2.41	0.50
1:B:421:VAL:CG1	1:B:425:GLY:HA2	2.41	0.50
1:B:429:PRO:CG	1:B:430:GLY:N	2.74	0.50
1:B:64:ASN:CG	1:B:334:VAL:HG13	2.31	0.50
1:A:610:ARG:C	1:A:610:ARG:HD2	2.32	0.50
1:A:98:HIS:HB3	1:A:157:LEU:HB2	1.94	0.50
1:A:107:THR:HG22	1:A:108:GLN:N	2.27	0.50
1:A:207:SER:HB2	1:A:208:ARG:CZ	2.42	0.50
1:A:647:LEU:HD12	1:A:901:LEU:HD23	1.94	0.50
1:B:467:PHE:C	1:B:467:PHE:CD1	2.85	0.50
1:B:651:ASN:HB2	1:B:775:SER:O	2.11	0.50
1:B:73:THR:O	1:B:74:THR:HB	2.12	0.50
1:B:1076:LEU:HB3	1:B:1079:ARG:HB2	1.94	0.50
1:B:1125:ALA:O	1:B:1127:GLU:N	2.45	0.50
1:B:484:ASP:HA	1:B:928:GLN:HE22	1.77	0.50
1:A:151:ASP:HB3	1:A:154:ARG:HB2	1.93	0.50
1:A:521:ARG:HD2	1:A:1011:ASN:O	2.11	0.50
1:A:733:LEU:HD22	1:A:759:ASP:HB3	1.94	0.50
1:A:948:LEU:HD22	1:A:955:HIS:CE1	2.46	0.50
1:B:1070:VAL:HG22	1:B:1122:LEU:CD1	2.41	0.50
1:B:421:VAL:HG11	1:B:425:GLY:HA2	1.94	0.50
1:B:151:ASP:HB3	1:B:154:ARG:HB2	1.94	0.49
1:A:1049:LEU:H	1:B:477:ILE:HG23	1.77	0.49
1:A:421:VAL:HG22	1:A:426:HIS:C	2.32	0.49
1:A:421:VAL:HG11	1:A:425:GLY:HA2	1.94	0.49
1:A:495:THR:O	1:A:495:THR:HG22	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:107:THR:HG22	1:B:108:GLN:N	2.28	0.49
1:A:1070:VAL:HG13	1:A:1122:LEU:HD11	1.94	0.49
1:A:99:GLY:HA3	1:A:156:LEU:HD23	1.92	0.49
1:B:277:ALA:HB3	1:B:321:ASP:OD1	2.12	0.49
1:B:879:ASN:HA	1:B:898:ASN:CG	2.33	0.49
1:A:174:THR:HG22	1:A:231:PHE:HB3	1.95	0.49
1:A:647:LEU:HG	1:A:778:LEU:HD11	1.94	0.49
1:B:31:ILE:HG23	1:B:32:GLU:N	2.26	0.49
1:B:348:PHE:HB3	1:B:352:ASP:CG	2.32	0.49
1:B:539:MET:CE	1:B:655:SER:H	2.25	0.49
1:B:647:LEU:HG	1:B:778:LEU:HD11	1.95	0.49
1:B:853:PRO:HB2	1:B:856:LEU:HB2	1.93	0.49
1:A:1068:VAL:HG12	1:A:1101:MET:HE1	1.94	0.49
1:A:619:ASN:O	1:A:623:VAL:HG13	2.12	0.49
1:A:654:MET:HE3	1:A:973:MET:SD	2.53	0.49
1:B:612:ALA:O	1:B:615:THR:HG23	2.12	0.49
1:B:857:LEU:HD22	1:B:861:ASP:HB3	1.95	0.49
1:B:739:ILE:HG22	1:B:739:ILE:O	2.11	0.49
1:A:879:ASN:HD22	1:A:898:ASN:HD21	1.60	0.49
1:B:471:ARG:HE	1:B:933:TRP:HZ2	1.60	0.49
1:B:610:ARG:HD2	1:B:610:ARG:C	2.33	0.49
1:A:125:PHE:CD2	1:A:255:ARG:HA	2.47	0.49
1:A:283:THR:CG2	1:A:420:GLN:HE21	2.10	0.49
1:A:553:ALA:HB2	1:A:575:TYR:H	1.78	0.49
1:A:680:VAL:HG13	1:A:985:ILE:HD11	1.95	0.49
1:B:807:ARG:NH1	1:B:873:LEU:HD11	2.27	0.49
1:A:975:ALA:HA	1:A:1031:ALA:HB3	1.93	0.49
1:A:467:PHE:CD1	1:A:467:PHE:C	2.86	0.49
1:A:1127:GLU:OE2	1:A:1128:ALA:HA	2.13	0.48
1:A:428:VAL:CB	1:A:429:PRO:CD	2.81	0.48
1:A:73:THR:O	1:A:74:THR:HB	2.11	0.48
1:B:847:LEU:HD23	1:B:852:LEU:HD12	1.95	0.48
1:A:67:VAL:HG22	1:A:86:THR:HG22	1.95	0.48
1:B:107:THR:CG2	1:B:470:GLU:OE2	2.60	0.48
1:A:1076:LEU:HB3	1:A:1079:ARG:HB2	1.94	0.48
1:A:879:ASN:HA	1:A:898:ASN:CG	2.34	0.48
1:B:1125:ALA:C	1:B:1127:GLU:N	2.66	0.48
1:B:89:HIS:CD2	1:B:660:PRO:HG3	2.48	0.48
1:B:1050:CYS:O	1:B:1054:ARG:HB2	2.13	0.48
1:B:29:GLU:C	1:B:31:ILE:H	2.17	0.48
1:A:29:GLU:C	1:A:31:ILE:H	2.17	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:107:THR:CG2	1:A:470:GLU:OE2	2.62	0.48
1:B:1069:PHE:HA	1:B:1101:MET:HE1	1.96	0.48
1:B:1091:LEU:O	1:B:1092:LEU:HD23	2.13	0.48
1:B:283:THR:CG2	1:B:420:GLN:HE21	2.19	0.48
1:B:476:VAL:C	1:B:477:ILE:HG13	2.33	0.48
1:A:611:GLU:O	1:A:615:THR:HG22	2.13	0.48
1:A:630:GLN:HG2	1:A:634:ASN:ND2	2.29	0.48
1:B:429:PRO:HD2	1:B:431:PHE:HD1	1.78	0.48
1:B:98:HIS:HB3	1:B:157:LEU:HB2	1.96	0.47
1:A:654:MET:O	1:A:773:VAL:HG13	2.14	0.47
1:B:125:PHE:CD2	1:B:255:ARG:HA	2.49	0.47
1:B:471:ARG:NE	1:B:933:TRP:CZ2	2.82	0.47
1:A:385:LEU:HB3	1:A:409:LEU:HB3	1.96	0.47
1:A:440:VAL:HG21	1:A:528:ALA:HB2	1.96	0.47
1:B:778:LEU:HD23	1:B:911:ILE:HG22	1.97	0.47
1:A:1050:CYS:O	1:A:1054:ARG:HB2	2.14	0.47
1:B:174:THR:HG23	1:B:196:VAL:HG13	1.95	0.47
1:B:24:ARG:HB3	1:B:191:VAL:HG22	1.96	0.47
1:A:131:ARG:HH12	1:A:212:GLU:CD	2.17	0.47
1:A:65:VAL:HG22	1:A:66:ALA:N	2.29	0.47
1:B:723:PHE:CB	1:B:999:GLN:HB2	2.45	0.47
1:A:1125:ALA:C	1:A:1127:GLU:N	2.67	0.47
1:A:503:THR:O	1:A:507:ARG:HG2	2.14	0.47
1:A:539:MET:CE	1:A:655:SER:H	2.27	0.47
1:A:538:THR:HG21	1:A:663:CYS:HA	1.95	0.47
1:A:857:LEU:O	1:A:858:SER:O	2.33	0.47
1:B:278:LEU:HD22	1:B:321:ASP:OD1	2.15	0.47
1:A:1005:SER:HA	4:A:2048:HOH:O	2.15	0.47
1:A:495:THR:O	1:A:496:ASP:HB3	2.14	0.47
1:B:632:MET:HB3	1:B:903:TYR:CZ	2.49	0.47
1:A:14:PRO:O	1:A:65:VAL:HG23	2.15	0.47
1:A:847:LEU:HD13	1:A:847:LEU:O	2.14	0.47
1:B:775:SER:HB2	1:B:1003:TRP:HB3	1.96	0.47
1:B:314:LEU:HD21	1:B:703:PHE:CD2	2.49	0.47
1:B:654:MET:O	1:B:773:VAL:HG13	2.15	0.47
1:A:1050:CYS:SG	1:B:476:VAL:CG2	3.03	0.47
1:A:462:LEU:O	1:A:465:MET:HB3	2.15	0.47
1:A:975:ALA:O	1:A:976:ARG:C	2.53	0.47
1:B:975:ALA:HA	1:B:1031:ALA:HB3	1.97	0.47
1:B:652:HIS:CE1	1:B:777:VAL:HG22	2.50	0.47
1:A:24:ARG:HB3	1:A:191:VAL:HG22	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1076:LEU:HD22	1:A:1079:ARG:HD3	1.97	0.46
1:A:138:GLU:OE2	1:A:234:ARG:HB2	2.14	0.46
1:B:485:VAL:O	1:B:489:VAL:HG23	2.15	0.46
1:B:471:ARG:HD2	1:B:959:TRP:O	2.15	0.46
1:B:975:ALA:O	1:B:976:ARG:C	2.53	0.46
1:A:1125:ALA:O	1:A:1127:GLU:N	2.47	0.46
1:A:222:GLY:O	1:A:225:PHE:HB2	2.16	0.46
1:A:1091:LEU:O	1:A:1092:LEU:HD23	2.15	0.46
1:A:369:ALA:HA	1:A:468:TYR:CD1	2.50	0.46
1:A:847:LEU:C	1:A:847:LEU:HD13	2.36	0.46
1:A:1069:PHE:HA	1:A:1101:MET:CE	2.46	0.46
1:A:203:MET:HE3	1:A:220:SER:HB2	1.98	0.46
1:A:831:LYS:HB3	1:A:837:GLN:C	2.36	0.46
1:A:864:THR:O	1:A:868:ILE:HG12	2.14	0.46
1:B:1069:PHE:HA	1:B:1101:MET:CE	2.45	0.46
1:B:83:LEU:HG	1:B:756:PHE:HB3	1.98	0.46
1:A:590:GLN:O	1:A:601:GLY:O	2.34	0.46
1:B:1068:VAL:HG12	1:B:1101:MET:CE	2.46	0.46
1:B:69:VAL:HA	1:B:198:PRO:HG2	1.97	0.46
1:B:590:GLN:O	1:B:601:GLY:O	2.34	0.46
1:B:1050:CYS:HB3	1:B:1054:ARG:NH2	2.26	0.46
1:B:14:PRO:O	1:B:65:VAL:HG23	2.15	0.46
1:B:552:TYR:O	1:B:553:ALA:HB2	2.15	0.46
1:A:183:LYS:HE3	1:A:192:HIS:NE2	2.31	0.46
1:A:319:ALA:HB2	1:A:686:LEU:CD1	2.46	0.46
1:B:122:HIS:ND1	1:B:449:GLU:OE1	2.48	0.46
1:A:69:VAL:HA	1:A:198:PRO:HG2	1.98	0.46
1:B:340:THR:HG22	1:B:345:TRP:NE1	2.28	0.46
1:A:473:ASP:HB2	1:A:518:LEU:HD21	1.98	0.45
1:A:816:GLY:O	1:A:820:LYS:HG3	2.15	0.45
1:A:507:ARG:HG3	1:A:507:ARG:HH11	1.80	0.45
1:B:1069:PHE:HD2	1:B:1122:LEU:CD2	2.29	0.45
1:B:150:LEU:O	1:B:152:PRO:HD3	2.17	0.45
1:B:613:LEU:HD23	1:B:613:LEU:C	2.36	0.45
1:B:708:GLN:HE22	1:B:711:LEU:HD23	1.82	0.45
1:A:32:GLU:H	1:A:32:GLU:HG3	1.43	0.45
1:A:340:THR:HG22	1:A:345:TRP:NE1	2.23	0.45
1:B:203:MET:CE	1:B:218:HIS:HD2	2.28	0.45
1:B:997:VAL:HG13	1:B:997:VAL:O	2.15	0.45
1:A:122:HIS:ND1	1:A:449:GLU:OE1	2.45	0.45
1:A:471:ARG:HD2	1:A:959:TRP:O	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:816:GLY:O	1:B:820:LYS:HG3	2.17	0.45
1:B:849:ARG:O	1:B:851:GLN:HG3	2.16	0.45
1:A:702:ASN:HB2	4:A:2031:HOH:O	2.17	0.45
1:B:630:GLN:HG2	1:B:634:ASN:ND2	2.32	0.45
1:B:718:MET:O	1:B:721:ASN:HB2	2.16	0.45
1:A:651:ASN:HB2	1:A:775:SER:C	2.37	0.45
1:A:85:LEU:HD12	1:A:85:LEU:N	2.32	0.45
1:B:108:GLN:O	1:B:109:ALA:C	2.54	0.45
1:A:471:ARG:NE	1:A:933:TRP:CZ2	2.84	0.45
1:A:485:VAL:O	1:A:489:VAL:HG23	2.16	0.45
1:B:743:SER:CB	1:B:746:ALA:HB3	2.46	0.45
1:A:108:GLN:O	1:A:109:ALA:C	2.55	0.45
1:A:718:MET:O	1:A:721:ASN:HB2	2.17	0.45
1:A:936:GLN:O	1:A:941:LEU:HA	2.16	0.45
1:B:952:VAL:CG1	1:B:953:ASP:N	2.80	0.45
1:A:1119:ASP:O	1:A:1122:LEU:HG	2.17	0.45
1:A:609:ASN:OD1	1:A:612:ALA:N	2.48	0.45
1:B:85:LEU:N	1:B:85:LEU:HD12	2.32	0.45
1:A:1069:PHE:HD2	1:A:1122:LEU:CD2	2.30	0.45
1:A:536:PHE:C	1:A:536:PHE:CD1	2.89	0.45
1:A:852:LEU:HD23	1:A:853:PRO:HD2	1.99	0.45
1:B:1119:ASP:OD1	1:B:1122:LEU:HD11	2.17	0.45
1:B:385:LEU:HB3	1:B:409:LEU:HB3	1.98	0.45
1:B:706:GLN:HG2	4:B:2034:HOH:O	2.16	0.45
1:A:319:ALA:CB	1:A:686:LEU:CD1	2.94	0.44
1:A:497:VAL:HA	1:A:498:PRO:HD3	1.83	0.44
1:A:624:VAL:O	1:A:628:VAL:HG23	2.16	0.44
1:A:723:PHE:HB3	1:A:999:GLN:HB2	1.99	0.44
1:B:519:ARG:HA	1:B:522:HIS:CD2	2.52	0.44
1:B:335:PHE:HB3	1:B:659:ASP:OD2	2.16	0.44
1:A:415:VAL:HG13	1:A:418:ASN:CG	2.38	0.44
1:A:613:LEU:C	1:A:613:LEU:HD23	2.38	0.44
1:A:362:GLY:HA3	1:A:956:PRO:O	2.18	0.44
1:B:521:ARG:HD2	1:B:1011:ASN:O	2.17	0.44
1:B:270:ASP:OD2	1:B:273:HIS:HB2	2.17	0.44
1:B:42:GLY:HA2	1:B:105:PRO:HG3	1.99	0.44
1:A:596:VAL:CG1	1:A:598:THR:HG22	2.46	0.44
1:B:478:VAL:O	1:B:478:VAL:HG12	2.17	0.44
1:B:596:VAL:HG12	1:B:598:THR:CG2	2.44	0.44
1:A:31:ILE:CG2	1:A:32:GLU:N	2.80	0.44
1:B:477:ILE:HD12	1:B:477:ILE:N	2.33	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:847:LEU:HD23	1:B:852:LEU:CD1	2.48	0.44
1:B:857:LEU:HD22	1:B:861:ASP:CB	2.47	0.44
1:A:270:ASP:OD2	1:A:273:HIS:HB2	2.18	0.44
1:A:952:VAL:CG1	1:A:953:ASP:N	2.79	0.44
1:B:415:VAL:HG13	1:B:418:ASN:CG	2.37	0.44
1:A:976:ARG:O	1:A:1030:ARG:HB2	2.18	0.44
1:A:985:ILE:HG22	1:A:987:LYS:HE3	1.99	0.44
1:B:201:LEU:HD22	1:B:744:LEU:HD21	2.00	0.44
1:A:1101:MET:O	1:A:1105:THR:HG22	2.18	0.44
1:B:467:PHE:O	1:B:471:ARG:HG2	2.17	0.44
1:B:652:HIS:CG	1:B:914:LEU:HD11	2.52	0.44
1:B:65:VAL:HG22	1:B:66:ALA:N	2.33	0.44
1:B:803:LYS:HA	1:B:910:PHE:CE2	2.52	0.44
1:B:852:LEU:O	1:B:853:PRO:C	2.55	0.44
1:B:370:GLY:CA	1:B:963:PHE:HZ	2.30	0.44
1:B:575:TYR:O	1:B:579:THR:HG23	2.17	0.44
1:B:612:ALA:HA	1:B:615:THR:CG2	2.48	0.44
1:A:1049:LEU:C	1:A:1051:GLU:N	2.71	0.43
1:A:42:GLY:HA2	1:A:105:PRO:HG3	1.99	0.43
1:A:549:LEU:HB2	1:A:575:TYR:CE2	2.53	0.43
1:A:917:ILE:HG22	1:A:963:PHE:CD2	2.53	0.43
1:B:1068:VAL:HG12	1:B:1101:MET:HE1	1.99	0.43
1:B:831:LYS:HD2	1:B:831:LYS:H	1.83	0.43
1:A:1058:SER:O	1:A:1060:GLY:N	2.51	0.43
1:A:408:PHE:HA	1:A:686:LEU:HD23	2.01	0.43
1:B:936:GLN:O	1:B:941:LEU:HA	2.18	0.43
1:A:658:LEU:HD12	1:A:768:PRO:HB2	2.01	0.43
1:B:1069:PHE:N	1:B:1101:MET:HE1	2.33	0.43
1:B:1078:PRO:HA	1:B:1116:TRP:CD1	2.53	0.43
1:B:636:VAL:HG23	1:B:643:PHE:HZ	1.83	0.43
1:A:67:VAL:HG21	1:A:165:PHE:CE1	2.53	0.43
1:B:354:ALA:C	1:B:356:ALA:H	2.20	0.43
1:B:524:LYS:HD3	1:B:524:LYS:HA	1.82	0.43
1:B:609:ASN:OD1	1:B:612:ALA:N	2.49	0.43
1:B:610:ARG:HG2	1:B:610:ARG:NH1	2.33	0.43
1:B:728:THR:HA	1:B:765:LEU:O	2.18	0.43
1:A:1049:LEU:HB2	1:B:477:ILE:HG23	2.00	0.43
1:A:1070:VAL:CG2	1:A:1122:LEU:HD13	2.48	0.43
1:A:96:VAL:HA	1:A:158:TYR:HB3	2.01	0.43
1:B:283:THR:OG1	1:B:420:GLN:HB3	2.17	0.43
1:B:869:LYS:O	1:B:873:LEU:HD23	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1127:GLU:O	1:A:1129:GLU:HG2	2.18	0.43
1:A:708:GLN:HE22	1:A:711:LEU:HD23	1.83	0.43
1:B:976:ARG:O	1:B:1030:ARG:HB2	2.18	0.43
1:B:96:VAL:HA	1:B:158:TYR:HB3	2.01	0.43
1:B:222:GLY:O	1:B:225:PHE:HB2	2.18	0.43
1:B:348:PHE:O	1:B:349:GLU:C	2.56	0.43
1:B:743:SER:HB3	1:B:746:ALA:HB3	2.00	0.43
1:A:970:ARG:CD	4:A:2047:HOH:O	2.67	0.43
1:B:199:LEU:HD12	1:B:199:LEU:HA	1.90	0.43
1:B:64:ASN:OD1	1:B:334:VAL:HG13	2.18	0.43
1:B:657:THR:HB	1:B:659:ASP:H	1.82	0.43
1:B:776:ARG:HG2	1:B:778:LEU:O	2.19	0.43
1:B:369:ALA:CB	1:B:471:ARG:HB2	2.49	0.43
1:B:53:VAL:HG13	1:B:59:SER:HA	2.01	0.43
1:A:469:LEU:HD12	1:A:469:LEU:HA	1.75	0.43
1:A:881:ILE:HG12	1:A:911:ILE:HD11	1.99	0.43
1:B:183:LYS:HE3	1:B:192:HIS:NE2	2.33	0.43
1:B:778:LEU:CD2	1:B:911:ILE:HG22	2.49	0.43
1:A:740:CYS:HA	1:A:754:SER:HA	1.99	0.43
1:B:1076:LEU:HD22	1:B:1079:ARG:HD3	2.00	0.43
1:B:29:GLU:O	1:B:32:GLU:HG3	2.19	0.43
1:B:493:ASN:HB2	1:B:504:PHE:CE1	2.54	0.43
1:A:174:THR:HG23	1:A:196:VAL:HG13	2.00	0.42
1:A:471:ARG:HE	1:A:933:TRP:HZ2	1.66	0.42
1:A:467:PHE:O	1:A:471:ARG:HG2	2.18	0.42
1:A:581:ARG:O	1:A:584:ALA:HB3	2.19	0.42
1:A:610:ARG:HG2	1:A:610:ARG:NH1	2.33	0.42
1:B:536:PHE:C	1:B:536:PHE:CD1	2.92	0.42
1:B:12:LYS:HD3	1:B:732:ALA:HB3	2.01	0.42
1:B:847:LEU:HD13	1:B:847:LEU:C	2.39	0.42
1:A:150:LEU:O	1:A:152:PRO:HD3	2.20	0.42
1:A:53:VAL:HG13	1:A:59:SER:HA	2.01	0.42
1:A:410:VAL:HB	1:A:411:PRO:HD2	2.00	0.42
1:A:612:ALA:HA	1:A:615:THR:CG2	2.49	0.42
1:A:882:ASN:HB3	4:A:2043:HOH:O	2.18	0.42
1:B:13:VAL:HG22	1:B:65:VAL:HA	2.00	0.42
1:B:503:THR:O	1:B:507:ARG:HG2	2.19	0.42
1:B:71:SER:HB2	1:B:81:VAL:HG13	2.01	0.42
1:B:359:ASN:OD1	1:B:956:PRO:HA	2.20	0.42
1:B:985:ILE:HG22	1:B:987:LYS:HE3	2.02	0.42
1:A:90:TYR:CE2	1:A:160:VAL:HG12	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:89:HIS:NE2	1:A:660:PRO:HG3	2.34	0.42
1:A:698:VAL:O	1:A:698:VAL:HG13	2.19	0.42
1:A:803:LYS:HA	1:A:910:PHE:CE2	2.54	0.42
1:B:596:VAL:CG1	1:B:598:THR:HG22	2.43	0.42
1:B:847:LEU:HD13	1:B:847:LEU:O	2.19	0.42
1:B:632:MET:HG3	1:B:903:TYR:CD2	2.54	0.42
1:B:881:ILE:HG12	1:B:911:ILE:HD11	2.01	0.42
1:B:917:ILE:HG22	1:B:963:PHE:CD2	2.54	0.42
1:A:54:GLY:CA	1:A:342:ILE:HD11	2.47	0.42
1:A:575:TYR:O	1:A:579:THR:HG23	2.19	0.42
1:B:1052:GLN:O	1:B:1056:ILE:HG13	2.19	0.42
1:A:279:PRO:HG2	1:A:282:ILE:HB	2.02	0.42
1:A:589:LEU:O	1:A:590:GLN:HB2	2.20	0.42
1:A:607:ILE:HA	1:A:612:ALA:CB	2.50	0.42
1:B:159:LEU:CG	1:B:161:VAL:HG22	2.37	0.42
1:B:352:ASP:CG	1:B:357:ARG:HE	2.18	0.42
1:B:581:ARG:O	1:B:584:ALA:HB3	2.20	0.42
1:A:718:MET:O	1:A:719:PHE:C	2.58	0.42
1:B:31:ILE:CG2	1:B:32:GLU:N	2.82	0.42
1:B:410:VAL:HB	1:B:411:PRO:HD2	2.01	0.42
1:B:469:LEU:HD12	1:B:469:LEU:HA	1.75	0.42
1:B:924:PRO:HA	1:B:925:PRO:HD2	1.95	0.42
1:A:601:GLY:O	1:A:602:ARG:HB2	2.19	0.42
1:A:833:PRO:HD3	1:A:853:PRO:HG2	2.02	0.42
1:B:279:PRO:HG2	1:B:282:ILE:HB	2.02	0.42
1:B:762:ARG:HG3	1:B:762:ARG:HH11	1.85	0.42
1:B:1069:PHE:CA	1:B:1101:MET:HE1	2.50	0.42
1:B:668:LEU:C	1:B:668:LEU:HD13	2.39	0.42
1:B:67:VAL:HG23	1:B:69:VAL:HG13	2.02	0.42
1:B:804:PRO:HD2	1:B:910:PHE:CZ	2.55	0.42
1:A:1123:GLU:O	1:A:1126:HIS:HB3	2.20	0.41
1:A:596:VAL:HG12	1:A:598:THR:CG2	2.48	0.41
1:B:406:ARG:CD	1:B:690:HIS:HD2	2.33	0.41
1:B:870:LYS:HE2	1:B:874:ASP:OD2	2.19	0.41
1:A:1068:VAL:HG12	1:A:1101:MET:CE	2.49	0.41
1:A:1069:PHE:HA	1:A:1101:MET:HE1	2.02	0.41
1:A:83:LEU:HG	1:A:756:PHE:HB3	2.02	0.41
1:B:589:LEU:O	1:B:590:GLN:HB2	2.20	0.41
1:B:607:ILE:HA	1:B:612:ALA:CB	2.50	0.41
1:B:778:LEU:HD23	1:B:778:LEU:HA	1.93	0.41
1:B:879:ASN:HA	1:B:898:ASN:OD1	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:223:GLU:HA	1:A:223:GLU:OE1	2.21	0.41
1:A:29:GLU:O	1:A:32:GLU:HG3	2.20	0.41
1:A:348:PHE:O	1:A:349:GLU:C	2.58	0.41
1:A:602:ARG:HG2	1:B:443:THR:O	2.19	0.41
1:A:750:ALA:HB1	1:A:751:PRO:HD2	2.01	0.41
1:B:1101:MET:O	1:B:1105:THR:HG22	2.20	0.41
1:B:494:GLN:CA	1:B:494:GLN:NE2	2.59	0.41
1:B:601:GLY:O	1:B:602:ARG:HB2	2.21	0.41
1:B:948:LEU:O	1:B:948:LEU:HD13	2.20	0.41
1:A:1030:ARG:HD3	1:A:1030:ARG:HH11	1.76	0.41
1:A:131:ARG:HB2	1:A:134:ASP:OD2	2.21	0.41
1:A:98:HIS:HD2	1:A:157:LEU:HD13	1.84	0.41
1:A:823:HIS:HB2	1:A:840:PRO:HB3	2.03	0.41
1:B:651:ASN:HB2	1:B:775:SER:C	2.41	0.41
1:A:408:PHE:HB3	1:A:530:ARG:HD2	2.02	0.41
1:B:1058:SER:O	1:B:1060:GLY:N	2.54	0.41
1:B:174:THR:CG2	1:B:175:PHE:N	2.83	0.41
1:B:714:ARG:HG2	1:B:714:ARG:HH11	1.85	0.41
1:A:53:VAL:N	1:A:340:THR:O	2.47	0.41
1:A:778:LEU:HD22	1:A:906:HIS:CE1	2.56	0.41
1:B:32:GLU:H	1:B:32:GLU:HG3	1.44	0.41
1:B:707:PHE:C	1:B:709:PRO:HD2	2.40	0.41
1:B:831:LYS:HA	1:B:838:PRO:HA	2.03	0.41
1:A:1078:PRO:HA	1:A:1116:TRP:CD1	2.56	0.41
1:A:67:VAL:HG23	1:A:69:VAL:HG13	2.02	0.41
1:B:1124:VAL:O	1:B:1127:GLU:HB3	2.21	0.41
1:B:258:ASP:OD1	1:B:262:ARG:NH1	2.53	0.41
1:A:1050:CYS:SG	1:B:476:VAL:HG21	2.61	0.41
1:A:1124:VAL:O	1:A:1127:GLU:HB3	2.21	0.41
1:A:203:MET:CE	1:A:218:HIS:CD2	3.03	0.41
1:A:477:ILE:H	1:A:477:ILE:HD12	1.86	0.41
1:B:42:GLY:HA2	1:B:105:PRO:CG	2.50	0.41
1:B:90:TYR:CE2	1:B:160:VAL:HG12	2.54	0.41
1:B:266:HIS:CE1	1:B:273:HIS:CE1	3.08	0.41
1:A:279:PRO:HA	4:A:2013:HOH:O	2.20	0.41
1:B:624:VAL:O	1:B:628:VAL:HG23	2.20	0.41
1:B:921:SER:HA	1:B:960:THR:O	2.20	0.41
1:B:53:VAL:CG1	1:B:59:SER:HA	2.51	0.41
1:A:354:ALA:C	1:A:356:ALA:H	2.23	0.41
1:A:776:ARG:HG2	1:A:778:LEU:O	2.21	0.41
1:A:890:GLU:HG2	1:A:968:LEU:HD13	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:723:PHE:HB2	1:A:999:GLN:HB2	2.02	0.41
1:B:1031:ALA:HA	1:B:1035:CYS:HB2	2.03	0.41
1:B:1119:ASP:O	1:B:1122:LEU:HG	2.20	0.41
1:B:177:HIS:CD2	1:B:180:GLY:HA3	2.56	0.41
1:B:39:ALA:HB3	1:B:48:VAL:CG1	2.50	0.41
1:A:13:VAL:O	1:A:13:VAL:HG13	2.20	0.40
1:A:524:LYS:HD3	1:A:524:LYS:HA	1.81	0.40
1:A:714:ARG:HH11	1:A:714:ARG:HG2	1.86	0.40
1:B:1054:ARG:HD2	1:B:1093:GLU:OE1	2.21	0.40
1:B:1127:GLU:CD	1:B:1127:GLU:C	2.80	0.40
1:A:1054:ARG:HD2	1:A:1093:GLU:OE1	2.20	0.40
1:A:451:LEU:HA	1:A:451:LEU:HD12	1.93	0.40
1:A:519:ARG:HA	1:A:522:HIS:CD2	2.55	0.40
1:A:71:SER:HB2	1:A:81:VAL:HG13	2.04	0.40
1:B:1109:LEU:HD12	1:B:1109:LEU:HA	1.98	0.40
1:B:354:ALA:C	1:B:356:ALA:N	2.74	0.40
1:B:415:VAL:C	1:B:417:ALA:H	2.24	0.40
1:B:899:GLN:OE1	1:B:899:GLN:HA	2.22	0.40
1:A:24:ARG:HH21	1:A:27:PRO:HB3	1.85	0.40
1:A:707:PHE:C	1:A:709:PRO:HD2	2.42	0.40
1:B:131:ARG:HA	1:B:132:PRO:HD3	1.95	0.40
1:B:225:PHE:CZ	1:B:744:LEU:HD13	2.55	0.40
1:B:86:THR:OG1	1:B:762:ARG:NH1	2.54	0.40
1:A:15:PRO:HB3	1:A:85:LEU:CD2	2.51	0.40
1:B:507:ARG:NH1	1:B:507:ARG:HG3	2.37	0.40
1:A:415:VAL:C	1:A:417:ALA:H	2.24	0.40
1:B:98:HIS:HD2	1:B:157:LEU:HD13	1.84	0.40
1:B:393:PRO:HG3	1:B:399:HIS:CE1	2.56	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	1007/1136 (89%)	912 (91%)	81 (8%)	14 (1%)	11	43
1	B	1011/1136 (89%)	912 (90%)	82 (8%)	17 (2%)	9	39
All	All	2018/2272 (89%)	1824 (90%)	163 (8%)	31 (2%)	10	42

All (31) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	428	VAL
1	A	429	PRO
1	A	858	SER
1	A	1128	ALA
1	B	428	VAL
1	B	429	PRO
1	B	1126	HIS
1	B	1128	ALA
1	A	601	GLY
1	A	1077	GLY
1	A	1117	SER
1	A	1126	HIS
1	B	477	ILE
1	B	601	GLY
1	B	755	SER
1	B	1077	GLY
1	B	1117	SER
1	A	473	ASP
1	A	882	ASN
1	B	473	ASP
1	B	756	PHE
1	B	882	ASN
1	A	1054	ARG
1	B	1054	ARG
1	B	738	ALA
1	A	491	ASP
1	A	643	PHE
1	A	938	GLY
1	B	938	GLY
1	B	763	VAL
1	B	838	PRO

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	818/887 (92%)	763 (93%)	55 (7%)	16	49
1	B	819/887 (92%)	763 (93%)	56 (7%)	16	48
All	All	1637/1774 (92%)	1526 (93%)	111 (7%)	16	48

All (111) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	32	GLU
1	A	34	LEU
1	A	101	ARG
1	A	104	ASP
1	A	118	ARG
1	A	127	ASP
1	A	136	LYS
1	A	146	GLU
1	A	161	VAL
1	A	173	ASN
1	A	174	THR
1	A	199	LEU
1	A	201	LEU
1	A	253	ARG
1	A	255	ARG
1	A	278	LEU
1	A	336	ASP
1	A	340	THR
1	A	342	ILE
1	A	347	LEU
1	A	351	GLN
1	A	372	VAL
1	A	421	VAL
1	A	432	GLU
1	A	436	THR
1	A	469	LEU
1	A	477	ILE

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Mol	Chain	Res	Type
1	A	505	ASP
1	A	512	HIS
1	A	538	THR
1	A	539	MET
1	A	610	ARG
1	A	615	THR
1	A	620	VAL
1	A	647	LEU
1	A	649	GLU
1	A	657	THR
1	A	686	LEU
1	A	698	VAL
1	A	721	ASN
1	A	773	VAL
1	A	807	ARG
1	A	811	LEU
1	A	829	ASN
1	A	831	LYS
1	A	853	PRO
1	A	950	ASP
1	A	952	VAL
1	A	960	THR
1	A	977	PRO
1	A	1025	VAL
1	A	1038	SER
1	A	1092	LEU
1	A	1111	ARG
1	A	1127	GLU
1	B	10	THR
1	B	32	GLU
1	B	34	LEU
1	B	101	ARG
1	B	104	ASP
1	B	118	ARG
1	B	127	ASP
1	B	136	LYS
1	B	146	GLU
1	B	161	VAL
1	B	173	ASN
1	B	174	THR
1	B	199	LEU
1	B	201	LEU

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Mol	Chain	Res	Type
1	B	253	ARG
1	B	278	LEU
1	B	336	ASP
1	B	340	THR
1	B	342	ILE
1	B	347	LEU
1	B	351	GLN
1	B	372	VAL
1	B	421	VAL
1	B	432	GLU
1	B	436	THR
1	B	469	LEU
1	B	477	ILE
1	B	494	GLN
1	B	495	THR
1	B	505	ASP
1	B	512	HIS
1	B	538	THR
1	B	539	MET
1	B	610	ARG
1	B	615	THR
1	B	620	VAL
1	B	647	LEU
1	B	649	GLU
1	B	657	THR
1	B	672	LEU
1	B	686	LEU
1	B	698	VAL
1	B	721	ASN
1	B	749	THR
1	B	773	VAL
1	B	807	ARG
1	B	811	LEU
1	B	831	LYS
1	B	950	ASP
1	B	952	VAL
1	B	960	THR
1	B	977	PRO
1	B	1025	VAL
1	B	1092	LEU
1	B	1111	ARG
1	B	1127	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (40) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	98	HIS
1	A	102	HIS
1	A	177	HIS
1	A	215	ASN
1	A	218	HIS
1	A	266	HIS
1	A	420	GLN
1	A	450	HIS
1	A	614	HIS
1	A	618	ASN
1	A	619	ASN
1	A	630	GLN
1	A	634	ASN
1	A	677	ASN
1	A	690	HIS
1	A	748	GLN
1	A	823	HIS
1	A	837	GLN
1	A	841	GLN
1	A	879	ASN
1	A	1084	GLN
1	B	98	HIS
1	B	102	HIS
1	B	177	HIS
1	B	215	ASN
1	B	218	HIS
1	B	266	HIS
1	B	399	HIS
1	B	420	GLN
1	B	450	HIS
1	B	494	GLN
1	B	618	ASN
1	B	619	ASN
1	B	630	GLN
1	B	634	ASN
1	B	677	ASN
1	B	690	HIS
1	B	879	ASN
1	B	1002	ASN
1	B	1084	GLN

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 10 ligands modelled in this entry, 10 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 [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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	1029/1136 (90%)	-0.39	4 (0%) 92 79	13, 34, 68, 79	0
1	B	1031/1136 (90%)	-0.34	6 (0%) 89 72	12, 33, 66, 80	0
All	All	2060/2272 (90%)	-0.37	10 (0%) 91 75	12, 34, 67, 80	0

All (10) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	1122	LEU	3.9
1	B	1129	GLU	3.4
1	A	751	PRO	2.9
1	A	494	GLN	2.7
1	B	352	ASP	2.6
1	A	223	GLU	2.6
1	A	1122	LEU	2.2
1	B	805	ASP	2.2
1	B	1038	SER	2.0
1	B	1108	ALA	2.0

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. 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(Å ²)	Q<0.9
3	HG	A	2135	1/1	0.71	0.24	24,24,24,24	1
3	HG	A	2134	1/1	0.76	0.15	85,85,85,85	1
3	HG	B	2135	1/1	0.87	0.23	25,25,25,25	1
3	HG	B	2134	1/1	0.94	0.11	58,58,58,58	1
3	HG	B	2132	1/1	0.97	0.04	57,57,57,57	1
3	HG	B	2133	1/1	0.98	0.05	66,66,66,66	1
3	HG	A	2133	1/1	0.98	0.06	59,59,59,59	1
3	HG	A	2132	1/1	0.99	0.04	49,49,49,49	1
2	ZN	B	2131	1/1	0.99	0.07	29,29,29,29	0
2	ZN	A	2131	1/1	1.00	0.10	35,35,35,35	0

6.5 Other polymers [i](#)

There are no such residues in this entry.